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Supporting Information

"Ga-Substituted Pnictinidenes and Gallapnictenes: Suitable Synthons for Various Open-Shell and Closed-Shell Species"

Julia Krüger

Universität Duisburg-Essen

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Supporting Information

Syntheses, Structures, and Bonding Analyses of Carbene-Stabilized Stibinidenes

Julia Krüger, Christoph Wölper, Lukas John, Lijuan Song,
Peter R. Schreiner* and Stephan Schulz*

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Content

A) Syntheses and Spectroscopic Characterization

Synthesis of IDipp-SbX_3 (X = Cl, Br). IDipp (30 mg, 0.077 mmol) and 0.077 mmol SbX_3 (X = Cl 18 mg, Br 28 mg) were dissolved in 0.5 mL of benzene in a J Young NMR tube. IDipp-SbX_3 is formed immediately.

IDipp-$SbCl_3$: **^{1}H-NMR (C_6D_6, 300 MHz, 25 °C) δ [ppm]:** 7.10-7.25 (m, 6 H, C_6H_3), 6.55 (s, 2 H, NC*H*), 3.20 (sept, $^3J_{HH}$ = 6.7 Hz, 4 H, C*H*(CH_3)$_2$), 1.50 (d, 12 H, $^3J_{HH}$ = 6.6 Hz, CH(C*H*$_3$)$_2$), 0.97 (d, 12 H, $^3J_{HH}$ = 6.6 Hz, CH(C*H*$_3$)$_2$). **^{13}C{^{1}H}-NMR (C_6D_6, 300 MHz, 25 °C) *δ* [ppm]:** 146.9 (C), 133.1 (C_6H_3), 131.7 (C_6H_3), 125.0 (N*C*H), 124.5 (C_6H_3), 29.2 (*C*H(CH_3)$_2$), 26.3 (CH(*C*H$_3$)$_2$), 23.4 (CH(*C*H$_3$)$_2$).

IDipp-$SbBr_3$: **^{1}H-NMR (C_6D_6, 300 MHz, 25 °C) δ [ppm]:** 7.10-7.24 (m, 6 H, C_6H_3), 6.56 (s, 2 H, NC*H*), 3.27 (sept, $^3J_{HH}$ = 6.7 Hz, 4 H, C*H*(CH_3)$_2$), 1.56 (d, 12 H, $^3J_{HH}$ = 6.6 Hz, CH(C*H*$_3$)$_2$), 0.92 (d, 12 H, $^3J_{HH}$ = 6.6 Hz, CH(C*H*$_3$)$_2$). **^{13}C{^{1}H}-NMR (C_6D_6, 300 MHz, 25 °C) *δ* [ppm]:** 147.0 (C), 133.4 (C_6H_3), 132.3 (C_6H_3), 126.2 (N*C*H), 124.9 (C_6H_3), 29.4 (*C*H(CH_3)$_2$), 26.7 (CH(*C*H$_3$)$_2$), 23.6 (CH(*C*H$_3$)$_2$).

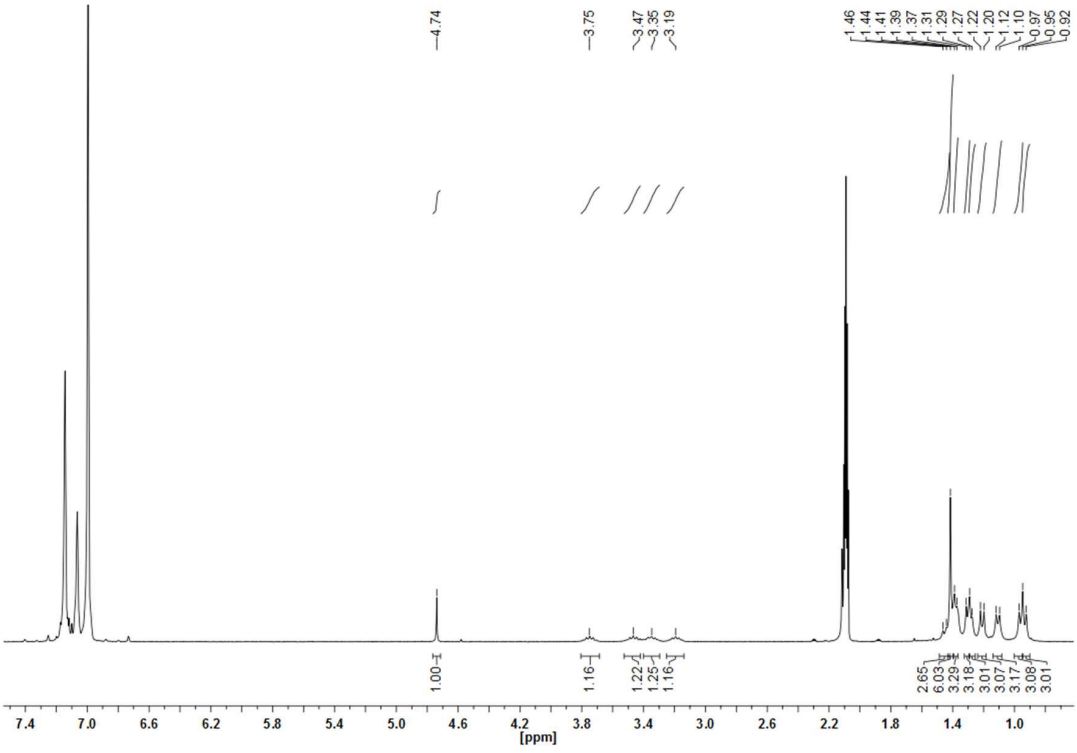

Fig. S1. ^{1}H NMR spectrum $[LGa(Cl)]_2SbCl$ (**1**) in toluene-d_8 at −50 °C.

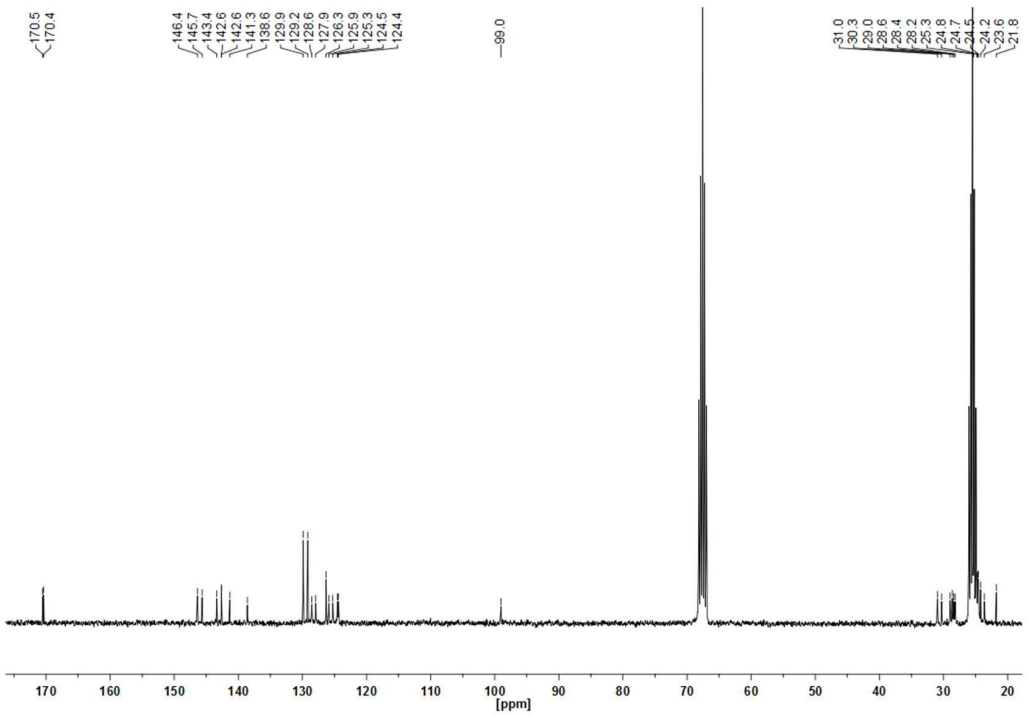

Fig. S2. ^{13}C NMR spectrum $[LGa(Cl)]_2SbCl$ (**1**) in THF-d_8 at −50 °C.

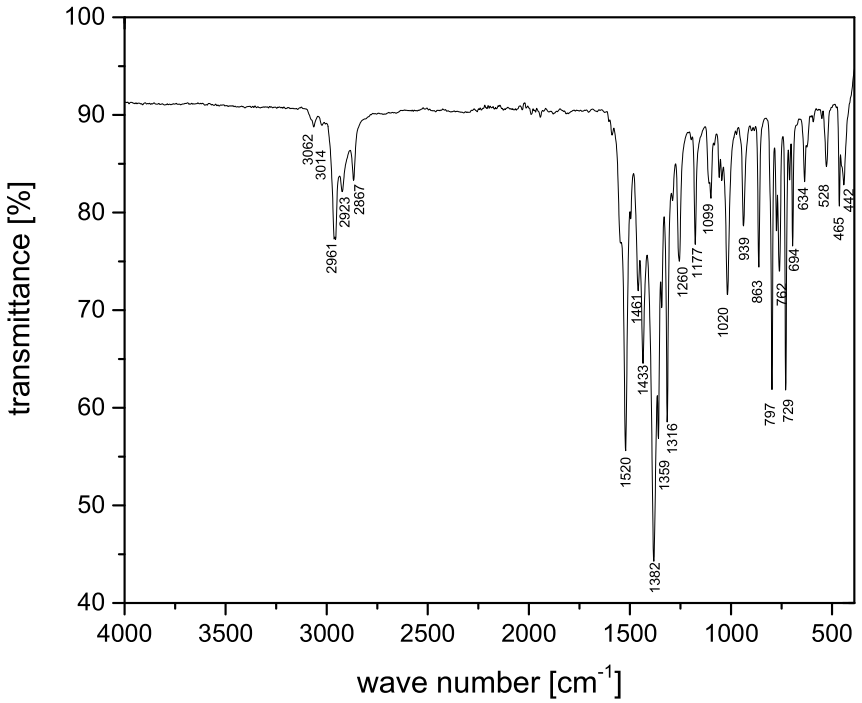

Fig. S3. IR spectrum of $[L(Cl)Ga]_2SbCl$ (**1**).

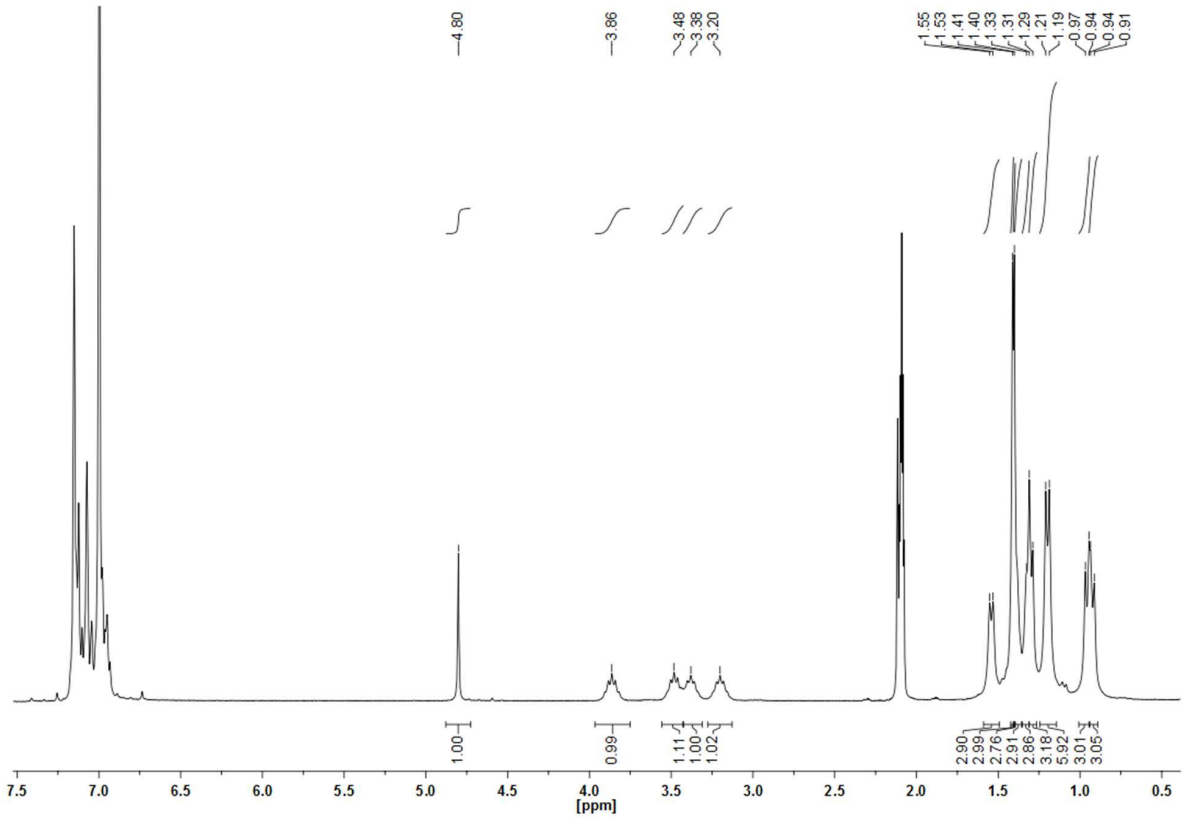

Fig. S4. ^{1}H NMR spectrum of $[LGa(Br)]_2SbBr$ (**2**) in toluene-d_8 at −50 °C.

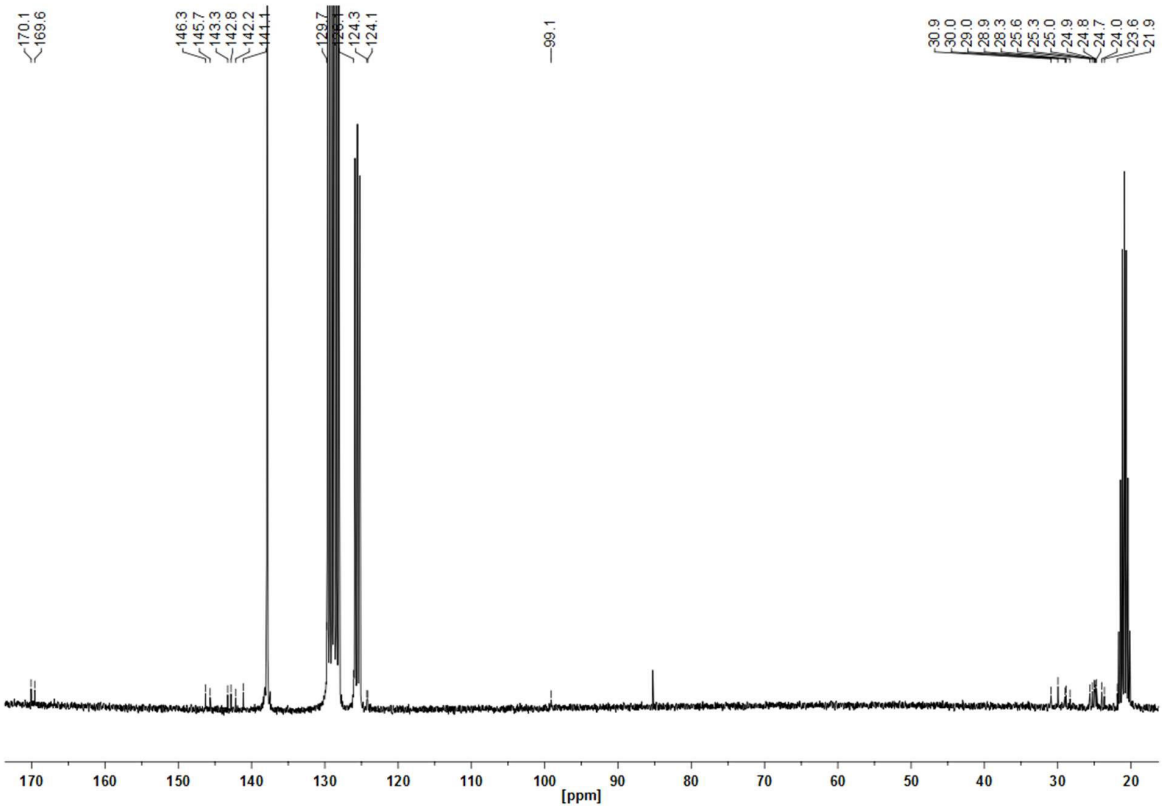

Fig. S5. ^{13}C NMR spectrum of $[LGa(Br)]_2SbBr$ (**2**) in toluene-d_8 at −50 °C.

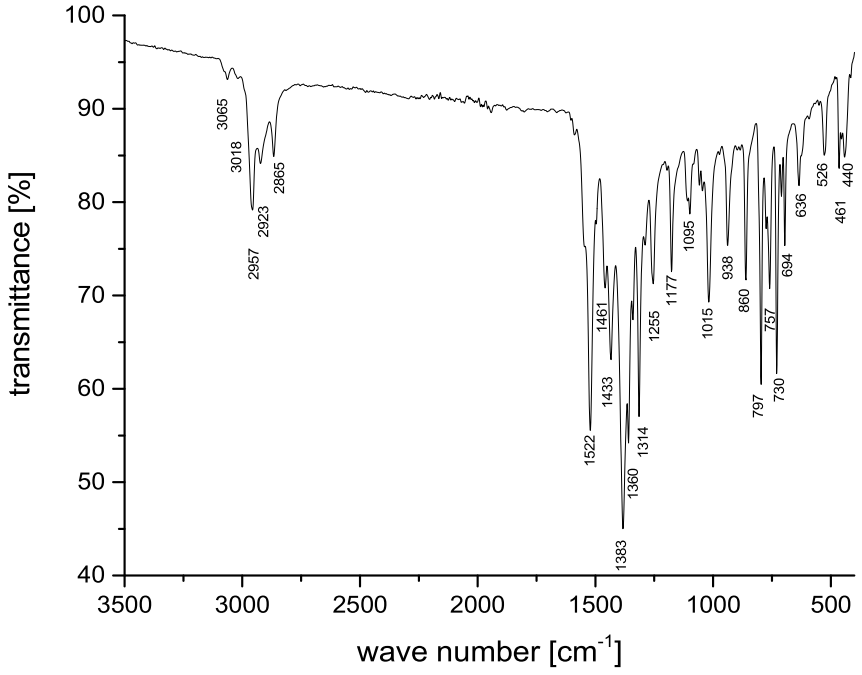

Fig. S6. IR spectrum of $[LGa(Br)]_2SbBr$ (**2**).

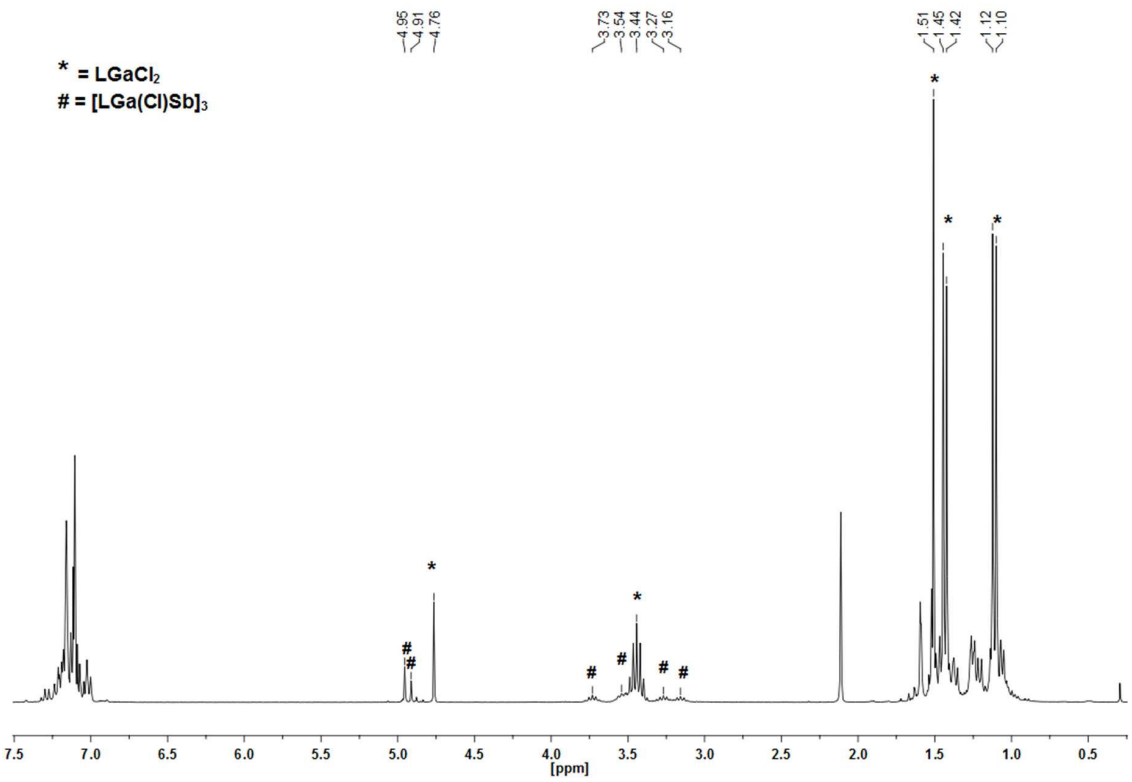

Fig. S7. *In situ* ^{1}H NMR spectrum of an isolated sample $[L(Cl)Ga]_2SbCl$ (**1**) warmed to 0 °C.

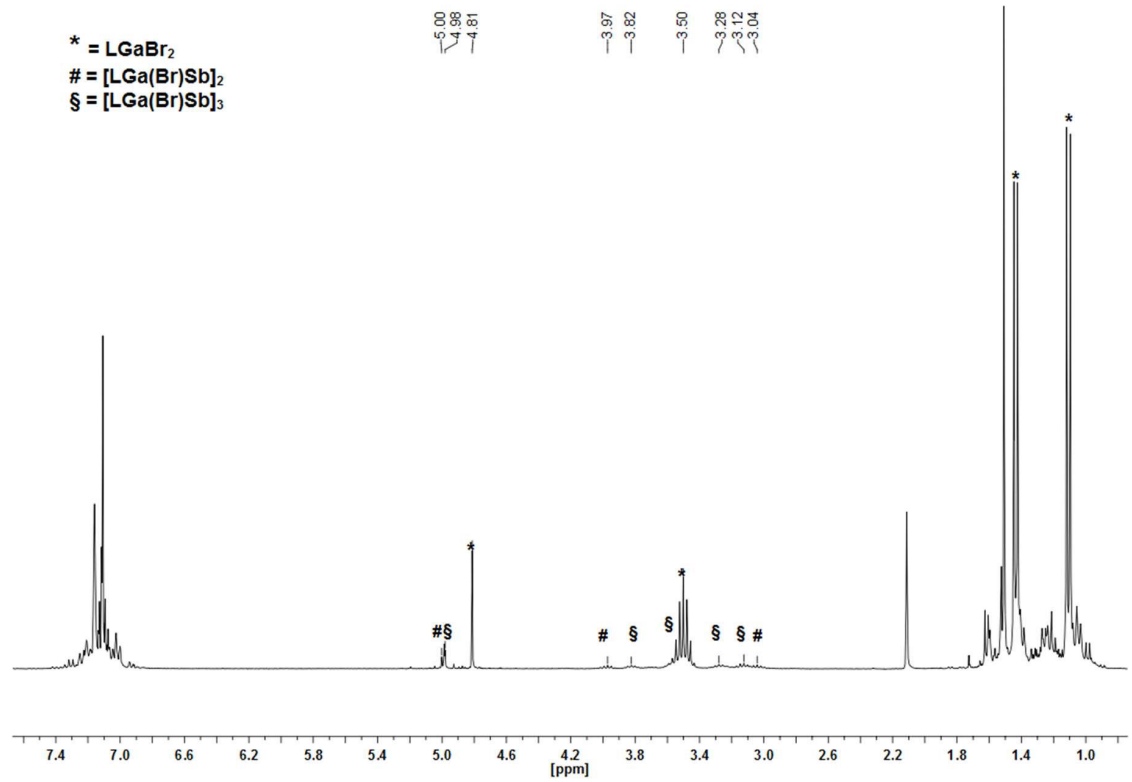

Fig. S8. *In situ* ^{1}H NMR spectrum of an isolated sample $[L(Br)Ga]_2SbBr$ (**2**) at ambient temperature in C_6D_6. The intensity of the product signal (#) is relatively low due to its poor solubility in benzene.

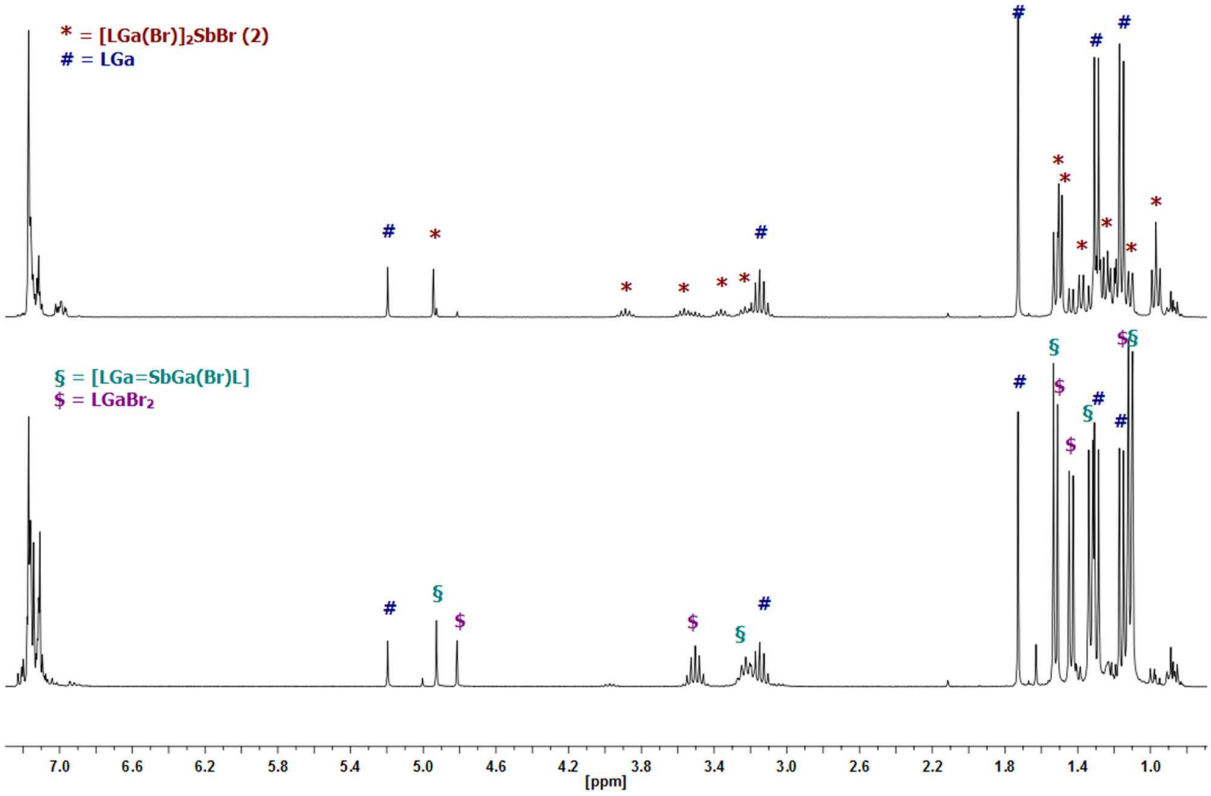

Fig. S9. *In situ* ^{1}H NMR spectrum of the reaction of an isolated sample [L(Br)Ga]$_2$SbBr (**2**) with one equivalent of LGa in C_6D_6.

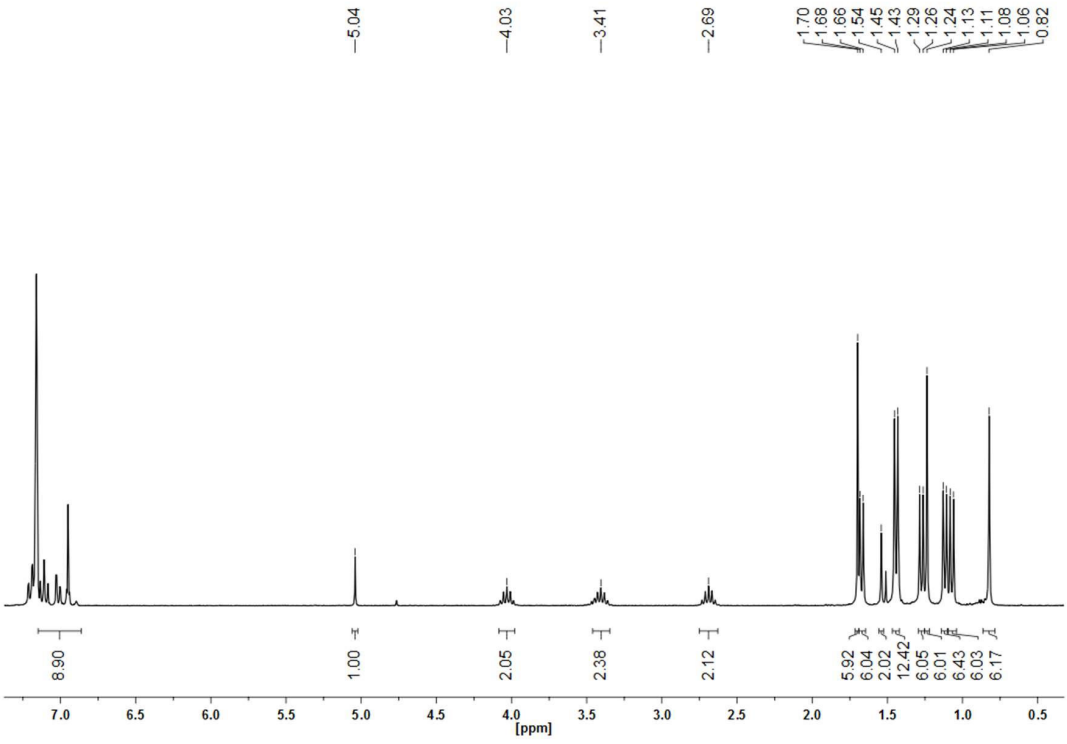

Fig. S10. ^{1}H NMR spectrum of ^{Me}CAAC-SbGa(Cl)L (**3**) in C_6D_6.

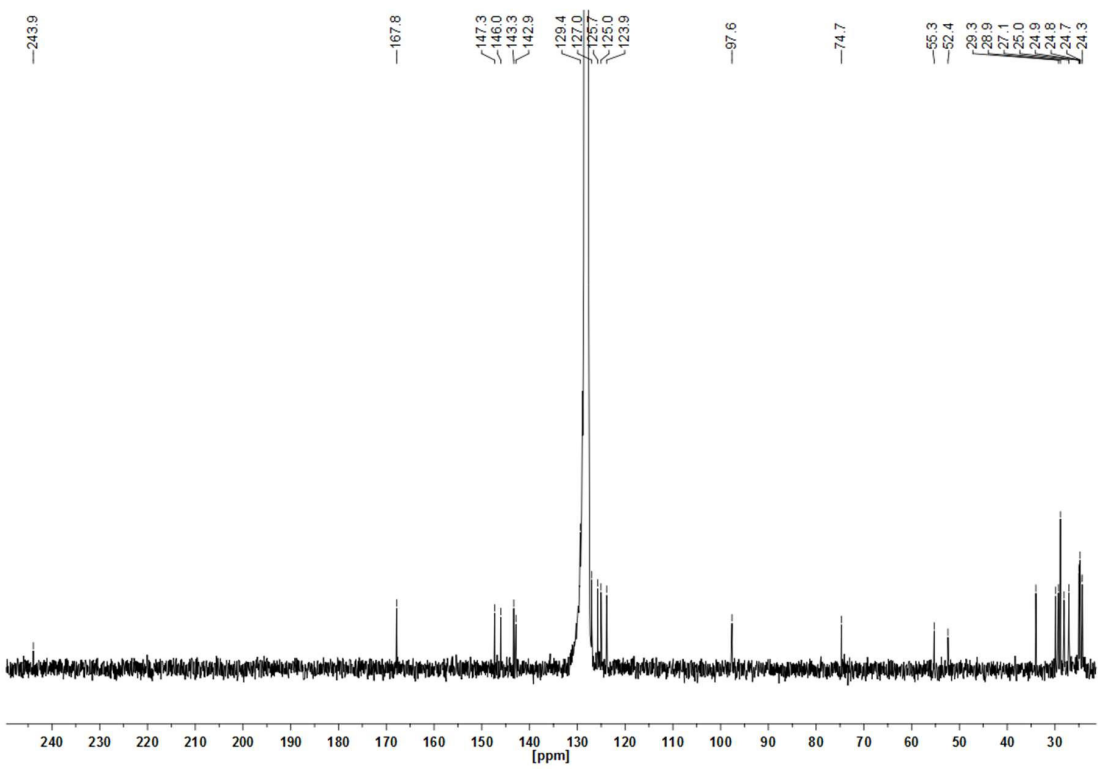

Fig. S11. ^{13}C NMR spectrum of ^{Me}CAAC-SbGa(Cl)L (**3**) in C_6D_6.

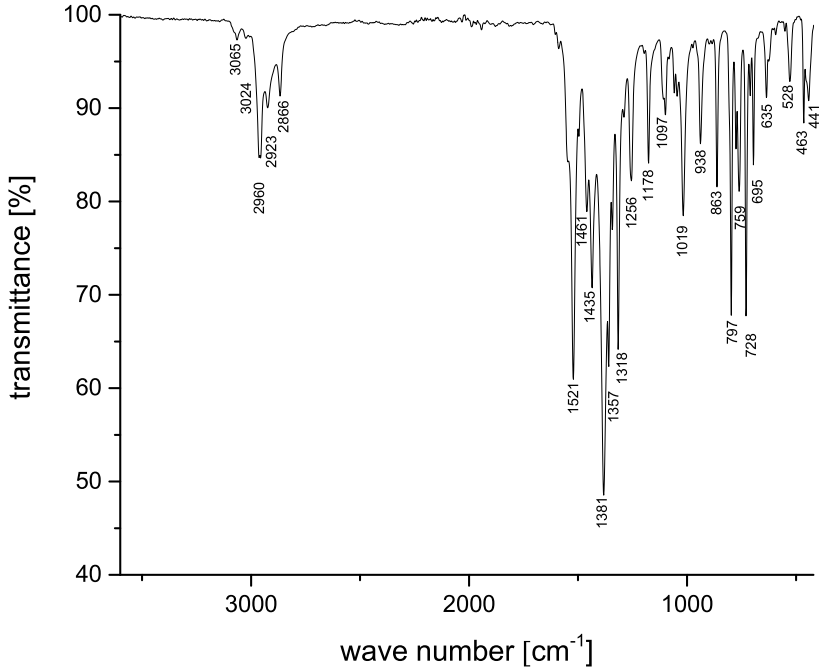

Fig. S12. IR spectrum of ^{Me}CAAC-SbGa(Cl)L (**3**).

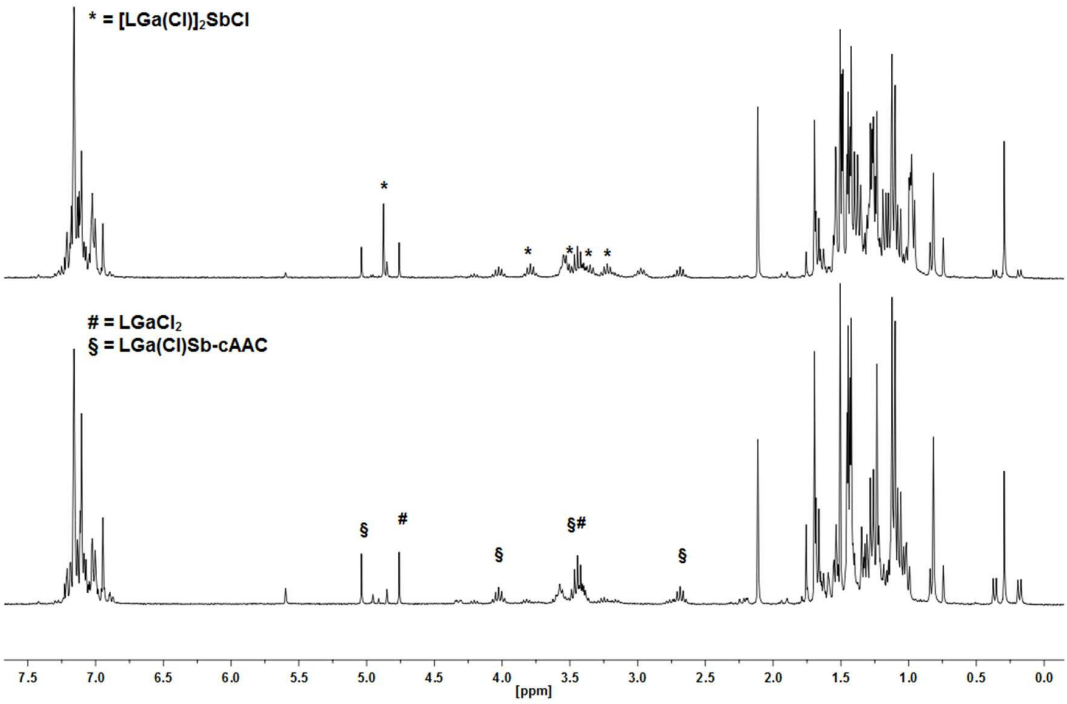

Fig. S13. *In situ* ^{1}H NMR spectrum of the reaction of [L(Cl)Ga]$_2$SbCl (**1**) with ^{Me}CAAC at the beginning and after 24 h in C_6D_6.

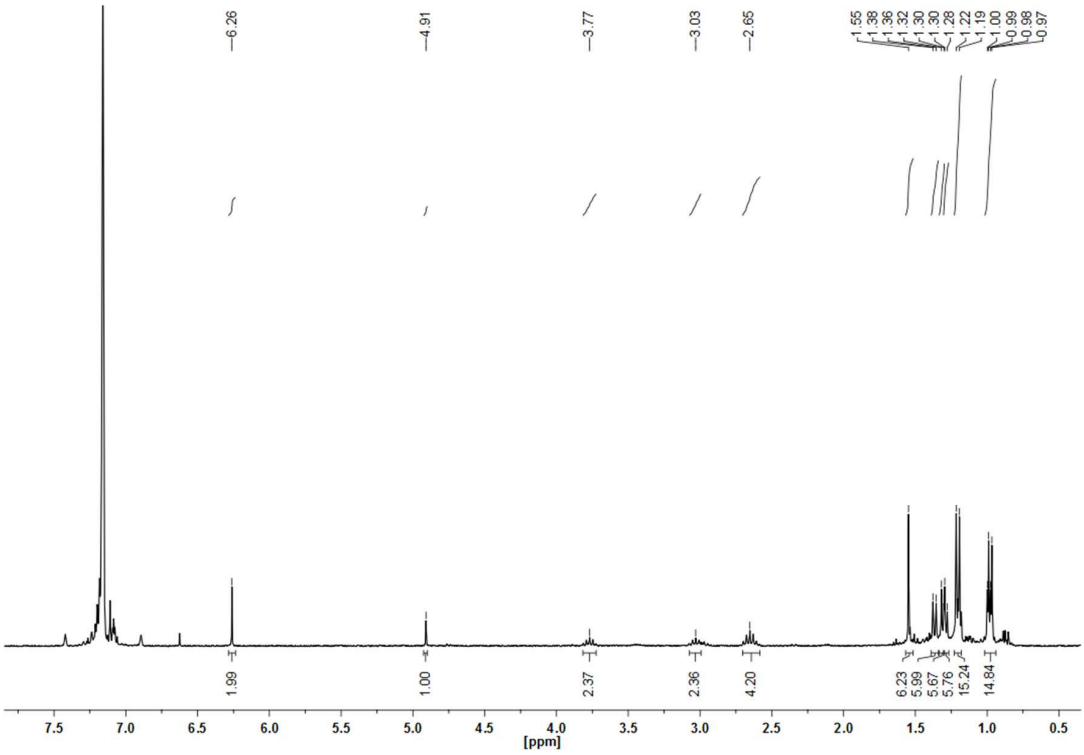

Fig. S14. ^{1}H NMR spectrum of IDipp-SbGa(Cl)L (**5**) in C_6D_6.

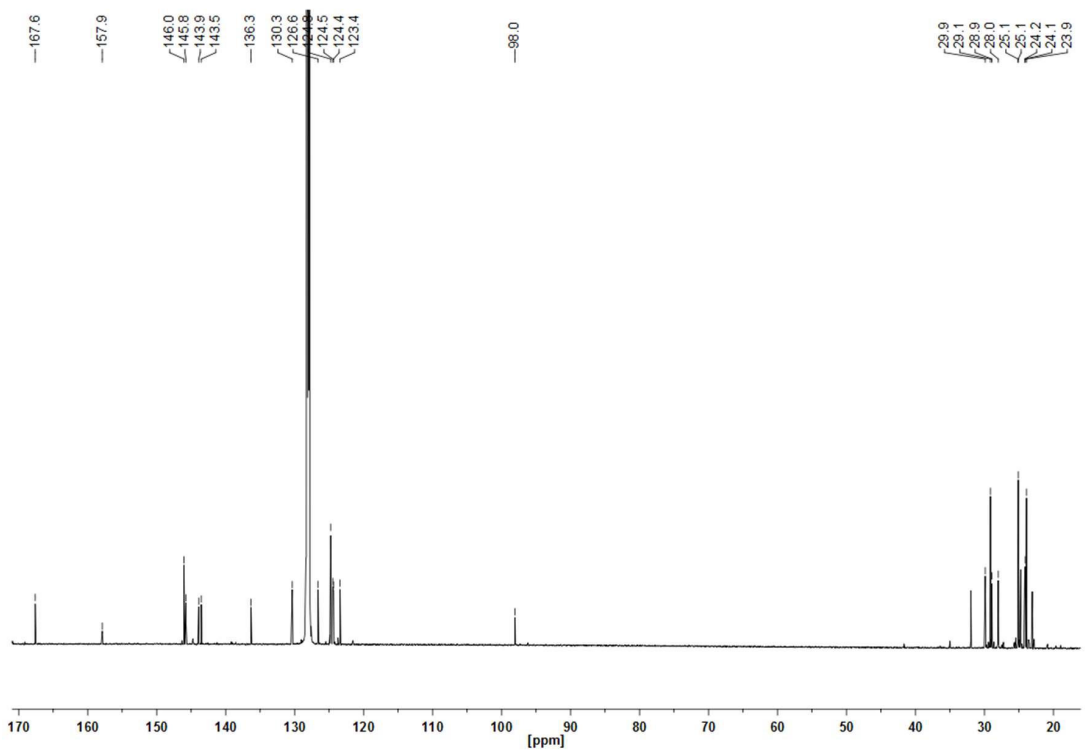

Fig. S15. ^{13}C NMR spectrum of IDipp-SbGa(Cl)L (**5**) in C_6D_6.

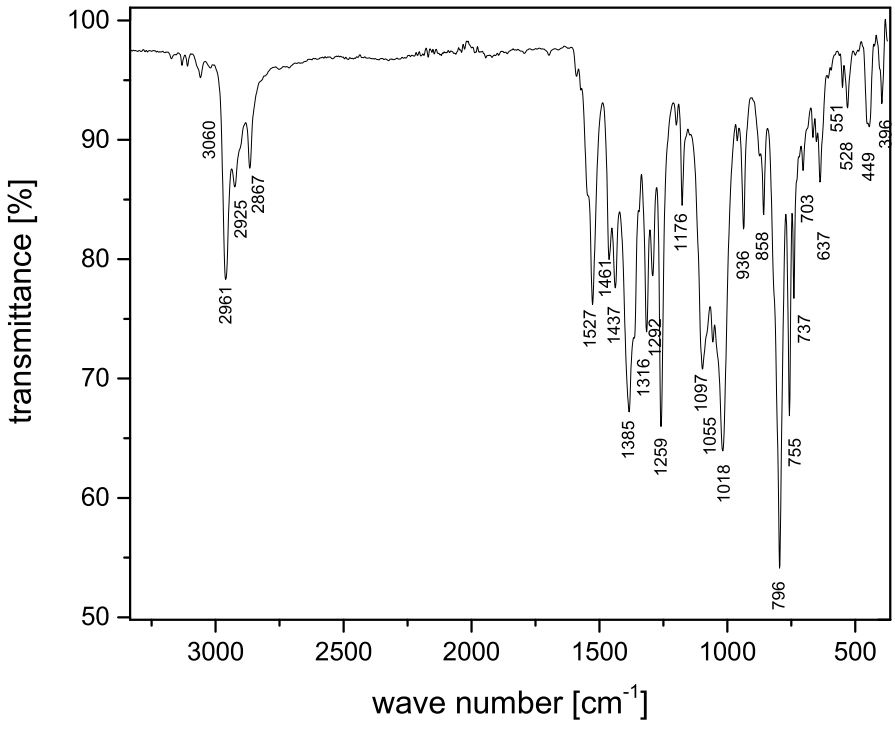

Fig. S16. IR spectrum of IDipp-SbGa(Cl)L (**5**).

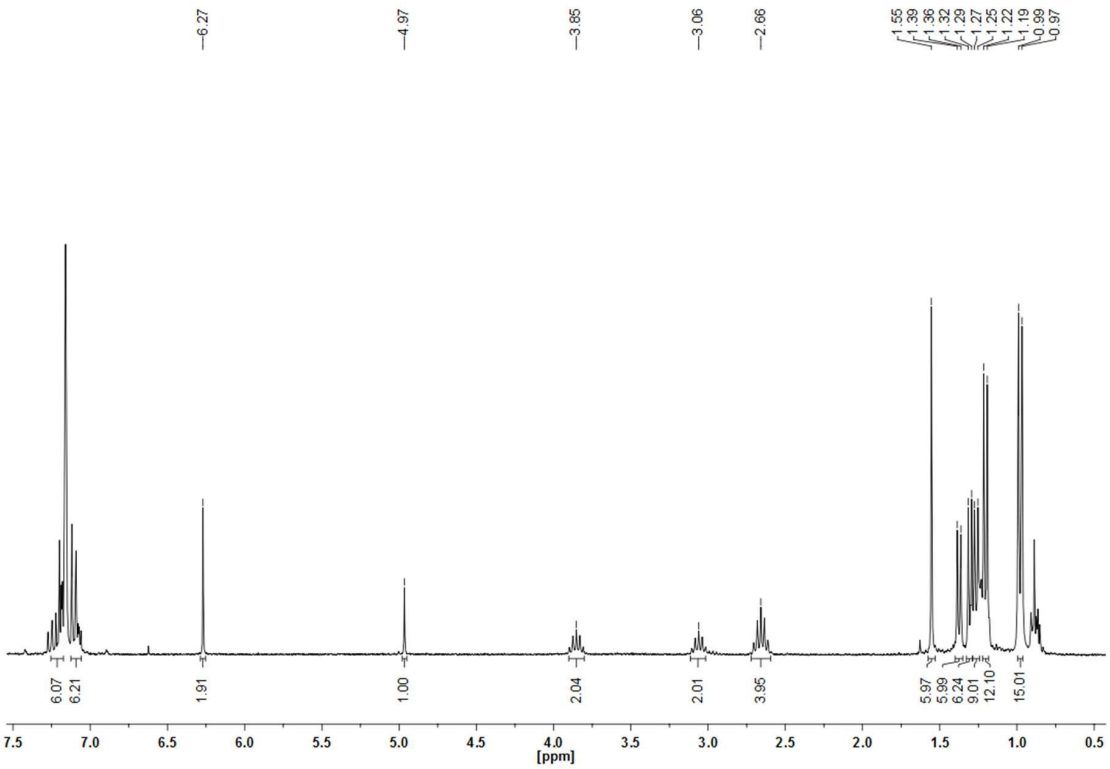

Fig. S17. ^{1}H NMR spectrum of IDipp-SbGa(Br)L (**6**) in C_6D_6.

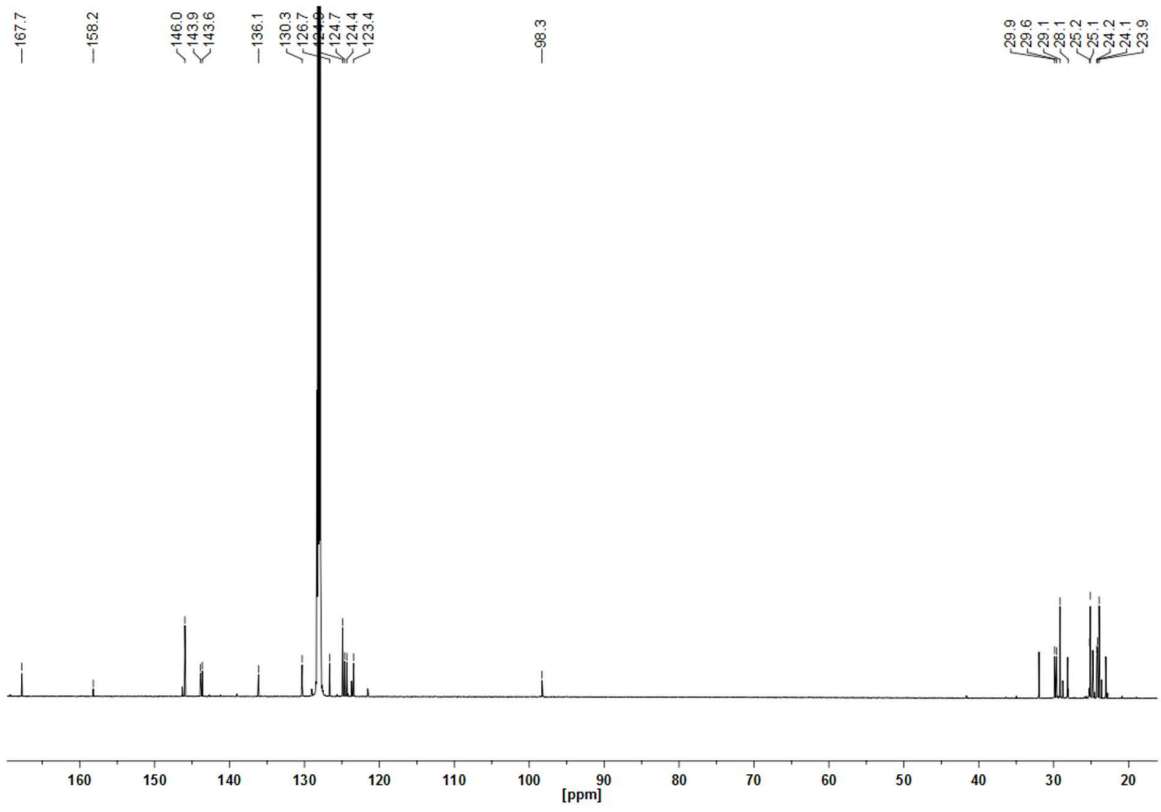

Fig. S18. ^{13}C NMR spectrum of IDipp-SbGa(Br)L (**6**) in C_6D_6.

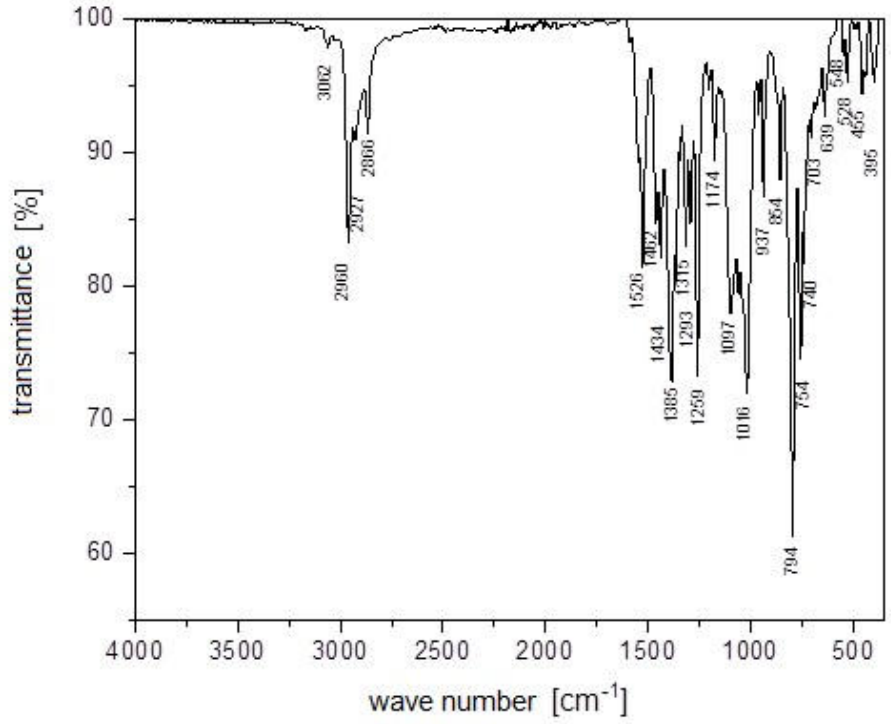

Fig. S19. IR spectrum of IDipp-SbGa(Br)L (**6**).

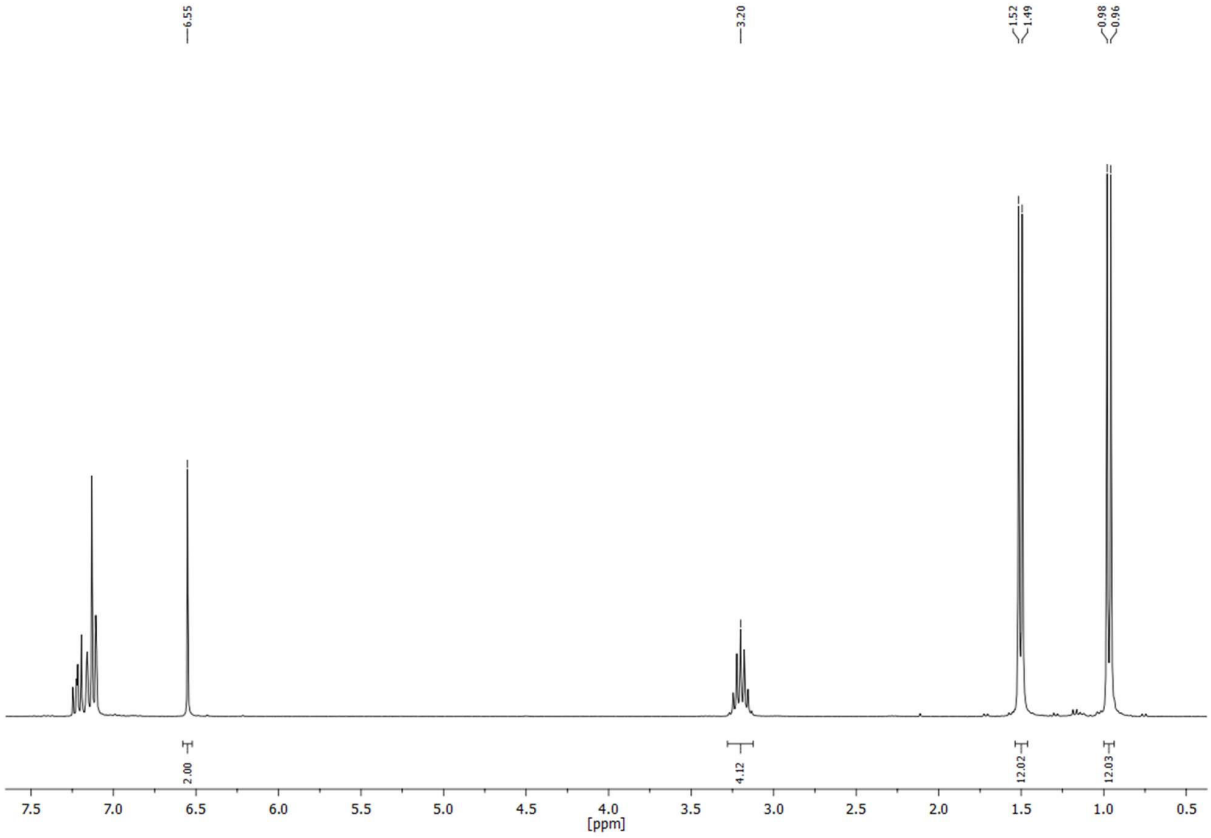

Fig. S20. ^{1}H NMR spectrum of IDipp-$SbCl_3$ in C_6D_6.

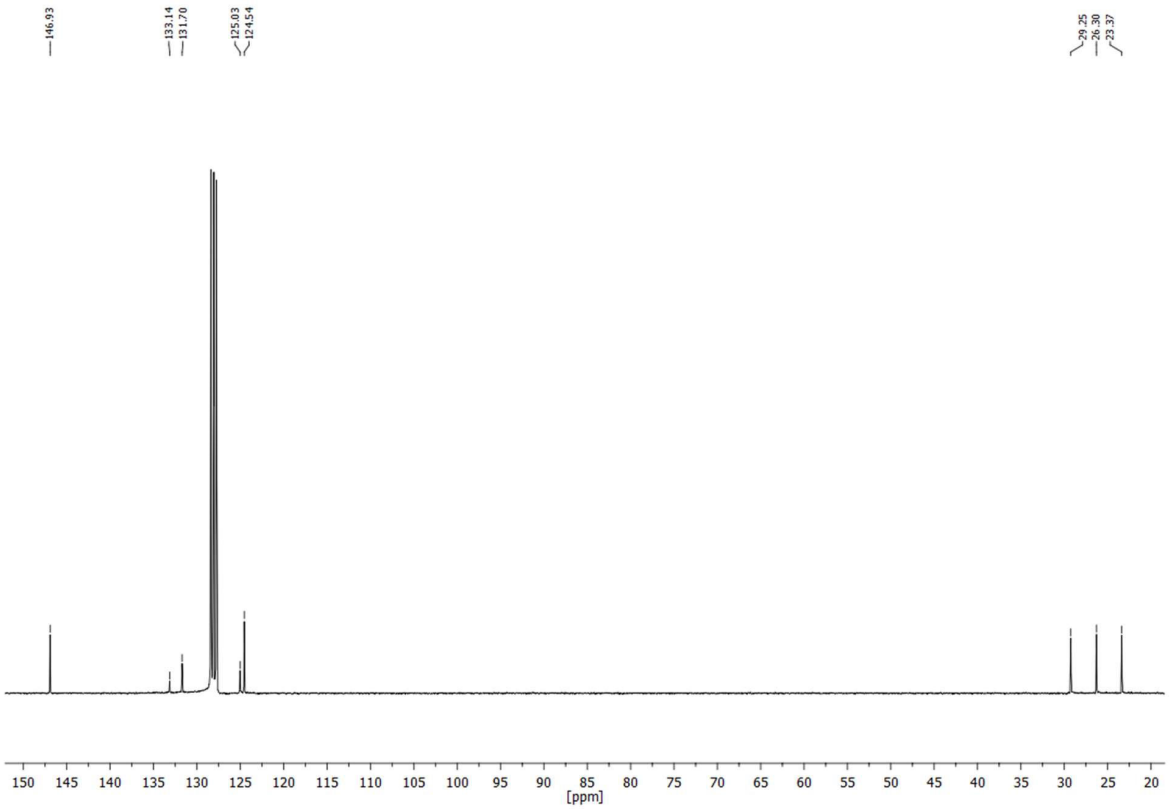

Fig. S21. ^{13}C NMR spectrum of IDipp-$SbCl_3$ in C_6D_6.

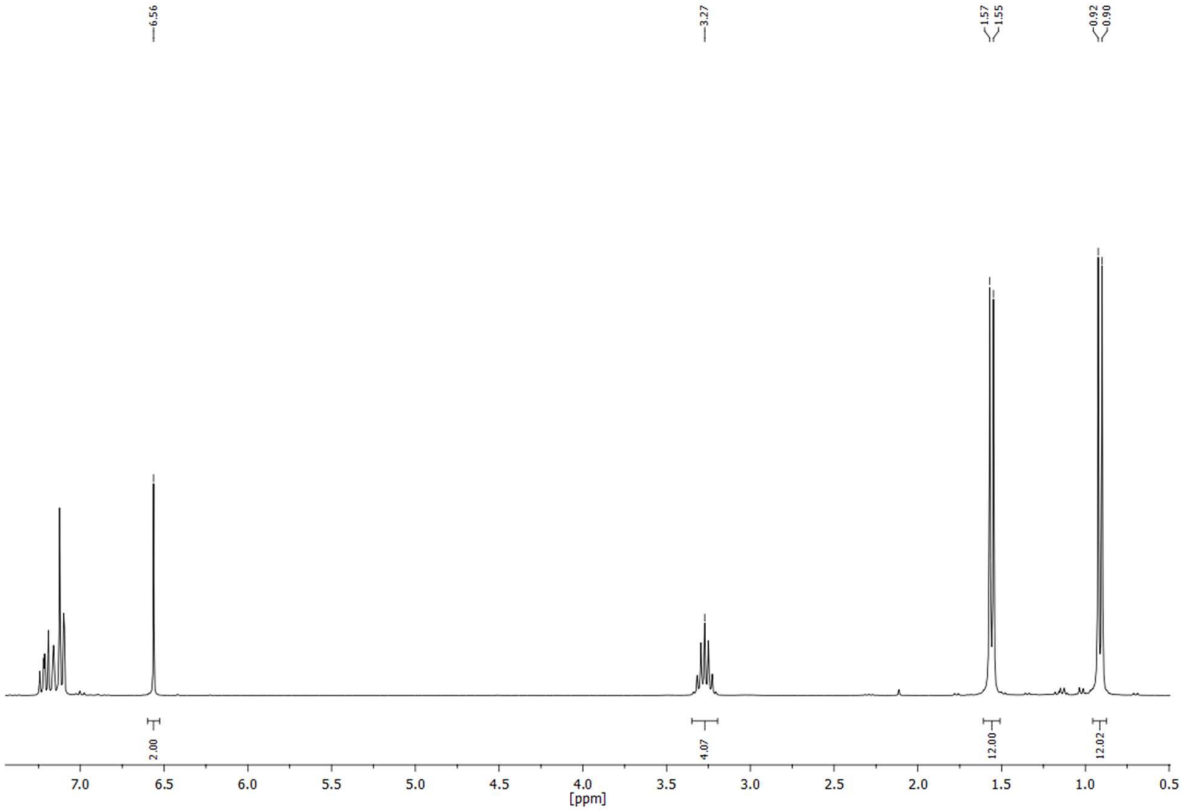

Fig. S22. ^{1}H NMR spectrum of IDipp-$SbBr_3$ in C_6D_6.

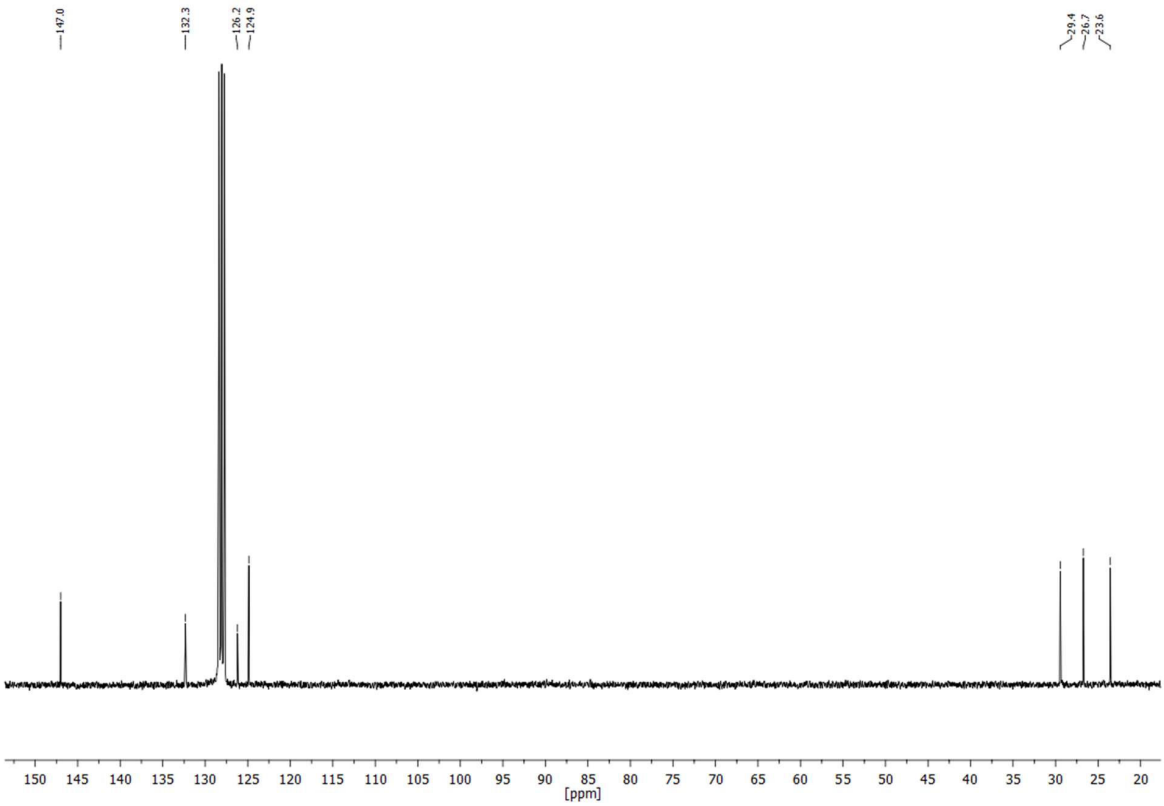

Fig. S23. ^{13}C NMR spectrum of IDipp-$SbBr_3$ in C_6D_6.

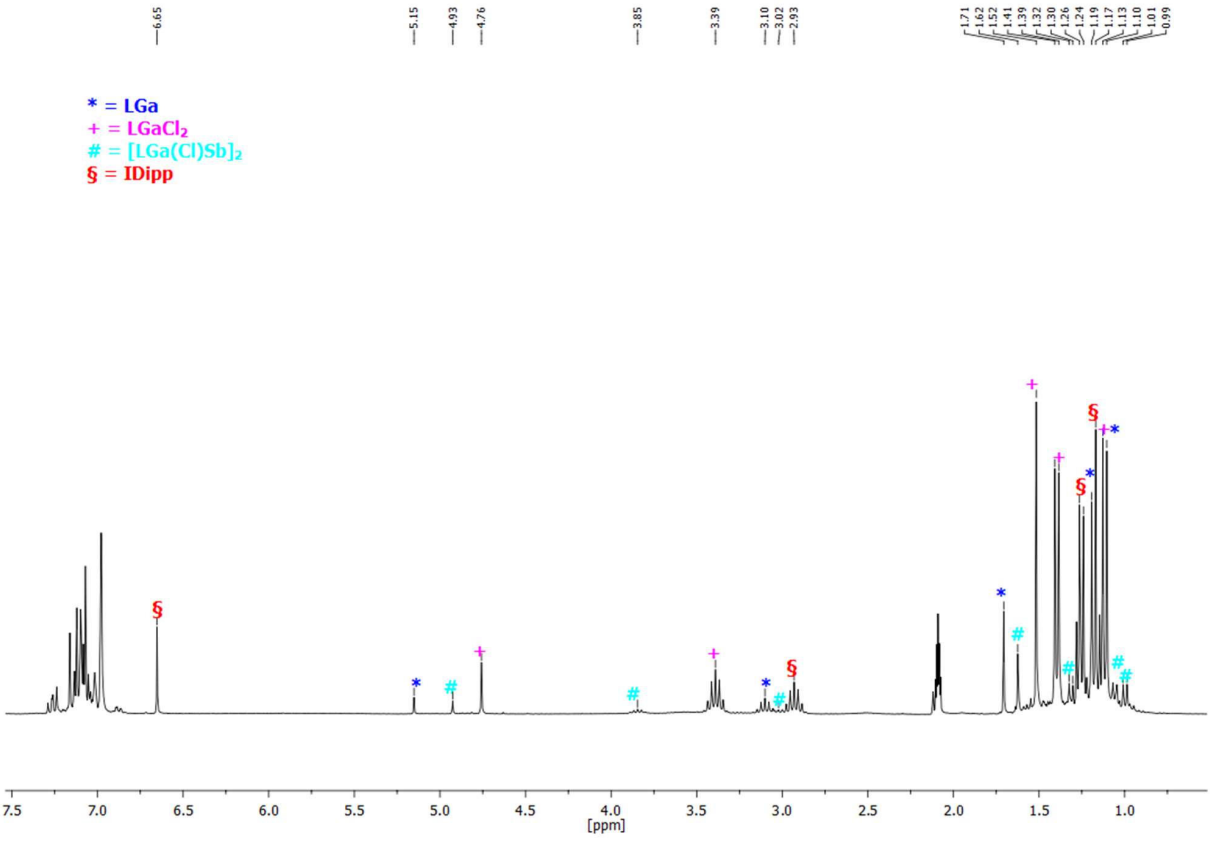

Fig. S24. *In situ* ^1H NMR spectrum of the reaction of two equivalent LGa with IDipp-$SbCl_3$ in toluene-d_8.

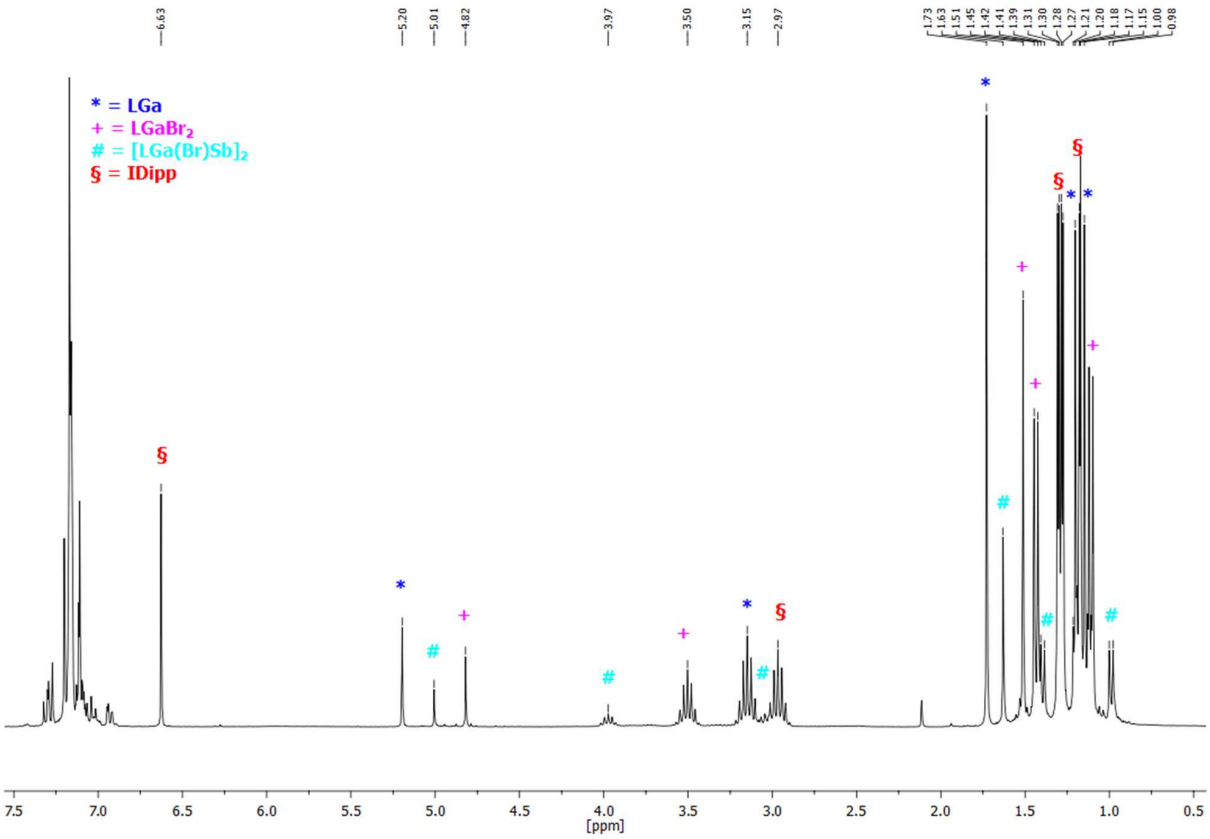

Fig. S25. *In situ* ^{1}H NMR spectrum of the reaction of two equivalent LGa with IDipp-$SbBr_3$ in C_6D_6.

Table S1. ^{1}H NMR chemical shifts of **3 - 6** in C_6D_6.

	ligand resonances (L)				carbene resonances			
	γ*-C*H	**C*H*Me$_2$**	**CH*Me*$_2$**	**C*Me***	**C*H*$_2$**	**C*H*Me$_2$**	**CH*Me*$_2$**	**C*Me*$_2$**
3	5.00	4.03, 3.41	1.67, 1.27, 1.12, 1.07	1.70	1.54	2.69	1.44,	0.82, 1.24
	γ*-C*H	**C*H*Me$_2$**	**CH*Me*$_2$**	**C*Me***	**NC*H***	**C*H*Me$_2$**	**CH*Me*$_2$**	
5	4.91	3.03; 3.77	1.37, 1.31, 1.29, 1.19, 0.99	1.55	6.26	2.65	0.98, 1.20	
6	4.97	3.85, 3.06	1.38, 1.31, 1.29, 1.27, 0.98	1.55	6.27	2.66	0.98, 1.21	

Table S2. ^{13}C NMR chemical shifts of **3 - 6** in C_6D_6 and those reported for ^{Cy}CAAC-SbCl[a] and DAC-SbPh[b].

	3	**5**	**6**	**^{Cy}CAAC-SbCl**	**DAC-SbPh**
C(Carbene)	243.9	157.9	158.2	241.3	205.6

[a] Kretschmer, R.; Ruiz, D. A.; Moore, C. E.; Rheingold, A. L.; Bertrand, G. *Angew. Chem. Int. Ed*. **2014**, *53*, 8176-8179; *Angew. Chem*. **2014**, *126*, 8315-8318.
[b] Dorsey, C. L.; Mushinski, R. M.; Hudnall, T. W. *Chem. Eur. J*. **2014**, *20*, 8914-8917.

B) Single Crystal X-ray Diffraction

Single-crystal X-ray analyses. The crystals were mounted on nylon loops in inert oil. Data of **2** to **5** were collected on a Bruker AXS D8 Venture diffractometer with Photon II detector (mono-chromated $Cu_{K\alpha}$ radiation, λ = 1.54178 Å, micro-focus source) at 123(2), 120(2), 120(2) and131(2) K, respectively. Data of **6** were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) at 100(2) K. The structures were solved by Direct Methods (SHELXS-97)[1] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2017)[2,3]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX2/3). Hydrogen atoms were refined using a riding model or rigid methyl groups. In **2** the central Sb-Br unit is disordered over two positions. The ADP of the toluene molecule suggest disorder however it was not possible to separate different orientations. RIGU restraints were applied to the solvent's ADP. In **3** the molecule is disordered over a mirror plane. RIGU restraints were applied to all ADP. Lowering the symmetry did not resolve the disorder. The crystal of **4** was a non-merohedral twin and the model was refined against HKLF5 data. As vast parts of the molecule are disordered RIGU restraints were applied to all ADP. The aromatic C--C bond lengths were restrained to be equal (SADI). **5** contains a highly disordered benzene molecule, whose electron density was removed by a Platon/SQUEEZE run. It was included in the sum formula for completeness.[4] In **6** a dipp group is disordered over two positions. RIGU and ISOR restraints were applied to the ADP of the corresponding atoms. The bond lengths within the phenyl ring were restrained to be equal (SADI). The structure contains two highly disordered n-hexane molecules that could not be modelled properly. The final refinement was done with a solvent free dataset from a SQUEEZE/Platon run. The solvent molecules were included in the sum formula for completeness. The unit cell parameters suggest pseudo-merohedral twinning however the obvious twin laws yielded a BASF of 0. Consequently, the high R_{int} is likely caused by the weak diffraction of the tiny crystal.

CCDC-1877414 (**2**), -1877415 (**3**), -1877416 (**4**), -1877417 (**5**) and -1877418 (**6**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

References

[1] Sheldrick, G. M. *Acta Crystallogr.* 1990, **A46**, 467-473.
[2] Sheldrick, G. M. SHELXL-2017, Program for the Refinement of Crystal Structures University of Göttingen, Göttingen (Germany) **2014**. (see also: Sheldrick, G. M. *Acta Crystallogr*. **2008**, *A64*, 112-122.)
[3] shelXle, *A Qt GUI for SHELXL*, Hübschle, C. B.; Sheldrick, G. M.; Dittrich, B. *J. Appl. Cryst.* **2011**, *44*, 1281-1284.
[4] Spek, A.L. *Acta Cryst*. **2015**, *C71*, 9-18.

Table S3. Crystallographic Data of **2** - **6**.

	2	**3**	**4**	**5**	**6**
Empirical formula	$C_{65}H_{90}Br_3Ga_2N_4Sb$	$C_{49}H_{72}ClGaN_3Sb$	$C_{49}H_{72}BrGaN_3Sb$	$C_{62}H_{83}ClGaN_4Sb$	$C_{62}H_{91}BrGaN_4Sb$
M	1428.32	930.01	974.47	1111.24	1163.76
Crystal size [mm]	0.122×0.062×0.027	0.151×0.108×0.076	0.122×0.047×0.041	0.332×0.231×0.211	0.063×0.061×0.047
T [K]	123(2)	120(2)	120(2)	131(2)	100(2)
Crystal system	monoclinic	orthorhombic	orthorhombic	monoclinic	monoclinic
Space group	$P2_1/c$	*Pnma*	*Pnma*	$P2_1/n$	$P2_1/c$
a [Å]	13.9460(5)	10.0803(3)	10.1139(3)	12.8959(5)	17.7535(19)
b [Å]	24.3834(11)	19.1276(7)	19.1231(6)	15.5258(6)	17.693(2)
c [Å]	19.1527(8)	24.5267(8)	24.5563(6)	31.0579(12)	38.637(4)
α [°]	90	90	90	90	90
β [°]	91.365(2)	90	90	98.7069(11)	90.929(7)
γ [°]	90	90	90	90	90
V [Å^3]	6511.0(5)	4729.0(3)	4749.4(2)	6146.7(4)	12134(2)
Z	4	4	4	4	8
D_{calc} [g·cm^{-3}]	1.457	1.306	1.363	1.201	1.274
μ(CuK_α [mm^{-1}])	6.689	5.997	6.440	4.702	1.587
Transmissions	0.75/0.53	0.75/0.66	0.75/0.48	0.75/0.47	0.75/0.63
F(000)	2904	1944	2016	2328	4864
Index ranges	-17 ≤ *h* ≤ 16	-10 ≤ *h* ≤ 12	0 ≤ *h* ≤ 12	-16 ≤ *h* ≤ 16	-23 ≤ *h* ≤ 23
	-31 ≤ *k* ≤ 30	-24 ≤ *k* ≤ 23	0 ≤ *k* ≤ 24	-19 ≤ *k* ≤ 19	-23 ≤ *k* ≤ 23
	-24 ≤ *l* ≤ 24	-31 ≤ *l* ≤ 28	0 ≤ *l* ≤ 31	-39 ≤ *l* ≤ 39	-51 ≤ *l* ≤ 51
ϑ_{max} [°]	80.404	79.045	79.414	79.356	28.458
Reflections collected	125208	48321	5782	146208	241231
Independent reflections	14083	5271	5782	13276	30382
R_{int}	0.1740	0.0430	0.1010	0.0471	0.1478
Refined parameters	716	508	454	587	1284
R_1 [$I > 2\sigma(I)$]	0.0931	0.0387	0.0698	0.0317	0.0668
wR_2 [all data]	0.2611	0.0913	0.1905	0.0889	0.1679
GooF	1.428	1.153	1.070	1.029	1.037
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	2.217/-1.731	1.257/-0.941	1.594/-0.701	1.716/-0.518	2.402/-1.433

C) Quantum chemical calculations

1. Structure optimization and bond analysis

The geometric parameters of the species under study were fully optimized in the gas phase at the PBE0-D3/def2-TZVP theoretical level as implemented in the ORCA 4.0 program[1–4] with a corresponding small-core relativistic effective core potential for Sb[5] employing ultrafine grid. The stationary points were characterized as minima on the potential energy surface by vibrational analysis (the number of imaginary frequencies (NImag) was equal to zero) and the structures obtained were used for the subsequent calculations. NBO analysis was performed with the NBO 6.0 program.[6,7]

References

[1] J. P. Perdew, M. Ernzerhof, K. Burke, *J. Chem. Phys*, **1996**, *105*, 9982–9985.
[2] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.*, **2010**, *132*, 154104.
[3] F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, **2006**, *8*, 1057.
[4] F. Neese, *Wiley Inderdisip. Rev. – Comput. Mol. Sci*., **2012**, *2*, 73–78.
[5] K. A. Peterson, D. Figgen, E. Goll, H. Stoll, M. Dolg, *J. Chem. Phys.*, **2003**, *119*, 11113–11123.
[6] A. E. Reed, L. A. Curtiss and F. Weinhold, *Chem. Rev.*, **1988**, *88*, 899–926.
[7] E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, F. Weinhold, **2013**, http://nbo6.chem.wisc.edu/

Cartesian coordinates of the species considered (Å, PBE0-D3/def2-TZVP optimization level).

LGaClSb-^{Me}CAAC, {L= HC[C(Me)N(2,6-*i*Pr$_2$C$_6$H$_3$)]$_2$}, 3'

Ga	3.18517115360477	4.79983483628387	14.75755743298440
Cl	1.08686531308396	5.12532166983436	15.48631523197114
Sb	3.82250796739022	4.26343677195021	12.30516213781744
N	3.85027612339452	3.22042738264602	15.74805916274243
N	4.13657915380780	6.10406051851659	15.91827767911174
N	2.71688620178745	5.30199421340872	9.76229747276433
C	4.43603623287502	5.80344505321264	17.16845209054610
C	4.34165880020276	4.51431286804150	17.70839282499128
H	4.59180237399210	4.43432017789178	18.75733934495574
C	4.15799196463516	3.30551201799707	17.03497307648785
C	4.91854220283035	6.87764171697904	18.09902981980387
H	5.37915224491583	7.70444472936173	17.56130151355217
H	5.62781061302683	6.47016806138809	18.81867638272844
H	4.06774563134996	7.27645679093914	18.65742026176293
C	4.31541899293245	2.04560716912959	17.83441010787714
H	4.78603385530285	1.25494551832912	17.25245816049229
H	3.32239635043196	1.68252710051301	18.11810675682152
H	4.88795202544584	2.22389573541783	18.74261956609531
C	4.41114513645076	7.38023552566249	15.34364391194569
C	5.55830711308972	7.49097929704679	14.53545877934249
C	5.77180411574328	8.67864501376614	13.84955325080885
H	6.64370055428431	8.78336718115563	13.21703945874140
C	4.88064768884213	9.73266972978276	13.95290460472127
H	5.06141484364171	10.64808414985056	13.40107105598679
C	3.77360086937024	9.61757179628815	14.77002539145419
H	3.08573014641032	10.45155061686931	14.85692471990459
C	3.52000360244147	8.45290385571093	15.49263226404280
C	6.56450394315358	6.36496218561733	14.46291802431772
H	6.00168467954571	5.42761829588711	14.49818305463495
C	7.36663096422071	6.36064216531776	13.17622024274464
H	6.70493068411823	6.34040404496982	12.31156451218303
H	8.00030826814919	5.47429643181178	13.13370760492383
H	8.02467676724168	7.23043565915907	13.10022996436862
C	7.50215573607461	6.39075047925074	15.66641380048709
H	8.22831014597474	5.57519150910251	15.60187434859183
H	6.96473733373982	6.28472214444412	16.60754404192929
H	8.05812446340303	7.33217668068910	15.69911362460194
C	2.32961720450113	8.41418956988243	16.42880373069278
H	2.29809236203427	7.42773781729087	16.89558922975455
C	2.46918432807965	9.47205428077792	17.52464022149065
H	2.32752098410548	10.47451762138005	17.11121410288590
H	3.44930783062997	9.44708207143591	18.00421002562431
H	1.70767414277854	9.32443924431242	18.29443728606758
C	0.99486829630675	8.61610310575088	15.71763133161306
H	0.95336204555918	9.59201321432190	15.22541139359814
H	0.18300984007506	8.57638823485494	16.44870499170619
H	0.81024125192176	7.83869851810043	14.97978060116156
C	3.95850259130071	1.98261018194758	15.04333875917371
C	5.20371628799326	1.60165391011032	14.51201285398263
C	5.27111122261596	0.43670765871899	13.75548982152197
H	6.22329599421927	0.12849659026217	13.33806303555462

C	4.14706914196486	-0.33178133230454	13.51476544618170
H	4.21895255314513	-1.23024825205220	12.91331756159175
C	2.93155685892312	0.05553028436655	14.04446466860130
H	2.04705641281111	-0.54039546366712	13.84875427455543
C	2.81343681307370	1.20758037519710	14.81392095882659
C	6.47029470313746	2.39290385735009	14.75705565045262
H	6.18928499233128	3.33303618843707	15.23734369107489
C	7.21155556688839	2.72763780921516	13.46680175825866
H	6.58842716815874	3.31108286591822	12.78651424186817
H	7.53038683422743	1.82409646113143	12.94225681406427
H	8.11078838679583	3.30500688079503	13.69317798877278
C	7.40569856057546	1.64456677404884	15.70403538748086
H	7.76587568888279	0.72419125163859	15.23662806814212
H	6.91487982856064	1.36977385813855	16.63868753648072
H	8.27637797618784	2.25935705216372	15.94626320380020
C	1.46149941823357	1.59613914461222	15.35950131383174
H	1.58895432712840	2.48189813172116	15.98298367013226
C	0.86702847684612	0.49440703595734	16.22857408179612
H	0.61995766001439	-0.39046914935372	15.63662819480737
H	-0.05289644945964	0.84677619924001	16.70230444814924
H	1.55863250217962	0.18470794126076	17.01605537677126
C	0.50943051909970	1.97431862220288	14.23013419388579
H	0.95376939430536	2.73231871787422	13.58233807243728
H	-0.41832745577557	2.38060530874602	14.63855022918538
H	0.26746036754309	1.10158521333674	13.61719341376169
C	2.65368341482622	5.45915975913804	11.08968783653661
C	1.64424425788690	6.54029957533078	11.41167227350502
C	1.46024951995331	7.24467520715332	10.06013797006301
H	0.43471093681589	7.58813008410400	9.91414058957056
H	2.11063933727663	8.12175118205964	10.02518919159416
C	1.88935721809931	6.26043046059363	8.97298411159725
C	0.33727494720280	5.89316211020834	11.88100805274810
H	-0.41906954718952	6.67068632406474	12.02018073731534
H	0.47648628912786	5.37719705933677	12.83095787425043
H	-0.04458598065267	5.17420178217777	11.15433141710725
C	2.14052836757055	7.51462078669039	12.46406448051633
H	3.12749406507242	7.90860618616474	12.21776634077103
H	2.20590519594559	7.03390864255951	13.43784830044386
H	1.44480213533136	8.35232228271192	12.55531279155247
C	0.72440831685999	5.54891597117710	8.30301703153115
H	0.12522776903758	6.27654055247213	7.75060040793260
H	0.07836772651305	5.04930296680655	9.02377516149571
H	1.08941079660572	4.80537604258602	7.59261594937646
C	2.70622482227178	6.96293972265121	7.90672207665538
H	3.09381506019830	6.25685389524025	7.17087708450989
H	3.53450712750381	7.51181666182916	8.35086285496043
H	2.06609317812687	7.67832438340975	7.38562756260534
C	3.43919669776522	4.24358891554275	9.11907906302406
C	4.73890079075018	4.47924170201555	8.63485647456556
C	5.35303369532059	3.48286315791339	7.88365339755463
H	6.34861483388519	3.65594395395747	7.49299608511397
C	4.73413447535066	2.27113848712289	7.65215402199314
H	5.23018060188329	1.50687172582748	7.06499026193427
C	3.49639985982890	2.02281062246843	8.21241280407747

H	3.03734301441554	1.05094684177433	8.07465929124364
C	2.83098908900506	2.98061003831568	8.96864355565142
C	5.56337339141317	5.70139669565210	8.98486643737295
H	4.95696039297042	6.34826472749485	9.62400702401398
C	6.78766689902885	5.26912957150342	9.79364109234351
H	7.45802701444068	4.65606294488721	9.18602547378707
H	6.49334463127721	4.68659955908776	10.66695373237052
H	7.34820280111273	6.14401425664749	10.13062906632518
C	6.03545147941040	6.49827367956988	7.77110739147644
H	6.73289494463056	5.90975520018238	7.16933992591630
H	6.56957388637833	7.39098919453505	8.10560841722747
H	5.22047242447175	6.81317848093659	7.12206717401247
C	1.54121797034693	2.56122768959922	9.64775806541458
H	1.14030828832139	3.41692304015426	10.19367987986955
C	0.48742749599574	2.06872630189595	8.65923365955949
H	0.23007531589649	2.81905984734658	7.91215782567234
H	-0.42423239754458	1.79146852719299	9.19435099014892
H	0.83545569779363	1.17791031849515	8.13120316787579
C	1.81780661342964	1.45616674100865	10.67054588430248
H	0.89058537807266	1.17413038717664	11.17513805857144
H	2.53274980423737	1.77945324933599	11.42677932847290
H	2.21753107092334	0.56398561455074	10.18144304449504

LGaBrSb-^{Me}CAAC, {L= HC[C(Me)N(2,6-*i*Pr$_2$C$_6$H$_3$)]$_2$}, 4'

Ga	2.01578794601587	4.44829256713576	9.74762403615611
Br	4.28571665059432	4.46522075103336	8.96151081989098
N	1.06888343391285	5.79912342935108	8.64357112328398
C	0.76775452950495	5.55007066478573	7.38126954947455
C	0.35740513763206	6.67254196321154	6.47504843705983
H	1.19208160688439	6.90668422949835	5.80797841480071
H	0.11091262763563	7.57362012572564	7.03249279846107
H	-0.49027684580462	6.38323294899815	5.85375852975715
C	0.77410012370229	7.04783892833380	9.27423717667411
C	-0.49137166238409	7.24409433772710	9.85513866390230
C	-0.69890994992062	8.38596943138758	10.62102563326791
C	0.30237147917647	9.32069937500941	10.80185816717894
H	0.12677927910528	10.19318364800388	11.42017349869771
C	1.51957965996806	9.14524003884409	10.17140439574421
H	2.29208305656837	9.89762037252803	10.28589351811387
C	1.77444022812637	8.02346530288696	9.39110182347107
C	3.07574308063445	7.93132103936704	8.63116605263225
H	3.12693184625048	6.94980752688677	8.15727703327477
C	4.29536034649389	8.06207702446481	9.53463056913481
H	5.20658549994348	7.90309127691727	8.95349644554209
H	4.27345744080146	7.31854389928921	10.33342896519123
H	4.35377878929274	9.05580017519172	9.98778309112485
C	3.09746402614572	8.98908489165585	7.52852105965893
H	2.26672124998530	8.85983876656347	6.83198194482505
H	4.02927889718994	8.93150808955426	6.96002508171564
H	3.01717791238981	9.99435876370920	7.95148073238264
C	-1.64713687625320	6.29788250269371	9.61763502722705
H	-1.25516926853414	5.40288472383754	9.12945006510201
C	-2.34625252541702	5.86377786559004	10.90113431562686

H	-2.80931820088927	6.71165535388045	11.41163830518143
H	-1.64809796327162	5.38989258590416	11.59348871691376
H	-3.14137091437148	5.15019649198986	10.66932122454600
C	-2.65745106871710	6.95122416669559	8.67487111733645
H	-3.11857244861328	7.81760652031115	9.15701372901766
H	-3.45325396861582	6.24903318715078	8.41456175781707
H	-2.18976458490699	7.30062044934373	7.75254043976862
Sb	1.30075214965925	5.10961032035691	12.14771640986795
C	2.55356121219686	4.10895510394159	13.45075653178989
C	3.72388887210278	3.18272083786679	13.19008277775012
C	3.89842527238048	2.48653618082980	14.54286542893793
H	4.93889336203038	2.22244242631336	14.74035227997901
H	3.31367995081326	1.56332760454537	14.53881291243644
C	3.33492805212611	3.42469313353283	15.60433244162913
C	3.48607916841111	2.16241384309366	12.09455083280814
H	3.52395425210161	2.63086998589027	11.11239988993165
H	2.52284229286656	1.66288289051079	12.20427417697860
H	4.27487969609572	1.40551916190051	12.11834400035067
C	4.95233659324165	4.02690093794404	12.82837330271114
H	4.80940282635805	4.51828467723748	11.86515538951987
H	5.82801242161665	3.37531956218300	12.75840826169365
H	5.15961294567280	4.79399887319891	13.57442424607049
C	1.58402752651366	5.25156155677001	15.40385461201289
C	2.05200843100899	6.57224948950404	15.55412483409359
C	1.31910771730283	7.44096245003057	16.35474432792972
H	1.67871356648395	8.45336178476983	16.49565010951391
C	0.14462702765254	7.04873707847685	16.96501817953111
H	-0.40147101151456	7.74096027723471	17.59561270606451
C	-0.35225496032210	5.78432841700157	16.72398196740997
H	-1.30807899191751	5.49757279588790	17.14545659862629
C	0.33344833675983	4.87506081767200	15.92557698487667
C	3.25535014675878	7.13895071520456	14.82753475452572
H	3.72219139055272	6.33622006369437	14.25541025641519
C	4.29415170696165	7.74196959181495	15.76848724243528
H	5.13742103131192	8.13256143404561	15.19406772111630
H	4.67915949896224	7.01655128469891	16.48571823129603
H	3.87274901701703	8.57745846028498	16.33213041330325
C	2.78950280262618	8.20093315282143	13.82756134938144
H	3.63528388203431	8.56253684893810	13.23662923818721
H	2.35031460546980	9.05754899249812	14.34602598724198
H	2.04627984896792	7.79739009738168	13.13931196478411
C	-0.79048819645309	2.75166118959512	16.77949097561661
H	-1.25567065801367	1.82206485588633	16.44217434472360
H	-1.53041608053798	3.28204080664718	17.38387019638741
H	0.04784561610312	2.49847142154944	17.42633559550016
C	-1.63062917096713	3.92287421360030	14.75690183846203
H	-1.37523247113773	4.49508640589617	13.86444401041720
H	-2.32961543653146	4.51357820432278	15.35370561945528
H	-2.14262815865538	3.00917075886180	14.44889905322829
C	2.57907140811544	2.64072253992037	16.65894446502859
H	1.81959442165211	2.00660266188652	16.20541018624255
H	2.10905419139140	3.30011971158290	17.39001099251711
H	3.28598816718151	1.99773187167498	17.18916246837028
C	4.39224509687434	4.26526878994914	16.30202910131814

H	5.04674163392650	3.60850624841098	16.88038483513733
H	3.92244629781776	4.96874603927832	16.99154445018198
H	5.00682987110529	4.82831374627818	15.60208407556795
N	2.42400724109558	4.27444857162163	14.77503127207662
C	-0.37922510560219	3.58604250619999	15.57035568091110
H	0.28262286592317	2.99385899453730	14.93280254910759
C	0.80692740059771	4.27403523096141	6.81590405893363
H	0.53386732448946	4.22285083303850	5.77061332805976
H	-1.66390771534069	8.54404155580524	11.08906998182586
H	5.59088294099524	0.85323187984433	8.21724281988834
H	4.92966776477290	-0.11213042951034	9.53955244770999
C	4.79665833957936	0.81037891697891	8.96741692427050
H	4.11349232389810	-0.07091661925070	6.43107606859782
H	4.92562129010202	1.65983938523854	9.63545786684838
H	3.66634004672940	-1.23541310860555	7.67681623226552
C	3.39583440766200	-0.27529926815741	7.22921144449276
C	3.43703213234510	0.83677424117890	8.27788315125386
H	3.01328163488710	-1.20418218941172	9.93883503377244
H	2.40789074495466	-0.38698713199857	6.78054872826172
H	3.34155346316499	1.80233219625498	7.77689267049959
C	2.22234027743019	-0.46790650391002	10.02601339522928
C	2.28813978712721	0.68963386234178	9.25295514912352
C	1.18005737968451	-0.69677488034138	10.89908830647325
H	1.15444995162398	-1.60163428335288	11.49516749325783
H	1.51772557577015	1.50092687628711	6.10608755539233
H	0.27878261920814	0.99860628436085	7.25428637707253
C	1.25927276044640	1.63350909202830	9.38778210202119
C	0.62117273201544	1.82824062205110	6.63759979562724
N	1.31374862127323	2.89519036214726	8.72396616318813
C	0.94538322302020	3.04005863782605	7.46124562997172
C	0.15807491889199	0.23197782937764	11.00151642850792
C	0.17412996532230	1.40306702366899	10.25470199245435
H	-0.13816951857608	2.06587892390593	5.89462541226809
H	-0.66042293169113	0.04099294381654	11.68297355411495
H	-1.40972609460422	2.49748949404522	8.20697473679391
C	-0.96973398518753	2.38705030808631	10.34189666324710
C	-1.91243579495090	2.27644673647042	9.14723431913272
H	-0.53060018472952	3.39058222695323	10.32439755077472
H	-2.33978564687386	1.27225704361747	9.07884873909865
C	-1.74746785626228	2.27408830150513	11.63857683627296
H	-1.08088340862707	2.36001795931026	12.49727572767368
H	-2.29613948002970	1.33083622159074	11.70904778699735
H	-2.73577259593197	2.98740000379698	9.25630336756047
H	-2.47997315703274	3.07956562081840	11.69853382966240

LGaClSb-IDipp, {L= HC[C(Me)N(2,6-*i*Pr$_2$C$_6$H$_3$)]$_2$}, 5'

Sb	5.75941752948087	10.06302917021478	4.12986640708204
Ga	6.01605095472309	12.46642483253209	5.02701683653295
Cl	7.43446785823561	13.27915190469231	6.53786379244087
N	4.31504745414706	13.39482045521114	5.53852941170614
N	6.33807214198280	13.66466272947410	3.45281002059453
N	7.32364360575633	7.52343263598794	4.36517746154091
N	7.58607618119691	8.41129282989018	6.30557181568559

C	4.14298264604011	14.67559225921290	5.24811237286737
C	4.96809069178599	15.40457072285222	4.38733571509990
H	4.73562751694744	16.45588906286071	4.30209068270498
C	5.92084781076634	14.92365127014645	3.48923728001934
C	2.98972898938779	15.42880549472119	5.84643326459151
H	2.78816278107754	16.33342745335893	5.27608950402557
H	3.22914030042429	15.71689812157545	6.87208898749039
H	2.08862186332640	14.81795794854635	5.88924160421412
C	6.46551015035582	15.91244638714370	2.49944842407526
H	6.41376255313826	15.52882674813103	1.48012329823109
H	7.52064517680007	16.09996260568709	2.70976083296477
H	5.92466758269393	16.85471455827536	2.55787307553077
C	3.33223214383297	12.73109086208735	6.33402822695473
C	3.31534414509170	12.89105416026561	7.72726892052089
C	2.31768936891219	12.24783824856062	8.45384065237481
H	2.29310477433227	12.36338886406416	9.53145385454167
C	1.36446200127215	11.46642493896975	7.83186625758378
H	0.59618360972897	10.97360255789232	8.41669230715093
C	1.40244061313988	11.30545109244688	6.45837610680392
H	0.66047437095839	10.68245914437587	5.97494847172912
C	2.37773983787038	11.92685883050622	5.68866124956474
C	4.34721979466695	13.70915246404019	8.46930492746969
H	4.95160545150272	14.24695745314684	7.73655227230211
C	3.71991600411524	14.72481119075444	9.42061994682311
H	2.98205180966763	15.35964891825506	8.92554338215960
H	4.49498049847403	15.36874619443372	9.84303591618565
H	3.21659278697197	14.23047401757936	10.25539128128980
C	5.28825733262226	12.78689469552901	9.23302608170990
H	5.76589006551338	12.07355442214197	8.56507043842023
H	4.74311961609557	12.22760361788962	9.99900448055669
H	6.07850928915725	13.36093721038136	9.72317118620321
C	2.37097286961078	11.77619810469328	4.18550118477318
H	3.40942527856985	11.85768769327910	3.85461848467449
C	1.59080924068528	12.90521022722794	3.51598749110772
H	1.56561851372755	12.75917597361950	2.43332663227977
H	2.03970689828349	13.88029742274209	3.70875820893105
H	0.55924229017167	12.92611563196806	3.87827667252564
C	1.85476820701468	10.42218357041926	3.72350152433893
H	2.04200218507804	10.29926131814235	2.65443340639373
H	0.77711224451864	10.32165270131156	3.87776874433280
H	2.36241621329049	9.61261585422356	4.25011388768987
C	7.10913541787114	13.25212077375798	2.32166417891204
C	8.49439537298390	13.45784900909945	2.28510278819381
C	9.18364385799481	13.13391147721368	1.12065210467572
H	10.25455296273354	13.29653117086828	1.07787549478095
C	8.53158789267446	12.60385343598904	0.02494278985995
H	9.08530312041296	12.36106702589973	-0.87490423281720
C	7.17154868799171	12.36042008134396	0.09163207000760
H	6.66708379406994	11.91864569016529	-0.75895225701603
C	6.43975349617478	12.67310564271747	1.23045616182685
C	9.26065212300620	13.97730570889991	3.47736392043196
H	8.54222171957910	14.34314893577247	4.21309392623699
C	10.02833942831449	12.83286148873036	4.13169774899907
H	9.35463325266079	12.02342874429698	4.41830085228235

H	10.53776189070944	13.18336354898136	5.03074333236824
H	10.77677246024613	12.42729636276000	3.44436160564157
C	10.20846155398772	15.12022219237888	3.12953418240506
H	11.02704232757937	14.78560365805673	2.48723752043033
H	10.65377663681827	15.52599430838467	4.04095115558779
H	9.69651688174947	15.93432771112533	2.61142063700232
C	4.94806300780164	12.43123921404897	1.25853163539065
H	4.65996584960409	12.34444001808778	2.30885435608255
C	4.18303103677098	13.61785739663733	0.67526158789172
H	4.50126998565825	13.81118839406089	-0.35303034016284
H	4.34038803279497	14.52711006268611	1.25687555151042
H	3.10981356176362	13.41308377016833	0.66379468403745
C	4.54505990036066	11.13841357705700	0.56167537061945
H	3.48604579176347	10.93649132775344	0.74010699990983
H	5.12173311830431	10.29171143266871	0.93898437230778
H	4.68162989781054	11.20019578274270	-0.52110054466059
C	7.05948733388415	8.66128940470953	5.07528377868550
C	7.96525084405556	6.58578515028806	5.14167019546135
H	8.25316060887355	5.62660247500293	4.74916228000708
C	8.12713498140738	7.13763250496186	6.35592431134995
H	8.55879453141289	6.75066855036275	7.26134339754598
C	7.00800882072103	7.31471902807537	2.98851593533736
C	5.79239806273845	6.70795902474972	2.66323325517147
C	5.52975659221922	6.48608693197512	1.31700178165148
H	4.59557004219397	6.02166786456245	1.02531075460158
C	6.43910826411333	6.86338361735897	0.34354901639431
H	6.21242902013215	6.68815444153699	-0.70196698604425
C	7.63203992348233	7.46792658560198	0.69731635389086
H	8.33210157127139	7.76794327681951	-0.07370114205285
C	7.94390433209190	7.70653483122603	2.03051848750828
C	4.80077196845128	6.29917271643396	3.72711045420139
H	5.05746244880007	6.84069205098737	4.64093340292712
C	3.37422692743502	6.69241415119194	3.36665607119085
H	3.31782545836590	7.75375854743853	3.12119127905926
H	2.70945671836822	6.50190417942584	4.21255070497768
H	2.99549704653960	6.11822818867017	2.51737388008367
C	4.90169265284677	4.80399747659588	4.01938938735742
H	4.66236613608469	4.21840707869846	3.12766926426389
H	4.20184175295585	4.52011908814421	4.80935614435925
H	5.90687363296858	4.52463606185560	4.34230008692944
C	9.24513365926789	8.37291978586262	2.40473812530128
H	9.24859399296925	8.52312101559591	3.48634870202069
C	10.43658425672961	7.48600232163553	2.05555635560953
H	10.49422923250451	7.30972663975406	0.97828298766374
H	10.37034146917133	6.51338833636027	2.54925941472408
H	11.36899480454218	7.96365500699567	2.36626103521477
C	9.35818161694655	9.74749747493437	1.75993210336544
H	9.39500633102923	9.67812101590309	0.67011932719484
H	10.26998101302774	10.24942114063596	2.09114773210433
H	8.50590974942415	10.37255812344902	2.03089692766770
C	7.45331917138777	9.16487865318381	7.51480125748497
C	6.29948770066731	8.96148999217569	8.27595362911293
C	6.26547863753243	9.51727236137548	9.54901361052929
H	5.38628923090869	9.37558544901082	10.16648399322616

C	7.33185150378583	10.25250649593220	10.03035230919299
H	7.28646154744611	10.68315259698196	11.02401891457279
C	8.44533225693538	10.46971082864344	9.23869541016875
H	9.25647549015443	11.07645275128952	9.61861648034610
C	8.53770670488878	9.92630755020212	7.96243117479962
C	5.13491169762746	8.13934765958389	7.77592722149714
H	5.31474736219430	7.90103329404213	6.72604216316353
C	5.02105980065575	6.82574912316733	8.54411907633576
H	4.19912317918743	6.22427643694571	8.14754995524773
H	4.82440470180131	7.00520167098471	9.60440104728005
H	5.93883353343714	6.23758837120076	8.46921139304382
C	3.83642342009224	8.93324359029627	7.82289911840144
H	3.91777192792221	9.84289256613400	7.22654130704755
H	3.56640908152173	9.21456673991774	8.84342702385640
H	3.01593663078605	8.33803376548175	7.41463225212835
C	9.77928797643777	10.12854400943964	7.11964021203970
H	9.45985517545585	10.14397591927951	6.07245554989582
C	10.78027504129413	8.98563146029300	7.29903323650362
H	10.38249158167906	8.02361836779096	6.97876093440954
H	11.07545827660540	8.90155953704966	8.34854505249000
H	11.68028253833958	9.18302611521349	6.71125272780159
C	10.48295836550520	11.44709153729724	7.41150656274691
H	11.28218628897351	11.60029419366680	6.68392504409676
H	10.94867146916327	11.43904334233063	8.40061010851713
H	9.79532960725437	12.29003901947596	7.35200779081327

LGaBrSb-IDipp, {L= HC[C(Me)N(2,6-*i*Pr$_2$C$_6$H$_3$)]$_2$}, 6'

Sb	5.79824104452346	10.06865886805655	4.11389890686126
Ga	6.00386708847910	12.45746670995355	5.07324336925092
Br	7.47390769282488	13.30594513877118	6.74479384488049
N	4.28743701752751	13.37469026887688	5.58065546413296
N	6.33798946716775	13.67410321313526	3.51556517348043
N	7.32927513294934	7.50921834818773	4.32679881601700
N	7.61887805601690	8.38027888226075	6.27086247656276
C	4.11564244288502	14.65597417741210	5.29491577515693
C	4.95863545647922	15.39884944419021	4.46210903869901
H	4.72482314666219	16.45099646749298	4.38957631687013
C	5.92189619420333	14.93400068915161	3.56892182613724
C	2.94490915763974	15.40577455118675	5.86375662305988
H	2.69682267137317	16.25598609955684	5.23094007132297
H	3.20189170946285	15.78593287166152	6.85479982383790
H	2.06885729889744	14.76943089630258	5.97748237194644
C	6.47953854834896	15.93897544886563	2.60316193034152
H	6.42855860572537	15.57870949359233	1.57529967284270
H	7.53537883386351	16.11193851172006	2.82198629542786
H	5.94690287704991	16.88458701106411	2.68008280749907
C	3.29315989117468	12.69948474659017	6.35407601658682
C	3.23144248743132	12.86273020106660	7.74640370547929
C	2.22378239595407	12.20332229937702	8.44471423947079
H	2.16603308471952	12.32233930485557	9.52069497567323
C	1.30278867452121	11.40365743811206	7.79909964670870
H	0.52719146027249	10.89841527787032	8.36323534907059
C	1.38136236680874	11.24369188359864	6.42734215606929

H	0.66243622021971	10.61014093110935	5.92351890111287
C	2.36648905056676	11.88156285253211	5.68456260760638
C	4.21240829828922	13.70895034782835	8.52553846929971
H	4.85621385263316	14.23178731282839	7.81568717142288
C	3.51818260849631	14.74380248031739	9.40834426727844
H	2.79891576219849	15.35028773416582	8.85474686072851
H	4.25918329360330	15.41268959710878	9.85269214496221
H	2.97695490063653	14.26576672419199	10.22878843090857
C	5.11242070648361	12.82142031688430	9.37599839090613
H	5.64224445486459	12.09730746854382	8.76168531809917
H	4.52631866156167	12.27724283107396	10.12282081969389
H	5.86091516136427	13.42224509282341	9.89872306619102
C	2.39399619613271	11.73890629150226	4.18133483433331
H	3.43983096793092	11.81915531630506	3.87462984562556
C	1.63114333408793	12.87400170903874	3.50246745023800
H	1.63055972637899	12.73556265088615	2.41859572701024
H	2.07659266125968	13.84708029276358	3.71265807330457
H	0.59167479649336	12.89366729793841	3.84131734048652
C	1.88583462158466	10.38933047674331	3.69889058950492
H	2.09953884460434	10.27191599268579	2.63437464290500
H	0.80438692861769	10.29104932253169	3.82573236262492
H	2.37801719907031	9.57538021417986	4.23310163931639
C	7.10015988401406	13.27656206334312	2.37187157806498
C	8.48689532829122	13.47018970269934	2.32899348248533
C	9.16588317839191	13.16301381737388	1.15396080101101
H	10.23795560089353	13.31679721110622	1.10801001565567
C	8.50275585382052	12.66142922171955	0.05170932977242
H	9.04868943372032	12.43101336584410	-0.85609391652206
C	7.14051125549447	12.43295356899695	0.12156836523857
H	6.62546309632633	12.01639808852899	-0.73545078283791
C	6.41896102177962	12.73016990743894	1.27099601607122
C	9.26745807499146	13.96293459808531	3.52259823907093
H	8.55819728514631	14.31787647944863	4.27274140337464
C	10.03835932302882	12.80369095196552	4.14545333563870
H	9.36447478665504	11.99459370726292	4.43358168382260
H	10.56849951775762	13.13743173087593	5.03869693138170
H	10.77007976153689	12.40267124264784	3.43774036745489
C	10.21562131566844	15.10927173940289	3.18693121941654
H	11.02793252688508	14.78368290900272	2.53211958930813
H	10.66931498989147	15.49758083606724	4.10181185862976
H	9.70195636425567	15.93378016576241	2.68732761570633
C	4.92415129029174	12.50945455045188	1.29595552933549
H	4.63119526034599	12.42737583943864	2.34505326421889
C	4.18029956508912	13.70796718581576	0.70916878282272
H	4.50685713640529	13.89609757869445	-0.31747116507838
H	4.34979225830013	14.61474117573171	1.29132370578883
H	3.10401823165494	13.52080903274327	0.69219445823234
C	4.50493049144269	11.22356169529832	0.59540064241524
H	3.44170526548800	11.03813612647604	0.76628703438980
H	5.06649086842084	10.36728664780992	0.97411242155910
H	4.64929175996645	11.28444926252554	-0.48634251893636
C	7.08440902141708	8.64507426208346	5.04727169016317
C	7.96509978370974	6.55837143922521	5.09184463126609
H	8.23759927065004	5.59826068147407	4.69080142842141

C	8.14267712268180	7.09942260730664	6.30880494263948
H	8.57442742140344	6.69983861756517	7.20849170618443
C	6.99927631392204	7.31584333309896	2.95133327543462
C	5.77951622357670	6.71380945161378	2.63259085791316
C	5.50223141620044	6.50625364915779	1.28693189400472
H	4.56468133552025	6.04559210173123	1.00029763911638
C	6.40151936558388	6.89308341955577	0.30792334769468
H	6.16366621143340	6.72880035652344	-0.73689040086284
C	7.59846813980340	7.49348657858011	0.65524349944413
H	8.29038390097769	7.80118343065331	-0.12005763953899
C	7.92495809515505	7.71778712808358	1.98742940427152
C	4.79922630407940	6.29563924570847	3.70327844546230
H	5.06061785632751	6.83615444738389	4.61653145387994
C	3.36755953835524	6.68103947220527	3.35544455361589
H	3.30352388726167	7.74124442926508	3.10744299077190
H	2.71165580208066	6.48927272533274	4.20790909057976
H	2.98360411329930	6.10270272232494	2.51132269550933
C	4.91019715662330	4.79992866384672	3.98954200292920
H	4.66724157704258	4.21671739221175	3.09722691599588
H	4.21758453602087	4.50957213327333	4.78349537931731
H	5.91888033454222	4.52407553786995	4.30408713029508
C	9.23189294368624	8.37732904003769	2.35417072453793
H	9.24358290930774	8.52427985946171	3.43620465582695
C	10.41593308992608	7.48484139366754	1.99373735557721
H	10.46394937179439	7.31106308840897	0.91557035989707
H	10.34818496192807	6.51135952082311	2.48547476152956
H	11.35335217947381	7.95664789065850	2.29824974821875
C	9.34829170943917	9.75337003630029	1.71301630151000
H	9.37688665814242	9.68792009862703	0.62264139590980
H	10.26548538405837	10.24867601083745	2.03937058014794
H	8.50207390018731	10.38244089150068	1.99308460495553
C	7.53053732714606	9.14823475815048	7.47434216911682
C	6.37171171385064	9.01431559279505	8.24291329614742
C	6.36462168716935	9.60897440581016	9.49851140173289
H	5.48182436722583	9.52438332827925	10.12089231165468
C	7.46321008320806	10.31084136452668	9.95773477857921
H	7.43664802063289	10.77487697763621	10.93693099831563
C	8.58708945225117	10.44785758498270	9.16357492304626
H	9.42642751424276	11.02607932072387	9.52649213278343
C	8.65195194533130	9.86554882206964	7.90302137848923
C	5.17980748674820	8.21305299662953	7.77394131466874
H	5.32577089488591	7.97535755083771	6.71857262835863
C	5.07414573258736	6.89969872068796	8.54449976768506
H	4.23241754969490	6.30857538492682	8.17473153410267
H	4.91443626846815	7.08244808215880	9.61049186937245
H	5.98158868262204	6.30002005739772	8.44052001652001
C	3.89120670997144	9.01829613288183	7.85992752779023
H	3.96392503908740	9.93031204678649	7.26627286178815
H	3.64837402823932	9.29605569901119	8.88813782550119
H	3.05542579304046	8.43273388320582	7.46964547263955
C	9.90160833028427	9.98890205005594	7.05660160881645
H	9.58605040745672	9.97160960006111	6.00824320799833
C	10.86339440387883	8.82191695489718	7.28789728570542
H	10.43617248796399	7.86127742996739	7.00404722308245

H	11.14958821057482	8.77100676797388	8.34194510578366
H	11.77280917496028	8.96578338976107	6.69898771231358
C	10.65050532303643	11.29328581217940	7.29696963692751
H	11.44378293845449	11.39996231047908	6.55450470608465
H	11.12855820383245	11.30145337065370	8.28012448238747
H	9.98818061154921	12.15518604862564	7.22289246555208

Table S4. Computed (PBE0-D3/def2-TZVP) bond lengths [Å] and angles [°] of LGa(X)Sb-^{Me}CAAC (X = Cl **3'**, Br **4'**) and LGa(X)Sb-IDipp (X = Cl **5'**, Br **6'**).

	3'	4'	5'	6'
Ga–Sb	2.590	2.590	2.578	2.583
C–Sb	2.067	2.066	2.133	2.134
Ga–X	2.245	2.402	2.23	2.382
C-Sb-Ga	107.3	107.1	113.4	114.0
X-Ga-Sb	124.6	124.2	129.8	129.7

2. Reaction energies and dispersion interactions

All calculations were performed with the Gaussian 09 Program.[1] Geometries were optimized in gas phase at the BP86-D3/def2-SVP level of theory.[2-4] Geometry optimization were also carried out without the empirical dispersion correction (DFT-D3) as a reference to evaluate dispersion energy.[5] Frequency calculation was performed for each optimized structure to verify the stationary points as minima at the same level of theory. Single-point energies in solvent (benzene) were calculate by SMD model[6] under def2-TZVP basis set. All the energies discussed are enthalpies at 298 K and 1 atm in kcal/mol. The molecular orbitals were computed at the BP86-D3/def2-SVP theoretical level. Non-covalent interaction (NCI) analysis were performed by NCIPLOT program.[7]

References

[1] Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Jr; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., *Gaussian 09 Revision E.01*, Gaussian, Inc., Wallingford CT, 2013.

[2] Becke, A. D., Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **1988,** *38*, 3098-3100.

[3] Perdew, J. P., Density-functional approximation for the correlation energy of the inhomogeneous electron gas. *Phys. Rev. B* **1986,** *33*, 8822-8824.

[4] Weigend, F.; Ahlrichs, R., Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005,** *7*, 3297-3305.

[5] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H., A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010,** *132*, 154104.

[6] Marenich, A. V., Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B.* **2009**, *113*, 6378–6396.

[7] Contreras-García, J.; Johnson, E. R.; Keinan, S.; Chaudret, R.; Piquemal, J.-P.; Beratan, D. N.; Yang, W., NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. *J. Chem. Theory Comput.* **2011,** *7*, 625-632.

Figure S26. Selected bond lengths [Å] for **3'** - **6'** from optimization with dispersion corrections, X-ray crystal structure (in bracket), and optimization without dispersion corrections (parentheses).

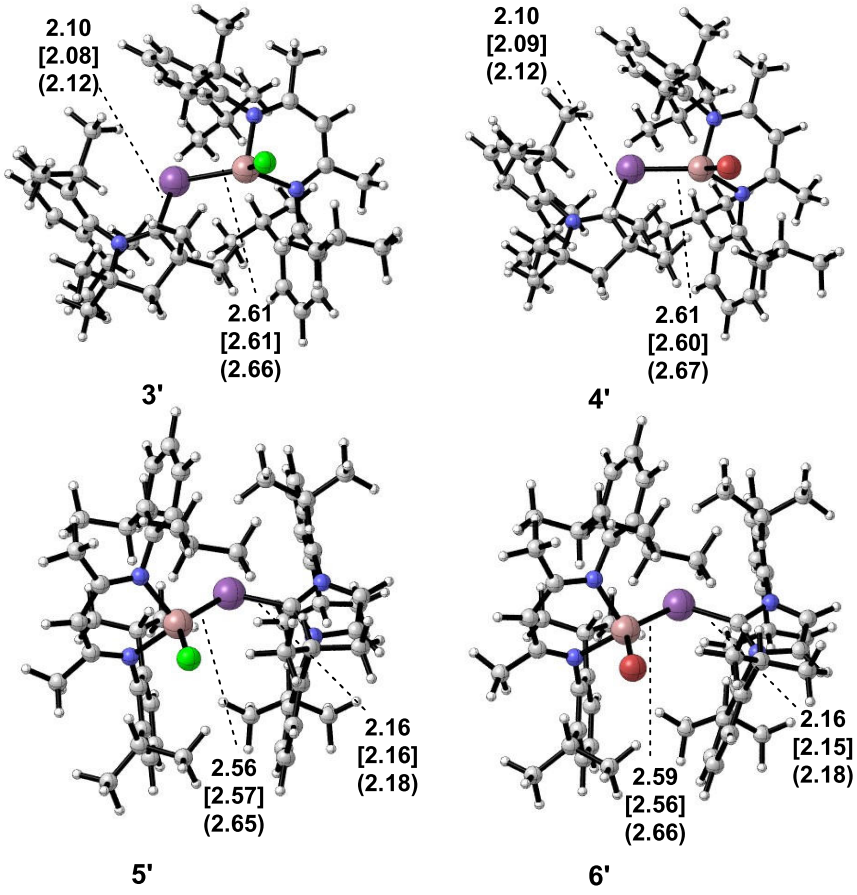

Figure S27. Non-covalent interaction (NCI) plots (s = 0.3 au, –0.1 < r < +0.1 au) of [LGa(Cl)Sb-^{Me}CAAC] **3'**, [LGa(Cl)Sb-IDipp] **5'**, and distibene [L(Cl)Ga]$_2$Sb$_2$. Red: repulsion; blue: attraction, green: non-covalent interactions.

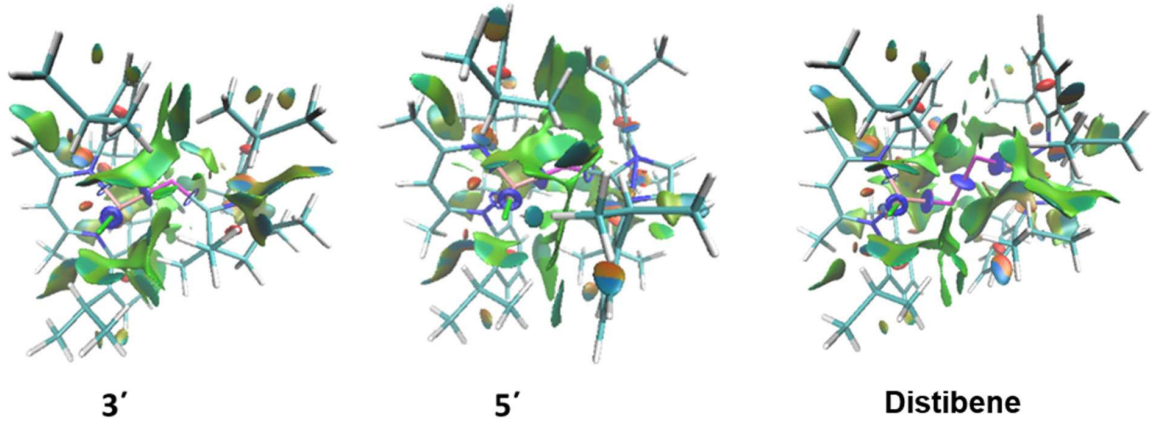

Table S5. Reaction energies in benzene solution (ΔH_0: kcal mol^{-1}) with and without LD corrections (D3(BJ)) for the formation of carbene-stabilized stibinidenes (**3'** – **6'**) and distibenes $[L(X)Ga]_2Sb_2$ from stibinidenes L(X)GaSb at the BP86/def2-SVP level of theory.

	ΔH_0 (D3(BJ))	ΔH_0	E_{disp}
3′	–67.4	–37.4	–30.1
4′	–67.7	–37.1	–30.6
5′	–52.5	–16.0	–36.6
6′	–53.0	–15.4	–37.5
$[L(Cl)Ga]_2Sb_2$	–86.5	–54.0	–32.5
$[L(Br)Ga]_2Sb_2$	–87.1	–53.5	–33.6

Cartesian Coordinates (Å, BP86-D3/def2-SVP level)
LGa

E = -3163.47115028 G = -3162.924 E+ZPE = -3162.854868

Ga	0.005179	-0.204445	-1.018056
N	-1.429201	-0.222893	0.531007
N	1.450176	-0.132315	0.528918
C	-1.250063	-0.313043	1.860759
C	0.020895	-0.366500	2.473819
H	0.024644	-0.455877	3.568327
C	1.287527	-0.243122	1.857202
C	-2.470188	-0.333701	2.758687
H	-3.049545	0.606071	2.645810
H	-2.191181	-0.455729	3.821602
H	-3.158538	-1.153353	2.467345
C	2.508076	-0.231718	2.758216
H	3.112753	-1.150034	2.608067
H	2.220833	-0.172666	3.824442
H	3.174893	0.618843	2.512233
C	-2.750666	-0.053996	0.008758
C	-3.500579	-1.191085	-0.397095
C	-4.755717	-0.984232	-1.002106
H	-5.348556	-1.853839	-1.326593
C	-5.261482	0.308675	-1.198723
H	-6.244096	0.450565	-1.675388
C	-4.512848	1.420719	-0.787164
H	-4.914838	2.434053	-0.944225
C	-3.252883	1.263877	-0.178269
C	-2.942839	-2.599841	-0.216526
H	-2.101930	-2.528323	0.504612
C	-3.976198	-3.578769	0.367961
H	-4.412988	-3.194207	1.312937
H	-3.504383	-4.560340	0.581949
H	-4.813811	-3.765315	-0.336724
C	-2.359942	-3.123591	-1.544796
H	-3.149091	-3.192505	-2.323307
H	-1.912621	-4.131748	-1.415070
H	-1.571349	-2.442690	-1.931345
C	-2.429059	2.481471	0.234577
H	-1.621176	2.121334	0.904267
C	-3.252847	3.518236	1.018383
H	-4.036242	3.987317	0.386705
H	-2.599148	4.334713	1.390075
H	-3.758419	3.058896	1.892884
C	-1.749813	3.118718	-0.994649
H	-1.118468	2.379455	-1.533563
H	-1.103054	3.970735	-0.696449
H	-2.505675	3.493958	-1.716746
C	2.756505	0.075760	-0.009660
C	3.630472	-1.027603	-0.209602
C	4.901429	-0.781014	-0.763476
H	5.596022	-1.620522	-0.920247
C	5.291641	0.514907	-1.129956

H	6.291369	0.689392	-1.557739
C	4.398387	1.584949	-0.976102
H	4.702051	2.592479	-1.297214
C	3.115632	1.389023	-0.428124
C	3.161790	-2.451304	0.079896
H	2.342634	-2.390519	0.825939
C	4.259661	-3.351778	0.669109
H	5.071681	-3.549146	-0.062101
H	3.838147	-4.336581	0.958774
H	4.722705	-2.897515	1.569859
C	2.555569	-3.066670	-1.198881
H	1.727018	-2.438339	-1.591442
H	2.154714	-4.083560	-1.002630
H	3.320883	-3.142301	-1.999867
C	2.125329	2.543701	-0.282398
H	1.111575	2.109544	-0.443159
C	2.130097	3.135165	1.141029
H	1.844132	2.381061	1.899622
H	1.408112	3.975427	1.217773
H	3.137287	3.523575	1.403001
C	2.312737	3.643368	-1.337058
H	3.251772	4.215458	-1.180177
H	1.476556	4.370453	-1.282095
H	2.334203	3.222406	-2.362741

^{Me}CAAC

E = -834.976580738 G = -834.575582 E+ZPE = -834.52509

N	-0.592580	-0.087293	0.062742
C	-1.335205	-0.133428	-1.024754
C	0.844706	0.059446	-0.002163
C	1.645395	-1.111415	-0.043166
C	3.044911	-0.954606	-0.012177
H	3.689601	-1.846021	-0.037101
C	3.628693	0.319540	0.028984
H	4.724732	0.422226	0.065214
C	2.818775	1.461998	-0.019117
H	3.286301	2.457902	-0.050519
C	1.413227	1.357633	-0.051918
C	1.021759	-2.482960	-0.280484
H	-0.020557	-2.447560	0.091378
C	0.930016	-2.727863	-1.802484
H	0.328688	-1.926750	-2.280846
H	0.448327	-3.706062	-2.014639
H	1.940448	-2.732232	-2.263489
C	1.739662	-3.628478	0.447811
H	2.763102	-3.796320	0.051372
H	1.182606	-4.578736	0.313363
H	1.826946	-3.431167	1.536438
C	0.554398	2.591830	-0.306753
H	-0.476956	2.357839	0.015418
C	1.012229	3.838410	0.465031
H	2.003173	4.202305	0.120608

H	1.086185	3.642246	1.554924
H	0.293320	4.670175	0.314085
C	0.485958	2.841662	-1.828817
H	1.496182	3.043928	-2.243603
H	-0.162359	3.714919	-2.054622
H	0.066112	1.950196	-2.338540
C	-2.779822	-0.266068	-0.549568
C	-1.293155	-0.163808	1.443192
C	-3.477973	1.083258	-0.840859
H	-3.008160	1.919935	-0.284071
H	-3.418157	1.326497	-1.920624
H	-4.548194	1.034283	-0.547078
C	-3.483428	-1.389958	-1.331820
H	-3.484905	-1.166463	-2.417653
H	-2.963549	-2.360310	-1.188859
H	-4.535187	-1.508309	-0.992390
C	-1.256486	1.209370	2.134221
H	-0.212457	1.545678	2.297184
H	-1.788598	1.984239	1.549748
H	-1.746990	1.136770	3.126560
C	-0.624251	-1.193805	2.362254
H	-0.678095	-2.217895	1.946102
H	0.440909	-0.943562	2.543575
H	-1.142874	-1.201383	3.342918
C	-2.706454	-0.578576	0.982116
H	-3.495921	-0.060667	1.563601
H	-2.843343	-1.667745	1.145172

IDipp

E = -1159.31247371 G = -1158.821781 E+ZPE = -1158.760053

N	1.058518	-0.184368	0.538850
N	-1.073948	-0.085243	0.518159
C	0.005566	-0.051829	-0.339370
C	0.657799	-0.292611	1.877674
H	1.372444	-0.395176	2.700591
C	-0.709525	-0.227532	1.864073
H	-1.444316	-0.259874	2.675365
C	2.441647	-0.130779	0.145969
C	3.113875	-1.337975	-0.160842
C	4.477440	-1.255496	-0.506064
H	5.031035	-2.173954	-0.752368
C	5.136744	-0.018000	-0.544006
H	6.203951	0.025832	-0.813334
C	4.442809	1.164179	-0.248812
H	4.969159	2.129542	-0.295065
C	3.078569	1.133013	0.102971
C	2.288893	2.416417	0.336691
H	1.399018	2.154567	0.946941
C	3.076128	3.489007	1.106062
H	3.933914	3.877036	0.517196
H	3.472589	3.096872	2.065300
H	2.421395	4.355734	1.333033

C	1.772802	2.950082	-1.016761
H	2.621351	3.230145	-1.676511
H	1.139422	3.850207	-0.869458
H	1.172161	2.175453	-1.535549
C	-2.438660	0.070997	0.088383
C	-3.291353	-1.060194	0.109938
C	-4.638375	-0.869264	-0.257513
H	-5.330681	-1.723871	-0.249624
C	-5.105598	0.394124	-0.646738
H	-6.161833	0.523741	-0.931197
C	-4.232146	1.490396	-0.689081
H	-4.609402	2.471723	-1.011945
C	-2.878600	1.354647	-0.322651
C	-2.731573	-2.445890	0.421331
H	-1.954951	-2.325272	1.206731
C	-3.777213	-3.433288	0.959029
H	-3.285917	-4.378298	1.269379
H	-4.529692	-3.699166	0.186855
H	-4.319335	-3.023882	1.836430
C	-2.023917	-3.003607	-0.833082
H	-1.241745	-2.305853	-1.193597
H	-2.754925	-3.151849	-1.655856
H	-1.546561	-3.982060	-0.614298
C	-1.912147	2.534477	-0.349190
H	-0.934021	2.117766	-0.670047
C	-1.725266	3.132251	1.061058
H	-1.377934	2.370064	1.786828
H	-2.679066	3.556445	1.441617
H	-0.971469	3.947518	1.041818
C	-2.299573	3.622924	-1.359762
H	-1.491308	4.379888	-1.428804
H	-3.224578	4.162611	-1.063374
H	-2.457807	3.201331	-2.373388
C	2.352691	-2.657989	-0.205009
H	1.505250	-2.573862	0.508649
C	1.746577	-2.845269	-1.613046
H	1.094543	-1.985926	-1.872436
H	2.550952	-2.913457	-2.375992
H	1.142368	-3.775289	-1.662638
C	3.198127	-3.870648	0.214003
H	4.003232	-4.087063	-0.519515
H	3.673212	-3.718492	1.205189
H	2.563243	-4.778706	0.272485

^{Me}CAAC^{H}

E = -289.756891587 G = -289.632474 E+ZPE = -289.601637

C	-1.620711	1.008535	0.169914
C	-1.820011	-0.476001	-0.101962
C	0.593038	-0.056391	-0.019411
C	1.194697	-0.450354	1.341151
H	1.789582	0.383486	1.770937
H	0.397572	-0.710774	2.067039

H	1.868872	-1.325273	1.234497
C	1.692236	0.275249	-1.035086
H	1.253474	0.610728	-1.996943
H	2.363624	1.077626	-0.659823
H	2.322270	-0.616258	-1.233612
C	-0.450703	-1.078989	-0.532239
H	-0.262923	-2.095305	-0.131815
H	-0.395803	-1.146432	-1.638909
N	-0.310214	1.143604	0.179859
H	0.137057	2.046173	0.390423
H	-2.629590	-0.643747	-0.842726
H	-2.203907	-0.917748	0.847726

IDipp^{H}

E = -226.027676282 G = -225.984592 E+ZPE = -225.958268

C	0.001090	-1.287682	-0.000033
C	0.685262	0.942614	0.000003
H	1.400621	1.771792	-0.001029
C	-0.686892	0.941484	0.000009
H	-1.403698	1.769467	0.000974
N	1.054685	-0.403504	0.000042
H	2.021908	-0.728104	0.000706
N	-1.053948	-0.405158	-0.000080
H	-2.020746	-0.731021	-0.000249

LGaCl$_2$

E = -4083.82438026 G = -4083.274706 E+ZPE = -4083.203421

Ga	-0.004292	-0.619325	-0.553942
Cl	-0.097706	-2.792740	-0.891296
N	1.467677	-0.230811	0.655345
N	-1.472544	-0.114220	0.626235
C	1.261326	-0.293276	1.986127
C	-0.023277	-0.352170	2.572257
H	-0.039040	-0.429825	3.666977
C	-1.286704	-0.162034	1.960108
C	2.464792	-0.275593	2.898717
H	3.094782	0.616028	2.709732
H	2.164164	-0.288496	3.961737
H	3.108655	-1.154673	2.691663
C	-2.483612	0.005243	2.866940
H	-3.116144	-0.905778	2.836453
H	-2.169757	0.178575	3.912150
H	-3.127859	0.841722	2.532266
C	2.758614	0.135020	0.134154
C	3.706632	-0.864552	-0.205128
C	4.962324	-0.447381	-0.691645
H	5.714158	-1.207612	-0.956794
C	5.267884	0.910602	-0.846212
H	6.256723	1.214825	-1.223751
C	4.306604	1.881696	-0.532848

H	4.544975	2.947636	-0.673007
C	3.035702	1.517836	-0.048891
C	3.397636	-2.352343	-0.084798
H	2.382071	-2.454214	0.348923
C	4.387174	-3.077658	0.846820
H	4.414665	-2.619376	1.857509
H	4.100551	-4.143336	0.964536
H	5.422068	-3.052797	0.444784
C	3.361468	-3.009781	-1.478377
H	4.359695	-2.974789	-1.964309
H	3.053138	-4.072569	-1.399455
H	2.636133	-2.499035	-2.141545
C	2.002098	2.593250	0.275494
H	1.030953	2.080576	0.432281
C	2.347260	3.336008	1.581405
H	3.321343	3.862768	1.494600
H	1.570862	4.093472	1.817749
H	2.414320	2.644238	2.444942
C	1.817435	3.578377	-0.891110
H	1.511650	3.043824	-1.811688
H	1.032306	4.322047	-0.643739
H	2.747708	4.145003	-1.104964
C	-2.759716	0.229715	0.077085
C	-3.765670	-0.761912	-0.070919
C	-5.020208	-0.359775	-0.573617
H	-5.816154	-1.111729	-0.691119
C	-5.267871	0.969448	-0.934250
H	-6.256558	1.262143	-1.321154
C	-4.246639	1.923719	-0.823871
H	-4.439318	2.960588	-1.135790
C	-2.975275	1.576746	-0.328768
C	-3.526541	-2.235436	0.244433
H	-2.505858	-2.334730	0.666460
C	-4.531447	-2.788587	1.273603
H	-5.566743	-2.791183	0.872030
H	-4.276968	-3.835572	1.539297
H	-4.544607	-2.193099	2.209986
C	-3.562903	-3.070742	-1.051485
H	-2.825268	-2.697081	-1.787278
H	-3.314921	-4.130926	-0.837358
H	-4.570384	-3.040254	-1.517992
C	-1.868283	2.622217	-0.220620
H	-0.906302	2.083052	-0.338192
C	-1.845857	3.297674	1.164678
H	-1.651092	2.569497	1.976805
H	-1.044449	4.064885	1.209105
H	-2.812410	3.800874	1.379671
C	-1.928690	3.662534	-1.348821
H	-2.819703	4.320327	-1.268774
H	-1.036640	4.318789	-1.310253
H	-1.944678	3.169027	-2.340968
Cl	0.107442	0.550293	-2.391243

LGaBr$_2$

E = -8311.86490984 G = -8311.317341 E+ZPE = -8311.24467

Ga	-0.003889	-0.531158	-0.364748
N	1.464276	-0.097957	0.842297
N	-1.480623	0.046590	0.783024
C	1.245278	-0.172145	2.170576
C	-0.047069	-0.213159	2.740947
H	-0.076229	-0.294895	3.835203
C	-1.301259	0.008033	2.118632
C	2.438881	-0.208385	3.095855
H	3.175931	0.576567	2.837778
H	2.135987	-0.094850	4.152352
H	2.965253	-1.179073	2.977654
C	-2.495530	0.221741	3.019356
H	-3.151486	-0.672790	3.005247
H	-2.178716	0.406974	4.061632
H	-3.117144	1.068106	2.667415
C	2.752223	0.286924	0.327378
C	3.721836	-0.692362	-0.007677
C	4.968368	-0.251146	-0.496993
H	5.735631	-0.996813	-0.759165
C	5.245050	1.111657	-0.658701
H	6.226233	1.435050	-1.040253
C	4.264811	2.063793	-0.345345
H	4.482130	3.133378	-0.488144
C	3.003099	1.675350	0.142689
C	3.447533	-2.185425	0.118677
H	2.439462	-2.307931	0.565346
C	4.462510	-2.887508	1.040393
H	4.498958	-2.418690	2.045817
H	4.193999	-3.956414	1.170962
H	5.490525	-2.850890	0.621901
C	3.410102	-2.844482	-1.273936
H	4.402911	-2.789441	-1.769074
H	3.122697	-3.912958	-1.192824
H	2.670186	-2.346618	-1.931313
C	1.951667	2.725903	0.488525
H	0.972698	2.205884	0.528847
C	2.201670	3.333528	1.883350
H	3.192251	3.834193	1.926543
H	1.425282	4.088548	2.126944
H	2.178069	2.562151	2.678123
C	1.842879	3.821559	-0.583138
H	1.622998	3.382748	-1.576576
H	1.025874	4.526296	-0.326219
H	2.773280	4.421642	-0.663152
C	-2.761347	0.406638	0.226694
C	-3.794853	-0.561773	0.111078
C	-5.043550	-0.140369	-0.390395
H	-5.858738	-0.875139	-0.481742
C	-5.262221	1.184407	-0.783587
H	-6.246785	1.491688	-1.169642

C	-4.216278	2.114183	-0.705840
H	-4.384776	3.147891	-1.041234
C	-2.950337	1.747754	-0.210894
C	-3.593678	-2.034784	0.451901
H	-2.571374	-2.155661	0.865504
C	-4.601999	-2.546361	1.498916
H	-5.641233	-2.527874	1.108140
H	-4.371399	-3.595790	1.776381
H	-4.589975	-1.938762	2.427358
C	-3.669872	-2.887932	-0.830759
H	-2.944809	-2.535549	-1.589749
H	-3.433703	-3.948903	-0.607837
H	-4.686617	-2.847317	-1.276003
C	-1.823682	2.773103	-0.130508
H	-0.872395	2.211830	-0.233195
C	-1.791167	3.480308	1.238516
H	-1.606784	2.767833	2.066969
H	-0.980152	4.237859	1.265881
H	-2.751148	4.000856	1.440896
C	-1.863240	3.785673	-1.284655
H	-2.736376	4.468430	-1.216901
H	-0.954006	4.418450	-1.268199
H	-1.898805	3.267650	-2.263973
Br	0.190083	0.604053	-2.379227
Br	-0.129559	-2.868926	-0.568033

[L(Cl)Ga]$_2$SbCl

E = -7947.94731052 G = -7946.817078 E+ZPE = -7946.703557

Ga	-1.920058	-0.431961	-0.565665
Cl	-1.552587	-1.871133	-2.256259
N	-3.008456	1.015362	-1.340750
N	-3.425917	-1.288415	0.422371
C	-4.317682	0.772172	-1.587078
C	-5.022823	-0.367946	-1.133711
H	-6.050336	-0.465193	-1.507611
C	-4.650322	-1.284041	-0.123245
C	-5.117597	1.800027	-2.361512
H	-5.261220	2.713613	-1.750625
H	-6.111514	1.396647	-2.628617
H	-4.591376	2.124181	-3.277348
C	-5.673724	-2.297104	0.336475
H	-5.540114	-3.229664	-0.253136
H	-6.707037	-1.937405	0.174852
H	-5.535882	-2.563909	1.401479
C	-2.499006	2.306098	-1.737208
C	-1.965474	2.487041	-3.044814
C	-1.699567	3.809781	-3.454081
H	-1.301806	3.991170	-4.461996
C	-1.925394	4.900534	-2.603681
H	-1.722365	5.923866	-2.956715
C	-2.353356	4.685276	-1.288651
H	-2.462490	5.540060	-0.605575

C	-2.630605	3.385342	-0.822175
C	-1.644555	1.305344	-3.966341
H	-1.148455	0.547096	-3.324813
C	-2.869935	0.614140	-4.599179
H	-3.516402	0.120023	-3.851072
H	-2.523845	-0.182027	-5.289734
H	-3.480463	1.331343	-5.189250
C	-0.646088	1.675063	-5.074130
H	-1.096495	2.354086	-5.829993
H	-0.330920	0.756942	-5.608257
H	0.263714	2.155840	-4.664191
C	-3.026113	3.148979	0.635794
H	-2.610219	2.156704	0.913012
C	-4.550137	3.095259	0.863808
H	-5.046929	4.002259	0.457550
H	-4.770384	3.054081	1.950648
H	-5.016508	2.202630	0.404319
C	-2.385627	4.168894	1.591885
H	-1.293064	4.246011	1.429940
H	-2.545051	3.848509	2.641259
H	-2.833583	5.179763	1.483949
C	-3.096236	-1.991318	1.628015
C	-2.606714	-3.322407	1.573046
C	-2.112809	-3.902729	2.759903
H	-1.718899	-4.930910	2.730086
C	-2.102490	-3.192179	3.964868
H	-1.696604	-3.655945	4.877522
C	-2.613651	-1.886627	4.008953
H	-2.606184	-1.335942	4.960278
C	-3.121156	-1.261545	2.854523
C	-2.585176	-4.125491	0.279619
H	-2.965668	-3.473266	-0.531691
C	-3.494019	-5.366743	0.373697
H	-3.121161	-6.084735	1.134786
H	-3.528208	-5.899240	-0.599766
H	-4.532139	-5.096685	0.655513
C	-1.150782	-4.517467	-0.105532
H	-0.497465	-3.627777	-0.185651
H	-1.128074	-5.015202	-1.095729
H	-0.700608	-5.208886	0.637518
C	-3.698180	0.149366	2.915881
H	-3.406296	0.655494	1.970844
C	-5.240896	0.113653	2.961479
H	-5.678516	-0.331029	2.048587
H	-5.649189	1.140590	3.057572
H	-5.592379	-0.477348	3.833706
C	-3.158867	0.986951	4.083549
H	-3.522478	0.610443	5.063346
H	-3.513092	2.033830	3.988103
H	-2.052139	1.007163	4.090758
Ga	1.991267	0.264596	-0.412833
Cl	1.449453	1.313739	-2.309134
N	3.333383	1.418167	0.464196
N	3.273997	-1.140642	-0.966360

C	4.620411	1.389395	0.067873
C	5.167532	0.369708	-0.741380
H	6.228450	0.487040	-0.997883
C	4.577861	-0.854622	-1.133998
C	5.542143	2.496878	0.527623
H	5.486794	2.637182	1.625227
H	6.588930	2.294379	0.236907
H	5.225002	3.460516	0.078157
C	5.485242	-1.881476	-1.773989
H	5.398365	-1.818750	-2.878491
H	6.541553	-1.700562	-1.502500
H	5.201988	-2.912855	-1.489862
C	2.931573	2.327868	1.504677
C	2.493718	3.637313	1.186705
C	2.112568	4.482773	2.247617
H	1.762696	5.502397	2.021563
C	2.167411	4.049694	3.578195
H	1.868594	4.728466	4.392448
C	2.581097	2.742929	3.870966
H	2.589298	2.397473	4.915584
C	2.951862	1.854934	2.845184
C	2.373992	4.121235	-0.252187
H	2.792499	3.334042	-0.911601
C	3.158251	5.421985	-0.505707
H	4.231220	5.320601	-0.238845
H	3.098608	5.706850	-1.576794
H	2.749494	6.268700	0.085481
C	0.892789	4.287303	-0.634692
H	0.421240	5.111162	-0.058378
H	0.783305	4.518503	-1.712625
H	0.315328	3.363962	-0.437821
C	3.331855	0.411752	3.160750
H	3.134001	-0.175775	2.238691
C	4.834819	0.261404	3.467085
H	5.126935	0.898752	4.328674
H	5.079705	-0.790989	3.721750
H	5.462428	0.548324	2.600527
C	2.472721	-0.192650	4.283392
H	1.392700	-0.026295	4.095882
H	2.650161	-1.285265	4.356985
H	2.717874	0.244648	5.274168
C	2.763572	-2.451317	-1.264011
C	2.424417	-2.808893	-2.596884
C	1.931899	-4.109788	-2.826812
H	1.654633	-4.401600	-3.851772
C	1.797065	-5.034224	-1.785866
H	1.421295	-6.048478	-1.992001
C	2.125081	-4.660942	-0.475238
H	2.001559	-5.386017	0.341904
C	2.593836	-3.366755	-0.184009
C	2.593090	-1.856732	-3.777373
H	3.024293	-0.909848	-3.392437
C	3.545947	-2.436209	-4.843430
H	3.100765	-3.323617	-5.341023

H	3.747981	-1.681922	-5.632211
H	4.517966	-2.755341	-4.415170
C	1.237735	-1.503847	-4.413456
H	0.553448	-1.053759	-3.672402
H	1.383862	-0.779356	-5.240624
H	0.740043	-2.405418	-4.829349
C	2.953379	-2.973785	1.247001
H	2.757764	-1.883199	1.337907
C	4.453197	-3.177153	1.538409
H	5.088478	-2.544022	0.889533
H	4.683624	-2.911222	2.591138
H	4.746503	-4.236585	1.380228
C	2.088411	-3.680536	2.302280
H	2.322458	-4.763741	2.373077
H	2.272728	-3.240176	3.303036
H	1.006134	-3.574231	2.085464
Sb	0.061053	-0.605236	1.157907
Cl	-0.292638	1.598894	2.185057

[L(Br)Ga]$_2$SbBr

E = -14290.011777 G = -14288.884465 E+ZPE = -14288.768974

Ga	-1.958166	0.328615	0.424129
N	-2.883759	-0.997597	1.554727
N	-3.566007	0.802954	-0.661566
C	-4.207330	-0.839780	1.787477
C	-5.028637	0.106028	1.129430
H	-6.055063	0.183836	1.511284
C	-4.770331	0.806254	-0.071383
C	-4.894508	-1.763150	2.773256
H	-5.013073	-2.770269	2.325780
H	-5.897809	-1.376189	3.029922
H	-4.304591	-1.904488	3.695757
C	-5.907874	1.584571	-0.692841
H	-5.915135	2.607898	-0.260077
H	-6.887482	1.119823	-0.473198
H	-5.783302	1.688464	-1.787006
C	-2.226265	-2.108115	2.200752
C	-1.684784	-1.947916	3.509376
C	-1.219802	-3.109419	4.159483
H	-0.803057	-3.028533	5.172387
C	-1.264135	-4.365812	3.541089
H	-0.900551	-5.255757	4.078596
C	-1.726260	-4.482355	2.225770
H	-1.704646	-5.462183	1.727978
C	-2.205512	-3.358346	1.524498
C	-1.545465	-0.575352	4.180976
H	-1.109827	0.092697	3.406718
C	-2.863388	0.082878	4.639579
H	-3.532264	0.342150	3.799062
H	-2.631757	1.034851	5.159696
H	-3.414683	-0.565148	5.354410
C	-0.566951	-0.589649	5.365890

H	-0.967286	-1.169018	6.225617
H	-0.401751	0.446786	5.720437
H	0.419386	-1.010645	5.087240
C	-2.662328	-3.489347	0.070534
H	-2.351614	-2.550799	-0.438760
C	-4.190549	-3.621292	-0.092694
H	-4.589057	-4.443174	0.539701
H	-4.438100	-3.863556	-1.146734
H	-4.728463	-2.688136	0.159460
C	-1.966250	-4.641628	-0.671247
H	-0.867223	-4.601393	-0.547910
H	-2.186514	-4.573865	-1.755866
H	-2.324951	-5.633940	-0.323330
C	-3.343762	1.245413	-2.009666
C	-3.029344	2.602485	-2.283804
C	-2.634943	2.948560	-3.593059
H	-2.379247	3.996554	-3.815627
C	-2.551490	1.985741	-4.603521
H	-2.221323	2.270500	-5.614776
C	-2.899838	0.655309	-4.327569
H	-2.846692	-0.092671	-5.131015
C	-3.310519	0.257626	-3.041348
C	-3.104927	3.689350	-1.219704
H	-3.369715	3.206194	-0.257534
C	-4.191513	4.729763	-1.557514
H	-3.937647	5.293263	-2.480540
H	-4.293453	5.466849	-0.733620
H	-5.180889	4.257104	-1.721141
C	-1.741506	4.366070	-1.017637
H	-0.960793	3.626116	-0.759674
H	-1.780696	5.091098	-0.179688
H	-1.415888	4.911162	-1.928908
C	-3.753081	-1.178958	-2.772983
H	-3.331048	-1.468910	-1.786664
C	-5.291236	-1.274421	-2.669832
H	-5.694351	-0.719864	-1.803122
H	-5.605012	-2.332349	-2.557246
H	-5.768835	-0.873412	-3.588780
C	-3.251505	-2.189213	-3.814213
H	-3.752280	-2.047720	-4.795697
H	-3.484427	-3.220107	-3.477141
H	-2.156199	-2.121939	-3.957633
Ga	2.022380	0.018040	0.329801
N	3.508979	-1.084516	-0.378652
N	3.122861	1.643504	0.646720
C	4.774874	-0.840922	0.016802
C	5.179294	0.345809	0.662764
H	6.241957	0.398208	0.934201
C	4.447104	1.542237	0.849442
C	5.834827	-1.881456	-0.269588
H	5.833474	-2.173316	-1.338433
H	6.839896	-1.514394	0.006696
H	5.621519	-2.807674	0.302380
C	5.237584	2.753503	1.294821

H	5.348558	2.736545	2.398926
H	6.254166	2.738241	0.858259
H	4.734810	3.700940	1.026239
C	3.256593	-2.178499	-1.278303
C	2.998233	-3.480154	-0.780134
C	2.775371	-4.513037	-1.712257
H	2.563709	-5.529737	-1.345223
C	2.813855	-4.269934	-3.090926
H	2.641699	-5.093299	-3.801866
C	3.048199	-2.971534	-3.564602
H	3.041863	-2.778788	-4.647810
C	3.254118	-1.903355	-2.673067
C	2.897152	-3.767614	0.711657
H	3.190072	-2.845499	1.254059
C	3.832469	-4.903762	1.164139
H	4.890690	-4.704338	0.893869
H	3.780221	-5.030674	2.265497
H	3.551564	-5.875124	0.704839
C	1.437286	-4.068260	1.096034
H	1.091227	-5.017024	0.632887
H	1.324998	-4.159971	2.194662
H	0.756954	-3.259851	0.764712
C	3.438981	-0.479767	-3.188463
H	3.133747	0.196473	-2.361634
C	4.916321	-0.163893	-3.494658
H	5.318084	-0.861408	-4.260124
H	5.023701	0.870033	-3.884281
H	5.550344	-0.246061	-2.589853
C	2.540368	-0.164261	-4.395295
H	1.484421	-0.439026	-4.195408
H	2.579659	0.919621	-4.628649
H	2.867081	-0.705710	-5.308050
C	2.441013	2.905003	0.753880
C	2.083480	3.432908	2.024542
C	1.390407	4.660297	2.057887
H	1.091917	5.077750	3.032055
C	1.079445	5.356832	0.886332
H	0.542542	6.316640	0.939385
C	1.446484	4.825868	-0.357742
H	1.198791	5.377154	-1.275682
C	2.117701	3.593469	-0.452671
C	2.447107	2.755696	3.342686
H	2.983628	1.813679	3.107541
C	3.367823	3.652303	4.198055
H	2.826308	4.553564	4.555374
H	3.720309	3.101007	5.094741
H	4.256137	4.005110	3.637596
C	1.198753	2.366438	4.152409
H	0.538611	1.699430	3.569747
H	1.498521	1.837534	5.080301
H	0.608590	3.261191	4.443806
C	2.555168	3.048765	-1.810468
H	2.513310	1.939563	-1.744654
C	4.019990	3.419165	-2.117035

H	4.717509	2.994614	-1.369711
H	4.320036	3.030877	-3.112646
H	4.153078	4.521703	-2.123809
C	1.633447	3.468554	-2.965205
H	1.705599	4.555531	-3.180106
H	1.919506	2.932509	-3.892611
H	0.572394	3.226475	-2.753849
Sb	-0.002597	0.404126	-1.331040
Br	-1.615848	2.258296	1.811576
Br	-0.103839	-2.080012	-2.077924
Br	1.606170	-0.833286	2.507665

LClGaSb

E = -3864.04284283 G = -3863.495609 E+ZPE = -3863.422652

Sb	0.361113	1.039376	-2.378113
Ga	-0.034943	-0.615405	-0.394043
Cl	-0.185001	-2.799403	-0.879043
N	1.388313	-0.511103	0.969378
N	-1.527539	-0.320215	0.869558
C	1.146397	-0.865253	2.243033
C	-0.159045	-0.995991	2.769536
H	-0.217453	-1.302744	3.822269
C	-1.392764	-0.641589	2.169178
C	2.318426	-1.146604	3.156093
H	3.165885	-0.463102	2.955795
H	2.031600	-1.078005	4.221737
H	2.687102	-2.177147	2.962284
C	-2.618214	-0.618929	3.055058
H	-3.242583	-1.515278	2.862083
H	-2.338208	-0.612925	4.124249
H	-3.254832	0.260314	2.835462
C	2.674644	-0.054926	0.525952
C	3.607777	-0.956398	-0.047658
C	4.825246	-0.434692	-0.531562
H	5.562458	-1.120904	-0.977422
C	5.108284	0.934607	-0.463939
H	6.063707	1.321570	-0.851562
C	4.166771	1.815016	0.088588
H	4.390309	2.891790	0.127667
C	2.936806	1.345115	0.585833
C	3.320266	-2.447143	-0.170365
H	2.324617	-2.638453	0.279054
C	4.358744	-3.294600	0.589261
H	4.428935	-2.996873	1.655866
H	4.087281	-4.370109	0.549840
H	5.373250	-3.190403	0.149069
C	3.230166	-2.866103	-1.650291
H	4.204874	-2.738249	-2.167966
H	2.931104	-3.930909	-1.735588
H	2.469979	-2.264724	-2.187361
C	1.925833	2.305340	1.205713
H	0.931387	1.818406	1.126035

C	2.202868	2.516583	2.707912
H	3.208939	2.960063	2.865209
H	1.451201	3.201944	3.152367
H	2.161681	1.563880	3.270064
C	1.847144	3.652049	0.471160
H	1.638531	3.511389	-0.609645
H	1.036786	4.275878	0.900419
H	2.786869	4.235043	0.566335
C	-2.779702	0.143562	0.338435
C	-3.801259	-0.778899	-0.016598
C	-5.012386	-0.264180	-0.523920
H	-5.817516	-0.964242	-0.797500
C	-5.204106	1.110333	-0.700646
H	-6.158336	1.489636	-1.098666
C	-4.168108	2.003057	-0.390713
H	-4.316364	3.079796	-0.557156
C	-2.941649	1.543854	0.125546
C	-3.620421	-2.290703	0.079781
H	-2.624567	-2.490763	0.525526
C	-4.696186	-2.955470	0.961127
H	-5.707820	-2.857978	0.513384
H	-4.487775	-4.039470	1.075416
H	-4.743637	-2.508583	1.975681
C	-3.613448	-2.919225	-1.328426
H	-2.828606	-2.466171	-1.964097
H	-3.402992	-4.006798	-1.264995
H	-4.595006	-2.787427	-1.831714
C	-1.817990	2.522281	0.457444
H	-0.864543	2.002926	0.207602
C	-1.765569	2.856242	1.961090
H	-1.556972	1.960211	2.577155
H	-0.963078	3.594587	2.168637
H	-2.727846	3.294485	2.300564
C	-1.862706	3.802616	-0.389288
H	-2.721713	4.451964	-0.118254
H	-0.940972	4.396263	-0.229886
H	-1.934504	3.569874	-1.471691

LBrGaSb

E = -5978.06287541 G = -5977.518148 E+ZPE = -5977.443492

Sb	0.269712	0.807184	-2.514722
Br	-0.251435	-2.918133	-0.433597
Ga	-0.028734	-0.538619	-0.295619
N	-1.497329	-0.026560	0.931186
N	1.424859	-0.247360	1.007994
C	-1.346360	-0.208170	2.255012
C	-0.107124	-0.524260	2.868523
H	-0.154083	-0.720674	3.947751
C	1.192272	-0.454244	2.317995
C	-2.549843	-0.063914	3.158739
H	-3.212027	0.757556	2.822947
H	-3.156277	-0.993026	3.129383

H	-2.242953	0.113990	4.205701
C	2.376402	-0.618147	3.242919
H	3.128528	0.179189	3.083211
H	2.066768	-0.621568	4.303852
H	2.888832	-1.577800	3.018256
C	-2.741643	0.423197	0.367754
C	-2.853390	1.795221	-0.004805
C	-4.067358	2.240777	-0.560920
H	-4.175088	3.295840	-0.849970
C	-5.143375	1.363231	-0.754368
H	-6.086370	1.732982	-1.186596
C	-5.006372	0.014414	-0.412291
H	-5.845208	-0.677772	-0.586574
C	-3.809646	-0.487535	0.140681
C	-1.698170	2.767974	0.218086
H	-0.761927	2.207882	-0.008986
C	-1.738589	3.979706	-0.724802
H	-1.822532	3.667980	-1.786063
H	-2.588970	4.655314	-0.494692
H	-0.811807	4.576360	-0.619092
C	-1.608595	3.221795	1.688790
H	-2.551713	3.714989	2.005631
H	-1.416139	2.373247	2.373073
H	-0.781692	3.949617	1.822806
C	-3.701475	-1.982431	0.421799
H	-2.706948	-2.177039	0.873459
C	-3.762420	-2.778659	-0.897406
H	-2.980796	-2.441762	-1.605489
H	-3.595306	-3.858933	-0.707409
H	-4.752328	-2.664161	-1.388314
C	-4.787849	-2.476317	1.397239
H	-5.802738	-2.387427	0.955146
H	-4.627280	-3.545989	1.645333
H	-4.793154	-1.901730	2.346183
C	2.719677	0.156143	0.534864
C	3.017807	1.548521	0.500422
C	4.282037	1.951565	0.029259
H	4.532397	3.023432	0.005594
C	5.223780	1.012832	-0.413690
H	6.207357	1.346974	-0.779422
C	4.903247	-0.349909	-0.400557
H	5.638466	-1.084586	-0.765041
C	3.653233	-0.805006	0.065712
C	2.012252	2.589507	0.981980
H	1.023218	2.089202	1.026727
C	1.893952	3.772437	0.008127
H	1.621196	3.426873	-1.011037
H	1.113834	4.480942	0.353555
H	2.841099	4.345884	-0.068916
C	2.342522	3.076146	2.407120
H	1.599656	3.827025	2.748831
H	2.335462	2.242199	3.136245
H	3.347365	3.548140	2.442397
C	3.324536	-2.290097	0.013721

H	2.334638	-2.435768	0.491801
C	3.189497	-2.751412	-1.450784
H	4.158524	-2.670858	-1.988158
H	2.847590	-3.805325	-1.500295
H	2.444505	-2.135001	-1.994377
C	4.347583	-3.147417	0.780773
H	5.357385	-3.098080	0.320834
H	4.446951	-2.818649	1.836306
H	4.034979	-4.212253	0.782688

3'

E = -4699.14053673 G = -4698.160326 E+ZPE = -4698.065153

Sb	-0.917374	0.373047	0.304168
Ga	1.559844	0.296023	-0.523166
Cl	2.147647	0.270968	-2.717654
N	3.167181	-0.667285	0.206043
N	2.211793	2.091033	0.068783
N	-3.174569	-1.412003	-0.604934
C	4.340992	-0.031936	0.361642
C	4.512334	1.367433	0.224859
H	5.547949	1.725144	0.302994
C	3.521192	2.369856	0.160017
C	5.580635	-0.829443	0.711298
H	6.271834	-0.226519	1.329935
H	6.120423	-1.111761	-0.216466
H	5.332595	-1.766383	1.244383
C	3.962495	3.816514	0.184472
H	3.246846	4.452477	0.740316
H	3.989724	4.201872	-0.857676
H	4.973359	3.929210	0.618644
C	3.037619	-2.078018	0.424723
C	3.471888	-3.016712	-0.552057
C	3.250029	-4.386481	-0.298543
H	3.578557	-5.126817	-1.045101
C	2.615536	-4.821691	0.870140
H	2.451815	-5.896981	1.043511
C	2.182292	-3.882112	1.816979
H	1.678273	-4.227323	2.731483
C	2.378779	-2.503869	1.613901
C	4.146029	-2.609267	-1.860266
H	4.245030	-1.504922	-1.865812
C	5.549920	-3.235061	-1.992245
H	6.183487	-3.033188	-1.105165
H	6.070384	-2.834939	-2.887271
H	5.491087	-4.338013	-2.109255
C	3.280469	-2.982083	-3.080011
H	2.306992	-2.458431	-3.051254
H	3.100825	-4.077396	-3.127405
H	3.789815	-2.679507	-4.018555
C	1.926810	-1.483053	2.651819
H	1.587077	-0.586042	2.089939
C	3.096433	-1.040812	3.552406

H	2.756832	-0.284288	4.290589
H	3.917895	-0.587178	2.964026
H	3.512317	-1.904965	4.112611
C	0.727758	-1.957273	3.479341
H	0.340039	-1.125530	4.099972
H	0.991958	-2.788209	4.167681
H	-0.094748	-2.294234	2.817328
C	1.199974	3.073430	0.322043
C	0.621744	3.804583	-0.748097
C	-0.460458	4.660759	-0.462147
H	-0.926902	5.227948	-1.283206
C	-0.960658	4.787873	0.839851
H	-1.813928	5.454334	1.041307
C	-0.382064	4.054339	1.886075
H	-0.791786	4.144755	2.902938
C	0.694530	3.179076	1.651006
C	1.131788	3.665310	-2.176780
H	1.971923	2.942504	-2.162800
C	0.054899	3.069405	-3.101127
H	-0.327521	2.111701	-2.695205
H	0.477597	2.865944	-4.106247
H	-0.803563	3.764240	-3.219674
C	1.658530	5.006214	-2.722788
H	0.846806	5.760535	-2.802669
H	2.091448	4.872049	-3.736191
H	2.444408	5.434546	-2.066865
C	1.296850	2.348665	2.782501
H	1.718486	1.435074	2.311837
C	2.466759	3.082243	3.468620
H	2.123955	4.039338	3.916277
H	3.283061	3.313100	2.757651
H	2.895796	2.457678	4.280015
C	0.255470	1.894124	3.816643
H	0.721674	1.202501	4.548392
H	-0.586654	1.363291	3.327723
H	-0.159955	2.745717	4.395542
C	-1.828799	-1.224434	-0.711408
C	-4.039844	-0.510602	0.116017
C	-4.357781	-0.783284	1.477993
C	-5.279956	0.058777	2.131083
H	-5.543959	-0.148623	3.179798
C	-5.848677	1.159375	1.481076
H	-6.572845	1.800654	2.007754
C	-5.465438	1.460103	0.169190
H	-5.874608	2.355322	-0.324345
C	-4.549883	0.652840	-0.534523
C	-3.689066	-1.888817	2.291197
H	-3.022482	-2.452556	1.606756
C	-2.803267	-1.275012	3.395116
H	-2.033436	-0.609184	2.956982
H	-2.286302	-2.072856	3.966859
H	-3.410871	-0.684303	4.112472
C	-4.706085	-2.863431	2.917843
H	-5.320315	-2.355849	3.690970

H	-4.180387	-3.703574	3.417821
H	-5.401481	-3.289148	2.168622
C	-4.099881	1.116762	-1.918031
H	-3.380929	0.369776	-2.308472
C	-5.272550	1.242863	-2.910851
H	-5.965730	2.055603	-2.608091
H	-5.866637	0.311327	-2.988077
H	-4.895244	1.493767	-3.924118
C	-3.353729	2.464179	-1.819105
H	-4.029531	3.272247	-1.467446
H	-2.964046	2.758644	-2.814641
H	-2.494649	2.398905	-1.120964
C	-1.260937	-2.267439	-1.675933
C	-3.713751	-2.597266	-1.373082
C	-1.016465	-1.609285	-3.056795
H	-1.923227	-1.103154	-3.442658
H	-0.205067	-0.857517	-2.997740
H	-0.713842	-2.383819	-3.793343
C	0.042150	-2.904820	-1.178862
H	0.873181	-2.176085	-1.204393
H	-0.048715	-3.270406	-0.137245
H	0.333180	-3.753111	-1.831498
C	-4.506187	-2.144965	-2.611366
H	-5.396712	-1.560009	-2.309690
H	-3.897896	-1.528419	-3.298107
H	-4.859319	-3.035409	-3.169935
C	-4.630378	-3.465763	-0.503340
H	-4.096459	-3.858897	0.381367
H	-5.519347	-2.897981	-0.161697
H	-4.986998	-4.329941	-1.099889
C	-2.398805	-3.323891	-1.724736
H	-2.455685	-3.834416	-2.706729
H	-2.200248	-4.100560	-0.956694

4'

E = -6813.16056386 G = -6812.181273 E+ZPE = -6812.085572

Sb	-1.004372	0.378155	0.345664
Ga	1.504064	0.277627	-0.386665
N	3.046441	-0.740943	0.414309
N	2.150362	2.047294	0.290449
N	-3.253059	-1.391917	-0.631736
C	4.220795	-0.128509	0.644879
C	4.426296	1.268583	0.532971
H	5.464252	1.602661	0.664608
C	3.460880	2.294089	0.444868
C	5.422119	-0.951942	1.060840
H	6.092272	-0.363305	1.715015
H	6.003906	-1.249236	0.163962
H	5.123496	-1.881604	1.580703
C	3.933248	3.728980	0.522426
H	3.229671	4.361212	1.097464
H	3.972731	4.150187	-0.505060

H	4.943391	3.802962	0.965905
C	2.884373	-2.151178	0.623351
C	3.357754	-3.096569	-0.329274
C	3.117921	-4.464327	-0.081726
H	3.477654	-5.208327	-0.809874
C	2.429530	-4.893502	1.057973
H	2.254205	-5.967487	1.227686
C	1.956210	-3.948340	1.979362
H	1.409080	-4.288044	2.870828
C	2.167529	-2.571461	1.780774
C	4.090840	-2.701419	-1.608464
H	4.179604	-1.595929	-1.625180
C	5.504224	-3.317405	-1.668795
H	6.095069	-3.104089	-0.755586
H	6.063099	-2.921600	-2.542214
H	5.458116	-4.421762	-1.777967
C	3.288216	-3.102187	-2.861827
H	2.294101	-2.618257	-2.871544
H	3.149278	-4.203145	-2.916596
H	3.821755	-2.779464	-3.779641
C	1.673129	-1.549691	2.797499
H	1.390775	-0.640555	2.224241
C	2.793664	-1.143839	3.774305
H	2.423992	-0.392436	4.503071
H	3.657280	-0.697425	3.243491
H	3.159766	-2.023631	4.344726
C	0.411978	-2.002290	3.541430
H	0.017009	-1.173349	4.160675
H	0.605537	-2.859095	4.221081
H	-0.381258	-2.290842	2.823077
C	1.153658	3.048274	0.535474
C	0.652265	3.849016	-0.523811
C	-0.410264	4.732763	-0.246713
H	-0.815849	5.353814	-1.060951
C	-0.963346	4.824646	1.036332
H	-1.799620	5.514475	1.230124
C	-0.456869	4.027641	2.073244
H	-0.903888	4.094137	3.076089
C	0.598154	3.124613	1.846587
C	1.216136	3.759224	-1.935745
H	2.044121	3.022031	-1.920440
C	0.164122	3.221915	-2.922556
H	-0.232450	2.244692	-2.582654
H	0.613936	3.071742	-3.925348
H	-0.688491	3.926405	-3.025251
C	1.784986	5.111096	-2.407272
H	0.988359	5.880110	-2.497661
H	2.262430	5.005979	-3.403829
H	2.545209	5.504835	-1.701302
C	1.135157	2.245512	2.973432
H	1.545929	1.332721	2.492363
C	2.301855	2.926353	3.717105
H	1.971457	3.882018	4.176965
H	3.148391	3.149712	3.040294

H	2.684639	2.269774	4.526294
C	0.047010	1.800487	3.961931
H	0.466497	1.077305	4.691148
H	-0.796219	1.309445	3.435186
H	-0.358434	2.651667	4.548207
C	-1.903074	-1.214383	-0.692567
C	-4.145500	-0.470000	0.027892
C	-4.531531	-0.708615	1.378304
C	-5.484217	0.149780	1.963153
H	-5.799903	-0.030648	3.002509
C	-6.018581	1.233462	1.258115
H	-6.767598	1.887376	1.731700
C	-5.569529	1.501603	-0.040009
H	-5.952130	2.384065	-0.575873
C	-4.621050	0.676863	-0.676325
C	-3.901134	-1.790120	2.252410
H	-3.195311	-2.365381	1.618470
C	-3.078753	-1.142208	3.385652
H	-2.296016	-0.475755	2.972353
H	-2.580970	-1.920798	3.999035
H	-3.728618	-0.544679	4.059023
C	-4.943125	-2.756069	2.850321
H	-5.602270	-2.232599	3.574263
H	-4.438777	-3.576782	3.401783
H	-5.593262	-3.209159	2.077247
C	-4.098499	1.107666	-2.044639
H	-3.374760	0.342754	-2.387098
C	-5.218006	1.234406	-3.096649
H	-5.918895	2.055101	-2.836755
H	-5.814206	0.306266	-3.195665
H	-4.787130	1.473627	-4.091135
C	-3.334793	2.443762	-1.927918
H	-4.017432	3.271162	-1.640324
H	-2.872453	2.707853	-2.900609
H	-2.527065	2.378117	-1.170920
C	-1.311715	-2.266162	-1.633402
C	-3.772158	-2.589304	-1.395622
C	-1.032284	-1.614868	-3.010680
H	-1.930385	-1.116859	-3.425923
H	-0.229141	-0.856096	-2.930632
H	-0.701565	-2.390044	-3.734121
C	-0.021651	-2.901446	-1.102514
H	0.807846	-2.169908	-1.109298
H	-0.136717	-3.266129	-0.063061
H	0.287038	-3.750137	-1.746293
C	-4.538157	-2.156322	-2.657362
H	-5.433101	-1.563053	-2.385360
H	-3.914044	-1.554539	-3.342903
H	-4.882523	-3.055861	-3.206576
C	-4.706278	-3.446689	-0.533408
H	-4.190908	-3.825318	0.368686
H	-5.603726	-2.875935	-0.220625
H	-5.047661	-4.320782	-1.124356
C	-2.449458	-3.320272	-1.706787

H	-2.480404	-3.836669	-2.686798
H	-2.272577	-4.093099	-0.929477
Br	2.266062	0.312357	-2.687890

5'

E = -5023.45586843 G = -5022.386528 E+ZPE = -5022.280909

Sb	0.841933	0.063993	-0.791012
Ga	-1.354166	0.644699	0.428697
Cl	-2.107630	0.049437	2.468829
N	-3.050280	0.522601	-0.668220
N	-1.450397	2.653057	0.522176
N	3.345746	-1.349797	0.169675
N	1.792350	-2.246563	1.419129
C	-4.015541	1.450191	-0.543078
C	-3.852753	2.660901	0.170432
H	-4.755803	3.276887	0.271983
C	-2.649852	3.266445	0.587353
C	-5.359489	1.226442	-1.205557
H	-5.916650	2.177092	-1.294841
H	-5.974190	0.520581	-0.611049
H	-5.244817	0.774014	-2.209522
C	-2.719086	4.694687	1.086157
H	-2.092154	5.368362	0.467926
H	-2.313562	4.759374	2.116591
H	-3.759546	5.068349	1.082964
C	-3.295630	-0.649680	-1.458399
C	-4.104510	-1.701947	-0.946171
C	-4.332586	-2.826074	-1.765620
H	-4.955334	-3.649345	-1.381700
C	-3.779589	-2.918676	-3.048087
H	-3.969893	-3.807073	-3.670500
C	-2.969843	-1.881666	-3.531824
H	-2.527291	-1.961778	-4.535398
C	-2.711760	-0.737179	-2.754326
C	-4.693894	-1.673136	0.461085
H	-4.528684	-0.663033	0.886884
C	-6.205495	-1.970459	0.481346
H	-6.775532	-1.309989	-0.204751
H	-6.610465	-1.832534	1.505359
H	-6.420447	-3.017933	0.181965
C	-3.932424	-2.656348	1.362877
H	-2.857073	-2.408607	1.390597
H	-4.041769	-3.699133	0.996734
H	-4.306926	-2.611944	2.406611
C	-1.879445	0.411122	-3.312290
H	-1.353081	0.869295	-2.447630
C	-2.778049	1.504826	-3.922149
H	-2.161408	2.319592	-4.355012
H	-3.446135	1.958622	-3.164160
H	-3.409678	1.085871	-4.733839
C	-0.804908	-0.040897	-4.309581
H	-0.129552	0.804815	-4.550154

H	-1.245011	-0.395039	-5.265841
H	-0.184039	-0.854183	-3.884047
C	-0.283587	3.489320	0.600461
C	0.298463	3.807003	1.854330
C	1.312414	4.783637	1.894789
H	1.756972	5.056742	2.864568
C	1.772848	5.399630	0.723624
H	2.562713	6.165460	0.774564
C	1.251073	5.008486	-0.517224
H	1.644913	5.461244	-1.440388
C	0.222165	4.050806	-0.603559
C	-0.095576	3.045119	3.109758
H	-1.056109	2.527370	2.909600
C	0.958711	1.949005	3.363130
H	1.081676	1.303831	2.467821
H	0.658113	1.309434	4.214307
H	1.948963	2.397959	3.592118
C	-0.289829	3.936039	4.346501
H	0.658349	4.415005	4.671471
H	-0.660845	3.332020	5.200268
H	-1.025963	4.745179	4.157074
C	-0.356718	3.657756	-1.958296
H	-0.914936	2.710480	-1.804458
C	-1.369360	4.706654	-2.459087
H	-0.891279	5.705316	-2.551135
H	-2.230600	4.802501	-1.768488
H	-1.769663	4.426308	-3.455355
C	0.738974	3.387846	-3.002912
H	0.287999	3.005881	-3.942367
H	1.463040	2.631512	-2.635010
H	1.301380	4.309322	-3.263254
C	1.988659	-1.267820	0.458801
C	3.963021	-2.357511	0.902666
H	5.029606	-2.573451	0.794709
C	2.994913	-2.921074	1.683173
H	3.027184	-3.760016	2.382036
C	3.974647	-0.601613	-0.882897
C	4.046322	-1.187509	-2.170576
C	4.636699	-0.421917	-3.195677
H	4.709124	-0.842856	-4.210791
C	5.121877	0.868952	-2.942210
H	5.572765	1.453969	-3.759333
C	5.035841	1.421037	-1.655054
H	5.417007	2.437008	-1.469376
C	4.455765	0.697514	-0.595867
C	3.509616	-2.586422	-2.455322
H	3.073667	-2.979410	-1.514829
C	2.376420	-2.558234	-3.496692
H	1.554275	-1.898925	-3.149363
H	1.963934	-3.577333	-3.649662
H	2.731205	-2.185867	-4.480709
C	4.644243	-3.544844	-2.865627
H	5.121615	-3.224783	-3.815875
H	4.251438	-4.572120	-3.015391

H	5.437126	-3.588870	-2.090602
C	4.367762	1.283540	0.805917
H	3.731504	0.603786	1.409336
C	5.762236	1.327119	1.462005
H	6.450047	1.993269	0.898917
H	6.226920	0.319772	1.498128
H	5.693108	1.712247	2.500946
C	3.682751	2.656971	0.806766
H	4.256149	3.412546	0.230046
H	3.581775	3.039451	1.841673
H	2.665372	2.585088	0.372040
C	0.551972	-2.829429	1.873540
C	-0.113745	-3.714842	0.987442
C	-1.171576	-4.481808	1.508623
H	-1.701074	-5.183283	0.846212
C	-1.557528	-4.361975	2.850146
H	-2.389391	-4.969657	3.238714
C	-0.909471	-3.449039	3.690479
H	-1.241135	-3.342131	4.733398
C	0.166541	-2.665539	3.227037
C	0.326335	-3.899146	-0.459759
H	1.013833	-3.067564	-0.710147
C	1.100163	-5.219064	-0.637674
H	1.456634	-5.323504	-1.684294
H	0.461865	-6.098563	-0.407331
H	1.986347	-5.260150	0.029582
C	-0.855416	-3.771253	-1.430506
H	-1.361697	-2.794789	-1.298783
H	-1.610709	-4.572445	-1.290833
H	-0.501919	-3.824766	-2.480358
C	0.909866	-1.729696	4.177625
H	1.387721	-0.946282	3.551571
C	2.020814	-2.473650	4.951811
H	2.799505	-2.891585	4.285756
H	1.590911	-3.311568	5.540589
H	2.525728	-1.783665	5.659893
C	-0.029310	-1.033585	5.177516
H	0.536670	-0.285928	5.770688
H	-0.460415	-1.755052	5.903368
H	-0.858905	-0.519331	4.655970

6‘

E = -7137.47641771 G = -7136.408674 E+ZPE = -7136.30197

Sb	0.963234	0.157189	-0.839379
Br	-2.200906	-0.298004	2.388199
Ga	-1.310150	0.556409	0.329633
N	-1.450164	2.545186	0.597706
N	-2.988690	0.500510	-0.821884
N	3.471917	-1.247287	0.118086
N	1.917362	-2.222421	1.307724
C	-2.669543	3.112571	0.722351
C	-3.846777	2.523892	0.224631

H	-4.769896	3.099194	0.379108
C	-3.967855	1.398284	-0.627611
C	-2.784104	4.467576	1.388990
H	-2.364496	4.420554	2.414869
H	-3.838082	4.796912	1.443551
H	-2.194062	5.237359	0.852166
C	-5.293758	1.261830	-1.350383
H	-5.644953	2.253417	-1.695871
H	-6.061289	0.865719	-0.653513
H	-5.233633	0.573969	-2.212761
C	-0.313997	3.414897	0.727719
C	0.106490	4.139976	-0.420845
C	1.097458	5.129009	-0.268689
H	1.422756	5.707282	-1.147821
C	1.666252	5.395881	0.984078
H	2.425307	6.186774	1.090311
C	1.291054	4.625106	2.091859
H	1.771513	4.804116	3.066576
C	0.316550	3.613888	1.982540
C	-0.512916	3.876922	-1.788711
H	-1.074968	2.924229	-1.706561
C	-1.531316	4.968603	-2.170982
H	-1.051936	5.970546	-2.196283
H	-2.370819	5.009791	-1.448556
H	-1.963290	4.771348	-3.174257
C	0.562433	3.699602	-2.873785
H	1.137449	4.634144	-3.042990
H	0.095604	3.424020	-3.841948
H	1.279969	2.900910	-2.593739
C	0.018869	2.704654	3.163049
H	-0.913197	2.146048	2.937944
C	-0.192428	3.453007	4.488396
H	-0.486888	2.741049	5.287100
H	-0.991762	4.218678	4.403002
H	0.730481	3.968190	4.830501
C	1.155972	1.669524	3.271598
H	1.254523	1.096254	2.325821
H	0.960335	0.959381	4.096168
H	2.128473	2.170248	3.465687
C	-3.175321	-0.601329	-1.721121
C	-2.503865	-0.577170	-2.977284
C	-2.670432	-1.667582	-3.851054
H	-2.157455	-1.663473	-4.823704
C	-3.481309	-2.757082	-3.504305
H	-3.598422	-3.602693	-4.200034
C	-4.136238	-2.766758	-2.268193
H	-4.770994	-3.625279	-1.997320
C	-4.000729	-1.701549	-1.354097
C	-1.695402	0.641296	-3.404404
H	-1.227109	1.054368	-2.484845
C	-2.623214	1.735625	-3.968994
H	-2.034128	2.612580	-4.308058
H	-3.347751	2.090503	-3.210393
H	-3.196638	1.351095	-4.838619

C	-0.563519	0.313035	-4.386731
H	0.082963	1.200798	-4.535013
H	-0.951104	0.016933	-5.384471
H	0.075332	-0.505049	-3.998289
C	-4.739882	-1.776315	-0.020970
H	-4.572456	-0.823717	0.521300
C	-6.256755	-1.975108	-0.210560
H	-6.698675	-1.219174	-0.890181
H	-6.779626	-1.908648	0.766372
H	-6.484110	-2.975032	-0.637535
C	-4.153839	-2.889611	0.861756
H	-3.077323	-2.721093	1.041251
H	-4.281539	-3.887555	0.389554
H	-4.654893	-2.910083	1.852116
C	2.107029	-1.211198	0.378361
C	4.103171	-2.249476	0.846884
H	5.178398	-2.429468	0.761065
C	3.135132	-2.860406	1.590652
H	3.179103	-3.706858	2.279602
C	4.095055	-0.482280	-0.926794
C	4.173860	-1.059386	-2.218511
C	4.767826	-0.286424	-3.235659
H	4.847525	-0.701633	-4.252575
C	5.249489	1.003560	-2.971571
H	5.705389	1.593826	-3.782137
C	5.152159	1.548589	-1.682587
H	5.528747	2.564743	-1.489210
C	4.566911	0.817945	-0.630709
C	3.645175	-2.458702	-2.515146
H	3.183492	-2.850382	-1.586691
C	2.543330	-2.433021	-3.589766
H	1.711574	-1.771474	-3.270657
H	2.134280	-3.452166	-3.750773
H	2.927932	-2.066669	-4.564749
C	4.791572	-3.417689	-2.890195
H	5.298406	-3.097962	-3.825229
H	4.402962	-4.444913	-3.050948
H	5.559570	-3.461635	-2.090560
C	4.465433	1.398246	0.772239
H	3.805480	0.728310	1.361052
C	3.807783	2.785018	0.768288
H	3.696032	3.163990	1.803225
H	2.796595	2.735078	0.316831
H	4.406626	3.532399	0.206463
C	5.848952	1.410522	1.452769
H	6.559765	2.064958	0.904659
H	6.292269	0.393675	1.491522
H	5.769924	1.791332	2.492613
C	0.679569	-2.833934	1.728665
C	-0.026115	-3.614737	0.776361
C	-1.125151	-4.362520	1.235202
H	-1.688100	-4.979462	0.519199
C	-1.502541	-4.343436	2.584677
H	-2.367401	-4.935663	2.921672

C	-0.791518	-3.561615	3.500594
H	-1.104642	-3.542143	4.554877
C	0.317037	-2.790220	3.097623
C	0.437300	-3.746487	-0.669065
H	1.105685	-2.890421	-0.886228
C	-0.721242	-3.633251	-1.666201
H	-1.266648	-2.680317	-1.521068
H	-1.449663	-4.465795	-1.575930
H	-0.336707	-3.640805	-2.706068
C	1.251805	-5.041771	-0.854700
H	1.628724	-5.119701	-1.896433
H	0.632729	-5.940761	-0.648461
H	2.127461	-5.071572	-0.173043
C	1.102840	-1.993271	4.135041
H	1.708924	-1.242271	3.585186
C	0.181802	-1.238846	5.111661
H	0.780919	-0.576503	5.770392
H	-0.368335	-1.939274	5.774461
H	-0.562427	-0.626025	4.566485
C	2.064646	-2.903202	4.929923
H	2.798154	-3.419665	4.280561
H	1.497215	-3.684051	5.479210
H	2.636160	-2.310492	5.674703

[L(Br)GaSb]$_2$

E = -11956.272645 G = -11955.154145 E+ZPE = -11955.033044

Sb	0.471311	1.212426	0.299486
Br	-2.443783	0.589017	3.431393
Ga	-0.144829	0.665801	2.749010
N	0.638442	-0.958129	3.602872
N	0.718290	1.965620	3.963342
C	0.982226	-0.911200	4.903265
C	1.043250	0.282461	5.669223
H	1.270925	0.142362	6.734525
C	1.012851	1.626655	5.227364
C	1.339028	-2.202716	5.605468
H	1.959340	-2.851839	4.956769
H	0.416799	-2.774758	5.836300
H	1.875206	-2.010292	6.552593
C	1.304214	2.723403	6.226598
H	1.813979	3.581517	5.747871
H	1.910274	2.357358	7.076159
H	0.340835	3.105505	6.629338
C	0.713048	-2.174244	2.837381
C	1.813353	-2.347284	1.940197
C	1.842656	-3.498478	1.127549
H	2.671028	-3.637241	0.420254
C	0.827111	-4.463161	1.189694
H	0.863151	-5.344405	0.531330
C	-0.247469	-4.273405	2.061727
H	-1.061847	-5.013930	2.087191
C	-0.340354	-3.129783	2.883738

C	2.918724	-1.304232	1.832270
H	2.411885	-0.310602	1.872418
C	3.677033	-1.360183	0.498851
H	2.991807	-1.299645	-0.371786
H	4.282217	-2.285969	0.402693
H	4.377113	-0.505421	0.423980
C	3.890584	-1.363800	3.027842
H	4.367636	-2.363849	3.099248
H	3.383268	-1.151526	3.988528
H	4.697559	-0.612036	2.906180
C	-1.602279	-2.945726	3.719696
H	-1.515736	-1.986670	4.269662
C	-2.837543	-2.831415	2.802814
H	-2.713263	-2.011637	2.068523
H	-3.745695	-2.610608	3.400562
H	-3.012260	-3.775204	2.243588
C	-1.796269	-4.083396	4.741541
H	-1.967334	-5.057740	4.236673
H	-2.678951	-3.881334	5.383132
H	-0.914179	-4.208369	5.402692
C	1.012864	3.244266	3.384013
C	2.282102	3.415054	2.755251
C	2.537067	4.622102	2.077655
H	3.508645	4.767758	1.582534
C	1.569177	5.634092	2.007995
H	1.786784	6.570027	1.469801
C	0.322405	5.443518	2.614577
H	-0.442281	6.233726	2.548601
C	0.015325	4.250129	3.300293
C	3.343457	2.321469	2.815420
H	2.806609	1.362771	2.974238
C	4.144646	2.197117	1.510805
H	3.475733	2.050584	0.637031
H	4.832058	1.329181	1.564937
H	4.771595	3.092368	1.317562
C	4.282721	2.516798	4.022656
H	5.036607	1.703330	4.067802
H	3.727116	2.513151	4.980351
H	4.823777	3.484027	3.948692
C	-1.374063	4.059956	3.891506
H	-1.409338	3.051470	4.351635
C	-2.441073	4.082194	2.780377
H	-2.501549	5.080093	2.294914
H	-3.441172	3.836403	3.192176
H	-2.208543	3.330078	2.000416
C	-1.676155	5.095836	4.990228
H	-1.695744	6.129472	4.583541
H	-0.911503	5.069714	5.793864
H	-2.666638	4.898543	5.450813
Sb	-0.528505	-1.223689	-0.277445
Br	2.435973	-0.480109	-3.331095
Ga	0.121667	-0.645410	-2.714549
N	-0.674382	0.972832	-3.572396
N	-0.653104	-1.947470	-3.981897

C	-0.975700	0.937489	-4.882972
C	-0.971376	-0.244253	-5.670057
H	-1.167063	-0.092379	-6.740058
C	-0.909408	-1.594166	-5.251007
C	-1.350892	2.228170	-5.577148
H	-1.987723	2.861277	-4.928816
H	-0.436705	2.817540	-5.796765
H	-1.874974	2.033316	-6.530627
C	-1.122696	-2.681968	-6.279033
H	-1.668647	-3.543713	-5.848728
H	-1.661388	-2.308255	-7.169431
H	-0.131894	-3.063929	-6.607851
C	-0.807906	2.171846	-2.788386
C	-1.934784	2.288483	-1.915818
C	-2.021941	3.417497	-1.077380
H	-2.871486	3.510889	-0.387825
C	-1.035943	4.414589	-1.091137
H	-1.114156	5.277790	-0.412965
C	0.064408	4.281352	-1.941209
H	0.855647	5.046563	-1.927359
C	0.214130	3.161901	-2.787648
C	-3.004663	1.205379	-1.860822
H	-2.461446	0.232008	-1.917341
C	-3.793104	1.195878	-0.543784
H	-3.123673	1.141023	0.339276
H	-4.436910	2.094256	-0.437334
H	-4.460297	0.312484	-0.507980
C	-3.951018	1.262784	-3.076640
H	-4.463956	2.245960	-3.131319
H	-3.413561	1.097789	-4.030302
H	-4.730924	0.477661	-2.995576
C	1.501800	3.036710	-3.594773
H	1.462992	2.084199	-4.161511
C	2.717553	2.949356	-2.649625
H	2.596951	2.119533	-1.926217
H	3.646117	2.760582	-3.226545
H	2.851140	3.891348	-2.076395
C	1.680190	4.198472	-4.592036
H	1.803485	5.168792	-4.065787
H	2.585343	4.039720	-5.214263
H	0.810804	4.304192	-5.272924
C	-0.918398	-3.251200	-3.446293
C	-2.199115	-3.482721	-2.862245
C	-2.437133	-4.722124	-2.239435
H	-3.418061	-4.916126	-1.780717
C	-1.441718	-5.707810	-2.180153
H	-1.647185	-6.670730	-1.686564
C	-0.183074	-5.456251	-2.737810
H	0.604129	-6.224399	-2.676188
C	0.107730	-4.228189	-3.367414
C	-3.289150	-2.417480	-2.913641
H	-2.774599	-1.437544	-3.003013
C	-4.145392	-2.381624	-1.639085
H	-3.514993	-2.278683	-0.731437

H	-4.844485	-1.521898	-1.671370
H	-4.764508	-3.296008	-1.526174
C	-4.173273	-2.576691	-4.167017
H	-4.954531	-1.788748	-4.197651
H	-3.582380	-2.498453	-5.100150
H	-4.680599	-3.564827	-4.168328
C	1.511156	-3.971811	-3.897622
H	1.530457	-2.948107	-4.323958
C	2.532737	-3.994293	-2.744153
H	2.605358	-5.004203	-2.286025
H	3.540177	-3.704469	-3.106305
H	2.244430	-3.274972	-1.951870
C	1.894980	-4.960713	-5.013997
H	1.938973	-6.005390	-4.638632
H	1.161894	-4.938160	-5.846705
H	2.894016	-4.711816	-5.428779

$[L(Cl)GaSb]_2$

E = -7728.23175478 G = -7727.109269 E+ZPE = -7726.991124

Sb	-0.892604	-0.873663	-0.268918
Ga	-2.684790	0.777022	0.583565
Cl	-2.849450	1.266394	2.771014
N	-4.480270	0.147833	0.050823
N	-2.835718	2.554735	-0.292873
C	-5.485244	1.015641	-0.143022
C	-5.272460	2.404797	-0.309116
H	-6.179588	3.010883	-0.435614
C	-4.048913	3.103247	-0.482248
C	-6.903493	0.491852	-0.164727
H	-6.960427	-0.502269	-0.648594
H	-7.593878	1.191048	-0.672006
H	-7.252529	0.357295	0.882158
C	-4.130255	4.550110	-0.915276
H	-3.959187	5.214950	-0.043158
H	-5.121768	4.787006	-1.342695
H	-3.341687	4.790574	-1.654787
C	-4.603013	-1.270518	-0.117603
C	-4.816958	-2.114655	1.002824
C	-4.821852	-3.509874	0.799106
H	-4.995090	-4.175184	1.660088
C	-4.596914	-4.060075	-0.468283
H	-4.598969	-5.152829	-0.606417
C	-4.352745	-3.214836	-1.560356
H	-4.152041	-3.652826	-2.549507
C	-4.342422	-1.815208	-1.410209
C	-4.997813	-1.556429	2.407912
H	-4.928739	-0.451694	2.343805
C	-6.376526	-1.914852	2.993394
H	-7.199828	-1.565958	2.336231
H	-6.511330	-1.447009	3.990992
H	-6.495627	-3.012202	3.119413
C	-3.852377	-2.021398	3.328072

H	-3.878017	-3.121316	3.484279
H	-3.923473	-1.529228	4.319372
H	-2.867311	-1.755107	2.896032
C	-4.065748	-0.905767	-2.603857
H	-3.663896	0.045344	-2.195100
C	-5.364518	-0.559845	-3.359584
H	-5.847222	-1.479536	-3.753361
H	-5.151090	0.110800	-4.218078
H	-6.096541	-0.045873	-2.707307
C	-3.013085	-1.480626	-3.563697
H	-2.070717	-1.726977	-3.032516
H	-2.776133	-0.742516	-4.356305
H	-3.370316	-2.398801	-4.074969
C	-1.619851	3.259140	-0.598362
C	-1.056348	4.169320	0.337947
C	0.175764	4.779894	0.020709
H	0.623392	5.482045	0.741126
C	0.856035	4.480980	-1.162652
H	1.830501	4.945291	-1.377844
C	0.308392	3.552976	-2.060602
H	0.863698	3.298080	-2.973383
C	-0.927675	2.927169	-1.804568
C	-1.685877	4.461885	1.695985
H	-2.625132	3.878206	1.773380
C	-2.019132	5.956949	1.869260
H	-1.099019	6.578939	1.875449
H	-2.543643	6.129364	2.832075
H	-2.666555	6.339097	1.053264
C	-0.762624	3.979410	2.833530
H	-0.520108	2.904665	2.720818
H	-1.260670	4.108359	3.816561
H	0.188278	4.553370	2.851006
C	-1.483232	1.886584	-2.767969
H	-1.861610	1.055399	-2.123472
C	-2.681301	2.414534	-3.581818
H	-3.534183	2.700947	-2.937468
H	-3.044036	1.633990	-4.281937
H	-2.387358	3.299085	-4.185214
C	-0.419650	1.277449	-3.691290
H	-0.037473	2.015196	-4.428058
H	-0.856508	0.438372	-4.267718
H	0.443826	0.871967	-3.126156
Sb	0.931643	0.986451	0.417620
Ga	2.652894	-0.694991	-0.544870
Cl	2.733171	-1.018551	-2.773528
N	4.506951	-0.221786	-0.058056
N	2.742545	-2.555865	0.160055
C	5.467259	-1.156236	0.003290
C	5.182355	-2.541018	0.061705
H	6.057651	-3.203708	0.087653
C	3.930250	-3.183459	0.239544
C	6.913841	-0.715845	-0.007082
H	7.053834	0.229744	0.551483
H	7.583844	-1.492878	0.405425

H	7.220450	-0.515591	-1.056722
C	3.946004	-4.663227	0.552813
H	3.599735	-5.244653	-0.325872
H	4.961562	-5.005968	0.822282
H	3.247291	-4.900420	1.379419
C	4.725486	1.166344	0.222869
C	4.949185	2.091939	-0.828837
C	5.054735	3.459845	-0.503061
H	5.233722	4.189758	-1.308594
C	4.926669	3.904235	0.818271
H	5.009666	4.977292	1.052096
C	4.676160	2.979955	1.842835
H	4.553364	3.337294	2.876267
C	4.559006	1.604400	1.569204
C	5.046534	1.649331	-2.282829
H	4.915250	0.548847	-2.309715
C	6.423634	1.980365	-2.888586
H	7.247236	1.533991	-2.293695
H	6.498451	1.591021	-3.925445
H	6.600194	3.076418	-2.928936
C	3.901636	2.253350	-3.118582
H	3.980575	3.360318	-3.175705
H	3.919844	1.851190	-4.152167
H	2.916044	1.997885	-2.681880
C	4.263924	0.607955	2.686244
H	3.790882	-0.275693	2.208734
C	5.560878	0.114609	3.358337
H	6.114590	0.960665	3.818200
H	5.332500	-0.621307	4.157432
H	6.236683	-0.377200	2.632145
C	3.277769	1.155751	3.728927
H	2.337088	1.502335	3.252714
H	3.019481	0.365699	4.462957
H	3.705718	2.003470	4.303775
C	1.508909	-3.234137	0.449866
C	0.869591	-4.032597	-0.539170
C	-0.376489	-4.615646	-0.225330
H	-0.887175	-5.225796	-0.986213
C	-0.997329	-4.397215	1.007240
H	-1.987727	-4.829570	1.214361
C	-0.375945	-3.575530	1.959068
H	-0.887280	-3.376776	2.910791
C	0.876738	-2.980271	1.706967
C	1.426599	-4.222634	-1.946824
H	2.390292	-3.678993	-2.013710
C	1.673502	-5.708132	-2.277597
H	0.723086	-6.282109	-2.300126
H	2.147693	-5.809832	-3.275849
H	2.334631	-6.200192	-1.534520
C	0.483470	-3.590889	-2.991208
H	0.326185	-2.514114	-2.786585
H	0.919712	-3.676591	-4.007714
H	-0.507006	-4.093558	-2.996960
C	1.514601	-2.049606	2.731911

H	1.938076	-1.196087	2.149880
C	2.690013	-2.715669	3.475082
H	3.509944	-3.001527	2.788677
H	3.115566	-2.017940	4.225806
H	2.351968	-3.626278	4.012948
C	0.507158	-1.451204	3.723604
H	0.088638	-2.219345	4.407497
H	1.007497	-0.691172	4.355602
H	-0.335590	-0.948150	3.206648

[L(Cl)GaSb]$_3$

E = -11592.3778312 G = -11590.668851 E+ZPE = -11590.512206

Sb	-1.557072	0.075571	-0.877747
Sb	0.167572	-1.277316	0.996419
Ga	-3.655803	0.707012	0.718457
Ga	1.318130	-3.397688	-0.190489
Cl	-4.182497	-0.564868	2.502333
Cl	2.489289	-3.861962	-2.048417
N	-5.495924	0.959494	-0.119705
N	-3.663495	2.497145	1.572529
N	2.292773	-4.648962	1.068644
N	-0.177853	-4.656054	-0.451834
C	-6.356697	1.873784	0.363375
C	-6.064576	2.766588	1.420146
H	-6.907588	3.381963	1.762736
C	-4.802847	3.120300	1.929366
C	-7.732278	2.041983	-0.256409
H	-8.516747	1.725720	0.460713
H	-7.857328	1.457647	-1.184765
H	-7.908081	3.113607	-0.477013
C	-4.720946	4.301186	2.872351
H	-5.718827	4.744899	3.043227
H	-4.039458	5.082469	2.479884
H	-4.298138	3.982130	3.847182
C	-5.931389	0.029578	-1.117762
C	-5.371841	0.116634	-2.424371
C	-5.748775	-0.842870	-3.382488
H	-5.318036	-0.793143	-4.392859
C	-6.677847	-1.847536	-3.076359
H	-6.960367	-2.589951	-3.838646
C	-7.244258	-1.901262	-1.797394
H	-7.971405	-2.693051	-1.559517
C	-6.882787	-0.981331	-0.791197
C	-4.469650	1.284505	-2.806580
H	-3.842421	1.527215	-1.920620
C	-3.517218	0.978475	-3.969206
H	-2.787346	1.802401	-4.088892
H	-4.057476	0.871014	-4.933459
H	-2.939506	0.048964	-3.787363
C	-5.317002	2.539996	-3.097695
H	-5.907115	2.847061	-2.212543

H	-6.022466	2.351728	-3.934173
H	-4.665568	3.392219	-3.380966
C	-7.505979	-1.130672	0.595914
H	-7.170993	-0.278594	1.220392
C	-7.011225	-2.407667	1.301575
H	-7.512294	-2.522071	2.285467
H	-5.924339	-2.348210	1.490479
H	-7.224229	-3.316043	0.699679
C	-9.047377	-1.117042	0.532493
H	-9.475747	-1.087693	1.555880
H	-9.439056	-2.031786	0.039773
H	-9.438415	-0.246304	-0.030720
C	-2.431817	3.205330	1.739495
C	-2.014008	4.021773	0.653881
C	-0.841092	4.780441	0.813408
H	-0.490271	5.411076	-0.015762
C	-0.106027	4.723100	2.006668
H	0.811611	5.313168	2.114421
C	-0.513750	3.880025	3.048303
H	0.101400	3.817071	3.958417
C	-1.676805	3.093681	2.933303
C	-2.829951	4.093082	-0.634183
H	-3.489011	3.200051	-0.652783
C	-3.754041	5.327246	-0.642526
H	-4.345502	5.365589	-1.581292
H	-3.160621	6.263528	-0.573091
H	-4.469357	5.310953	0.203599
C	-1.953547	4.044713	-1.891739
H	-2.588505	3.990687	-2.800059
H	-1.286028	3.160900	-1.883828
H	-1.301700	4.934501	-1.992646
C	-2.076446	2.115837	4.031568
H	-3.114601	1.782816	3.823941
C	-2.042721	2.749491	5.432944
H	-2.658393	3.672021	5.481438
H	-1.010018	3.022742	5.736707
H	-2.431244	2.037011	6.189831
C	-1.194164	0.855145	3.967927
H	-1.498872	0.117909	4.738897
H	-0.122814	1.105448	4.121244
H	-1.286468	0.352853	2.983830
C	2.102291	-5.976260	0.976764
C	1.131489	-6.588582	0.145522
H	1.172929	-7.685496	0.098718
C	0.014430	-5.985069	-0.462791
C	2.927897	-6.925430	1.823294
H	2.258154	-7.618153	2.370971
H	3.567095	-6.393969	2.550688
H	3.577791	-7.546844	1.174215
C	-1.011316	-6.857871	-1.149132
H	-0.870849	-7.926846	-0.904129
H	-0.912210	-6.731060	-2.248699
H	-2.043614	-6.552392	-0.889351
C	3.337860	-4.078023	1.865221

C	2.974824	-3.366859	3.047146
C	3.982688	-2.687301	3.755428
H	3.721267	-2.136276	4.669809
C	5.313450	-2.697659	3.311357
H	6.084958	-2.142669	3.867613
C	5.659531	-3.433724	2.172490
H	6.710851	-3.463373	1.845148
C	4.694863	-4.152686	1.436121
C	1.542433	-3.418946	3.570957
H	0.870124	-3.362946	2.685646
C	1.254191	-4.769791	4.255874
H	0.210337	-4.798413	4.631229
H	1.935381	-4.925974	5.118816
H	1.382230	-5.619235	3.559218
C	1.166659	-2.252859	4.494293
H	1.412123	-1.273389	4.039925
H	1.681389	-2.318940	5.476335
H	0.075592	-2.263866	4.687398
C	5.158866	-5.037796	0.278351
H	4.264478	-5.517224	-0.166747
C	6.113192	-6.137736	0.795405
H	6.328831	-6.874354	-0.006742
H	5.697962	-6.683928	1.664570
H	7.083460	-5.701403	1.113911
C	5.840773	-4.253782	-0.854303
H	6.214427	-4.952420	-1.631674
H	6.706767	-3.667319	-0.482857
H	5.125678	-3.566505	-1.339701
C	-1.470149	-4.080543	-0.644431
C	-2.278257	-3.915505	0.516648
C	-3.521982	-3.284546	0.362646
H	-4.160862	-3.131517	1.240814
C	-3.941308	-2.810838	-0.887217
H	-4.915583	-2.321367	-0.984672
C	-3.117714	-2.956313	-2.011053
H	-3.459983	-2.564370	-2.981065
C	-1.865736	-3.594318	-1.914571
C	-1.816202	-4.423483	1.882017
H	-0.704706	-4.420084	1.866892
C	-2.256917	-5.881403	2.126406
H	-1.919354	-6.226099	3.126549
H	-1.837587	-6.577879	1.375638
H	-3.363953	-5.965540	2.090731
C	-2.271531	-3.526992	3.042280
H	-1.809651	-3.870514	3.990920
H	-3.371242	-3.553516	3.184733
H	-1.991406	-2.468181	2.875708
C	-0.969325	-3.726044	-3.139060
H	-0.102793	-4.358149	-2.855474
C	-1.697610	-4.412082	-4.309273
H	-2.117740	-5.394355	-4.008344
H	-1.000812	-4.578916	-5.157072
H	-2.538179	-3.792138	-4.687214
C	-0.394662	-2.362160	-3.563072

H	0.291917	-2.475889	-4.425296
H	0.190790	-1.898232	-2.745005
H	-1.198554	-1.649606	-3.846582
Sb	0.509470	1.549796	0.539902
Ga	2.314046	2.683875	-1.087629
Cl	1.490683	4.529880	-2.105241
N	3.796359	3.585446	-0.028087
N	3.500715	2.009556	-2.499013
C	4.948179	3.919013	-0.631421
C	3.523763	4.038052	1.303724
C	4.624074	2.688714	-2.826642
C	3.291509	0.763921	-3.178398
C	5.243655	3.626726	-1.984737
C	6.055217	4.613421	0.137738
C	3.450622	3.074204	2.348926
C	3.315266	5.423772	1.564509
C	5.310238	2.362245	-4.135750
C	4.080476	-0.339225	-2.757237
C	2.419376	0.683510	-4.290984
H	6.174071	4.067386	-2.368547
H	7.011269	4.079024	-0.030719
H	5.855049	4.661517	1.222592
H	6.191385	5.648147	-0.236813
C	3.139799	3.512463	3.649650
C	3.817236	1.619532	2.086506
C	3.042599	5.811967	2.893391
C	3.358565	6.501674	0.481103
H	6.088592	3.113183	-4.365986
H	4.574308	2.325702	-4.963496
H	5.783978	1.360064	-4.099305
C	4.030008	-1.515607	-3.523764
C	4.916671	-0.262599	-1.480407
C	2.381018	-0.528129	-5.009665
C	1.543739	1.866407	-4.678287
H	3.071594	2.776695	4.464129
C	2.943222	4.872663	3.926807
H	3.469619	1.365601	1.061125
C	5.350505	1.446853	2.096649
C	3.149578	0.632083	3.048071
H	2.883699	6.879141	3.114768
H	3.650654	6.021848	-0.474467
C	4.381159	7.608051	0.813210
H	4.637949	-2.382195	-3.228795
C	3.194035	-1.609338	-4.645698
H	4.968811	0.799705	-1.170587
C	6.366259	-0.733801	-1.682609
C	4.191930	-1.017471	-0.348601
H	1.714583	-0.617361	-5.881499
H	1.981134	2.774002	-4.212343
C	1.471910	2.103803	-6.195242
C	0.141330	1.688465	-4.070257
H	2.713008	5.201186	4.952357
H	5.623411	0.383819	1.935378
H	5.771893	1.765761	3.073355

H	5.835826	2.047452	1.302489
H	2.058168	0.815850	3.122586
H	3.584306	0.683657	4.068970
H	3.295076	-0.403486	2.685480
H	4.493818	8.299652	-0.047449
H	5.380828	7.199592	1.061058
H	4.050315	8.217027	1.681072
H	3.159780	-2.545605	-5.223541
H	6.932953	-0.659980	-0.730965
H	6.887064	-0.110241	-2.438603
H	6.421866	-1.786875	-2.020276
H	4.782311	-1.014281	0.589601
H	4.001973	-2.072084	-0.622760
H	3.206586	-0.552535	-0.141412
H	2.483232	2.203360	-6.641893
H	0.909162	3.035295	-6.412255
H	0.951519	1.276357	-6.722908
H	-0.492240	2.577133	-4.267108
H	0.197571	1.554724	-2.970179
H	-0.362361	0.789943	-4.484454
C	1.967971	7.120160	0.244292
H	2.027655	7.912608	-0.530432
H	1.262014	6.353626	-0.122179
H	1.560874	7.577820	1.170688

L(Br)GaSbGaL

E = -9141.63187591 G = -9140.506342 E+ZPE = -9140.393011

Ga	2.045055	0.190520	0.164143
N	2.890985	1.785322	0.923332
N	3.759410	-0.684059	-0.329014
C	4.232051	1.981196	0.954637
C	5.192525	1.003852	0.620608
H	6.239607	1.289589	0.784150
C	4.983089	-0.243616	-0.012052
C	4.752104	3.359342	1.304462
H	4.546860	4.052039	0.461536
H	5.843209	3.333882	1.479745
H	4.244119	3.792064	2.185876
C	6.183490	-1.094162	-0.353242
H	6.210125	-1.982110	0.313216
H	7.127548	-0.533084	-0.227813
H	6.119733	-1.485690	-1.387148
C	2.047145	2.919319	1.207020
C	1.629639	3.155305	2.544585
C	0.935247	4.352120	2.804685
H	0.597102	4.570966	3.827098
C	0.645415	5.263144	1.778379
H	0.105910	6.194940	2.008420
C	0.992988	4.964444	0.455800
H	0.708365	5.655621	-0.352837
C	1.685014	3.779279	0.139582
C	1.882682	2.122376	3.645287

H	1.708450	1.129826	3.171551
C	3.326487	2.124706	4.191362
H	4.073217	1.822901	3.432941
H	3.411622	1.407639	5.034475
H	3.604476	3.129083	4.576382
C	0.893632	2.250791	4.814366
H	1.064394	3.181353	5.396319
H	1.027467	1.403711	5.517933
H	-0.155752	2.241608	4.459005
C	1.976162	3.427882	-1.317311
H	2.579313	2.494532	-1.327776
C	2.803671	4.509340	-2.034848
H	2.250109	5.469918	-2.097060
H	3.038657	4.194082	-3.072799
H	3.763306	4.708916	-1.513861
C	0.663923	3.128942	-2.066254
H	0.097275	2.309160	-1.578877
H	0.868621	2.812179	-3.109341
H	0.007271	4.021266	-2.105786
C	3.564139	-1.820553	-1.184297
C	3.363080	-3.107265	-0.621691
C	3.070697	-4.173064	-1.495572
H	2.905702	-5.179152	-1.079273
C	2.960768	-3.967669	-2.876838
H	2.725339	-4.812905	-3.542480
C	3.129294	-2.681762	-3.410893
H	3.013410	-2.523081	-4.494088
C	3.418085	-1.582507	-2.581019
C	3.422978	-3.348146	0.883151
H	3.617493	-2.367768	1.367264
C	4.578931	-4.297302	1.257600
H	4.417865	-5.310396	0.832308
H	4.656796	-4.406128	2.359592
H	5.555958	-3.932463	0.877807
C	2.078653	-3.872592	1.421988
H	1.245768	-3.191525	1.153098
H	2.109057	-3.968070	2.527103
H	1.836829	-4.873597	1.007804
C	3.556978	-0.180071	-3.170263
H	3.491000	0.536251	-2.323907
C	4.935101	0.015909	-3.833289
H	5.764285	-0.153147	-3.117087
H	5.037092	1.046820	-4.232657
H	5.070993	-0.691990	-4.678426
C	2.413582	0.168325	-4.137902
H	2.426595	-0.467720	-5.047893
H	2.501548	1.223303	-4.471662
H	1.432322	0.044395	-3.634606
Ga	-1.760259	-0.028347	0.327896
N	-3.335843	0.672866	-0.715853
N	-2.820734	-1.489966	1.186577
C	-4.589977	0.484623	-0.277598
C	-4.926022	-0.348720	0.819664
H	-5.983110	-0.328771	1.118456

C	-4.131883	-1.329834	1.447354
C	-5.752211	1.159644	-0.977574
H	-5.470673	1.548607	-1.972995
H	-6.598298	0.453398	-1.085547
H	-6.112618	2.013582	-0.367359
C	-4.795052	-2.260785	2.439374
H	-4.356153	-2.106115	3.447212
H	-5.885122	-2.084668	2.493539
H	-4.610186	-3.322654	2.182005
C	-3.038143	1.507038	-1.844524
C	-3.090488	2.924530	-1.733326
C	-2.736638	3.694398	-2.860752
H	-2.777401	4.792972	-2.790267
C	-2.318231	3.095359	-4.053189
H	-2.032151	3.717717	-4.915635
C	-2.259681	1.697514	-4.143962
H	-1.931532	1.229832	-5.083400
C	-2.624894	0.881758	-3.057504
C	-3.488997	3.645963	-0.449445
H	-3.726556	2.881148	0.318082
C	-4.724429	4.546029	-0.651690
H	-5.584326	3.992915	-1.078975
H	-5.044568	4.987458	0.315356
H	-4.500165	5.388156	-1.340676
C	-2.309255	4.469170	0.095519
H	-2.037305	5.292473	-0.599502
H	-2.565319	4.921400	1.076081
H	-1.418092	3.835198	0.251126
C	-2.656318	-0.635600	-3.198665
H	-2.339536	-1.053022	-2.218465
C	-4.092482	-1.134092	-3.454604
H	-4.501504	-0.696074	-4.389630
H	-4.109228	-2.239129	-3.557603
H	-4.773441	-0.865275	-2.623821
C	-1.685283	-1.177794	-4.254963
H	-0.656666	-0.803010	-4.080320
H	-1.651099	-2.284598	-4.208348
H	-1.992811	-0.900267	-5.285549
C	-2.176664	-2.723571	1.536645
C	-1.517854	-2.877665	2.782354
C	-0.955703	-4.131977	3.093167
H	-0.449569	-4.267334	4.062181
C	-1.014945	-5.198534	2.188403
H	-0.569881	-6.171533	2.449469
C	-1.616157	-5.013254	0.935265
H	-1.630172	-5.842570	0.211734
C	-2.198464	-3.781225	0.583885
C	-1.349997	-1.711780	3.745496
H	-1.949866	-0.862257	3.359608
C	-1.839235	-2.030735	5.168925
H	-1.237150	-2.834494	5.643977
H	-1.760810	-1.131650	5.815068
H	-2.898528	-2.362718	5.173389
C	0.121153	-1.255905	3.746904

H	0.449274	-0.994254	2.719492
H	0.249294	-0.363254	4.389537
H	0.790572	-2.058557	4.123784
C	-2.845651	-3.588415	-0.783705
H	-2.864658	-2.494438	-0.972954
C	-4.309657	-4.072133	-0.797238
H	-4.931965	-3.520846	-0.065374
H	-4.762889	-3.922142	-1.799553
H	-4.371063	-5.154070	-0.551878
C	-2.037657	-4.243037	-1.915574
H	-2.043665	-5.351152	-1.844173
H	-2.475948	-3.980730	-2.900475
H	-0.981902	-3.901941	-1.903509
Sb	0.218939	-1.092709	-0.904821
Br	-1.553828	1.625026	2.062999

L(Br)GaSbGaL

E = -7027.61160921 G = -7026.483491 E+ZPE = -7026.372295

Ga	-1.966239	0.172429	-0.195918
N	-2.813126	1.719727	-1.050840
N	-3.680142	-0.694569	0.310916
C	-4.156627	1.886478	-1.131946
C	-5.110271	0.909779	-0.776835
H	-6.156264	1.167289	-0.987548
C	-4.901057	-0.293227	-0.064050
C	-4.692678	3.235512	-1.563519
H	-4.530913	3.969992	-0.746707
H	-5.776390	3.178037	-1.773791
H	-4.162581	3.638984	-2.445502
C	-6.097807	-1.137545	0.303601
H	-6.092384	-2.072340	-0.295693
H	-7.046224	-0.602834	0.112863
H	-6.055050	-1.450836	1.365209
C	-1.993794	2.866561	-1.357084
C	-1.559727	3.071277	-2.693820
C	-0.936629	4.297991	-2.992217
H	-0.593235	4.494541	-4.017628
C	-0.732532	5.270040	-2.001572
H	-0.253909	6.226728	-2.262169
C	-1.081265	5.000938	-0.672732
H	-0.855478	5.739199	0.112665
C	-1.699729	3.786264	-0.319015
C	-1.733787	1.982513	-3.753880
H	-1.550554	1.019898	-3.227146
C	-3.152311	1.914963	-4.359301
H	-3.923358	1.633821	-3.617068
H	-3.182386	1.151119	-5.164326
H	-3.440444	2.888619	-4.810363
C	-0.696366	2.089858	-4.882701
H	-0.868485	2.986145	-5.515748
H	-0.771284	1.207403	-5.551242
H	0.334021	2.128798	-4.478866

C	-1.986915	3.471091	1.146383
H	-2.523623	2.498713	1.186262
C	-2.895981	4.517586	1.815029
H	-2.410050	5.515435	1.849558
H	-3.124710	4.223319	2.860594
H	-3.859285	4.632076	1.275576
C	-0.665057	3.288823	1.915949
H	-0.047404	2.482590	1.470302
H	-0.858523	3.009846	2.971988
H	-0.062061	4.219389	1.914621
C	-3.493995	-1.769468	1.243721
C	-3.306324	-3.096168	0.778150
C	-3.033970	-4.098232	1.730583
H	-2.883709	-5.135301	1.391727
C	-2.925348	-3.792552	3.093477
H	-2.704330	-4.589485	3.820754
C	-3.077644	-2.468444	3.529914
H	-2.964329	-2.231831	4.598931
C	-3.351965	-1.430863	2.619749
C	-3.352322	-3.443696	-0.705966
H	-3.571747	-2.506225	-1.259095
C	-4.475187	-4.451200	-1.022439
H	-4.290388	-5.427828	-0.527380
H	-4.536787	-4.638313	-2.114881
H	-5.467307	-4.090075	-0.679291
C	-1.986820	-3.960483	-1.197716
H	-1.180170	-3.232146	-0.978079
H	-2.005972	-4.142112	-2.292145
H	-1.713066	-4.916608	-0.705033
C	-3.495465	0.010854	3.104574
H	-3.398496	0.666228	2.212441
C	-4.893904	0.262010	3.704374
H	-5.700330	0.049775	2.973814
H	-4.999251	1.319088	4.027154
H	-5.065500	-0.384489	4.591096
C	-2.383214	0.421845	4.083054
H	-2.428822	-0.150727	5.033160
H	-2.479242	1.497019	4.341579
H	-1.385693	0.264745	3.622194
Ga	1.774968	-0.002113	-0.398435
Cl	1.426475	1.429279	-2.116750
N	3.369424	0.823265	0.511855
N	2.848317	-1.467970	-1.224600
C	4.613727	0.637165	0.046210
C	4.937059	-0.259242	-1.003408
H	5.983347	-0.235641	-1.337486
C	4.145490	-1.294033	-1.541536
C	5.776641	1.393069	0.657168
H	5.522459	1.822824	1.643211
H	6.655467	0.727538	0.760728
H	6.073395	2.229991	-0.008910
C	4.798435	-2.270519	-2.496283
H	4.312721	-2.202840	-3.492010
H	5.878300	-2.062794	-2.610291

H	4.663913	-3.317322	-2.158180
C	3.089513	1.734353	1.583325
C	3.099886	3.138383	1.356900
C	2.767116	3.989003	2.431159
H	2.773841	5.078773	2.270697
C	2.412328	3.477824	3.684189
H	2.143312	4.160680	4.505343
C	2.393676	2.090778	3.888207
H	2.113921	1.691890	4.873934
C	2.736907	1.198515	2.855955
C	3.430041	3.754406	0.000620
H	3.701319	2.933914	-0.693694
C	4.614116	4.737924	0.084229
H	5.508811	4.279868	0.551995
H	4.896885	5.090941	-0.929561
H	4.352354	5.635678	0.683585
C	2.190613	4.443392	-0.592450
H	1.859164	5.292203	0.042773
H	2.407543	4.841075	-1.605683
H	1.350844	3.732899	-0.693693
C	2.808688	-0.302042	3.114411
H	2.488463	-0.802332	2.175309
C	4.260602	-0.745117	3.383740
H	4.670886	-0.228729	4.277296
H	4.307475	-1.838963	3.567451
H	4.923158	-0.520870	2.525078
C	1.866120	-0.781682	4.225834
H	0.826305	-0.444725	4.037621
H	1.858021	-1.889473	4.266087
H	2.181149	-0.418447	5.227021
C	2.226343	-2.735301	-1.478436
C	1.533185	-2.978622	-2.690525
C	1.003680	-4.265779	-2.911266
H	0.473434	-4.473862	-3.854169
C	1.125025	-5.275413	-1.948715
H	0.705074	-6.275420	-2.140126
C	1.754429	-4.999111	-0.726321
H	1.813738	-5.783682	0.043451
C	2.308050	-3.731968	-0.465210
C	1.293279	-1.870007	-3.705503
H	1.876272	-0.982785	-3.384694
C	1.740891	-2.247124	-5.128189
H	1.147725	-3.091731	-5.539152
H	1.611018	-1.385614	-5.815951
H	2.809277	-2.547238	-5.155289
C	-0.192293	-1.464006	-3.673712
H	-0.490187	-1.158367	-2.648958
H	-0.377354	-0.613122	-4.357997
H	-0.846256	-2.308211	-3.979624
C	2.984516	-3.434804	0.869516
H	2.967912	-2.331569	0.993004
C	4.465475	-3.862979	0.871155
H	5.047719	-3.329548	0.094549
H	4.936688	-3.640907	1.851588

H	4.562015	-4.953760	0.683264
C	2.229703	-4.044721	2.061129
H	2.286574	-5.153766	2.067631
H	2.672506	-3.692477	3.015637
H	1.159447	-3.753040	2.046254
Sb	-0.134946	-0.996245	0.991016

3^{H}

E = -4153.91130567 G = -4153.214831 E+ZPE = -4153.133015

Sb	0.099889	2.116841	0.340158
Ga	0.412251	-0.279804	-0.593649
Cl	0.103528	-0.722859	-2.788542
N	-0.401495	-1.944030	0.190730
N	2.271173	-0.839120	-0.226479
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C	1.686450	-3.178958	-0.046484
H	2.102299	-4.195840	-0.034276
C	2.623756	-2.135618	-0.197339
C	-0.377471	-4.371333	0.673791
H	0.269628	-4.939941	1.369654
H	-0.547995	-5.012950	-0.215518
H	-1.356367	-4.187756	1.153283
C	4.087124	-2.491056	-0.338013
H	4.728573	-1.821874	0.267991
H	4.394193	-2.345827	-1.396104
H	4.282280	-3.542283	-0.056829
C	-1.792260	-1.872383	0.528219
C	-2.788374	-2.339713	-0.376628
C	-4.143232	-2.156368	-0.026756
H	-4.924558	-2.516561	-0.714351
C	-4.512267	-1.518800	1.162643
H	-5.576716	-1.383763	1.411565
C	-3.519698	-1.049937	2.035652
H	-3.812486	-0.546844	2.968515
C	-2.153411	-1.217560	1.743334
C	-2.460471	-3.014027	-1.706484
H	-1.357482	-3.031923	-1.818784
C	-2.991728	-4.462015	-1.748834
H	-2.651381	-5.059351	-0.879872
H	-2.651824	-4.973483	-2.673480
H	-4.102407	-4.483031	-1.748034
C	-3.013227	-2.207466	-2.897791
H	-2.574567	-1.192609	-2.924455
H	-4.120152	-2.124850	-2.855006
H	-2.747722	-2.705606	-3.853332
C	-1.081415	-0.758348	2.724785
H	-0.233632	-0.383769	2.111630
C	-0.558235	-1.939757	3.564755
H	0.240961	-1.602088	4.257396
H	-0.130839	-2.737735	2.926737
H	-1.372720	-2.387630	4.172852
C	-1.528390	0.408519	3.613766

H	-0.667351	0.791893	4.196165
H	-2.311626	0.107574	4.342019
H	-1.914790	1.246204	2.998097
C	3.220218	0.210976	-0.005061
C	3.844302	0.865774	-1.097839
C	4.725019	1.930635	-0.820178
H	5.220004	2.449436	-1.656448
C	4.969795	2.346186	0.494750
H	5.658849	3.182878	0.690334
C	4.322543	1.706695	1.562206
H	4.502976	2.051496	2.591643
C	3.433612	0.638445	1.337701
C	3.549280	0.471072	-2.539150
H	2.882331	-0.414646	-2.515415
C	2.775343	1.593987	-3.257190
H	1.861475	1.867897	-2.692088
H	2.460457	1.264510	-4.268609
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H	4.575280	-0.264479	-4.330214
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C	2.730042	-0.055140	2.502170
H	1.817521	-0.531113	2.085306
C	3.597579	-1.183812	3.094208
H	4.555875	-0.781350	3.486464
H	3.838692	-1.955524	2.337824
H	3.068546	-1.687856	3.930295
C	2.280361	0.925490	3.596189
H	1.690701	0.391075	4.369356
H	1.644095	1.729146	3.171928
H	3.141192	1.397852	4.114762
C	-1.927456	2.160366	-0.203220
C	-2.711001	1.206876	-1.085502
C	-4.130043	3.103652	-0.467873
C	-4.184081	4.043898	-1.688770
H	-3.987351	5.094830	-1.389842
H	-3.424472	3.754985	-2.443181
H	-5.184338	4.006646	-2.167363
C	-5.193106	3.481727	0.571122
H	-5.112720	2.832018	1.466000
H	-5.087405	4.539656	0.893504
H	-6.209532	3.364331	0.143111
C	-4.185208	1.608741	-0.880347
H	-4.816529	1.446271	-1.775588
H	-4.611658	1.011665	-0.049041
N	-2.779156	3.152358	0.140765
H	-2.468354	3.976586	0.663196
H	-2.522393	0.148991	-0.829912
H	-2.368701	1.335304	-2.135288

E = -4090.16235389 G = -4089.550367 E+ZPE = -4089.471442

Sb	0.282437	1.128198	2.007839
Ga	0.051942	0.226872	-0.384766
Cl	-0.254775	1.699779	-2.156991
N	-1.297323	-1.139759	-0.910833
N	1.602343	-0.816481	-1.035435
C	-1.055462	-1.973587	-1.938276
C	0.218552	-2.127437	-2.538821
H	0.255087	-2.797083	-3.407974
C	1.470102	-1.670253	-2.066934
C	-2.188946	-2.820477	-2.473370
H	-1.822270	-3.566650	-3.201638
H	-2.948456	-2.182859	-2.969506
H	-2.714282	-3.342669	-1.648771
C	2.722054	-2.190444	-2.735877
H	3.368272	-2.718327	-2.006044
H	3.327051	-1.345706	-3.125033
H	2.480376	-2.878019	-3.566740
C	-2.573187	-1.152001	-0.249963
C	-3.685228	-0.463242	-0.804557
C	-4.926124	-0.554848	-0.141559
H	-5.799131	-0.033276	-0.564863
C	-5.064079	-1.281999	1.045749
H	-6.043271	-1.346360	1.545962
C	-3.943456	-1.906416	1.611199
H	-4.049899	-2.448009	2.562096
C	-2.682854	-1.847474	0.987418
C	-3.559522	0.432851	-2.031158
H	-2.548013	0.289739	-2.461195
C	-4.597710	0.116980	-3.122651
H	-4.557761	-0.946467	-3.437975
H	-4.418250	0.743903	-4.020773
H	-5.634092	0.320350	-2.779128
C	-3.651038	1.909080	-1.593815
H	-2.915143	2.126356	-0.795785
H	-4.662058	2.146461	-1.199055
H	-3.440327	2.586460	-2.447272
C	-1.466638	-2.520109	1.617080
H	-0.594885	-1.873234	1.373517
C	-1.194007	-3.908540	1.006067
H	-0.315761	-4.383715	1.491319
H	-0.978987	-3.847634	-0.078820
H	-2.066434	-4.581091	1.148467
C	-1.557809	-2.592321	3.147597
H	-0.602367	-2.957625	3.572515
H	-2.351986	-3.290962	3.486061
H	-1.760309	-1.590355	3.577476
C	2.884473	-0.610708	-0.421135
C	3.716394	0.464423	-0.831485
C	4.960678	0.628426	-0.191833
H	5.615255	1.459606	-0.498372
C	5.375017	-0.236860	0.828769
H	6.352811	-0.092607	1.314712
C	4.531656	-1.277354	1.239461
H	4.850715	-1.945530	2.055284

C	3.276069	-1.478794	0.634389
C	3.272396	1.463336	-1.891537
H	2.331051	1.087808	-2.339403
C	2.942203	2.816562	-1.230234
H	2.231542	2.676872	-0.389613
H	2.482705	3.509443	-1.964990
H	3.857353	3.294918	-0.819795
C	4.300130	1.622625	-3.025636
H	5.257020	2.053163	-2.660927
H	3.908210	2.303358	-3.809831
H	4.534375	0.649120	-3.505404
C	2.368710	-2.600516	1.128835
H	1.396146	-2.496736	0.606007
C	2.932459	-3.990315	0.775997
H	3.913395	-4.164441	1.267318
H	3.080027	-4.104920	-0.317132
H	2.240046	-4.792131	1.108357
C	2.101437	-2.473559	2.638772
H	1.418507	-3.276602	2.983204
H	1.636447	-1.496255	2.885151
H	3.037301	-2.557593	3.229416
C	-0.640250	2.999603	1.476824
C	-1.575104	5.072597	1.756744
H	-1.970125	5.929919	2.309243
C	-1.454431	4.843120	0.409254
H	-1.727328	5.463641	-0.449417
N	-1.074586	3.936061	2.386382
H	-1.047098	3.775804	3.393816
N	-0.882608	3.587539	0.264316
H	-0.655613	3.115323	-0.638037

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Supporting Information

Formation and Cleavage of a Sb—Sb Double Bond: From Carbene-Coordinated Distibenes to Stibinidenes

Julia Krüger, Christoph Wölper, Alexander A. Auer,* and Stephan Schulz*

Contents

Synthesis of $L^1Ga(Cl)^RNHC^{Me}$

$LGaCl_2$ (50 mg, 0.09mmol) and $^RNHC^{Me}$ (R = Me, Et, *i*Pr; 0.18 mmol) were weighed in a Schlenk flask, 2 mL toluene were added. The suspension was stirred over night at ambient temperature, yielding a white precipitate ($^RNHC^{Me}HCl$) that was filtered off and the solvent removed in vacuo. The residue was washed with 5 mL n-hexane and dried vacuum to give analytically pure powder of $L^1Ga(Cl)^RNHC^{Me}$.

$L^1Ga(Cl)^{Me}NHC^{Me}$: Yield 36 mg (0.056 mmol; 63 %). M.p. 161 °C (dec.). Anal. Calcd. for $C_{36}H_{52}N_4ClGa$: C, 66.93; H, 8.11; N, 8.67. Found: C, 67.1; H, 8.22; N, 8.15 %. **^{1}H-NMR (C_6D_6, 400 MHz, 25 °C) δ [ppm]:** 7.03-7.45 (m, 6 H, C_6H_3), 5.44 (s, 1 H, γ-C*H*), 4.30 (sept, 2 H, $^3J_{HH}$ = 6.8 Hz, C*H*(CH_3)$_2$), 3.97 (s, 1H, β-CH_2), 3.33 (s (br), 6H, NCH_3), 3.28 (s, 1 H, β-CH_2), 3.17 (sept, 1 H, $^3J_{HH}$ = 6.8 Hz, C*H*(CH_3)$_2$), 3.12 (sept, 1 H, $^3J_{HH}$ = 6.8 Hz, C*H*(CH_3)$_2$), 1.72-1.76 (m, 12 H, CCH_3, CH(CH_3)$_2$), 1.55 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 1.46 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 1.16 (s (br), 6H, C=CCH_3), 1.13 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 0.45 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 0.34 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$). **^{13}C{^{1}H}-NMR (C_6D_6, 100 MHz, 25 °C) δ [ppm]:** 155.1 (*C*CH_3), 149.7 (*C*$_6H_3$), 149.4 (*C*$_6H_3$), 146.8 (*C*$_6H_3$), 145.6 (*C*$_6H_3$), 143.3 (*C*$_6H_3$), 143.1 (*C*$_6H_3$), 126.8 (*C=C,* (br)), 125.9 (*C*$_6H_3$), 125.8 (*C*$_6H_3$), 125.0 (*C*$_6H_3$), 124.6 (*C*$_6H_3$), 123.2 (*C*$_6H_3$), 122.7 (*C*$_6H_3$), 102.5 (γ-*C*H), 80.8 (β-CH_2), 34.1 (NCH_3), 29.0 (*C*H(CH_3)$_2$), 28.8 (*C*H(CH_3)$_2$), 28.0 (*C*H(CH_3)$_2$), 27.4 (*C*H(CH_3)$_2$), 26.8 (CH(*C*H_3)$_2$), 26.7 (CH(*C*H_3)$_2$), 25.7 (CH(*C*H_3)$_2$), 25.1 (C*C*H_3), 24.8 (CH(*C*H_3)$_2$), 24.4 (CH(*C*H_3)$_2$), 24.2 (CH(*C*H_3)$_2$), 23.9 (C*C*H_3), 23.6 (CH(*C*H_3)$_2$), 7.7 (C=C*C*H_3). *The carbene ^{13}C signal could not be determined unambiguously. Probably it is superimposed by one of the C_6H_6 signals (most likely by the signal at 145.6 ppm) or is too low in intensity.* **IR *ν* [cm^{-1}]:** 3031, 2947, 2914, 2854, 1648, 1604, 1564, 1542, 1448, 1431, 1398, 1371, 1351, 1308, 1245, 1202, 1172, 1098, 1051, 1029, 968, 932, 906, 843, 799, 781, 759, 740, 706, 677, 657, 590, 541, 505, 429.

$L^1Ga(Cl)^{Et}NHC^{Me}$: Yield 27 mg (0.040 mmol; 45 %). M.p. 198 °C. Anal. Calcd. for $C_{38}H_{56}N_4ClGa$: C, 67.71; H, 8.37; N, 8.31. Found: C, 67.54; H, 8.45; N, 8.18 %. **^{1}H-NMR (C_6D_6, 400 MHz, 25 °C) δ [ppm]:** 7.06-7.45 (m, 6 H, C_6H_3), 5.41 (s, 1 H, γ-C*H*), 4.40 (m (br), 2 H, CH_2CH$_3$), 4.28 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 3.90 (m (br), 1 H, CH_2CH$_3$), 3.46 (m (br), 1 H, CH_2CH$_3$), 3.33 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 3.27 (s, 1H, β-CH_2), 3.15 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 1.70-1.75 (m, 12 H, CCH_3, CH(*C*H_3)$_2$), 1.55 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$), 1.43 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$), 1.40 (s (br), 3 H, C=CCH_3), 1.25 (s (br), 3 H, CH$_2$*C*H$_3$), 1.15 (s (br), 3 H, C=CCH_3), 1.13 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 0.66 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 0.61 (s (br), 3H, CH$_2$*C*H$_3$), 0.41 (d, 3 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$). **^{13}C{^{1}H}-NMR (C_6D_6, 100 MHz, 25 °C) δ [ppm]:** 154.9 (*C*CH_3), 149.6 (*C*$_6H_3$), 149.5 (*C*$_6H_3$), 146.8 (*C*$_6H_3$), 145.7 (Ga*C*), 145.6 (*C*$_6H_3$), 143.4 (*C*$_6H_3$), 143.1 (*C*$_6H_3$), 125.9 (*C*$_6H_3$), 125.6 (*C*$_6H_3$), 125.1 (*C*$_6H_3$), 124.7 (*C*$_6H_3$), 123.3 (*C*$_6H_3$), 122.8 (*C*$_6H_3$), 102.9 (γ-*C*H), 81.1 (β-CH_2), 44.0 (*C*H$_2$), 42.3 (*C*H$_2$), 29.0 (*C*H(CH_3)$_2$), 28.8 (*C*H(CH_3)$_2$), 27.8 (*C*H(CH_3)$_2$), 27.3 (*C*H(CH_3)$_2$), 26.9 (CH(*C*H_3)$_2$), 26.8 (CH(*C*H_3)$_2$), 26.2 (CH(*C*H_3)$_2$), 24.9 (CH(*C*H_3)$_2$), 24.8 (CH(*C*H_3)$_2$), 24.7 (CH(*C*H_3)$_2$), 24.4 (C*C*H_3), 24.2 (CH(*C*H_3)$_2$), 23.6 (CH(*C*H_3)$_2$), 16.5 (*C*H$_2$CH$_3$), 15.3 (*C*H$_2$CH$_3$), 8.1 (C=C*C*H_3), 7.6 (C=C*C*H_3). *Due to the broad signals of the $^{Et}NHC^{Me}$ in $L^1Ga(Cl)^{Et}NHC^{Me}$ the C=C signal could not be determined unambiguously.* **IR *ν* [cm^{-1}]:** 3040, 3023, 2954, 2913, 2853, 1639, 1609, 1562, 1546, 1521, 1450, 1431, 1397, 1367, 1347, 1310, 1238, 1198, 1171, 1091, 1026, 965, 902, 877, 796, 756, 718, 661, 641, 590, 551, 501, 469, 431.

$L^1Ga(Cl)^{iPr}NHC^{Me}$: Yield 31 mg (0.044 mmol; 49 %). M.p. 226 °C (dec.). Anal. Calcd. for $C_{40}H_{60}N_4ClGa$: C, 68.43; H, 8.61; N, 7.98. Found: C, 67.9; H, 8.83; N, 7.71 %. **^{1}H-NMR (C_6D_6, 400 MHz, 25 °C) δ [ppm]:**

7.11-7.45 (m, 6 H, C_6H_3), 5.64-5.74 (m, 2 H, $CH(CH_3)_2$), 5.74 (s, 1 H, γ-CH), 4.28 (sept, 2 H, $^3J_{HH}$ = 6.6 Hz, $CH(CH_3)_2$), 3.95 (s, 1H, β-CH_2), 3.55 (sept, 1 H, $^3J_{HH}$ = 6.6 Hz, $CH(CH_3)_2$), 3.30 (s, 1 H, β-CH_2), 3.19 (sept, 1 H, $^3J_{HH}$ = 6.6 Hz, $CH(CH_3)_2$), 1.73 (s, 3 H, CCH_3), 1.69 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 1.66 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 1.59 (s, 3 H, $C=CCH_3$), 1.57 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 1.49 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 1.42 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 1.39 (s, 3 H, $C=CCH_3$), 1.34 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 1.19 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 0.89 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 0.84 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 0.58 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$), 0.45 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, $CH(CH_3)_2$). **$^{13}C\{^1H\}$-NMR (C_6D_6, 100 MHz, 25 °C) δ [ppm]:** 154.4 (CCH_3), 149.6 (C_6H_3), 149.6 (C_6H_3), 146.6 (Ga*C*), 146.1 (C_6H_3), 145.5 (C_6H_3), 143.8 (C_6H_3), 143.2 (C_6H_3), 127.4 (*C*=*C*) 125.8 (C_6H_3), 125.4 (C_6H_3), 125.0 (C_6H_3), 124.8 (C_6H_3), 123.7 (C_6H_3), 122.9 (C_6H_3), 105.4 (γ-*C*H), 81.8 (β-CH_2), 53.4 ($CH(CH_3)_2$), 51.7 ($CH(CH_3)_2$), 29.0 ($CH(CH_3)_2$), 28.8 ($CH(CH_3)_2$), 27.8 ($CH(CH_3)_2$), 27.3 ($CH(CH_3)_2$), 27.2 ($CH(CH_3)_2$), 27.0 ($CH(CH_3)_2$), 26.2 ($CH(CH_3)_2$), 25.0 ($CH(CH_3)_2$), 24.8 ($CH(CH_3)_2$), 24.5 ($CH(CH_3)_2$), 24.5 (CCH_3), 23.7 ($CH(CH_3)_2$), 23.2 ($CH(CH_3)_2$), 22.3 ($CH(CH_3)_2$), 21.7 (CCH_3), 20.7 ($CH(CH_3)_2$), 10.1 ($C=CCH_3$), 10.1 ($C=CCH_3$). **IR ν [cm^{-1}]:** 3067, 3020, 2961, 2931, 2916, 2855, 1613, 1594, 1549, 1458, 1433, 1367, 1345, 1317, 1300, 1239, 1197, 1165, 1104, 1075, 1052, 1025, 960, 902, 883, 796, 757, 729, 656, 623, 594, 538, 429.

A) Spectroscopic Characterization

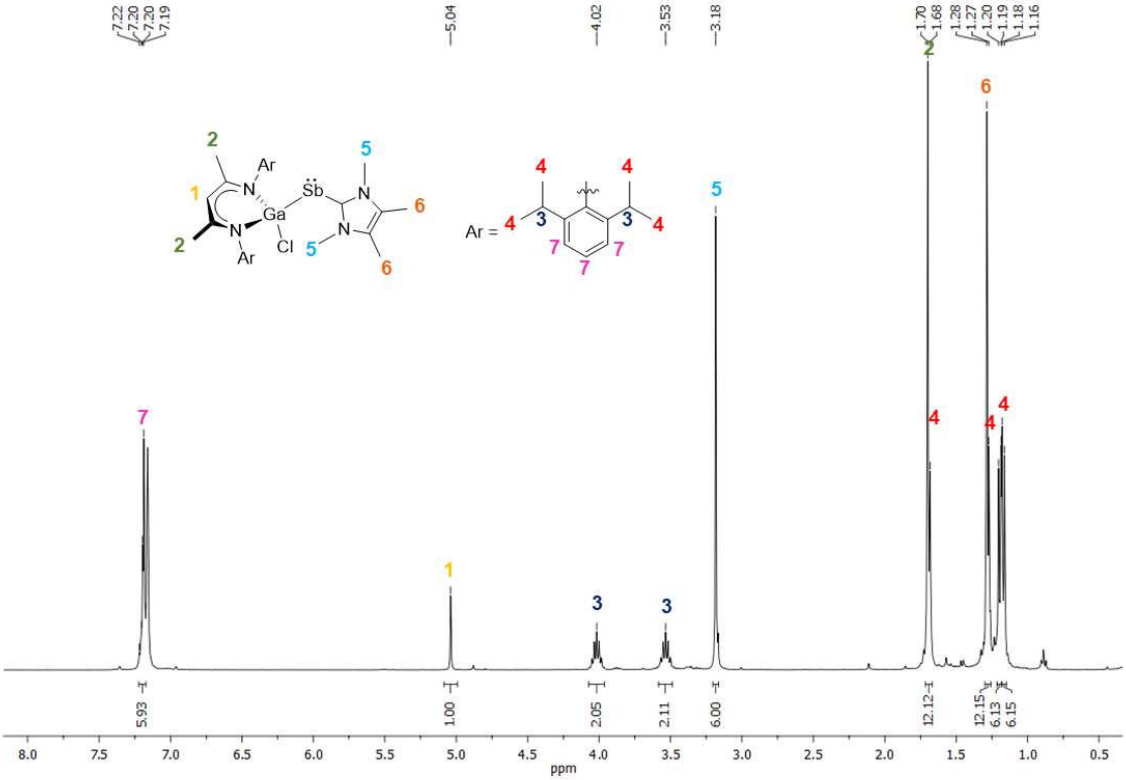

Figure S1. ^{1}H NMR spectrum of LGa(Cl)Sb-^{Me}NHC^{Me} (**1a**) in C_6D_6.

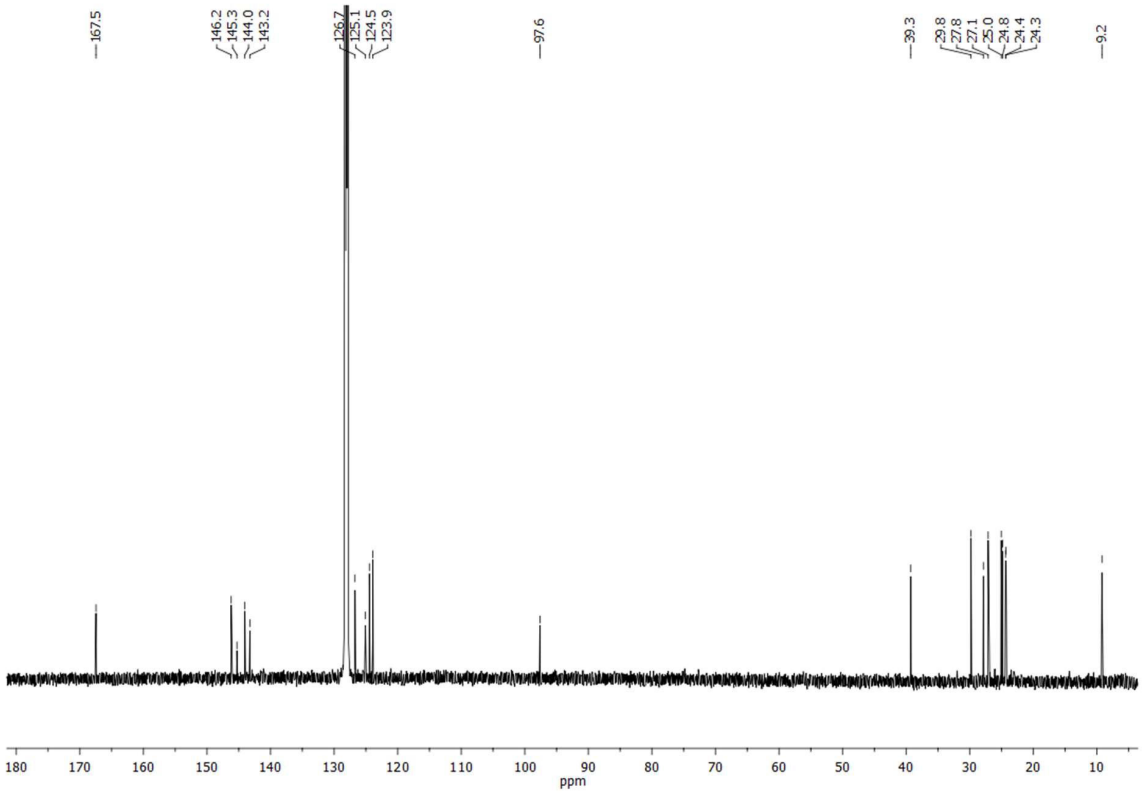

Figure S2. ^{13}C NMR spectrum of LGa(Cl)Sb-^{Me}NHC^{Me} (**1a**) in C_6D_6.

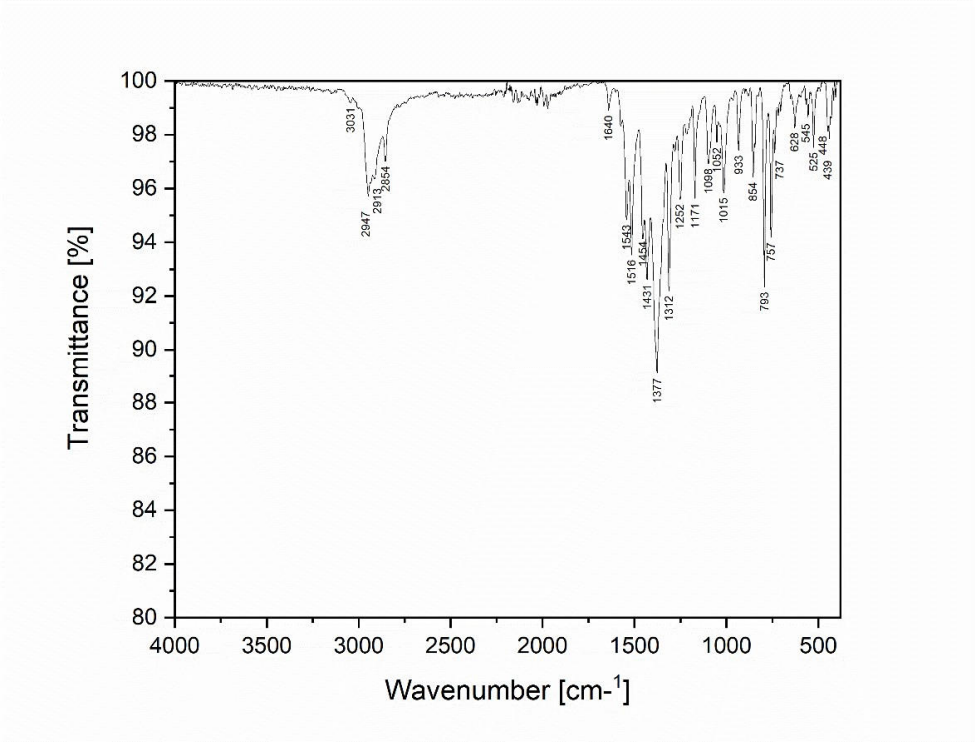

Figure S3. IR spectrum of LGa(Cl)Sb-^{Me}NHC^{Me} (**1a**) in C_6D_6.

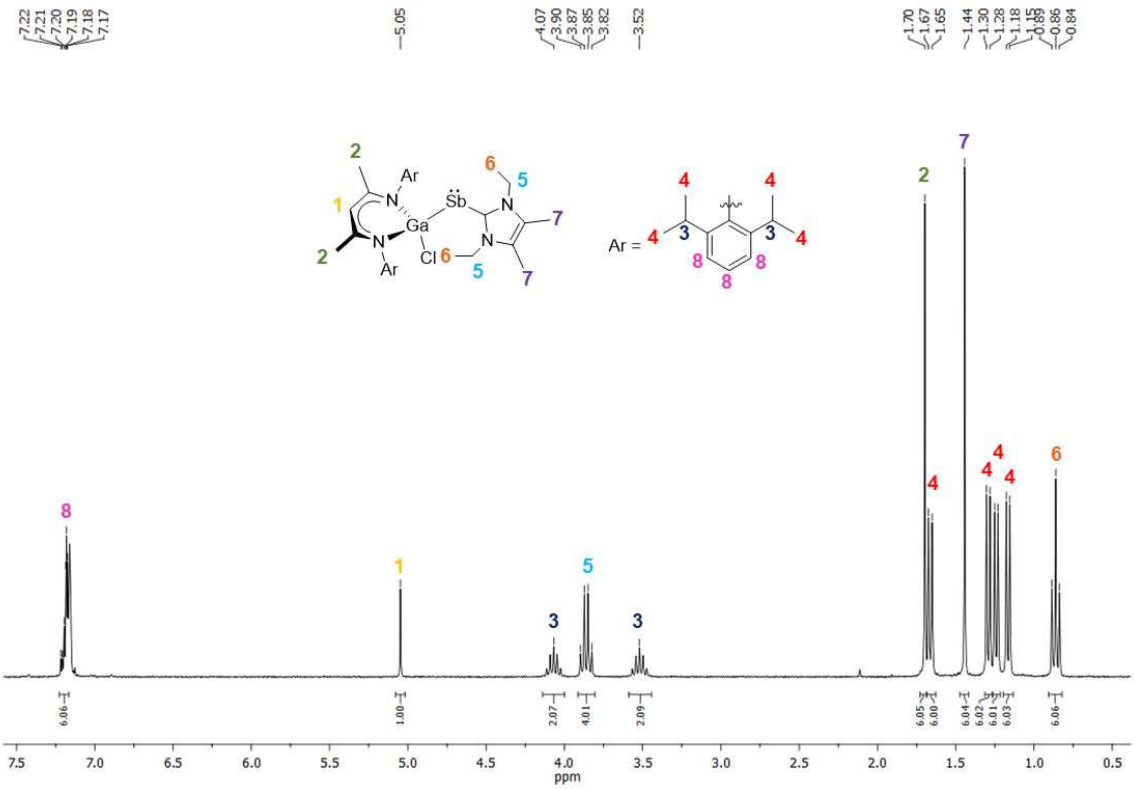

Figure S4. ^{1}H NMR spectrum of L(Cl)GaSb-^{Et}NHC^{Me} (**1b**) in C_6D_6.

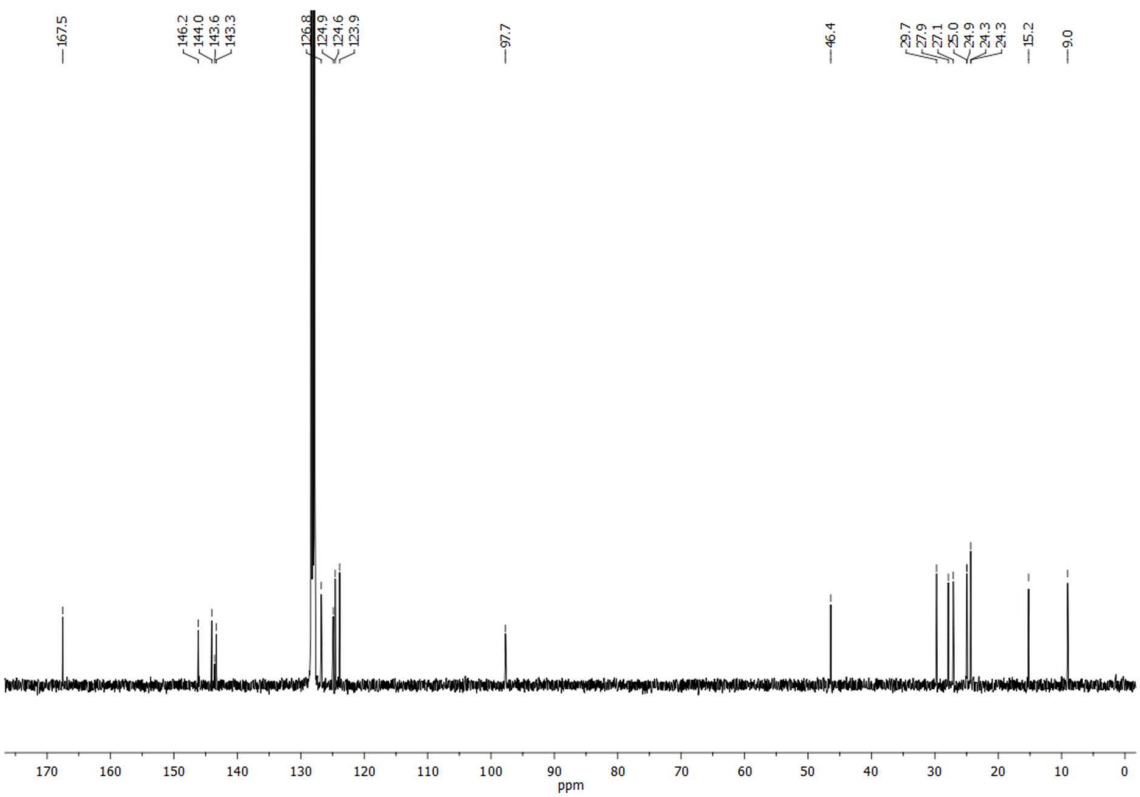

Figure S5. ^{13}C NMR spectrum of L(Cl)GaSb-$^{Et}NHC^{Me}$ (**1b**) in C_6D_6.

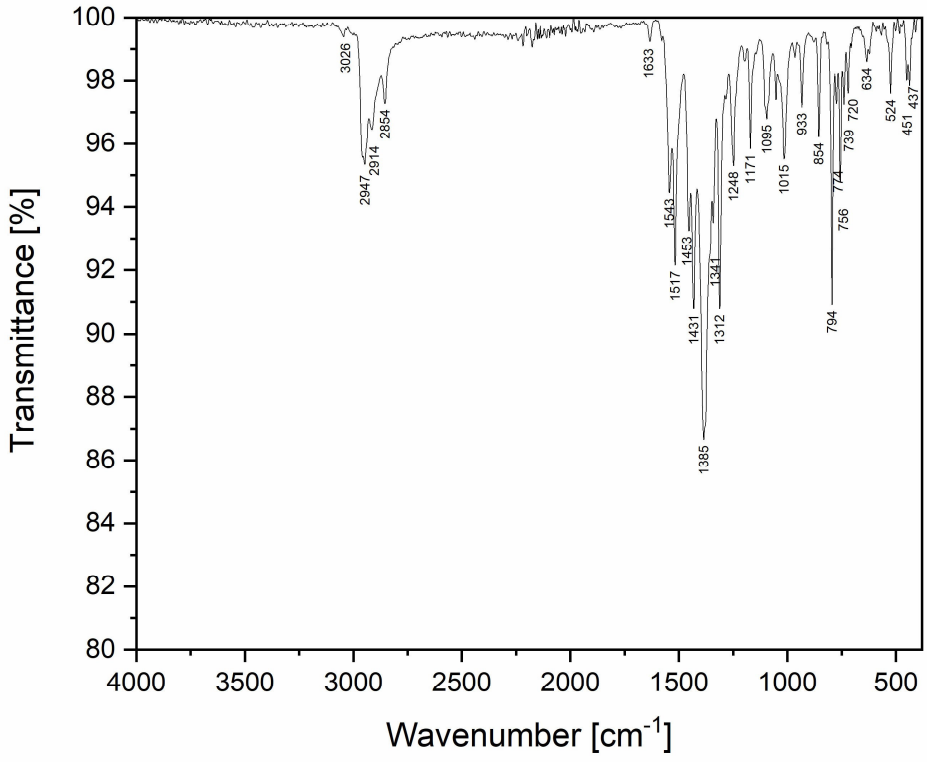

Figure S6. IR spectrum of L(Cl)GaSb-$^{Et}NHC^{Me}$ (**1b**).

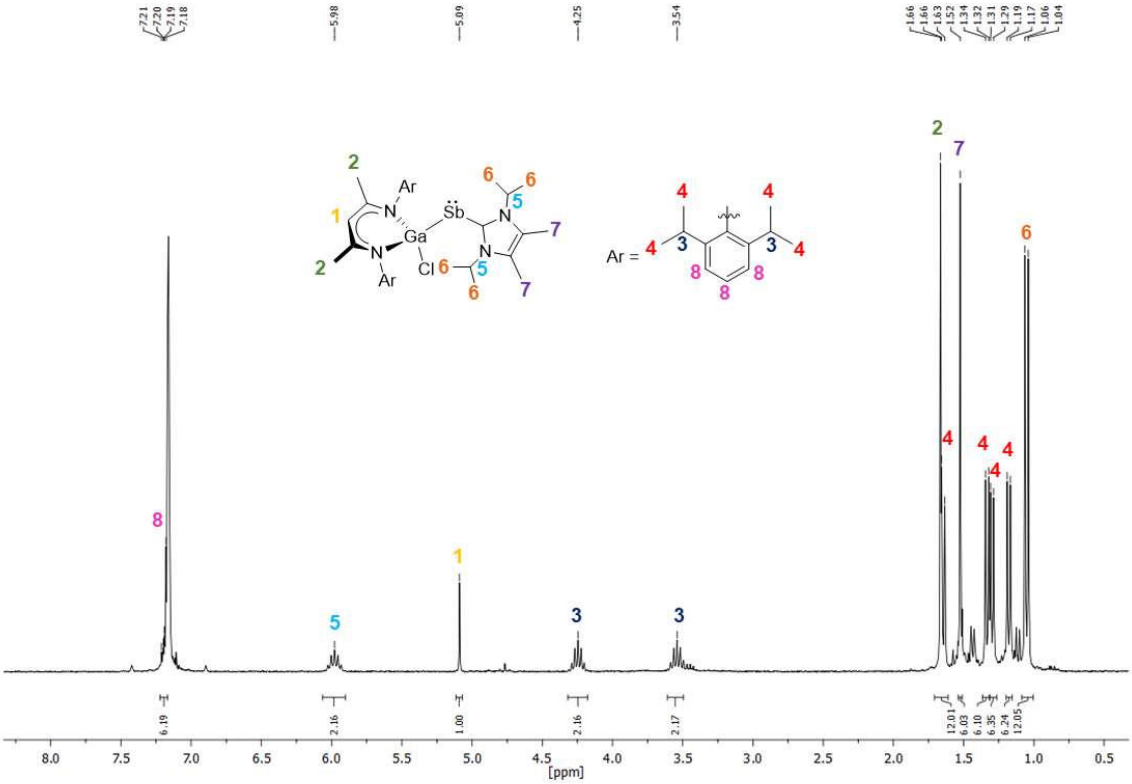

Figure S7. ^{1}H NMR spectrum of L(Cl)GaSb-$^{i\text{Pr}}$NHC$^{\text{Me}}$ (**1c**) in C_6D_6.

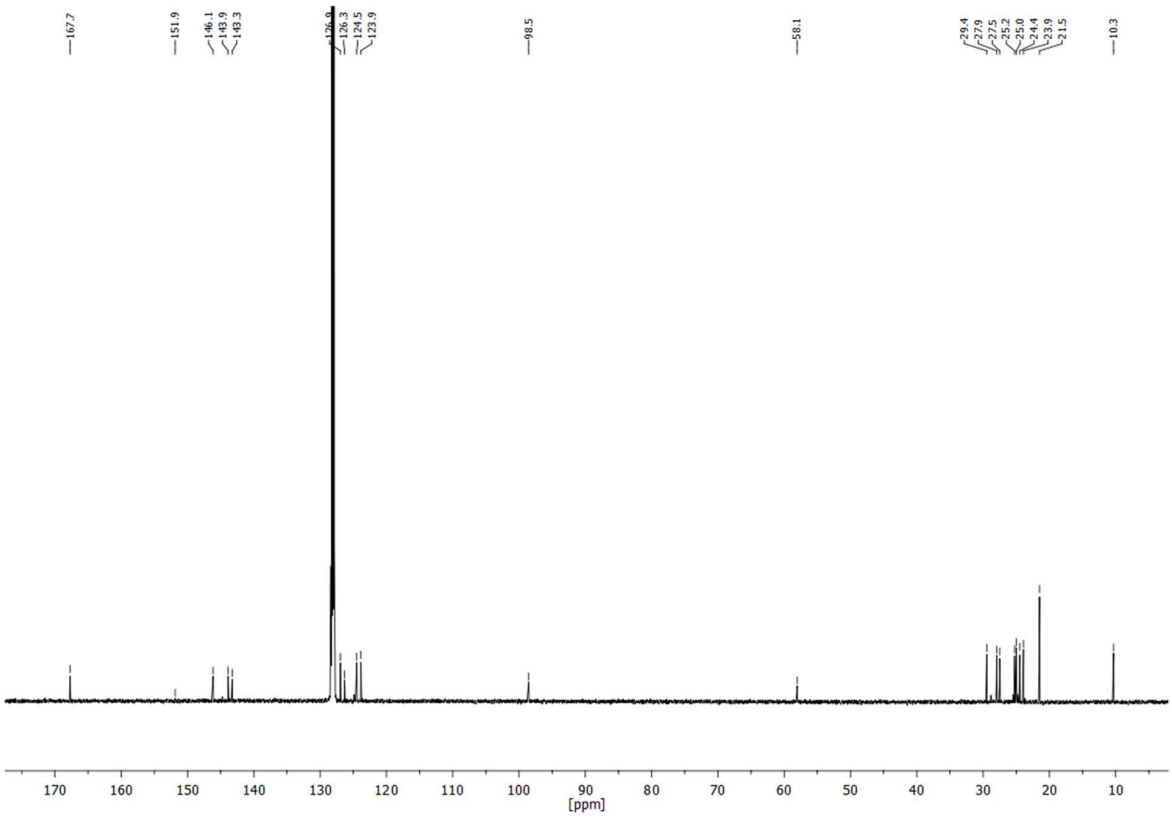

Figure S8. ^{13}C NMR spectrum of L(Cl)GaSb-$^{i\text{Pr}}$NHC$^{\text{Me}}$ (**1c**) in C_6D_6.

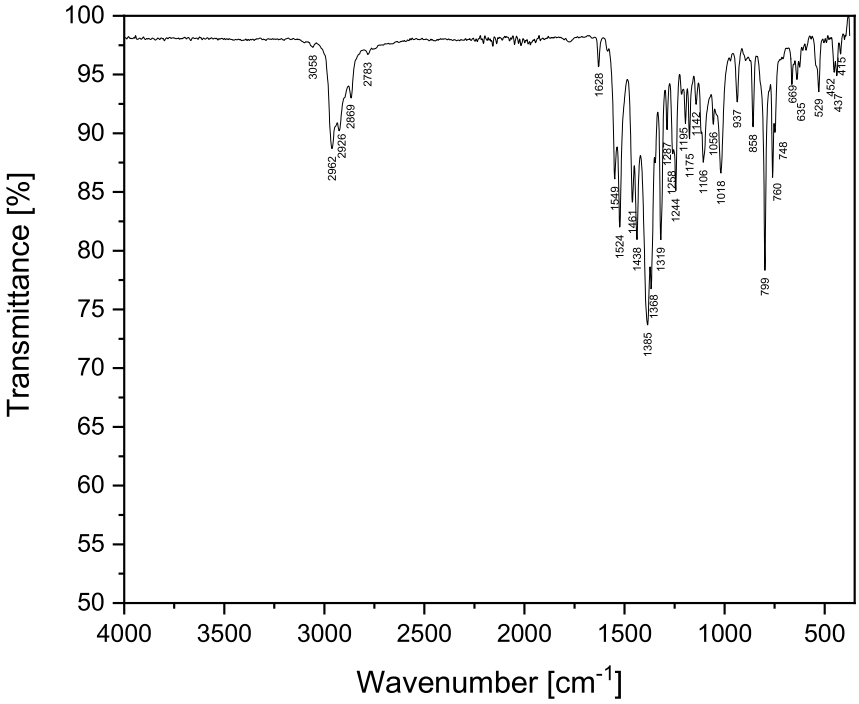

Figure S9. ATR-IR spectrum of L(Cl)GaSb-$^{i\text{Pr}}$NHC$^{\text{Me}}$ (**1c**).

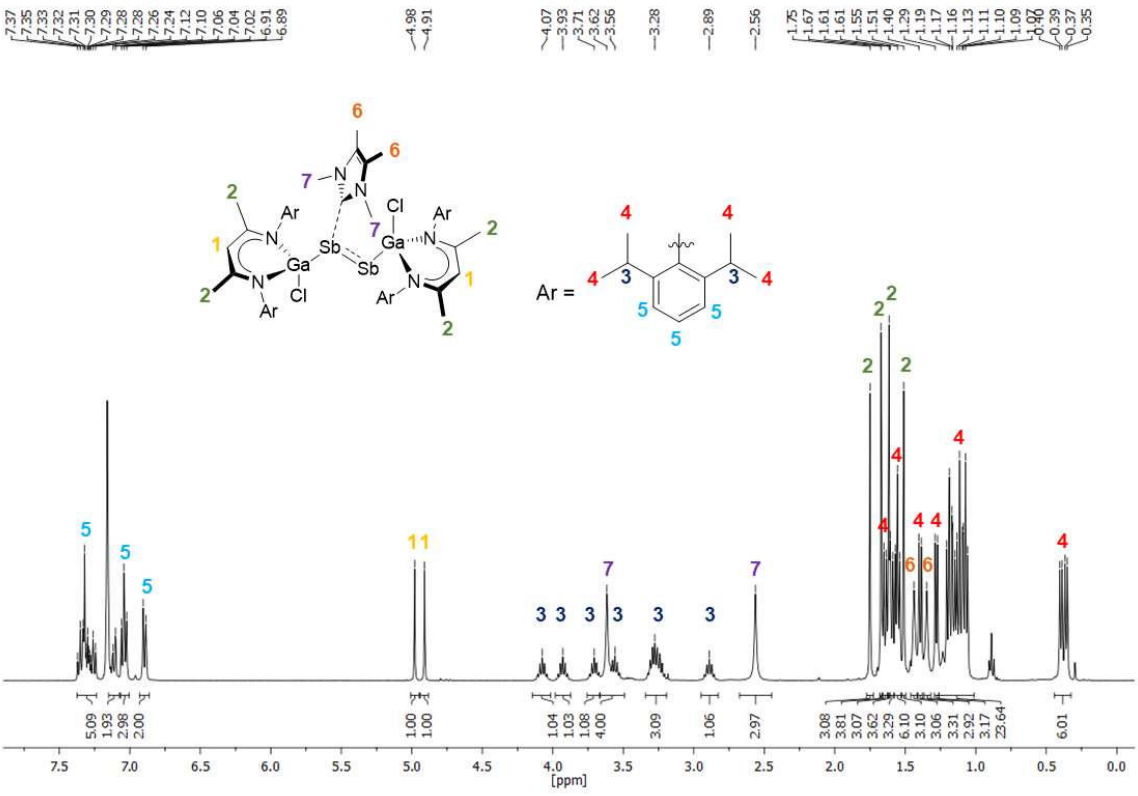

Figure S10. ^{1}H NMR spectrum of L(Cl)GaSbSb($^{\text{Me}}$NHC$^{\text{Me}}$)Ga(Cl)L (**2a**) in C_6D_6.

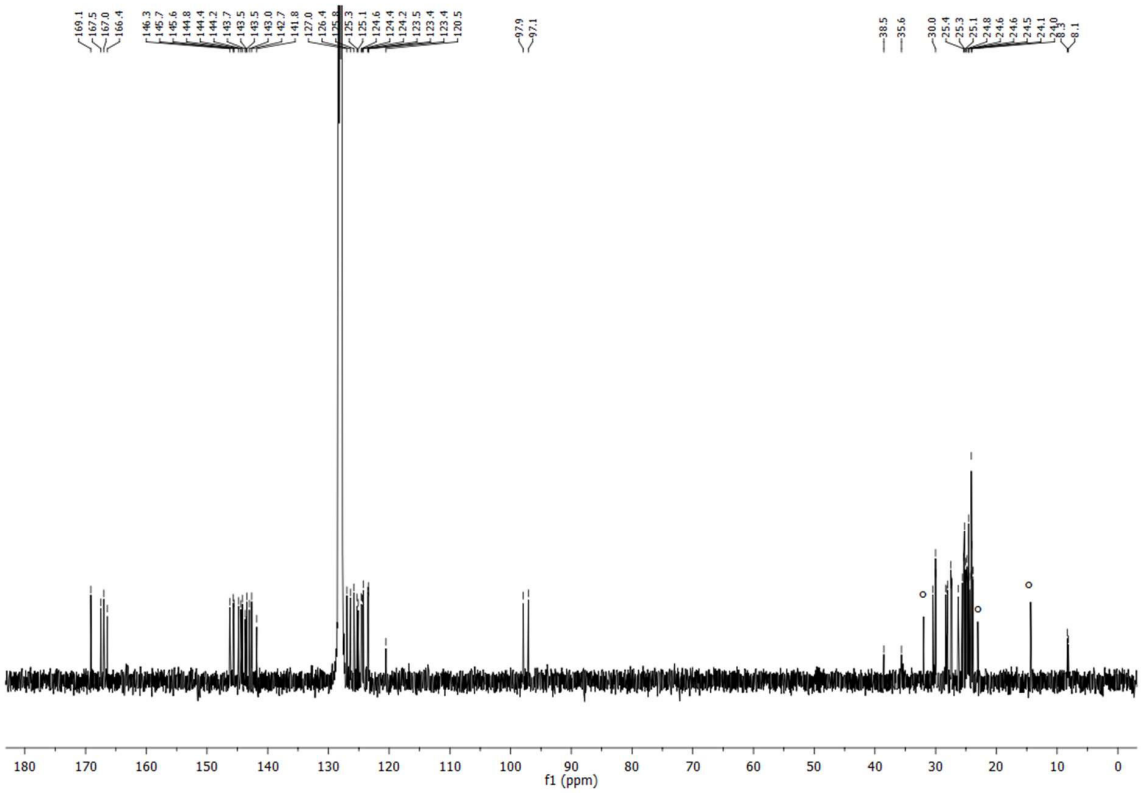

Figure S11. ^{13}C NMR spectrum of L(Cl)GaSbSb(^{Me}NHC^{Me})Ga(Cl)L (**2a**) in C_6D_6 (° = n-hexane).

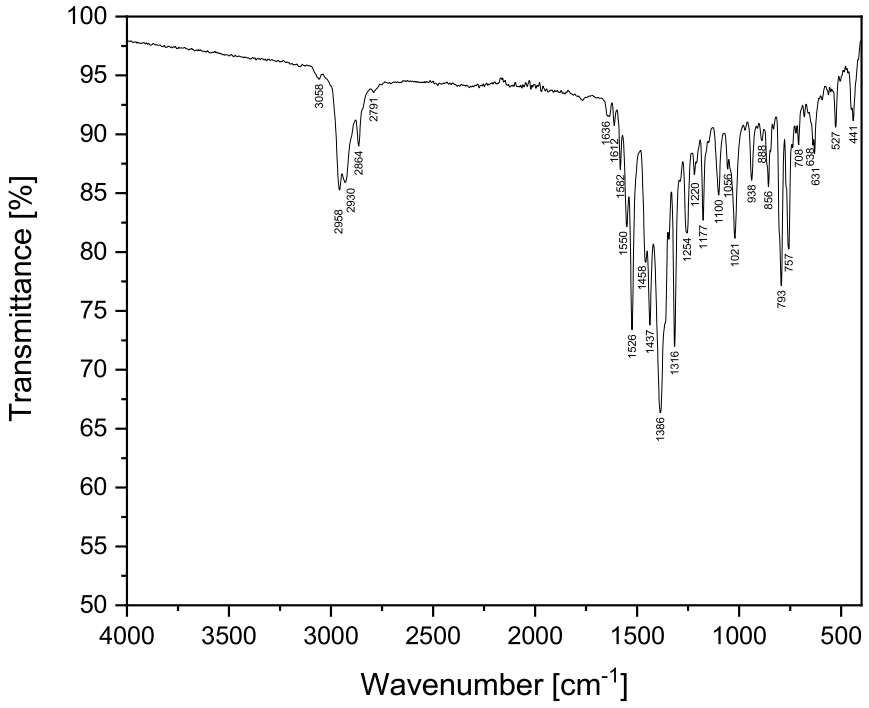

Figure S12. ATR-IR spectrum of L(Cl)GaSbSb(^{Me}NHC^{Me})Ga(Cl)L (**2a**).

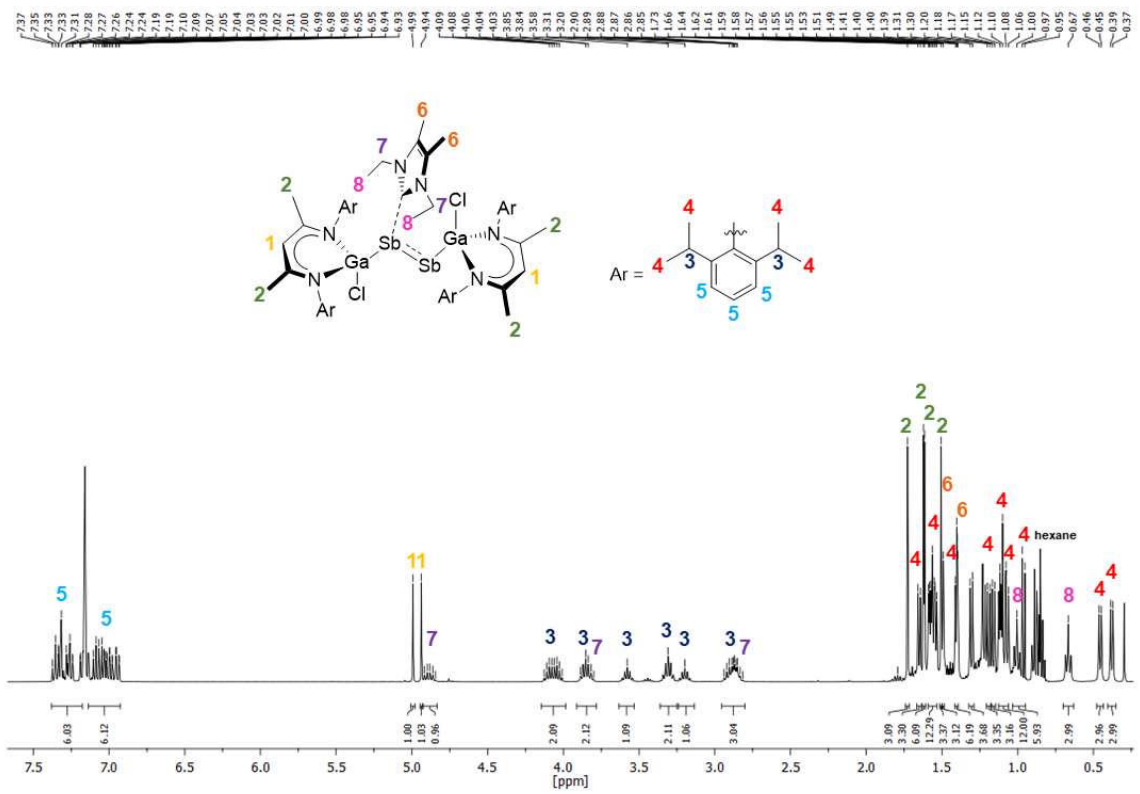

Figure S13. ^{1}H NMR spectrum of L(Cl)GaSbSb(^{Et}NHC^{Me})Ga(Cl)L (**2b**) in C_6D_6.

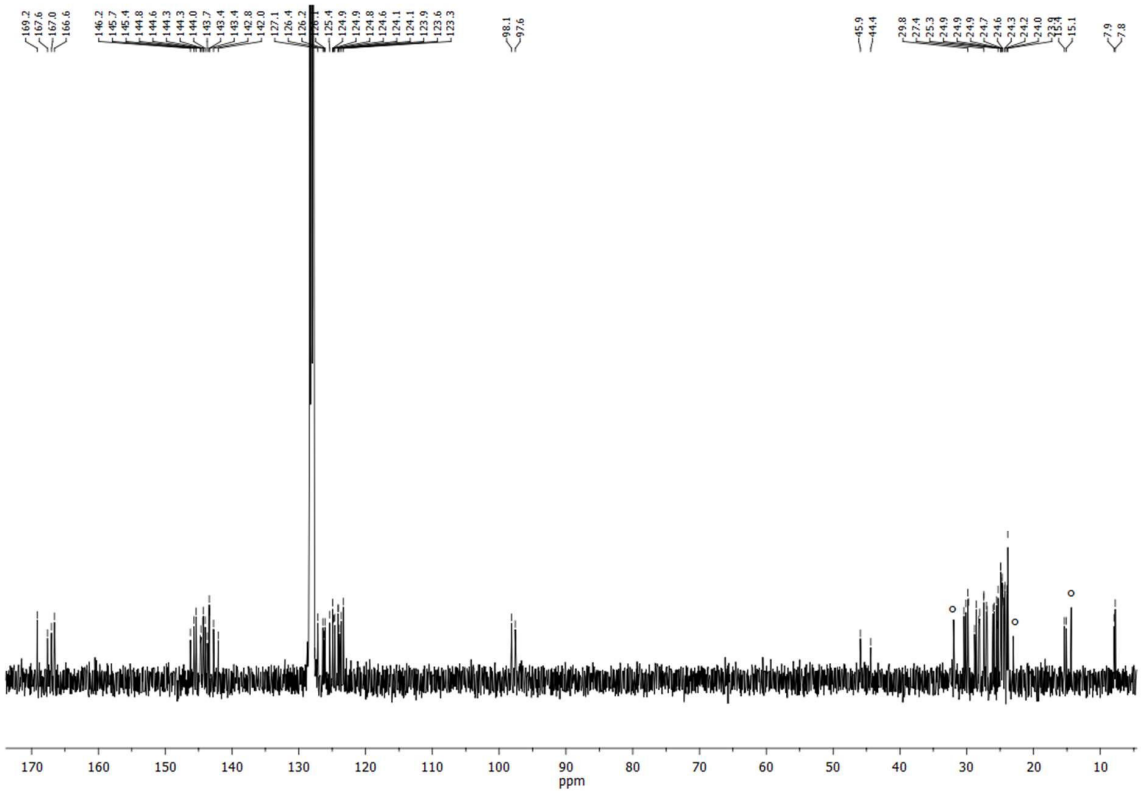

Figure S14. ^{13}C NMR spectrum of L(Cl)GaSbSb(^{Et}NHC^{Me})Ga(Cl)L (**2b**) in C_6D_6 (° = n-hexane).

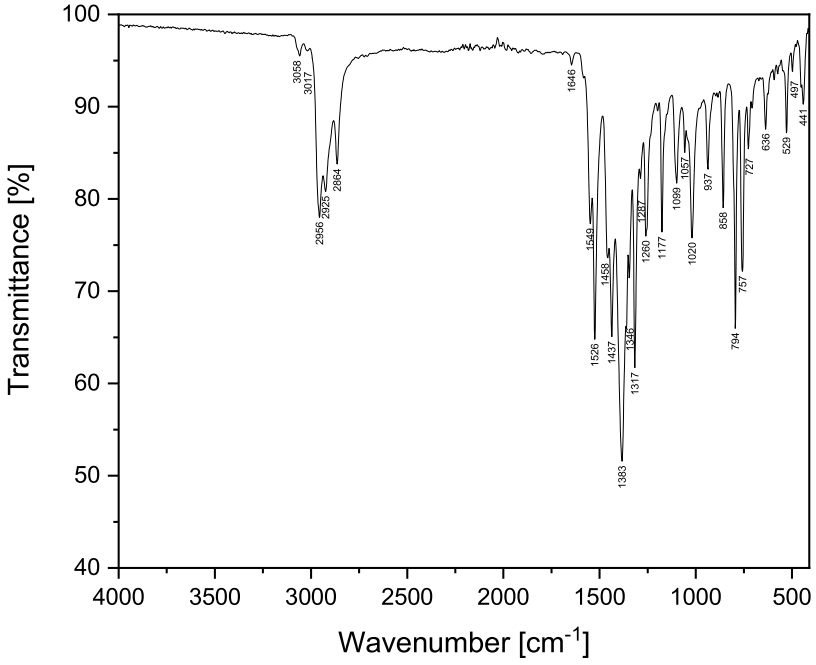

Figure S15. ATR-IR spectrum of L(Cl)GaSbSb(^{Et}NHC^{Me})Ga(Cl)L (**2b**).

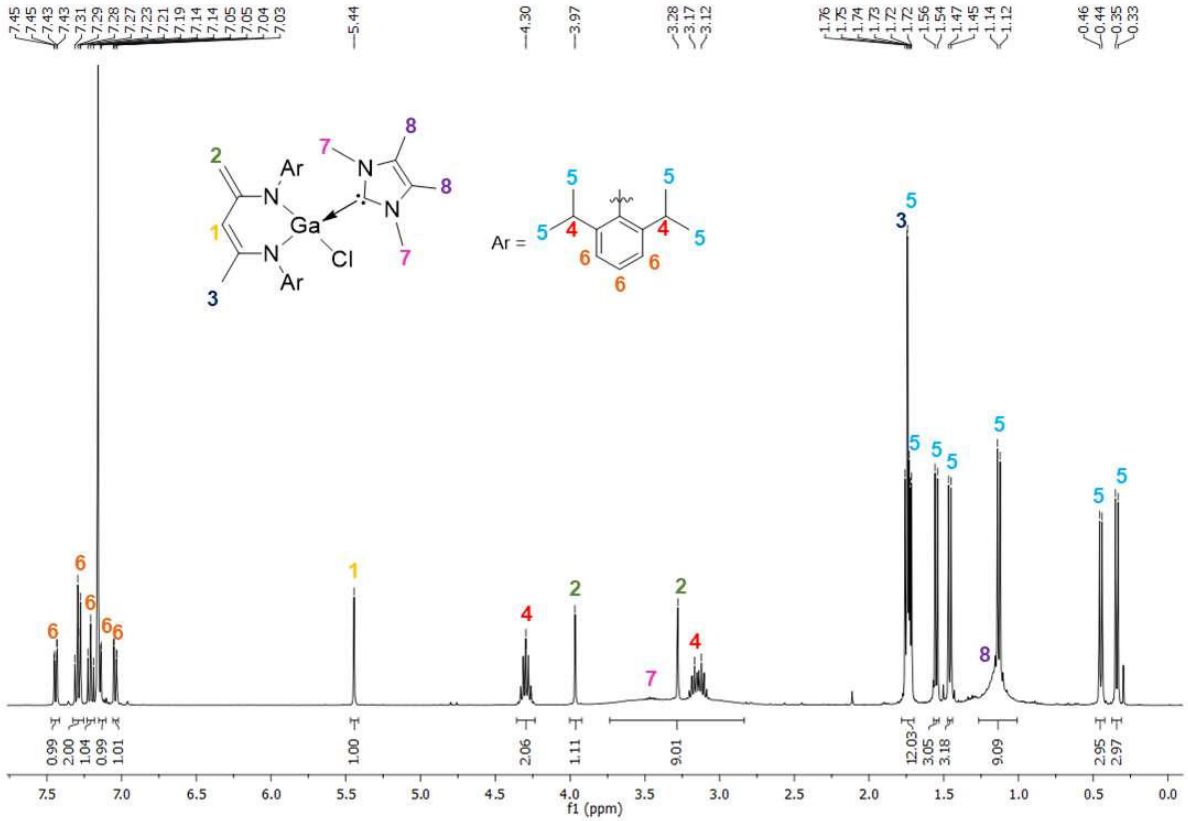

Figure S16. ^{1}H NMR spectrum of L^{1}Ga(Cl)^{Me}NHC^{Me} in C_6D_6.

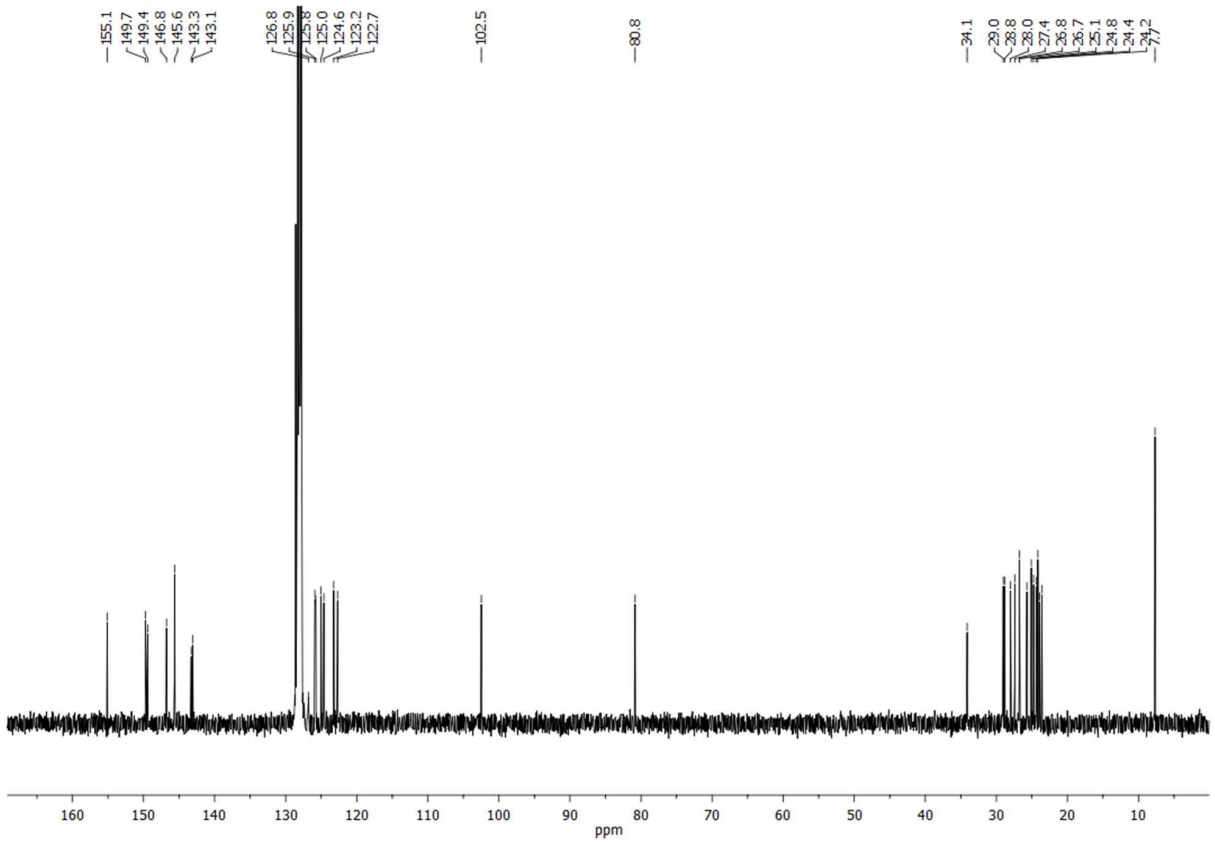

Figure S17. ^{13}C NMR spectrum of $L^1Ga(Cl)^{Me}NHC^{Me}$ in C_6D_6.

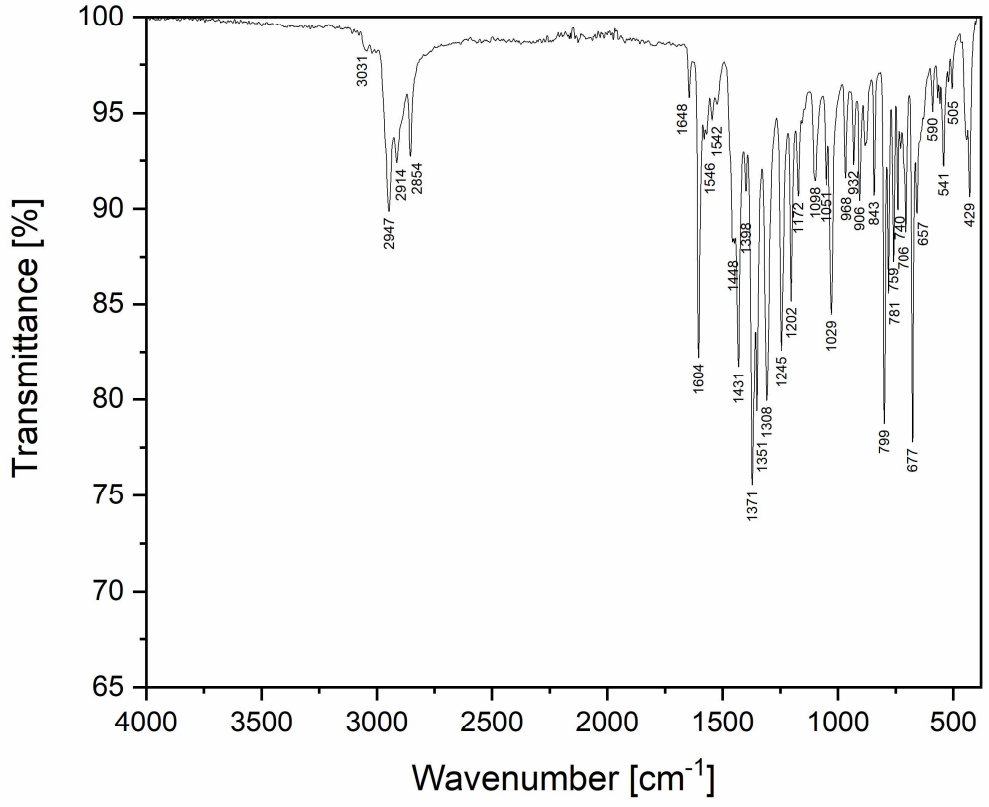

Figure S18. ATR-IR spectrum of $L^1Ga(Cl)^{Me}NHC^{Me}$.

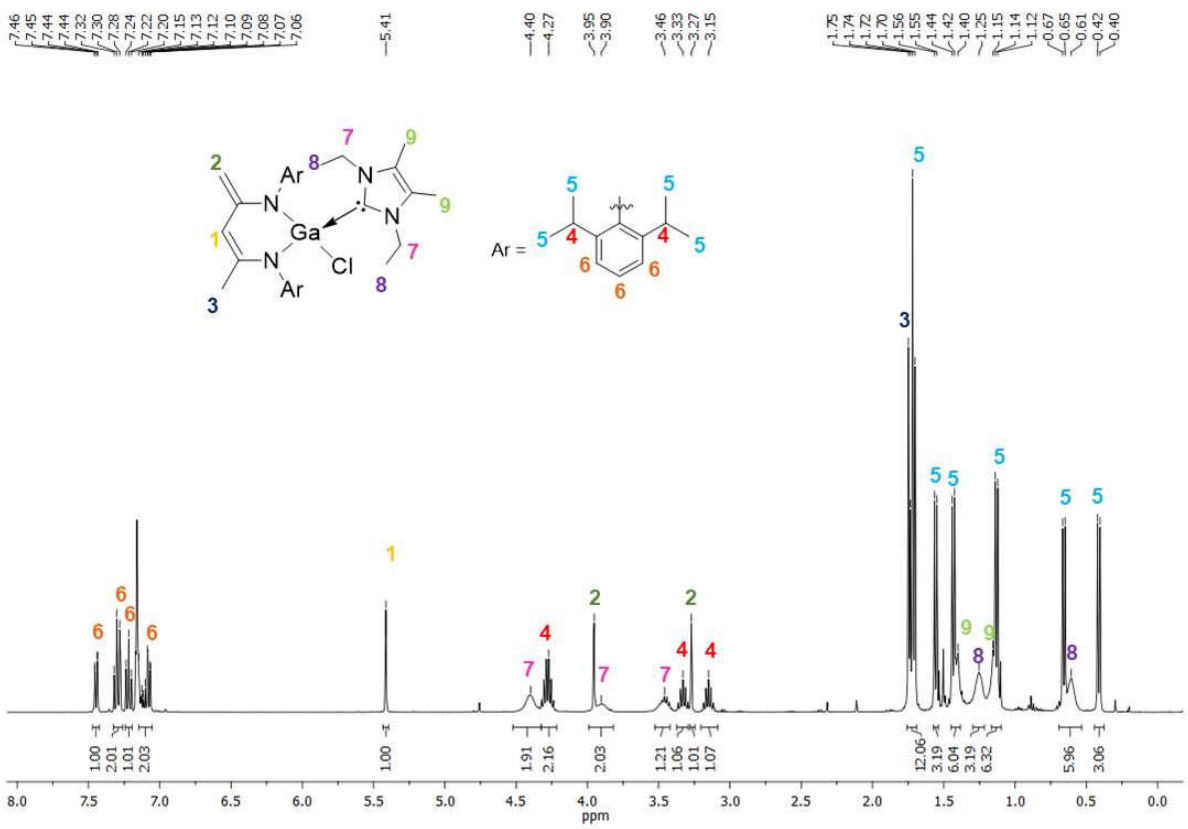

Figure S19. ^{1}H NMR spectrum of L^{1}Ga(Cl)^{Et}NHC^{Me} in C_6D_6.

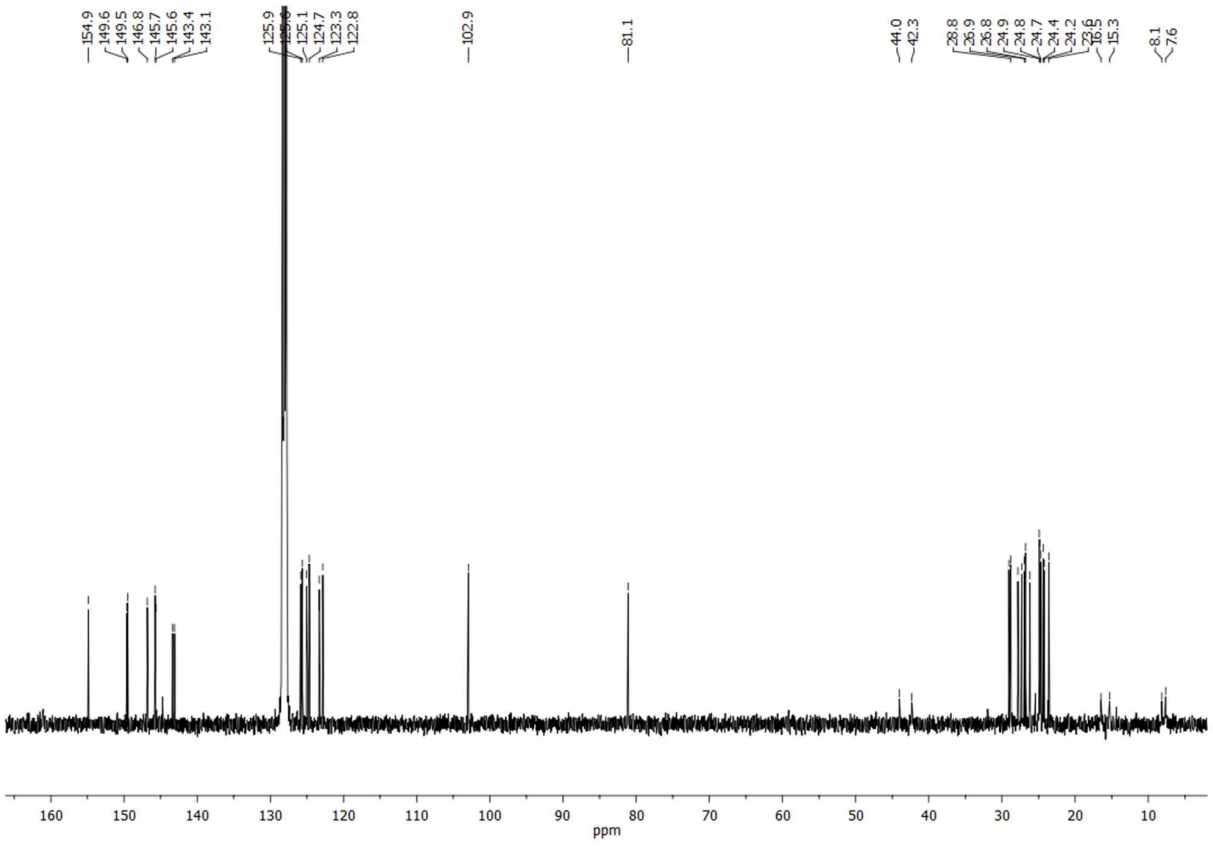

Figure S20. ^{13}C NMR spectrum of L^{1}Ga(Cl)^{Et}NHC^{Me} in C_6D_6.

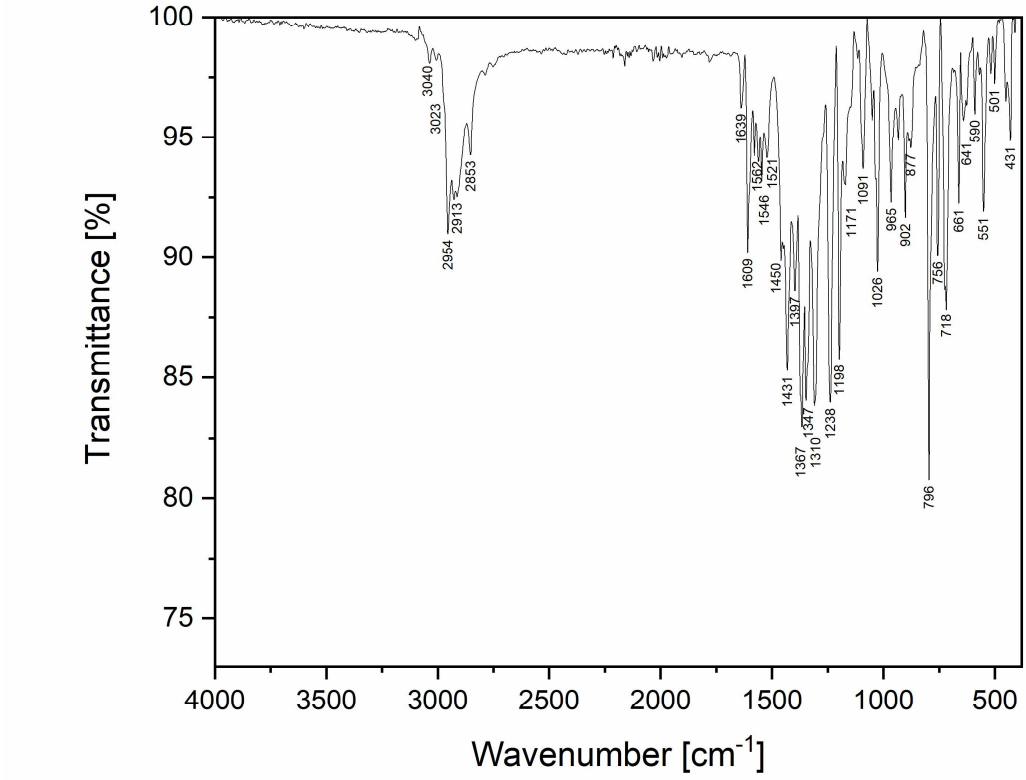

Figure S21. ATR-IR spectrum of $L^1Ga(Cl)^{Et}NHC^{Me}$.

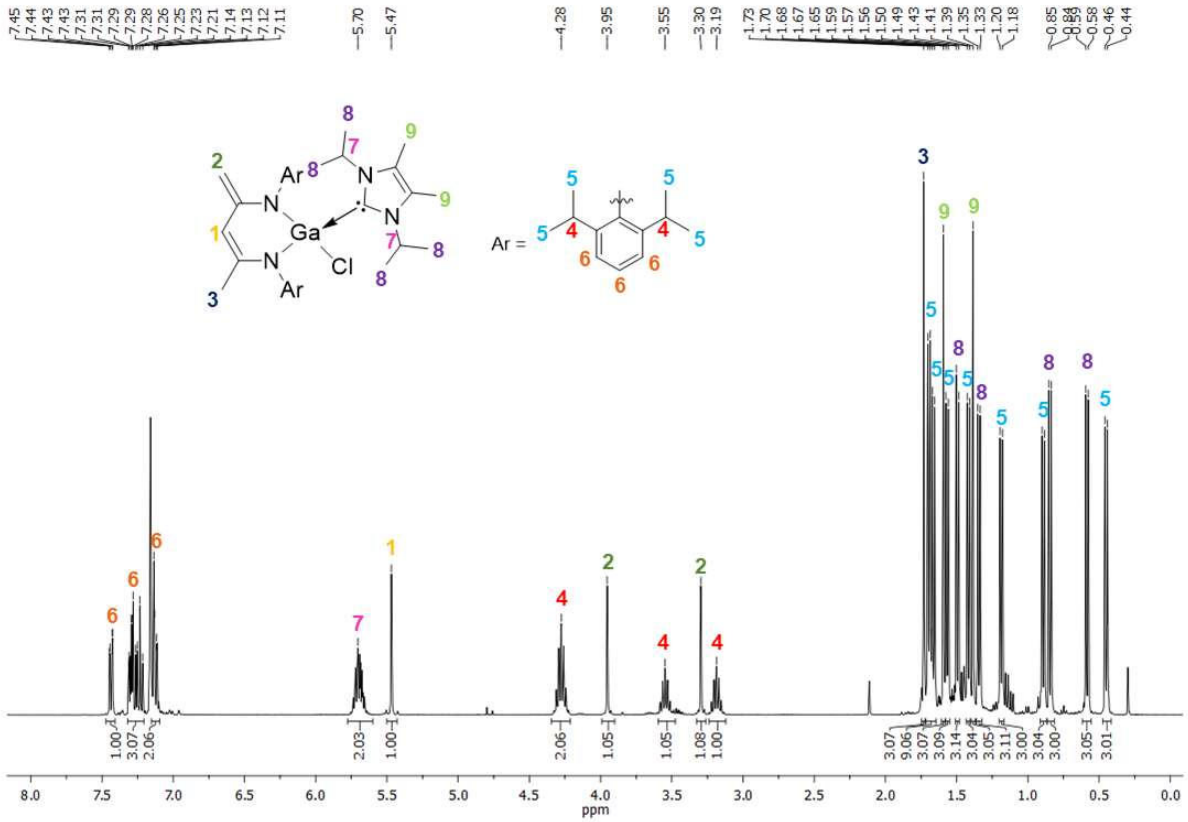

Figure S22. ^1H NMR spectrum of $L^1Ga(Cl)^{iPr}NHC^{Me}$ in C_6D_6.

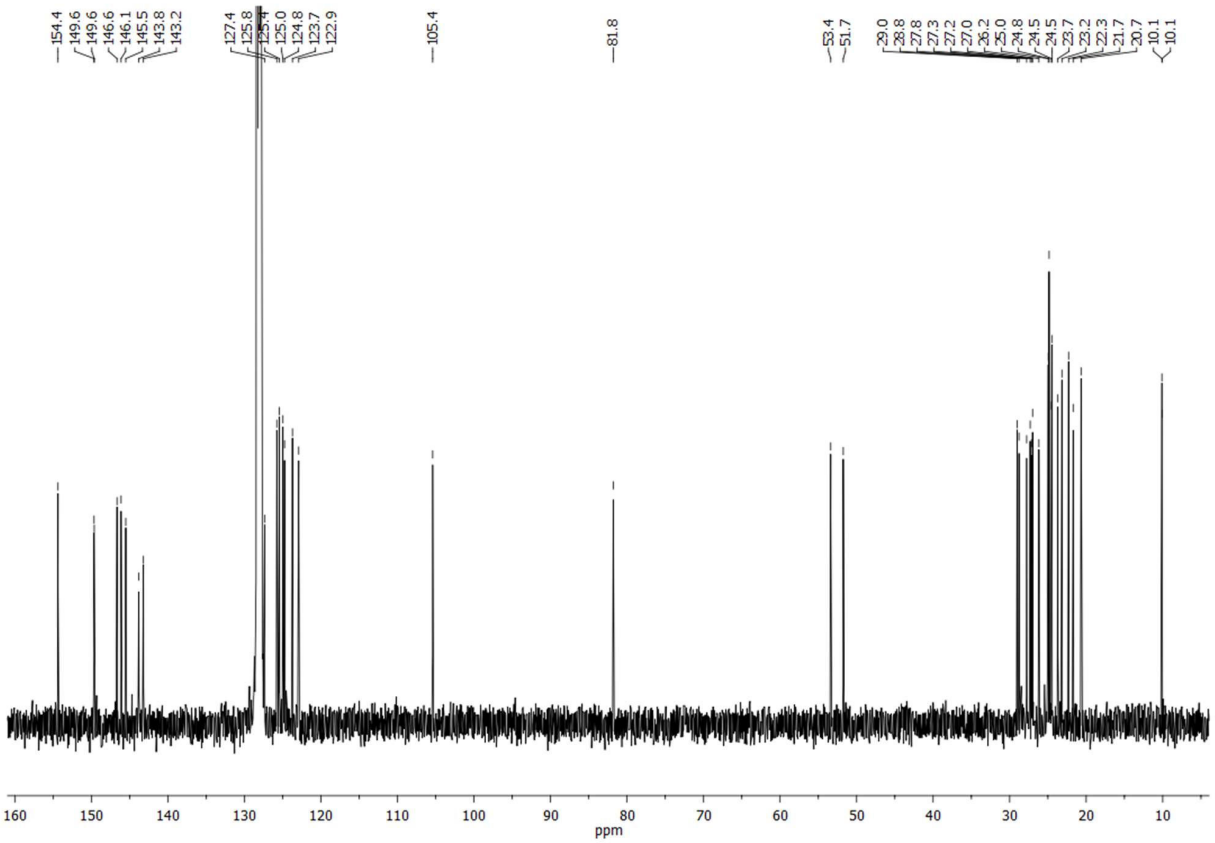

Figure S23. ^{13}C NMR spectrum of $L^1Ga(Cl)^{iPr}NHC^{Me}$ in C_6D_6.

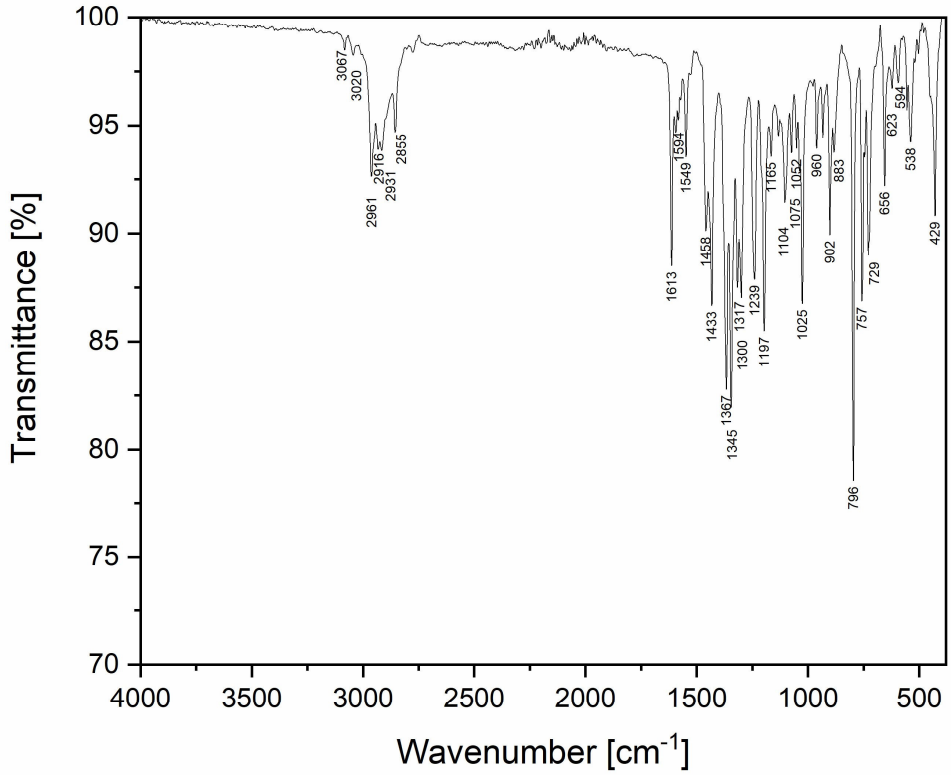

Figure S24. ATR-IR spectrum of $L^1Ga(Cl)^{iPr}NHC^{Me}$.

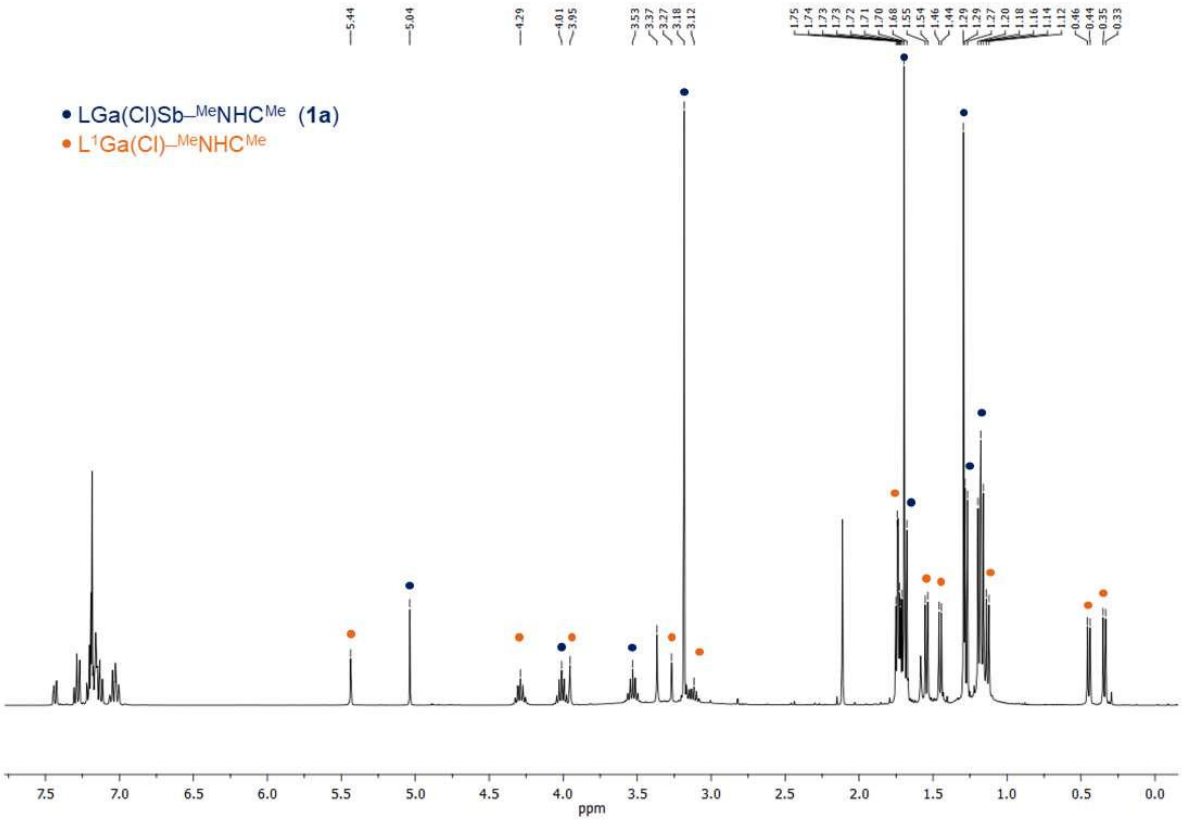

Figure S25. ^{1}H NMR spectrum of the reaction of $[LGa(Cl)]_2SbCl$ and 3 equivalents $^{Me}NHC^{Me}$ after 24 h at room temperature in C_6D_6.

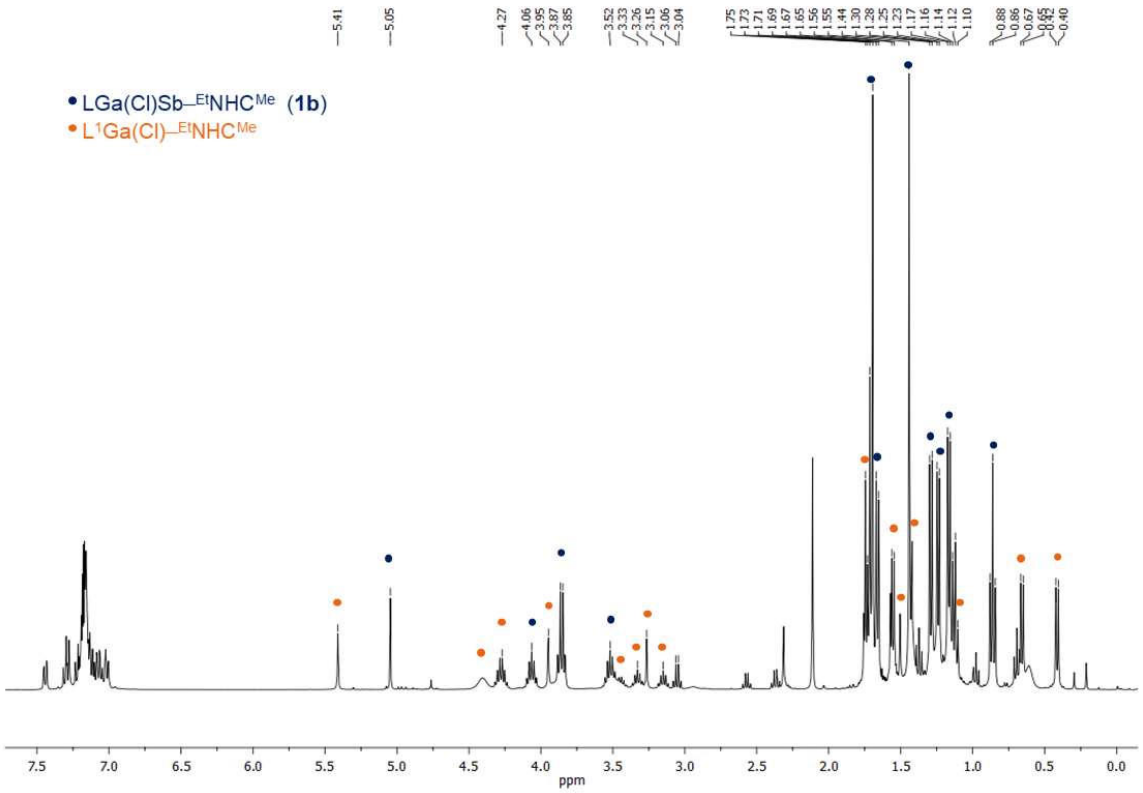

Figure S26. ^{1}H NMR spectrum of the reaction of $[LGa(Cl)]_2SbCl$ and 3 equivalents $^{Et}NHC^{Me}$ after 24 h at room temperature in C_6D_6.

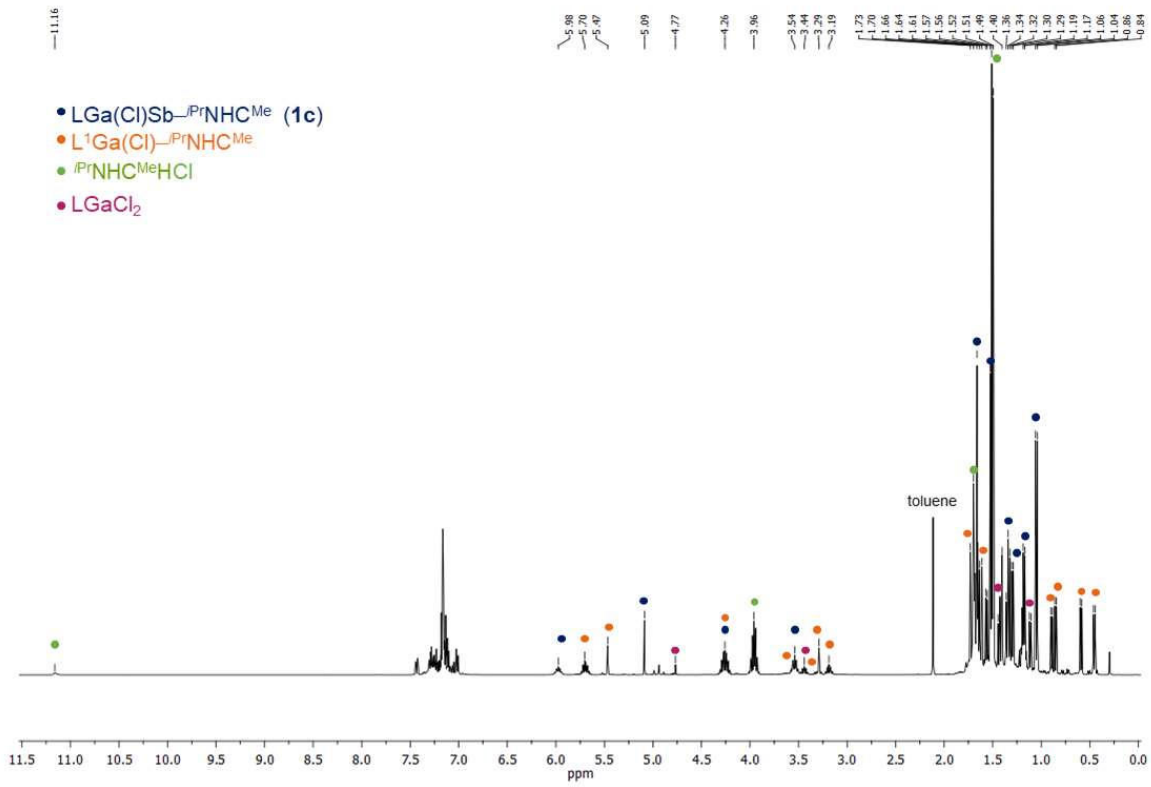

Figure S27. ^{1}H NMR spectrum of the reaction of $[LGa(Cl)]_2SbCl$ and 3 equivalents $^{i\text{Pr}}NHC^{Me}$ after 24 h at room temperature in C_6D_6.

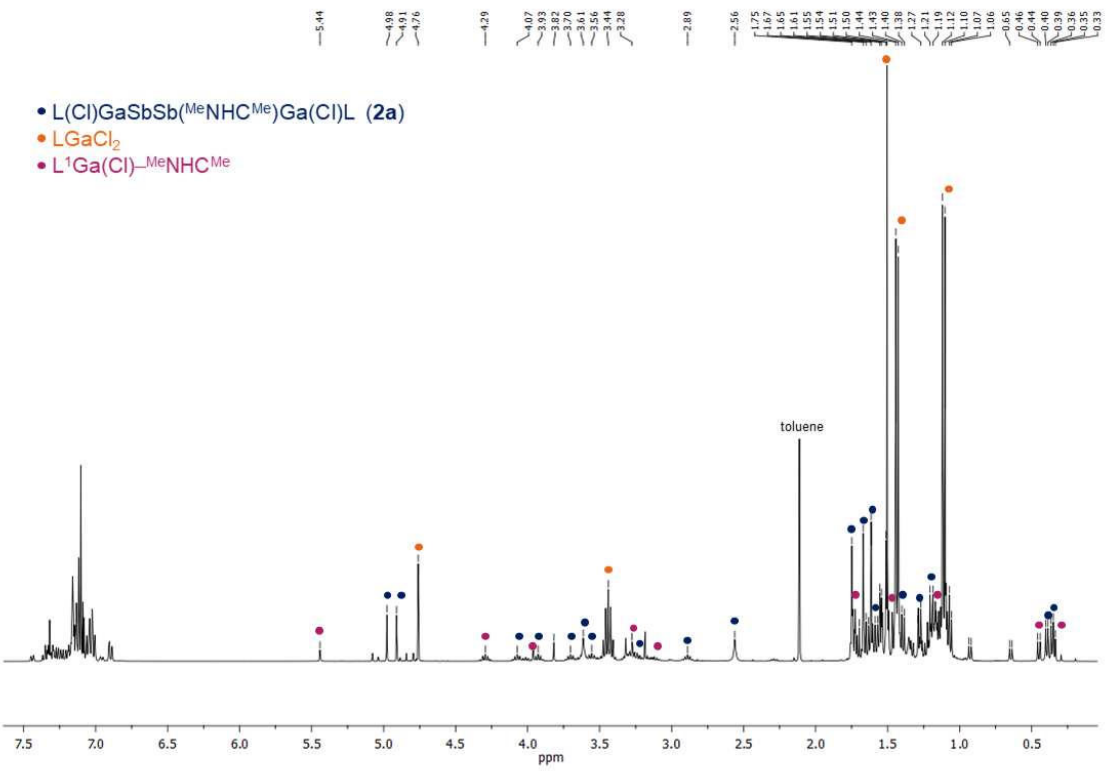

Figure S28. ^{1}H NMR spectrum of the reaction of $[LGa(Cl)]_2SbCl$ and 0.5 equivalents $^{Me}NHC^{Me}$ after 24 h at room temperature in C_6D_6.

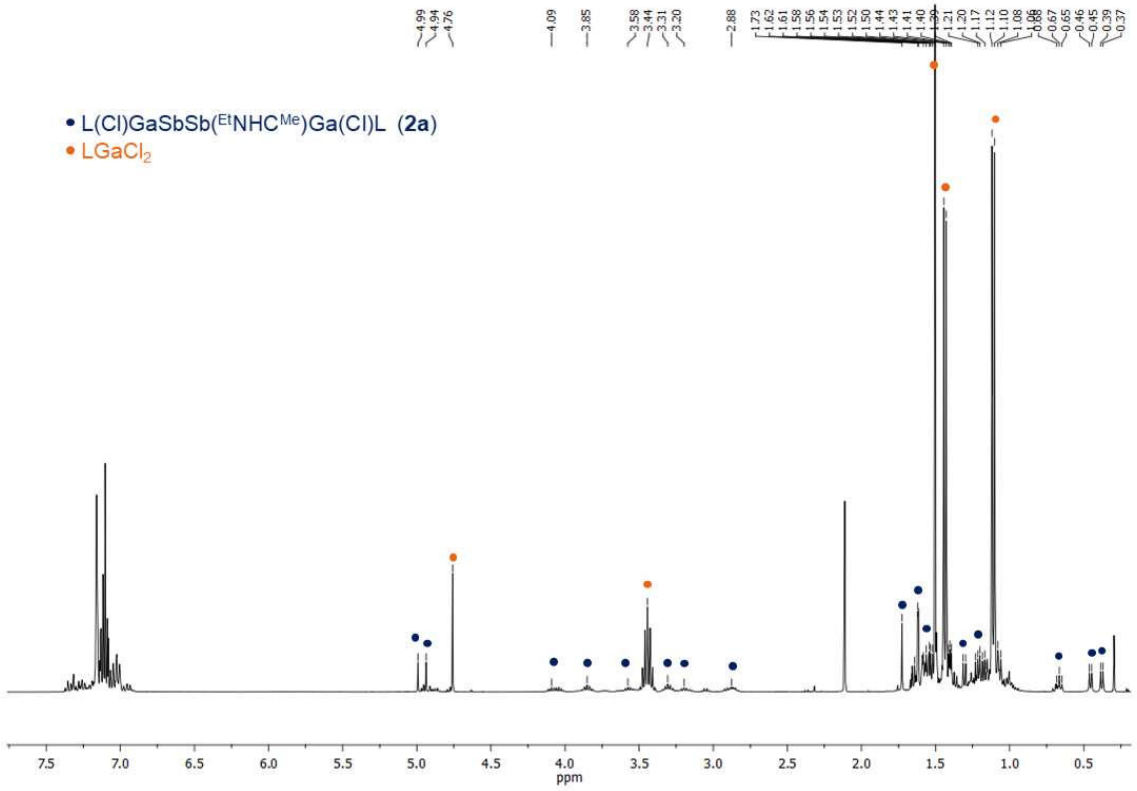

Figure S29. ^{1}H NMR spectrum of the reaction of [LGa(Cl)]$_2$SbCl and 0.5 equivalents ^{Et}NHC^{Me} after 2 d at room temperature in C_6D_6.

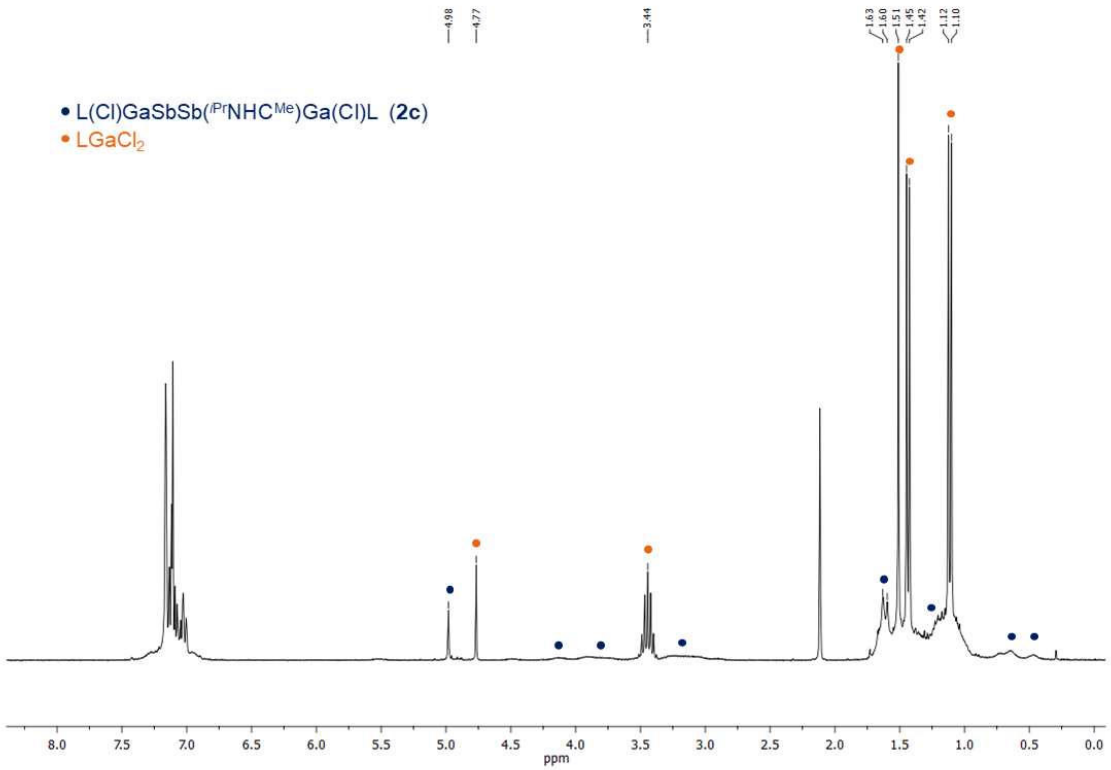

Figure S30. ^{1}H NMR spectrum of the reaction of [LGa(Cl)]$_2$SbCl and 0.5 equivalents ^{iPr}NHC^{Me} after 5 h at room temperature in C_6D_6.

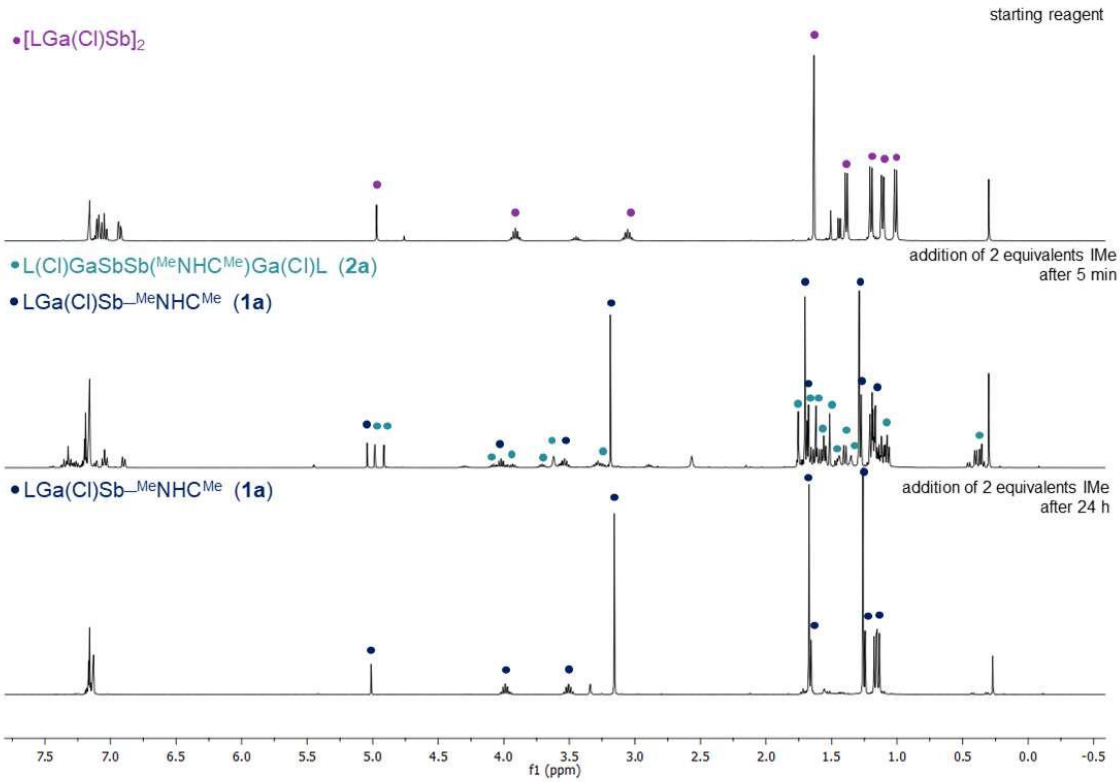

Figure S31. ^{1}H NMR spectra of the reaction of $[LGa(Cl)Sb]_2$ and 2 equivalents $^{Me}NHC^{Me}$ at room temperature in C_6D_6.

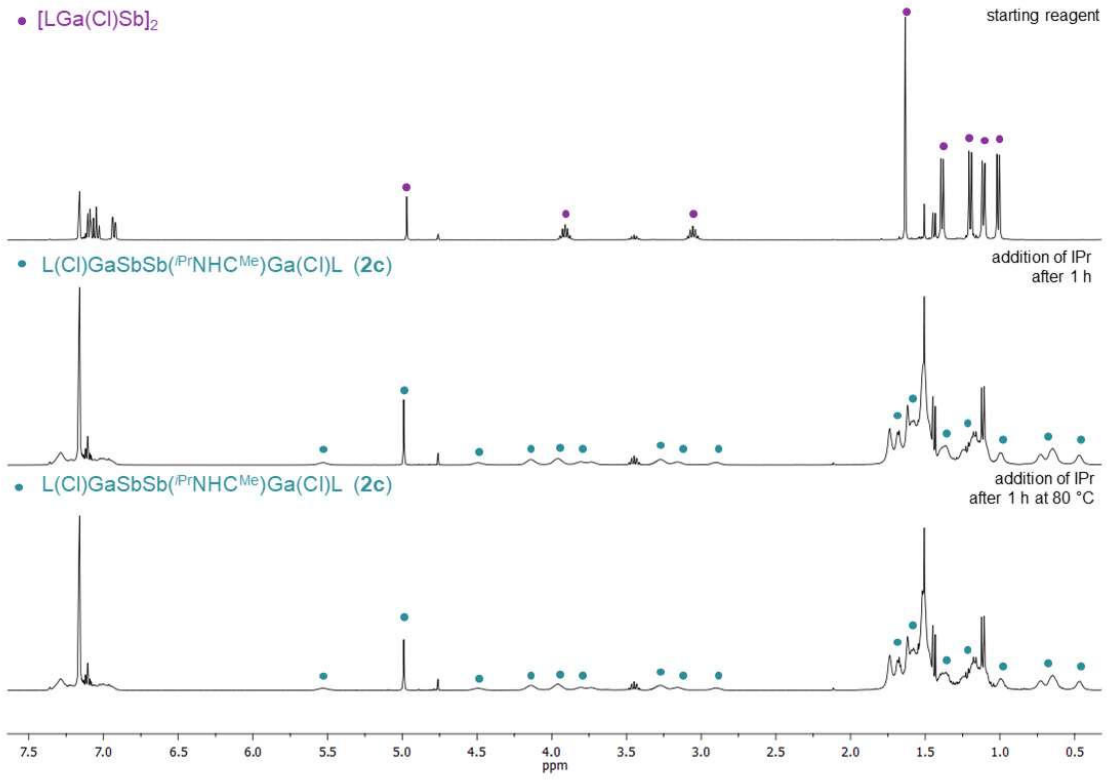

Figure S32. ^{1}H NMR spectra of the reaction of $[LGa(Cl)Sb]_2$ and $^{iPr}NHC^{Me}$ at room temperature and at 80 °C in C_6D_6.

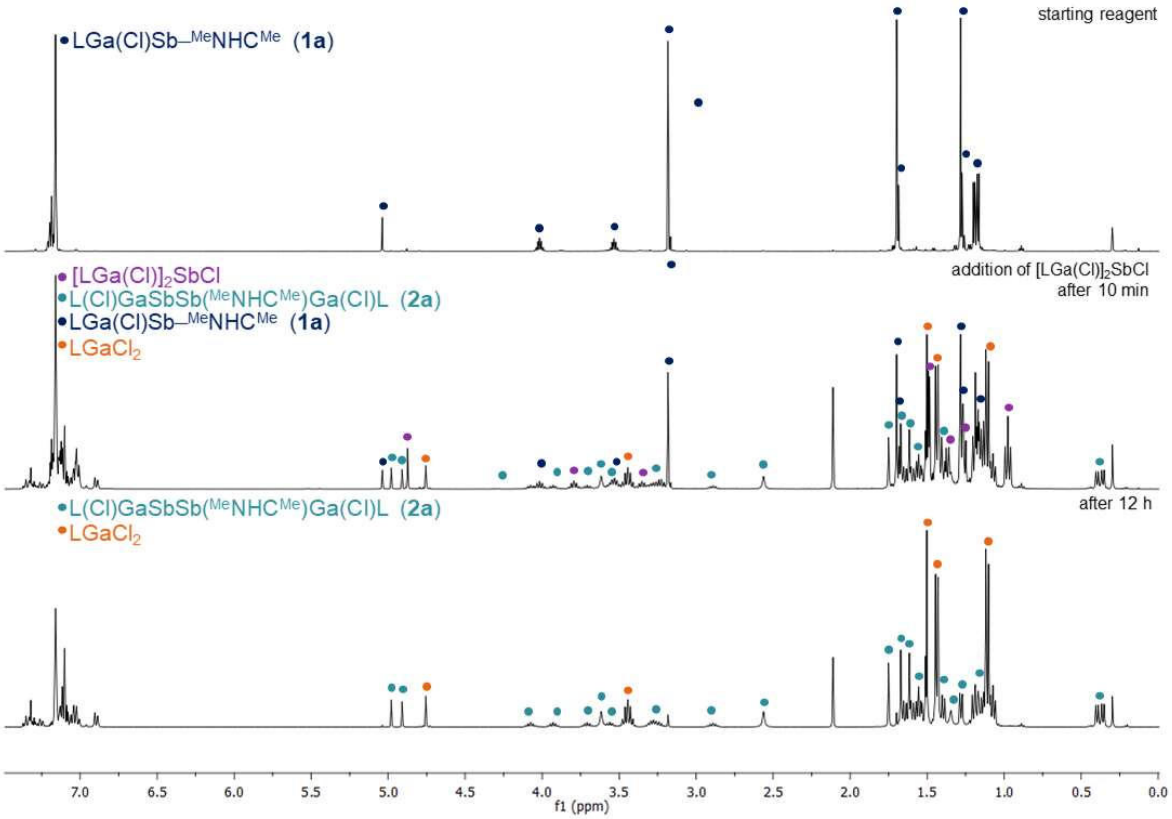

Figure S33. ^{1}H NMR spectra of the reaction of LGa(Cl)Sb-^{Me}NHC^{Me} (**1a**) and [LGa(Cl)]$_2$SbCl at room temperature in C_6D_6.

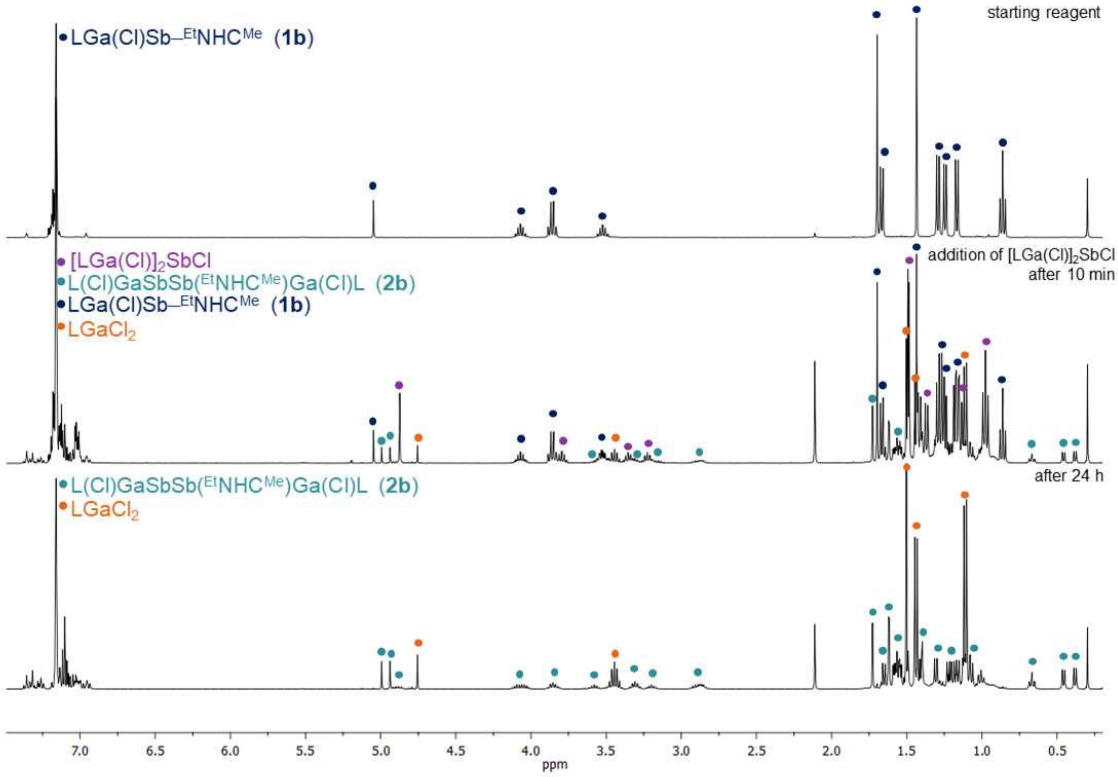

Figure S34. ^{1}H NMR spectra of the reaction of LGa(Cl)Sb-^{Et}NHC^{Me} (**1b**) and [LGa(Cl)]$_2$SbCl at room temperature in C_6D_6.

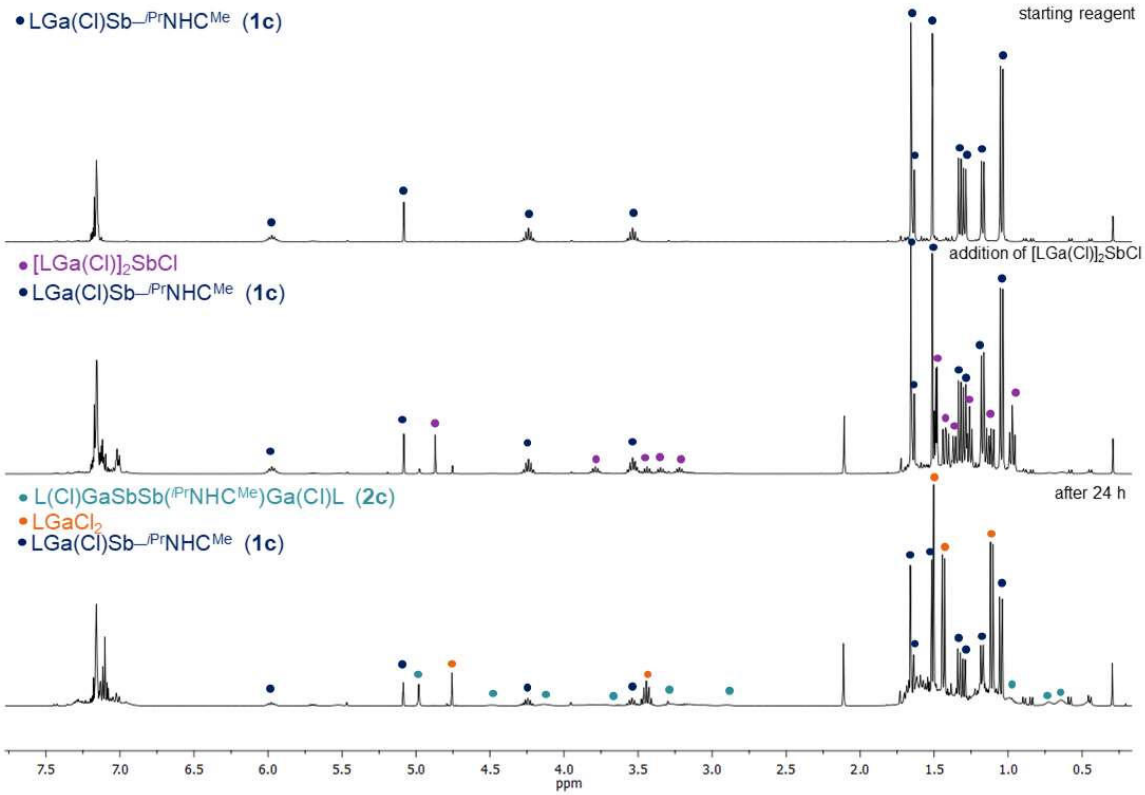

Figure S35. ^{1}H NMR spectra of the reaction of LGa(Cl)Sb-$^{i\text{Pr}}$NHC$^{\text{Me}}$ (**1c**) and [LGa(Cl)]$_2$SbCl at room temperature in C_6D_6.

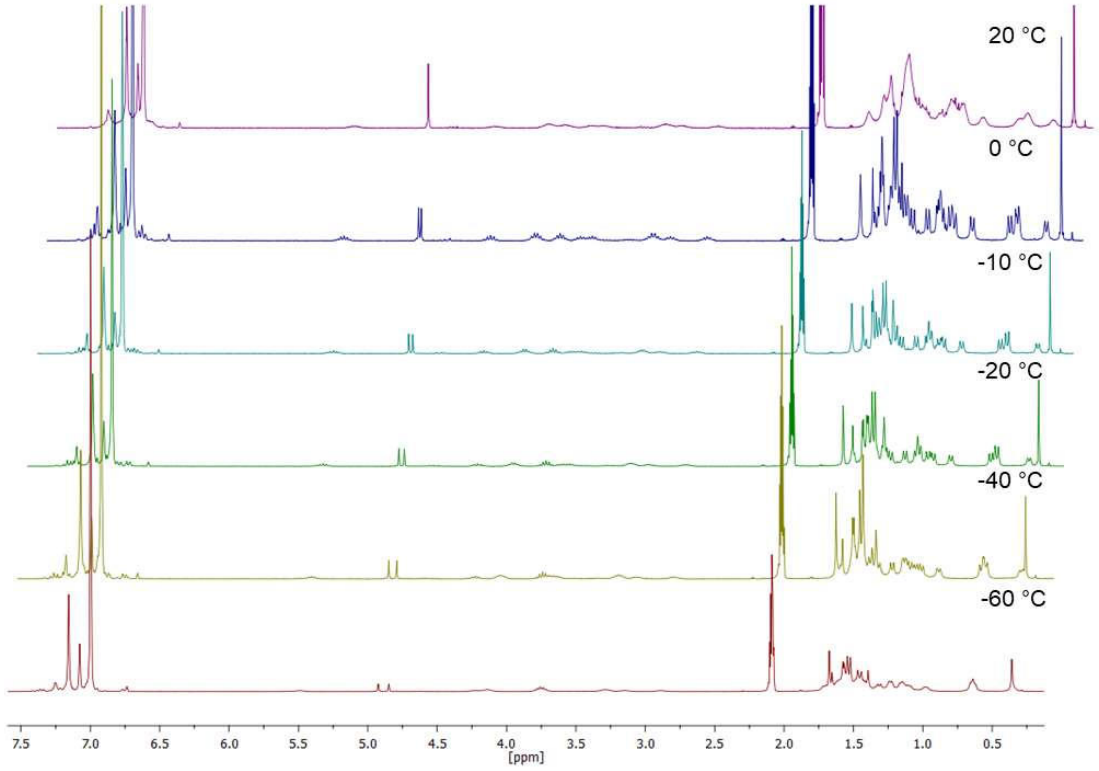

Figure S36. ^{1}H NMR spectra of L(Cl)GaSbSb($^{i\text{Pr}}$NHC$^{\text{Me}}$)Ga(Cl)L (**2c**) at low temperatures in Tol-d_8.

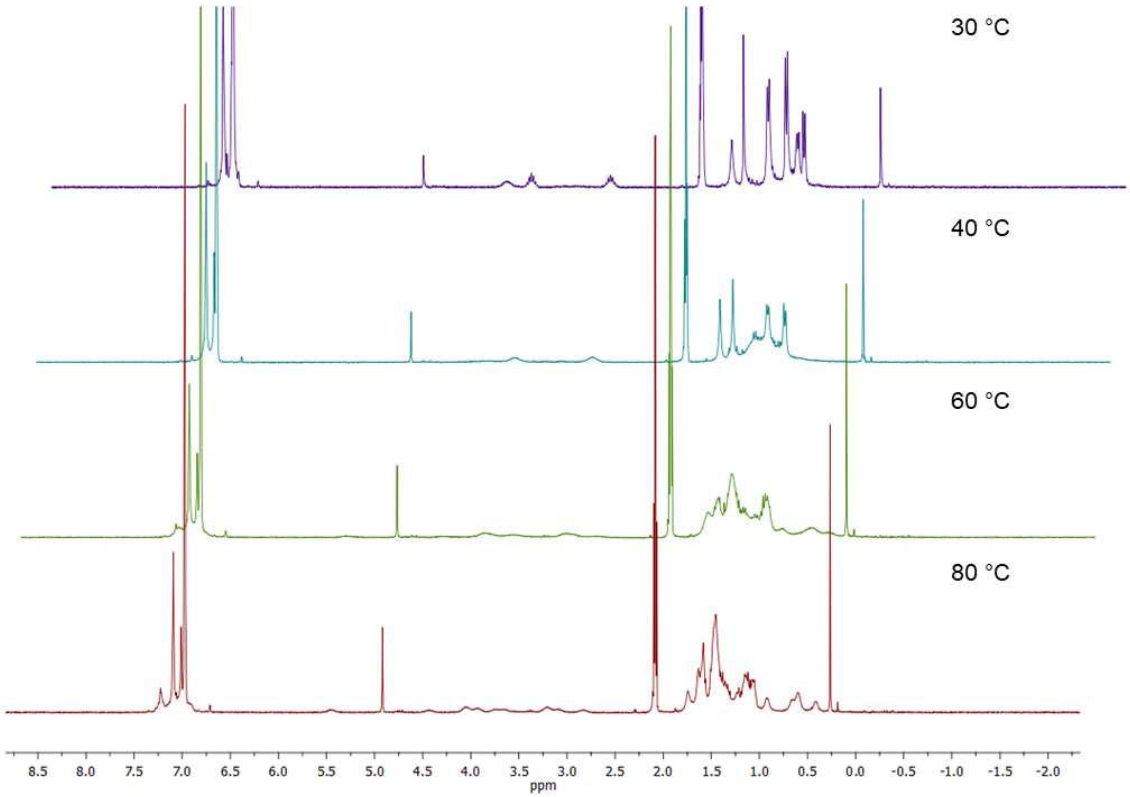

Figure S37. ^{1}H NMR spectra of L(Cl)GaSbSb($^{i\text{Pr}}$NHC$^{\text{Me}}$)Ga(Cl)L (**2c**) at high temperatures in Tol-d_8.

B) Single Crystal X-ray Diffraction

Table S1. Crystallographic details of LGa(Cl)Sb-^{R}NHC^{Me} (R = Me **1a**, Et **1b**, *i*Pr **1c**).

	1a·C$_6$H$_5$Me	**1b**	**1c**
Empirical formula	$C_{36}H_{53}ClGaN_4Sb$	$C_{38}H_{57}ClGaN_4Sb$	$C_{40}H_{61}ClGaN_4Sb$
M [g mol^{-1}]	768.74	796.79	824.84
Crystal size [mm]	0.702 × 0.224 × 0.033	0.132 × 0.126 × 0.061	0.257 × 0.194 × 0.084
T [K]	100(2)	100(2)	100(2)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P -1	C 2/c	C2/c
a [Å]	13.7869(7)	37.523(5)	38.426(5)
b [Å]	14.0433(8)	14.605(2)	14.5623(19)
c [Å]	19.2674(10)	14.951(2)	15.702(2)
α [°]	98.252(3)	90	90
β [°]	90.902(3)	107.971(2)	107.468(7)
γ [°]	91.190(3)	90	90
V [Å^3]	3690.3(3)	7793.5(19)	8381.2(19)
Z	4	8	8
D_{calcd} [g cm^{-3}]	1.384	1.358	1.307
μ(K_α [mm^{-1}])	1.563	1.483	1.382
Transmissions	0.75/0.51	0.75/0.65	0.75/0.63
F(000)	1584	3296	3424
Index ranges	-21 ≤ h ≤ 21	-53 ≤ h ≤ 51	-55 ≤ h ≤ 54
	-21 ≤ k ≤ 21	0 ≤ k ≤ 20	-20 ≤ k ≤ 20
	-29 ≤ l ≤ 29	0 ≤ l ≤ 21	-22 ≤ l ≤ 21
θ_{max} [°]	33.016	30.682	30.801
Reflections collected	254708	66692	156385
Independent reflections	27729	11641	13002
R_{int}	0.0476	0.0709	0.0570
Refined parameters	803	422	440
R_1 [$I > 2\sigma(I)$]	0.0355	0.0517	0.0353
wR_2 [all data]	0.0966	0.0900	0.0966
GooF	1.121	1.131	1.063
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	1.631/-0.791	1.427/-1.687	1.016/-0.906

Table S2. Crystallographic details of L(Cl)GaSbSb(^{R}NHC^{Me})Ga(Cl)L (R = Me **2a**,Et **2b**) and L^{1}(Cl)Ga–^{Me}NHC^{Me}.

	2a·3 C_6H_5Me	**2b·solvent**	L^{1}(Cl)Ga–^{Me}NHC^{Me}
Empirical formula	$C_{67}H_{98}Cl_2Ga_2N_6Sb_2$	$C_{82.50}H_{114}Cl_2Ga_2N_6Sb_2$	$C_{39.50}H_{56}ClGaN_4$
M [g mol^{-1}]	1441.35	1643.63	692.05
Crystal size [mm]	0.170 × 0.126 × 0.084	0.077 × 0.048 × 0.044	0.415 × 0.158 × 0.102
T [K]	100(2)	100(2)	100(2)
Crystal system	monoclinic	triclinic	monoclinic
Space group	$P2_1/c$	P-1	P 21/n
a [Å]			
b [Å]	22.5064(19)	14.441(4)	17.1559(15)
c [Å]	22.0453(15)	15.659(5)	13.1868(11)
α [°]	17.7735(14)	18.893(5)	17.9028(15)
β [°]	90	100.210(6)	90
γ [°]	112.844(4)	101.195(6)	109.450(2)
V [Å^3]	90	99.936(6)	90
Z	8126.8(11)	4029(2)	3819.1(6)
D_{calcd} [g cm^{-3}]	4	2	4
$\mu(K_\alpha$ [mm^{-1}])	1.178	1.355	1.204
Transmissions	1.415	1.436	1.855
F(000)	0.75/0.67	0.75/0.65	0.75/0.57
Index ranges	2960	1698	1476
	-30 ≤ h ≤ 30	-17 ≤ h ≤ 17	-20 ≤ h ≤ 21
	-27 ≤ k ≤ 29	-18 ≤ k ≤ 18	-16 ≤ k ≤ 16
θ_{max} [°]	-23 ≤ l ≤ 23	-22 ≤ l ≤ 22	-22 ≤ l ≤ 22
Reflections collected	28.366	25.279	79.890
Independent reflections	143296	104050	135556
R_{int}	20218	14339	8280
Refined parameters	0.0571	0.1855	0.0454
R_1 [$I > 2\sigma(I)$]	738	975	456
wR_2 [all data]	0.0376	0.0541	0.0254
GooF	0.0856	0.0983	0.0669
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	0.875/-0.780	0.825/-1.108	0.327/-0.414

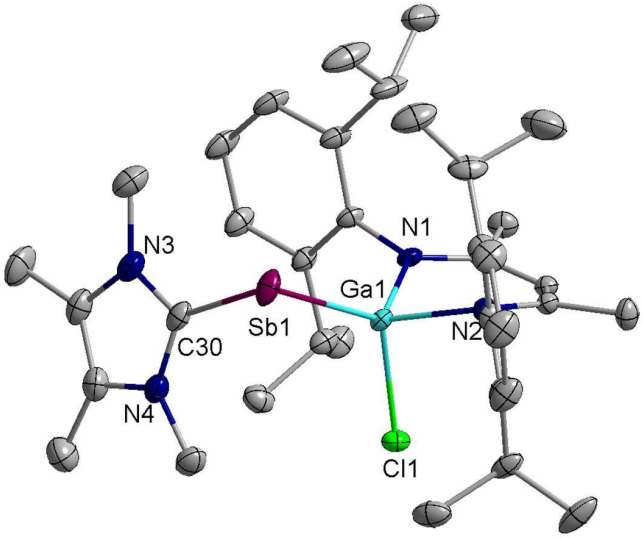

Figure S38. Solid state structure of LGa(Cl)Sb-^{Me}NHC^{Me} (**1a**). Hydrogen atoms and solvent molecules are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S3. Bond lengths [Å] for LGa(Cl)Sb-^{Me}NHC^{Me} (**1a**).

Sb11-C301	2.184(2)	C181-C231	1.406(2)	C12-C42	1.509(3)
Sb11-Ga11	2.5523(2)	C181-C191	1.407(3)	C22-C32	1.402(2)
Ga11-N21	1.9643(15)	C191-C201	1.398(3)	C32-C52	1.508(3)
Ga11-N11	1.9717(15)	C191-C241	1.518(3)	C62-C112	1.406(3)
Ga11-Cl11	2.2773(5)	C201-C211	1.386(3)	C62-C72	1.406(3)
N11-C11	1.337(2)	C211-C221	1.380(3)	C72-C82	1.398(3)
N11-C61	1.441(2)	C221-C231	1.401(3)	C72-C122	1.519(3)
N21-C31	1.333(2)	C231-C271	1.519(3)	C82-C92	1.383(3)
N21-C181	1.441(2)	C241-C261	1.531(3)	C92-C102	1.381(3)
N31-C301	1.351(2)	C241-C251	1.538(3)	C102-C112	1.393(3)
N31-C311	1.387(3)	C271-C281	1.530(3)	C112-C152	1.514(3)
N31-C331	1.463(3)	C271-C291	1.530(3)	C122-C142	1.522(3)
N41-C301	1.357(3)	C311-C321	1.356(3)	C122-C132	1.535(3)
N41-C321	1.386(3)	C311-C351	1.489(3)	C152-C172	1.529(4)
N41-C341	1.458(3)	C321-C361	1.491(3)	C152-C162	1.540(4)
C11-C21	1.398(3)	Sb12-C302	2.181(2)	C182-C192	1.409(3)
C11-C41	1.504(2)	Sb12-Ga12	2.5533(3)	C182-C232	1.411(3)
C21-C31	1.400(3)	Ga12-N22	1.9647(15)	C192-C202	1.394(3)
C31-C51	1.511(3)	Ga12-N12	1.9736(15)	C192-C242	1.517(3)
C61-C71	1.402(3)	Ga12-Cl12	2.2791(5)	C202-C212	1.378(3)
C61-C111	1.410(2)	N12-C12	1.331(2)	C212-C222	1.384(3)
C71-C81	1.395(3)	N12-C62	1.443(2)	C222-C232	1.396(3)
C71-C121	1.520(3)	N22-C32	1.330(2)	C232-C272	1.522(3)
C81-C91	1.382(3)	N22-C182	1.443(2)	C242-C262	1.534(3)
C91-C101	1.379(3)	N32-C302	1.349(3)	C242-C252	1.534(3)
C101-C111	1.398(3)	N32-C312	1.390(3)	C272-C282	1.520(4)
C111-C151	1.521(3)	N32-C332	1.458(3)	C272-C292	1.526(4)
C121-C131	1.532(3)	N42-C302	1.352(3)	C312-C322	1.360(3)

C121-C141	1.532(3)	N42-C322	1.387(3)	C312-C352	1.489(3)
C151-C171	1.521(3)	N42-C342	1.458(3)	C322-C362	1.494(4)
C151-C161	1.528(3)	C12-C22	1.400(2)		

Table S4. Bond angles [°] for LGa(Cl)Sb-^{Me}NHC^{Me} (**1a**).

C301-Sb11-Ga11	92.22(5)	C302-Sb12-Ga12	93.87(5)
N21-Ga11-N11	94.76(6)	N22-Ga12-N12	94.89(6)
N21-Ga11-Cl11	100.73(4)	N22-Ga12-Cl12	99.88(5)
N11-Ga11-Cl11	98.24(4)	N12-Ga12-Cl12	97.82(4)
N21-Ga11-Sb11	116.10(4)	N22-Ga12-Sb12	112.58(4)
N11-Ga11-Sb11	122.65(4)	N12-Ga12-Sb12	124.33(4)
Cl11-Ga11-Sb11	119.503(14)	Cl12-Ga12-Sb12	121.840(15)
C11-N11-C61	117.71(15)	C12-N12-C62	120.63(15)
C11-N11-Ga11	118.87(12)	C12-N12-Ga12	118.91(12)
C61-N11-Ga11	123.10(11)	C62-N12-Ga12	120.23(12)
C31-N21-C181	119.03(15)	C32-N22-C182	120.60(15)
C31-N21-Ga11	119.21(12)	C32-N22-Ga12	119.15(12)
C181-N21-Ga11	121.71(11)	C182-N22-Ga12	119.80(12)
C301-N31-C311	111.18(17)	C302-N32-C312	110.95(19)
C301-N31-C331	125.64(18)	C302-N32-C332	125.7(2)
C311-N31-C331	123.16(18)	C312-N32-C332	123.35(19)
C301-N41-C321	111.24(17)	C302-N42-C322	110.99(18)
C301-N41-C341	124.78(17)	C302-N42-C342	124.39(19)
C321-N41-C341	123.97(18)	C322-N42-C342	124.6(2)
N11-C11-C21	124.05(16)	N12-C12-C22	124.02(16)
N11-C11-C41	119.46(16)	N12-C12-C42	119.38(16)
C21-C11-C41	116.49(15)	C22-C12-C42	116.57(16)
C11-C21-C31	127.51(16)	C12-C22-C32	127.66(16)
N21-C31-C21	123.98(16)	N22-C32-C22	123.87(16)
N21-C31-C51	119.45(16)	N22-C32-C52	119.78(16)
C21-C31-C51	116.55(15)	C22-C32-C52	116.35(16)
C71-C61-C111	120.89(17)	C112-C62-C72	120.51(16)
C71-C61-N11	120.78(16)	C112-C62-N12	119.67(16)
C111-C61-N11	118.28(16)	C72-C62-N12	119.73(15)
C81-C71-C61	118.03(18)	C82-C72-C62	118.42(17)
C81-C71-C121	119.58(18)	C82-C72-C122	118.15(17)
C61-C71-C121	122.38(17)	C62-C72-C122	123.36(16)
C91-C81-C71	121.7(2)	C92-C82-C72	120.98(19)
C101-C91-C81	119.8(2)	C102-C92-C82	120.02(19)
C91-C101-C111	120.80(19)	C92-C102-C112	120.86(19)
C101-C111-C61	118.64(18)	C102-C112-C62	118.89(19)
C101-C111-C151	120.26(17)	C102-C112-C152	118.28(18)
C61-C111-C151	121.09(16)	C62-C112-C152	122.77(17)
C71-C121-C131	113.01(18)	C72-C122-C142	111.39(17)
C71-C121-C141	109.09(16)	C72-C122-C132	110.18(16)

C131-C121-C141	110.34(17)	C142-C122-C132	110.33(17)
C171-C151-C111	112.43(17)	C112-C152-C172	110.7(2)
C171-C151-C161	110.50(16)	C112-C152-C162	110.0(2)
C111-C151-C161	110.87(17)	C172-C152-C162	110.5(2)
C231-C181-C191	121.44(17)	C192-C182-C232	121.24(17)
C231-C181-N21	118.23(16)	C192-C182-N22	120.20(16)
C191-C181-N21	120.33(15)	C232-C182-N22	118.53(16)
C201-C191-C181	118.25(17)	C202-C192-C182	118.04(19)
C201-C191-C241	119.29(17)	C202-C192-C242	118.67(18)
C181-C191-C241	122.45(16)	C182-C192-C242	123.29(16)
C211-C201-C191	121.13(19)	C212-C202-C192	121.5(2)
C221-C211-C201	119.77(19)	C202-C212-C222	119.85(19)
C211-C221-C231	121.60(19)	C212-C222-C232	121.4(2)
C221-C231-C181	117.81(18)	C222-C232-C182	117.93(19)
C221-C231-C271	119.42(17)	C222-C232-C272	119.75(18)
C181-C231-C271	122.78(17)	C182-C232-C272	122.32(17)
C191-C241-C261	110.55(15)	C192-C242-C262	110.59(17)
C191-C241-C251	112.17(17)	C192-C242-C252	111.9(2)
C261-C241-C251	109.41(17)	C262-C242-C252	109.73(19)
C231-C271-C281	111.62(18)	C282-C272-C232	111.6(2)
C231-C271-C291	111.81(19)	C282-C272-C292	110.2(2)
C281-C271-C291	109.51(19)	C232-C272-C292	112.4(2)
N31-C301-N41	104.61(17)	N32-C302-N42	105.19(18)
N31-C301-Sb11	127.43(14)	N32-C302-Sb12	127.62(16)
N41-C301-Sb11	127.67(14)	N42-C302-Sb12	127.09(14)
C321-C311-N31	106.68(18)	C322-C312-N32	106.45(19)
C321-C311-C351	131.0(2)	C322-C312-C352	131.2(2)
N31-C311-C351	122.3(2)	N32-C312-C352	122.4(2)
C311-C321-N41	106.29(18)	C312-C322-N42	106.4(2)
C311-C321-C361	130.8(2)	C312-C322-C362	130.3(2)
N41-C321-C361	122.9(2)	N42-C322-C362	123.1(2)

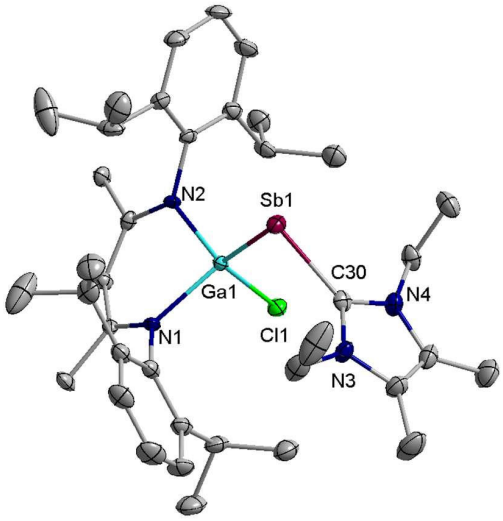

Figure S39. Solid state structure of LGa(Cl)Sb-^{Et}NHC^{Me} (**1b**). Hydrogen atoms are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S5. Bond lengths [Å] for LGa(Cl)Sb-^{Et}NHC^{Me} (**1b**).

Sb(1)-C(30)	2.183(4)	C(1)-C(4)	1.514(5)	C(18)-C(19)	1.405(6)
Sb(1)-Ga(1)	2.5380(5)	C(2)-C(3)	1.396(5)	C(19)-C(20)	1.390(6)
Ga(1)-N(2)	1.966(3)	C(3)-C(5)	1.505(5)	C(19)-C(24)	1.512(6)
Ga(1)-N(1)	1.986(3)	C(6)-C(11)	1.401(6)	C(20)-C(21)	1.375(6)
Ga(1)-Cl(1)	2.2700(10)	C(6)-C(7)	1.408(6)	C(21)-C(22)	1.375(7)
N(1)-C(1)	1.329(5)	C(7)-C(8)	1.395(6)	C(22)-C(23)	1.391(6)
N(1)-C(6)	1.446(5)	C(7)-C(12)	1.518(6)	C(23)-C(27)	1.513(6)
N(2)-C(3)	1.328(5)	C(8)-C(9)	1.372(7)	C(24)-C(25)	1.536(6)
N(2)-C(18)	1.448(5)	C(9)-C(10)	1.385(7)	C(24)-C(26)	1.541(6)
N(3)-C(30)	1.348(5)	C(10)-C(11)	1.392(6)	C(27)-C(29)	1.521(7)
N(3)-C(31)	1.389(5)	C(11)-C(15)	1.518(6)	C(27)-C(28)	1.524(7)
N(3)-C(33)	1.461(6)	C(12)-C(14)	1.528(6)	C(31)-C(32)	1.354(6)
N(4)-C(30)	1.346(5)	C(12)-C(13)	1.539(6)	C(31)-C(37)	1.492(6)
N(4)-C(32)	1.389(5)	C(15)-C(16)	1.514(7)	C(32)-C(38)	1.483(6)
N(4)-C(35)	1.463(5)	C(15)-C(17)	1.524(6)	C(33)-C(34)	1.508(8)
C(1)-C(2)	1.406(5)	C(18)-C(23)	1.405(5)	C(35)-C(36)	1.522(6)

Table S6. Bond angles [°] for LGa(Cl)Sb-^{Et}NHC^{Me} (**1b**).

C(30)-Sb(1)-Ga(1)	90.73(10)	C(6)-C(11)-C(15)	121.7(4)
N(2)-Ga(1)-N(1)	94.59(13)	C(7)-C(12)-C(14)	110.7(4)
N(2)-Ga(1)-Cl(1)	100.89(10)	C(7)-C(12)-C(13)	111.6(4)
N(1)-Ga(1)-Cl(1)	99.45(10)	C(14)-C(12)-C(13)	110.4(4)
N(2)-Ga(1)-Sb(1)	116.88(9)	C(16)-C(15)-C(11)	112.3(4)
N(1)-Ga(1)-Sb(1)	121.50(9)	C(16)-C(15)-C(17)	109.3(4)
Cl(1)-Ga(1)-Sb(1)	118.91(3)	C(11)-C(15)-C(17)	113.1(4)
C(1)-N(1)-C(6)	120.5(3)	C(23)-C(18)-C(19)	121.6(4)
C(1)-N(1)-Ga(1)	119.3(3)	C(23)-C(18)-N(2)	118.1(3)
C(6)-N(1)-Ga(1)	120.0(2)	C(19)-C(18)-N(2)	120.2(3)

C(3)-N(2)-C(18)	120.2(3)
C(3)-N(2)-Ga(1)	119.9(2)
C(18)-N(2)-Ga(1)	119.6(2)
C(30)-N(3)-C(31)	110.2(3)
C(30)-N(3)-C(33)	125.1(4)
C(31)-N(3)-C(33)	124.7(4)
C(30)-N(4)-C(32)	111.0(3)
C(30)-N(4)-C(35)	124.3(3)
C(32)-N(4)-C(35)	124.7(3)
N(1)-C(1)-C(2)	123.3(3)
N(1)-C(1)-C(4)	120.2(3)
C(2)-C(1)-C(4)	116.6(3)
C(3)-C(2)-C(1)	128.7(4)
N(2)-C(3)-C(2)	123.1(3)
N(2)-C(3)-C(5)	120.2(3)
C(2)-C(3)-C(5)	116.7(3)
C(11)-C(6)-C(7)	121.3(4)
C(11)-C(6)-N(1)	118.8(3)
C(7)-C(6)-N(1)	119.9(4)
C(8)-C(7)-C(6)	117.8(4)
C(8)-C(7)-C(12)	119.0(4)
C(6)-C(7)-C(12)	123.2(4)
C(9)-C(8)-C(7)	121.7(4)
C(8)-C(9)-C(10)	119.7(4)
C(9)-C(10)-C(11)	121.3(4)
C(10)-C(11)-C(6)	118.2(4)
C(10)-C(11)-C(15)	120.0(4)
C(20)-C(19)-C(18)	117.4(4)
C(20)-C(19)-C(24)	120.1(4)
C(18)-C(19)-C(24)	122.5(3)
C(21)-C(20)-C(19)	122.2(4)
C(22)-C(21)-C(20)	119.3(4)
C(21)-C(22)-C(23)	121.8(4)
C(22)-C(23)-C(18)	117.7(4)
C(22)-C(23)-C(27)	120.7(4)
C(18)-C(23)-C(27)	121.5(4)
C(19)-C(24)-C(25)	112.2(4)
C(19)-C(24)-C(26)	109.7(4)
C(25)-C(24)-C(26)	110.3(3)
C(23)-C(27)-C(29)	113.5(4)
C(23)-C(27)-C(28)	110.7(4)
C(29)-C(27)-C(28)	109.6(4)
N(4)-C(30)-N(3)	105.6(3)
N(4)-C(30)-Sb(1)	127.4(3)
N(3)-C(30)-Sb(1)	126.5(3)
C(32)-C(31)-N(3)	107.1(4)
C(32)-C(31)-C(37)	129.8(4)
N(3)-C(31)-C(37)	123.0(4)
C(31)-C(32)-N(4)	106.0(4)
C(31)-C(32)-C(38)	130.6(4)
N(4)-C(32)-C(38)	123.4(4)
N(3)-C(33)-C(34)	111.0(4)
N(4)-C(35)-C(36)	111.8(4)

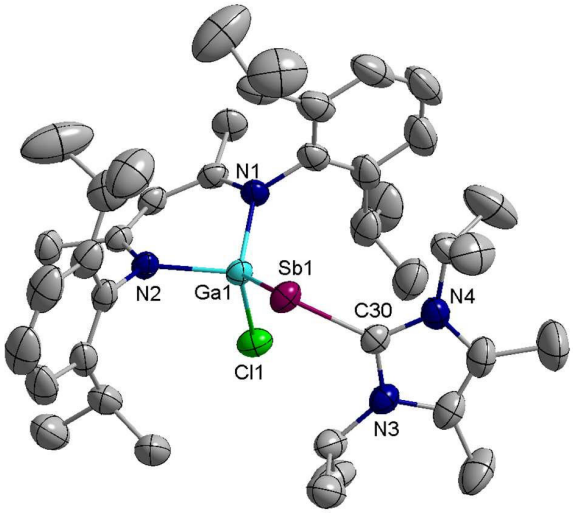

Figure S40. Solid state structure of LGa(Cl)Sb-$^{i\text{Pr}}$NHC$^{\text{Me}}$ (**1c**). Hydrogen atoms are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S7. Bond lengths [Å] for LGa(Cl)Sb-$^{i\text{Pr}}$NHC$^{\text{Me}}$ (**1c**).

Sb(1)-C(30)	2.194(3)	C(2)-C(3)	1.396(4)	C(19)-C(24)	1.496(5)
Sb(1)-Ga(1)	2.5528(4)	C(3)-C(5)	1.511(4)	C(20)-C(21)	1.355(6)
Ga(1)-N(2)	1.974(2)	C(6)-C(7)	1.401(4)	C(21)-C(22)	1.362(6)
Ga(1)-N(1)	1.989(2)	C(6)-C(11)	1.404(5)	C(22)-C(23)	1.402(5)
Ga(1)-Cl(1)	2.2561(8)	C(7)-C(8)	1.400(5)	C(23)-C(27)	1.498(5)
N(1)-C(1)	1.329(3)	C(7)-C(12)	1.507(5)	C(24)-C(25)	1.528(5)
N(1)-C(6)	1.447(4)	C(8)-C(9)	1.359(6)	C(24)-C(26)	1.539(5)
N(2)-C(3)	1.330(3)	C(9)-C(10)	1.371(6)	C(27)-C(28)	1.520(6)
N(2)-C(18)	1.447(3)	C(10)-C(11)	1.399(5)	C(27)-C(29)	1.531(6)
N(3)-C(30)	1.359(3)	C(11)-C(15)	1.509(5)	C(31)-C(32)	1.346(5)
N(3)-C(31)	1.387(4)	C(12)-C(13)	1.532(5)	C(31)-C(36)	1.502(5)
N(3)-C(33)	1.468(4)	C(12)-C(14)	1.539(5)	C(32)-C(37)	1.505(5)
N(4)-C(30)	1.353(4)	C(15)-C(17)	1.514(6)	C(33)-C(35)	1.515(5)
N(4)-C(32)	1.386(4)	C(15)-C(16)	1.517(6)	C(33)-C(34)	1.519(4)
N(4)-C(38)	1.482(4)	C(18)-C(23)	1.390(4)	C(38)-C(39)	1.491(5)
C(1)-C(2)	1.391(4)	C(18)-C(19)	1.411(4)	C(38)-C(40)	1.516(5)
C(1)-C(4)	1.523(4)	C(19)-C(20)	1.400(5)		

Table S8. Bond angles [°] for LGa(Cl)Sb-$^{i\text{Pr}}$NHC$^{\text{Me}}$ (**1c**).

C(30)-Sb(1)-Ga(1)	94.82(7)	C(7)-C(12)-C(14)	112.7(3)
N(2)-Ga(1)-N(1)	94.69(9)	C(13)-C(12)-C(14)	110.5(3)
N(2)-Ga(1)-Cl(1)	99.49(7)	C(11)-C(15)-C(17)	114.1(4)
N(1)-Ga(1)-Cl(1)	98.32(7)	C(11)-C(15)-C(16)	111.7(4)
N(2)-Ga(1)-Sb(1)	114.90(6)	C(17)-C(15)-C(16)	109.3(4)
N(1)-Ga(1)-Sb(1)	124.92(7)	C(23)-C(18)-C(19)	122.3(3)
Cl(1)-Ga(1)-Sb(1)	119.24(2)	C(23)-C(18)-N(2)	117.9(3)
C(1)-N(1)-C(6)	119.0(2)	C(19)-C(18)-N(2)	119.8(3)
C(1)-N(1)-Ga(1)	118.65(18)	C(20)-C(19)-C(18)	116.6(4)

C(6)-N(1)-Ga(1)	122.09(16)
C(3)-N(2)-C(18)	119.5(2)
C(3)-N(2)-Ga(1)	119.32(17)
C(18)-N(2)-Ga(1)	120.82(16)
C(30)-N(3)-C(31)	110.0(3)
C(30)-N(3)-C(33)	122.4(2)
C(31)-N(3)-C(33)	127.5(3)
C(30)-N(4)-C(32)	110.2(3)
C(30)-N(4)-C(38)	122.5(2)
C(32)-N(4)-C(38)	127.3(3)
N(1)-C(1)-C(2)	124.1(2)
N(1)-C(1)-C(4)	119.8(3)
C(2)-C(1)-C(4)	116.0(2)
C(1)-C(2)-C(3)	128.9(2)
N(2)-C(3)-C(2)	123.3(2)
N(2)-C(3)-C(5)	120.1(2)
C(2)-C(3)-C(5)	116.6(2)
C(7)-C(6)-C(11)	121.6(3)
C(7)-C(6)-N(1)	120.3(3)
C(11)-C(6)-N(1)	118.1(3)
C(8)-C(7)-C(6)	117.5(4)
C(8)-C(7)-C(12)	119.3(3)
C(6)-C(7)-C(12)	123.2(3)
C(9)-C(8)-C(7)	121.5(4)
C(8)-C(9)-C(10)	120.7(4)
C(9)-C(10)-C(11)	120.9(4)
C(10)-C(11)-C(6)	117.8(4)
C(10)-C(11)-C(15)	119.7(4)
C(6)-C(11)-C(15)	122.5(3)
C(7)-C(12)-C(13)	110.7(3)
C(20)-C(19)-C(24)	120.0(3)
C(18)-C(19)-C(24)	123.4(3)
C(21)-C(20)-C(19)	121.9(4)
C(20)-C(21)-C(22)	120.4(4)
C(21)-C(22)-C(23)	121.6(4)
C(18)-C(23)-C(22)	117.1(3)
C(18)-C(23)-C(27)	122.2(3)
C(22)-C(23)-C(27)	120.7(3)
C(19)-C(24)-C(25)	109.5(3)
C(19)-C(24)-C(26)	113.8(3)
C(25)-C(24)-C(26)	110.0(3)
C(23)-C(27)-C(28)	113.9(4)
C(23)-C(27)-C(29)	111.0(4)
C(28)-C(27)-C(29)	109.4(3)
N(4)-C(30)-N(3)	105.6(2)
N(4)-C(30)-Sb(1)	126.0(2)
N(3)-C(30)-Sb(1)	127.7(2)
C(32)-C(31)-N(3)	107.0(3)
C(32)-C(31)-C(36)	127.8(3)
N(3)-C(31)-C(36)	125.2(3)
C(31)-C(32)-N(4)	107.2(3)
C(31)-C(32)-C(37)	127.8(3)
N(4)-C(32)-C(37)	125.0(3)
N(3)-C(33)-C(35)	110.4(3)
N(3)-C(33)-C(34)	112.4(3)
C(35)-C(33)-C(34)	113.5(3)
N(4)-C(38)-C(39)	110.2(3)
N(4)-C(38)-C(40)	112.7(3)
C(39)-C(38)-C(40)	112.9(3)

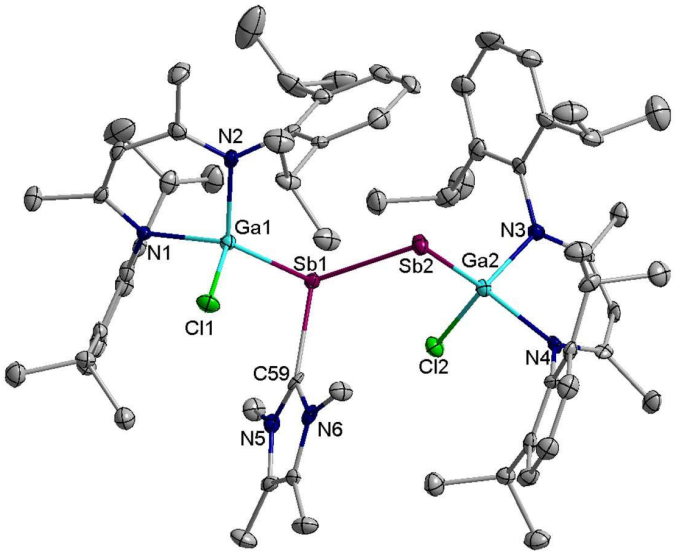

Figure S41. Solid state structure of L(Cl)GaSbSb(^{Me}NHC^{Me})Ga(Cl)L (**2a**). Hydrogen atoms and solvent molecules are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S9. Bond lengths [Å] for L(Cl)GaSbSb(^{Me}NHC^{Me})Ga(Cl)L (**2a**).

Sb(1)-C(59)	2.225(5)	C(12)-C(14)	1.528(7)	C(51)-C(52)	1.410(7)
Sb(1)-Ga(1)	2.6093(9)	C(15)-C(16)	1.507(8)	C(52)-C(56)	1.519(7)
Sb(1)-Sb(2)	2.7461(8)	C(15)-C(17)	1.537(7)	C(53)-C(55)	1.533(7)
Sb(2)-Ga(2)	2.5457(9)	C(18)-C(23)	1.404(7)	C(53)-C(54)	1.539(7)
Ga(1)-N(1)	1.955(4)	C(18)-C(19)	1.410(7)	C(56)-C(58)	1.521(7)
Ga(1)-N(2)	1.958(4)	C(19)-C(20)	1.376(8)	C(56)-C(57)	1.530(7)
Ga(1)-Cl(1)	2.2353(15)	C(19)-C(24)	1.530(7)	C(60)-C(61)	1.349(7)
Ga(2)-N(4)	1.982(4)	C(20)-C(21)	1.395(8)	C(60)-C(64)	1.483(7)
Ga(2)-N(3)	1.990(4)	C(21)-C(22)	1.372(8)	C(61)-C(65)	1.483(7)
Ga(2)-Cl(2)	2.2656(15)	C(22)-C(23)	1.378(8)	C11-C21	1.385(7)
N(1)-C(1)	1.337(6)	C(23)-C(27)	1.525(8)	C11-C61	1.391(7)
N(1)-C(6)	1.459(6)	C(24)-C(25)	1.522(8)	C11-C71	1.498(8)
N(2)-C(3)	1.331(6)	C(24)-C(26)	1.540(7)	C21-C31	1.374(7)
N(2)-C(18)	1.439(7)	C(27)-C(28)	1.507(8)	C31-C41	1.376(7)
N(3)-C(30)	1.334(6)	C(27)-C(29)	1.514(9)	C41-C51	1.382(7)
N(3)-C(35)	1.450(7)	C(30)-C(31)	1.382(7)	C51-C61	1.371(7)
N(4)-C(32)	1.328(6)	C(30)-C(33)	1.506(7)	C12-C22	1.369(12)
N(4)-C(47)	1.454(6)	C(31)-C(32)	1.399(7)	C12-C62	1.396(12)
N(5)-C(59)	1.339(6)	C(32)-C(34)	1.508(7)	C12-C72	1.500(13)
N(5)-C(60)	1.390(7)	C(35)-C(40)	1.400(7)	C22-C32	1.388(12)
N(5)-C(62)	1.469(6)	C(35)-C(36)	1.415(7)	C32-C42	1.372(13)
N(6)-C(59)	1.358(6)	C(36)-C(37)	1.389(8)	C42-C52	1.401(13)
N(6)-C(61)	1.381(7)	C(36)-C(41)	1.511(8)	C52-C62	1.402(12)
N(6)-C(63)	1.459(6)	C(37)-C(38)	1.369(8)	C13-C23	1.373(11)
C(1)-C(2)	1.403(7)	C(38)-C(39)	1.373(8)	C13-C63	1.390(11)
C(1)-C(4)	1.496(7)	C(39)-C(40)	1.391(8)	C13-C73	1.501(13)
C(2)-C(3)	1.395(7)	C(40)-C(44)	1.505(8)	C23-C33	1.386(12)
C(3)-C(5)	1.511(7)	C(41)-C(43)	1.524(8)	C33-C43	1.379(12)

C(6)-C(11)	1.407(7)	C(41)-C(42)	1.529(8)	C43-C53	1.383(11)
C(6)-C(7)	1.410(8)	C(44)-C(46)	1.530(7)	C53-C63	1.396(12)
C(7)-C(8)	1.388(7)	C(44)-C(45)	1.548(7)	C14-C64	1.382(13)
C(7)-C(12)	1.521(7)	C(47)-C(52)	1.389(7)	C14-C24	1.384(13)
C(8)-C(9)	1.373(7)	C(47)-C(48)	1.417(7)	C14-C74	1.506(15)
C(9)-C(10)	1.367(8)	C(48)-C(49)	1.399(7)	C24-C34	1.383(13)
C(10)-C(11)	1.396(7)	C(48)-C(53)	1.502(8)	C34-C44	1.399(13)
C(11)-C(15)	1.506(8)	C(49)-C(50)	1.381(8)	C44-C54	1.394(13)
C(12)-C(13)	1.525(7)	C(50)-C(51)	1.385(7)	C54-C64	1.381(13)

Table S10. Bond angles [°] for L(Cl)GaSbSb(^{Me}NHC^{Me})Ga(Cl)L (**2a**).

C(59)-Sb(1)-Ga(1)	91.44(12)	N(4)-C(32)-C(31)	122.7(5)
C(59)-Sb(1)-Sb(2)	105.92(13)	N(4)-C(32)-C(34)	119.7(5)
Ga(1)-Sb(1)-Sb(2)	99.75(3)	C(31)-C(32)-C(34)	117.6(4)
Ga(2)-Sb(2)-Sb(1)	88.37(3)	C(40)-C(35)-C(36)	121.2(5)
N(1)-Ga(1)-N(2)	96.13(18)	C(40)-C(35)-N(3)	120.7(5)
N(1)-Ga(1)-Cl(1)	101.71(12)	C(36)-C(35)-N(3)	118.1(5)
N(2)-Ga(1)-Cl(1)	101.28(12)	C(37)-C(36)-C(35)	117.2(5)
N(1)-Ga(1)-Sb(1)	113.48(11)	C(37)-C(36)-C(41)	120.1(5)
N(2)-Ga(1)-Sb(1)	122.70(12)	C(35)-C(36)-C(41)	122.7(5)
Cl(1)-Ga(1)-Sb(1)	117.67(5)	C(38)-C(37)-C(36)	122.1(6)
N(4)-Ga(2)-N(3)	93.27(17)	C(37)-C(38)-C(39)	120.0(6)
N(4)-Ga(2)-Cl(2)	99.83(13)	C(38)-C(39)-C(40)	121.0(6)
N(3)-Ga(2)-Cl(2)	100.76(13)	C(39)-C(40)-C(35)	118.4(5)
N(4)-Ga(2)-Sb(2)	116.71(11)	C(39)-C(40)-C(44)	119.1(5)
N(3)-Ga(2)-Sb(2)	121.59(13)	C(35)-C(40)-C(44)	122.4(5)
Cl(2)-Ga(2)-Sb(2)	119.61(4)	C(36)-C(41)-C(43)	112.1(5)
C(1)-N(1)-C(6)	120.4(4)	C(36)-C(41)-C(42)	111.2(5)
C(1)-N(1)-Ga(1)	120.7(3)	C(43)-C(41)-C(42)	110.1(5)
C(6)-N(1)-Ga(1)	118.8(3)	C(40)-C(44)-C(46)	111.7(5)
C(3)-N(2)-C(18)	121.7(4)	C(40)-C(44)-C(45)	112.4(5)
C(3)-N(2)-Ga(1)	119.0(4)	C(46)-C(44)-C(45)	109.6(5)
C(18)-N(2)-Ga(1)	119.1(3)	C(52)-C(47)-C(48)	122.5(5)
C(30)-N(3)-C(35)	118.0(4)	C(52)-C(47)-N(4)	120.7(5)
C(30)-N(3)-Ga(2)	121.2(4)	C(48)-C(47)-N(4)	116.7(5)
C(35)-N(3)-Ga(2)	120.8(3)	C(49)-C(48)-C(47)	117.0(5)
C(32)-N(4)-C(47)	119.3(4)	C(49)-C(48)-C(53)	120.9(5)
C(32)-N(4)-Ga(2)	121.7(3)	C(47)-C(48)-C(53)	122.1(5)
C(47)-N(4)-Ga(2)	118.9(3)	C(50)-C(49)-C(48)	121.8(5)
C(59)-N(5)-C(60)	111.8(4)	C(49)-C(50)-C(51)	119.9(5)
C(59)-N(5)-C(62)	124.2(5)	C(50)-C(51)-C(52)	120.9(5)
C(60)-N(5)-C(62)	123.9(4)	C(47)-C(52)-C(51)	117.9(5)
C(59)-N(6)-C(61)	111.0(4)	C(47)-C(52)-C(56)	123.7(5)
C(59)-N(6)-C(63)	126.2(5)	C(51)-C(52)-C(56)	118.4(5)
C(61)-N(6)-C(63)	122.7(4)	C(48)-C(53)-C(55)	113.1(4)
N(1)-C(1)-C(2)	122.1(5)	C(48)-C(53)-C(54)	112.4(5)

N(1)-C(1)-C(4)	120.6(5)	C(55)-C(53)-C(54)	109.6(5)
C(2)-C(1)-C(4)	117.3(5)	C(52)-C(56)-C(58)	110.3(4)
C(3)-C(2)-C(1)	129.3(5)	C(52)-C(56)-C(57)	112.9(5)
N(2)-C(3)-C(2)	124.5(5)	C(58)-C(56)-C(57)	109.8(5)
N(2)-C(3)-C(5)	119.5(5)	N(5)-C(59)-N(6)	104.4(5)
C(2)-C(3)-C(5)	116.0(5)	N(5)-C(59)-Sb(1)	122.5(4)
C(11)-C(6)-C(7)	121.8(5)	N(6)-C(59)-Sb(1)	132.9(4)
C(11)-C(6)-N(1)	117.9(5)	C(61)-C(60)-N(5)	105.9(5)
C(7)-C(6)-N(1)	120.3(4)	C(61)-C(60)-C(64)	131.6(5)
C(8)-C(7)-C(6)	117.2(5)	N(5)-C(60)-C(64)	122.4(5)
C(8)-C(7)-C(12)	119.5(5)	C(60)-C(61)-N(6)	106.9(5)
C(6)-C(7)-C(12)	123.3(5)	C(60)-C(61)-C(65)	130.5(5)
C(9)-C(8)-C(7)	122.0(6)	N(6)-C(61)-C(65)	122.5(5)
C(10)-C(9)-C(8)	119.8(5)	C21-C11-C61	118.3(6)
C(9)-C(10)-C(11)	121.9(5)	C21-C11-C71	120.2(5)
C(10)-C(11)-C(6)	117.2(5)	C61-C11-C71	121.4(5)
C(10)-C(11)-C(15)	121.3(5)	C31-C21-C11	121.1(5)
C(6)-C(11)-C(15)	121.5(5)	C21-C31-C41	120.0(6)
C(7)-C(12)-C(13)	111.6(5)	C31-C41-C51	119.6(6)
C(7)-C(12)-C(14)	110.8(4)	C61-C51-C41	120.3(6)
C(13)-C(12)-C(14)	110.2(5)	C51-C61-C11	120.6(5)
C(11)-C(15)-C(16)	111.5(5)	C22-C12-C62	120.0(14)
C(11)-C(15)-C(17)	113.1(5)	C22-C12-C72	120.6(11)
C(16)-C(15)-C(17)	110.2(5)	C62-C12-C72	119.2(11)
C(23)-C(18)-C(19)	120.9(5)	C12-C22-C32	123.3(16)
C(23)-C(18)-N(2)	118.5(5)	C42-C32-C22	116.4(17)
C(19)-C(18)-N(2)	120.5(5)	C32-C42-C52	122.2(18)
C(20)-C(19)-C(18)	118.2(5)	C42-C52-C62	120.0(17)
C(20)-C(19)-C(24)	119.1(5)	C12-C62-C52	117.6(15)
C(18)-C(19)-C(24)	122.7(5)	C23-C13-C63	115.4(12)
C(19)-C(20)-C(21)	121.6(5)	C23-C13-C73	122.3(10)
C(22)-C(21)-C(20)	118.8(6)	C63-C13-C73	122.3(9)
C(21)-C(22)-C(23)	122.3(5)	C13-C23-C33	122.9(12)
C(22)-C(23)-C(18)	118.1(5)	C43-C33-C23	121.2(13)
C(22)-C(23)-C(27)	120.6(5)	C33-C43-C53	117.4(13)
C(18)-C(23)-C(27)	121.3(5)	C43-C53-C63	120.4(12)
C(25)-C(24)-C(19)	110.0(5)	C13-C63-C53	122.7(13)
C(25)-C(24)-C(26)	110.4(5)	C64-C14-C24	121.7(18)
C(19)-C(24)-C(26)	111.2(5)	C64-C14-C74	119.4(14)
C(28)-C(27)-C(29)	110.2(5)	C24-C14-C74	118.8(13)
C(28)-C(27)-C(23)	113.9(5)	C34-C24-C14	122(2)
C(29)-C(27)-C(23)	111.5(5)	C24-C34-C44	115(2)
N(3)-C(30)-C(31)	122.9(5)	C54-C44-C34	123(2)
N(3)-C(30)-C(33)	119.9(5)	C64-C54-C44	120(2)
C(31)-C(30)-C(33)	117.2(4)	C54-C64-C14	117(2)

C(30)-C(31)-C(32)	129.3(5)	N(4)-C(32)-C(31)	122.7(5)

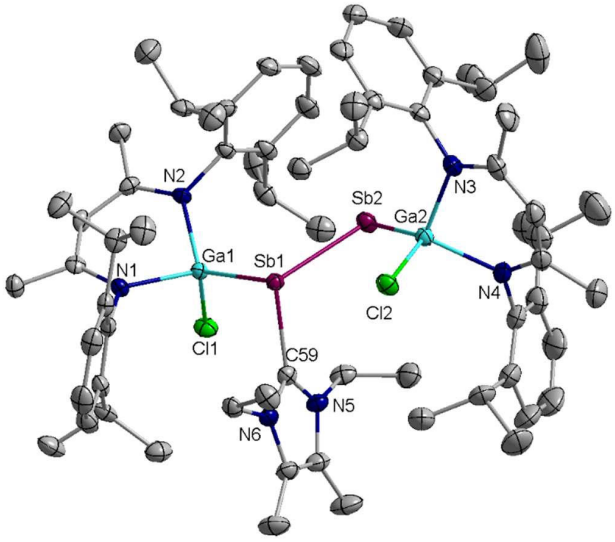

Figure S42. Solid state structure of L(Cl)GaSbSb(^{Et}NHC^{Me})Ga(Cl)L (**2b**). Hydrogen atoms and solvent molecules are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S11. Bond lengths [Å] for L(Cl)GaSbSb(^{Et}NHC^{Me})Ga(Cl)L (**2b**).

Sb(1)-C(59)	2.245(3)	C(6)-C(7)	1.407(4)	C(35)-C(40)	1.402(4)
Sb(1)-Ga(1)	2.6103(4)	C(7)-C(8)	1.386(4)	C(36)-C(37)	1.393(4)
Sb(1)-Sb(2)	2.7385(4)	C(7)-C(12)	1.529(4)	C(36)-C(41)	1.515(4)
Sb(2)-Ga(2)	2.5541(4)	C(8)-C(9)	1.379(5)	C(37)-C(38)	1.369(5)
Ga(1)-N(2)	1.954(2)	C(9)-C(10)	1.382(4)	C(38)-C(39)	1.372(4)
Ga(1)-N(1)	1.973(2)	C(10)-C(11)	1.390(4)	C(39)-C(40)	1.403(4)
Ga(1)-Cl(1)	2.2426(7)	C(11)-C(15)	1.514(4)	C(40)-C(44)	1.510(4)
Ga(2)-N(3)	1.985(2)	C(12)-C(13)	1.525(4)	C(41)-C(42)	1.522(5)
Ga(2)-N(4)	1.989(2)	C(12)-C(14)	1.532(4)	C(41)-C(43)	1.537(5)
Ga(2)-Cl(2)	2.2599(8)	C(15)-C(17)	1.527(4)	C(44)-C(46)	1.526(4)
N(1)-C(1)	1.337(3)	C(15)-C(16)	1.534(4)	C(44)-C(45)	1.529(4)
N(1)-C(6)	1.444(3)	C(18)-C(23)	1.391(4)	C(47)-C(48)	1.405(5)
N(2)-C(3)	1.331(3)	C(18)-C(19)	1.408(4)	C(47)-C(52)	1.406(5)
N(2)-C(18)	1.461(3)	C(19)-C(20)	1.391(4)	C(48)-C(49)	1.387(5)
N(3)-C(30)	1.329(4)	C(19)-C(24)	1.515(4)	C(48)-C(53)	1.513(5)
N(3)-C(35)	1.449(4)	C(20)-C(21)	1.365(5)	C(49)-C(50)	1.372(6)
N(4)-C(32)	1.335(4)	C(21)-C(22)	1.375(5)	C(50)-C(51)	1.375(6)
N(4)-C(47)	1.449(4)	C(22)-C(23)	1.391(4)	C(51)-C(52)	1.395(5)
N(5)-C(59)	1.355(4)	C(23)-C(27)	1.518(4)	C(52)-C(56)	1.517(5)
N(5)-C(60)	1.391(4)	C(24)-C(25)	1.521(4)	C(53)-C(54)	1.541(5)
N(5)-C(62)	1.461(4)	C(24)-C(26)	1.532(4)	C(53)-C(55)	1.541(5)
N(6)-C(59)	1.342(3)	C(27)-C(29)	1.530(4)	C(56)-C(57)	1.523(5)
N(6)-C(61)	1.385(4)	C(27)-C(28)	1.531(5)	C(56)-C(58)	1.526(5)
N(6)-C(64)	1.468(4)	C(30)-C(31)	1.394(4)	C(60)-C(61)	1.342(4)

C(1)-C(2)	1.397(4)	C(30)-C(33)	1.521(4)	C(60)-C(66)	1.496(4)
C(1)-C(4)	1.507(4)	C(31)-C(32)	1.390(5)	C(61)-C(67)	1.492(4)
C(2)-C(3)	1.396(4)	C(32)-C(34)	1.511(4)	C(62)-C(63)	1.514(4)
C(3)-C(5)	1.504(4)	C(35)-C(36)	1.401(4)	C(64)-C(65)	1.513(4)
C(6)-C(11)	1.407(4)				

Table S12. Bond angles [°] for L(Cl)GaSbSb(^{Et}NHC^{Me})Ga(Cl)L (**2b**).

C(59)-Sb(1)-Ga(1)	90.85(7)	C(20)-C(21)-C(22)	120.0(3)
C(59)-Sb(1)-Sb(2)	107.83(7)	C(21)-C(22)-C(23)	121.8(3)
Ga(1)-Sb(1)-Sb(2)	101.159(11)	C(22)-C(23)-C(18)	117.4(3)
Ga(2)-Sb(2)-Sb(1)	91.131(11)	C(22)-C(23)-C(27)	119.5(3)
N(2)-Ga(1)-N(1)	95.51(9)	C(18)-C(23)-C(27)	123.1(3)
N(2)-Ga(1)-Cl(1)	101.96(7)	C(19)-C(24)-C(25)	110.6(3)
N(1)-Ga(1)-Cl(1)	100.88(7)	C(19)-C(24)-C(26)	112.0(3)
N(2)-Ga(1)-Sb(1)	121.52(7)	C(25)-C(24)-C(26)	110.0(3)
N(1)-Ga(1)-Sb(1)	113.11(7)	C(23)-C(27)-C(29)	111.8(3)
Cl(1)-Ga(1)-Sb(1)	119.57(2)	C(23)-C(27)-C(28)	111.0(3)
N(3)-Ga(2)-N(4)	93.19(10)	C(29)-C(27)-C(28)	109.9(3)
N(3)-Ga(2)-Cl(2)	100.39(7)	N(3)-C(30)-C(31)	123.3(3)
N(4)-Ga(2)-Cl(2)	98.63(8)	N(3)-C(30)-C(33)	119.9(3)
N(3)-Ga(2)-Sb(2)	116.21(7)	C(31)-C(30)-C(33)	116.8(3)
N(4)-Ga(2)-Sb(2)	121.19(8)	C(32)-C(31)-C(30)	128.2(3)
Cl(2)-Ga(2)-Sb(2)	121.74(2)	N(4)-C(32)-C(31)	123.9(3)
C(1)-N(1)-C(6)	118.7(2)	N(4)-C(32)-C(34)	119.1(3)
C(1)-N(1)-Ga(1)	119.73(18)	C(31)-C(32)-C(34)	116.9(3)
C(6)-N(1)-Ga(1)	121.46(17)	C(36)-C(35)-C(40)	121.6(3)
C(3)-N(2)-C(18)	119.4(2)	C(36)-C(35)-N(3)	118.2(3)
C(3)-N(2)-Ga(1)	119.67(18)	C(40)-C(35)-N(3)	120.2(3)
C(18)-N(2)-Ga(1)	120.97(17)	C(37)-C(36)-C(35)	117.9(3)
C(30)-N(3)-C(35)	120.5(2)	C(37)-C(36)-C(41)	120.2(3)
C(30)-N(3)-Ga(2)	120.7(2)	C(35)-C(36)-C(41)	121.9(3)
C(35)-N(3)-Ga(2)	118.46(18)	C(38)-C(37)-C(36)	121.5(3)
C(32)-N(4)-C(47)	118.4(3)	C(37)-C(38)-C(39)	120.1(3)
C(32)-N(4)-Ga(2)	120.5(2)	C(38)-C(39)-C(40)	121.3(3)
C(47)-N(4)-Ga(2)	120.92(19)	C(35)-C(40)-C(39)	117.6(3)
C(59)-N(5)-C(60)	109.8(2)	C(35)-C(40)-C(44)	122.3(3)
C(59)-N(5)-C(62)	125.0(2)	C(39)-C(40)-C(44)	120.0(3)
C(60)-N(5)-C(62)	125.1(2)	C(36)-C(41)-C(42)	113.6(3)
C(59)-N(6)-C(61)	110.7(2)	C(36)-C(41)-C(43)	110.2(3)
C(59)-N(6)-C(64)	124.6(2)	C(42)-C(41)-C(43)	110.2(3)
C(61)-N(6)-C(64)	124.8(2)	C(40)-C(44)-C(46)	110.4(3)
N(1)-C(1)-C(2)	123.2(3)	C(40)-C(44)-C(45)	111.8(3)
N(1)-C(1)-C(4)	120.3(3)	C(46)-C(44)-C(45)	110.7(3)
C(2)-C(1)-C(4)	116.5(2)	C(48)-C(47)-C(52)	121.4(3)
C(3)-C(2)-C(1)	128.6(3)	C(48)-C(47)-N(4)	120.2(3)

N(2)-C(3)-C(2)	123.9(3)
N(2)-C(3)-C(5)	119.0(3)
C(2)-C(3)-C(5)	117.1(2)
C(11)-C(6)-C(7)	120.9(3)
C(11)-C(6)-N(1)	120.7(2)
C(7)-C(6)-N(1)	118.4(2)
C(8)-C(7)-C(6)	118.2(3)
C(8)-C(7)-C(12)	120.2(3)
C(6)-C(7)-C(12)	121.5(3)
C(9)-C(8)-C(7)	121.5(3)
C(8)-C(9)-C(10)	119.9(3)
C(9)-C(10)-C(11)	121.0(3)
C(10)-C(11)-C(6)	118.4(3)
C(10)-C(11)-C(15)	118.8(3)
C(6)-C(11)-C(15)	122.8(3)
C(13)-C(12)-C(7)	112.2(3)
C(13)-C(12)-C(14)	109.6(3)
C(7)-C(12)-C(14)	112.0(3)
C(11)-C(15)-C(17)	112.2(3)
C(11)-C(15)-C(16)	111.3(2)
C(17)-C(15)-C(16)	109.7(3)
C(23)-C(18)-C(19)	121.8(3)
C(23)-C(18)-N(2)	120.3(2)
C(19)-C(18)-N(2)	117.8(2)
C(20)-C(19)-C(18)	117.7(3)
C(20)-C(19)-C(24)	119.4(3)
C(18)-C(19)-C(24)	122.9(3)
C(21)-C(20)-C(19)	121.3(3)
C(52)-C(47)-N(4)	118.4(3)
C(49)-C(48)-C(47)	117.9(4)
C(49)-C(48)-C(53)	119.6(3)
C(47)-C(48)-C(53)	122.5(3)
C(50)-C(49)-C(48)	121.6(4)
C(49)-C(50)-C(51)	120.0(4)
C(50)-C(51)-C(52)	121.4(4)
C(51)-C(52)-C(47)	117.6(3)
C(51)-C(52)-C(56)	121.4(3)
C(47)-C(52)-C(56)	121.0(3)
C(48)-C(53)-C(54)	109.2(3)
C(48)-C(53)-C(55)	113.1(3)
C(54)-C(53)-C(55)	108.7(3)
C(52)-C(56)-C(57)	113.0(3)
C(52)-C(56)-C(58)	112.4(3)
C(57)-C(56)-C(58)	110.8(3)
N(6)-C(59)-N(5)	105.7(2)
N(6)-C(59)-Sb(1)	121.3(2)
N(5)-C(59)-Sb(1)	132.4(2)
C(61)-C(60)-N(5)	107.0(3)
C(61)-C(60)-C(66)	129.8(3)
N(5)-C(60)-C(66)	123.2(3)
C(60)-C(61)-N(6)	106.8(3)
C(60)-C(61)-C(67)	129.9(3)
N(6)-C(61)-C(67)	123.2(3)
N(5)-C(62)-C(63)	112.7(3)
N(6)-C(64)-C(65)	112.5(2)

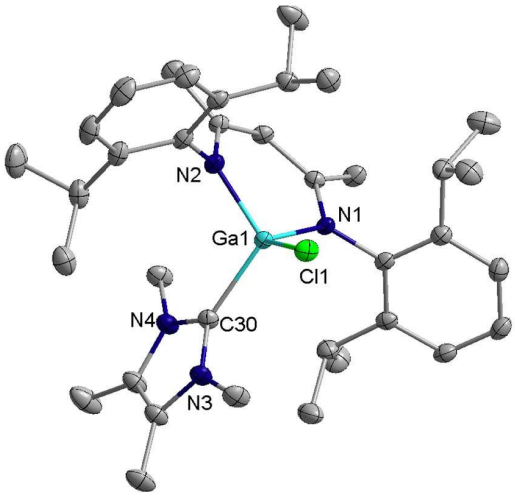

Figure S43. Solid state structure of L[1](Cl)Ga–[Me]NHC[Me]. Hydrogen atoms are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S13. Bond lengths [Å] for L[1](Cl)Ga–[Me]NHC[Me].

Ga(1)-N(1)	1.8830(9)	C(6)-C(7)	1.4082(16)	C(21)-C(22)	1.378(2)
Ga(1)-N(2)	1.8882(9)	C(6)-C(11)	1.4104(15)	C(22)-C(23)	1.3998(17)
Ga(1)-C(30)	2.0428(11)	C(7)-C(8)	1.3969(16)	C(23)-C(27)	1.5171(18)
Ga(1)-Cl(1)	2.2074(3)	C(7)-C(12)	1.5222(16)	C(24)-C(25)	1.5264(17)
N(1)-C(1)	1.3978(14)	C(8)-C(9)	1.3852(18)	C(24)-C(26)	1.5309(17)
N(1)-C(6)	1.4344(14)	C(9)-C(10)	1.3830(18)	C(27)-C(29)	1.5320(19)
N(2)-C(3)	1.3958(14)	C(10)-C(11)	1.3954(16)	C(27)-C(28)	1.5354(18)
N(2)-C(18)	1.4363(14)	C(11)-C(15)	1.5157(17)	C(31)-C(32)	1.3528(17)
N(3)-C(30)	1.3540(14)	C(12)-C(14)	1.5310(18)	C(31)-C(34)	1.4924(17)
N(3)-C(31)	1.3872(15)	C(12)-C(13)	1.5391(19)	C(32)-C(35)	1.4884(18)
N(3)-C(33)	1.4646(15)	C(15)-C(17)	1.5327(18)	C11-C21	1.382(7)
N(4)-C(30)	1.3529(15)	C(15)-C(16)	1.5330(18)	C11-C61	1.392(6)
N(4)-C(32)	1.3898(15)	C(18)-C(23)	1.4095(16)	C11-C71	1.497(7)
N(4)-C(36)	1.4652(14)	C(18)-C(19)	1.4123(16)	C21-C31	1.399(8)
C(1)-C(4)	1.3955(16)	C(19)-C(20)	1.3960(17)	C31-C41	1.366(8)
C(1)-C(2)	1.4365(16)	C(19)-C(24)	1.5207(16)	C41-C51	1.377(7)
C(2)-C(3)	1.3854(16)	C(20)-C(21)	1.386(2)	C51-C61	1.382(6)
C(3)-C(5)	1.4736(16)				

Table S14. Bond angles [°] for L[1](Cl)Ga–[Me]NHC[Me].

N(1)-Ga(1)-N(2)	102.69(4)	C(14)-C(12)-C(13)	110.35(11)
N(1)-Ga(1)-C(30)	113.12(4)	C(11)-C(15)-C(17)	110.48(11)
N(2)-Ga(1)-C(30)	111.83(4)	C(11)-C(15)-C(16)	111.92(10)
N(1)-Ga(1)-Cl(1)	112.23(3)	C(17)-C(15)-C(16)	110.38(11)
N(2)-Ga(1)-Cl(1)	109.39(3)	C(23)-C(18)-C(19)	120.56(10)
C(30)-Ga(1)-Cl(1)	107.55(3)	C(23)-C(18)-N(2)	120.12(10)
C(1)-N(1)-C(6)	116.69(9)	C(19)-C(18)-N(2)	119.32(10)
C(1)-N(1)-Ga(1)	119.76(7)	C(20)-C(19)-C(18)	118.50(11)
C(6)-N(1)-Ga(1)	123.55(7)	C(20)-C(19)-C(24)	119.89(11)
C(3)-N(2)-C(18)	118.31(9)	C(18)-C(19)-C(24)	121.60(10)

C(3)-N(2)-Ga(1)	118.90(7)	C(21)-C(20)-C(19)	121.21(12)
C(18)-N(2)-Ga(1)	121.59(7)	C(22)-C(21)-C(20)	119.94(12)
C(30)-N(3)-C(31)	111.16(10)	C(21)-C(22)-C(23)	121.20(12)
C(30)-N(3)-C(33)	127.07(10)	C(22)-C(23)-C(18)	118.58(12)
C(31)-N(3)-C(33)	121.72(10)	C(22)-C(23)-C(27)	119.75(11)
C(30)-N(4)-C(32)	111.21(10)	C(18)-C(23)-C(27)	121.67(11)
C(30)-N(4)-C(36)	125.92(10)	C(19)-C(24)-C(25)	111.58(11)
C(32)-N(4)-C(36)	122.81(10)	C(19)-C(24)-C(26)	112.86(10)
C(4)-C(1)-N(1)	120.76(10)	C(25)-C(24)-C(26)	109.65(10)
C(4)-C(1)-C(2)	118.50(10)	C(23)-C(27)-C(29)	111.52(10)
N(1)-C(1)-C(2)	120.73(10)	C(23)-C(27)-C(28)	112.14(12)
C(3)-C(2)-C(1)	131.41(10)	C(29)-C(27)-C(28)	110.02(11)
C(2)-C(3)-N(2)	122.99(10)	N(4)-C(30)-N(3)	104.61(10)
C(2)-C(3)-C(5)	118.87(10)	N(4)-C(30)-Ga(1)	122.77(8)
N(2)-C(3)-C(5)	118.08(10)	N(3)-C(30)-Ga(1)	132.61(8)
C(7)-C(6)-C(11)	119.88(10)	C(32)-C(31)-N(3)	106.63(10)
C(7)-C(6)-N(1)	119.74(10)	C(32)-C(31)-C(34)	130.83(12)
C(11)-C(6)-N(1)	120.32(10)	N(3)-C(31)-C(34)	122.52(11)
C(8)-C(7)-C(6)	119.00(11)	C(31)-C(32)-N(4)	106.39(10)
C(8)-C(7)-C(12)	118.48(11)	C(31)-C(32)-C(35)	130.40(12)
C(6)-C(7)-C(12)	122.45(10)	N(4)-C(32)-C(35)	123.21(11)
C(9)-C(8)-C(7)	121.34(12)	C21-C11-C61	116.6(5)
C(10)-C(9)-C(8)	119.36(11)	C21-C11-C71	122.4(5)
C(9)-C(10)-C(11)	121.35(11)	C61-C11-C71	121.0(4)
C(10)-C(11)-C(6)	119.06(11)	C11-C21-C31	122.0(6)
C(10)-C(11)-C(15)	118.96(10)	C41-C31-C21	119.8(4)
C(6)-C(11)-C(15)	121.98(10)	C31-C41-C51	119.4(6)
C(7)-C(12)-C(14)	112.11(11)	C41-C51-C61	120.4(5)
C(7)-C(12)-C(13)	110.03(10)	C51-C61-C11	121.7(4)

D) Quantum Chemical Calculations

Computational Details

All quantum chemical calculations were employed with the ORCA quantum chemistry package (version 4.12).[1] The geometry optimization for ^{Me}NHC^{Me}, ^{Et}NHC^{Me}, $^{i\text{Pr}}$NHC^{Me}, ^{Dipp}NHC^{H}, ^{Me}cAAC, ^{Cy}cAAC and DAC were calculated with B3LYP functional by using def2-TZVPP basis set[2] and atom-pairwise dispersion correction with Becke-Johnson damping Scheme (D3BJ).[3] Natural bond orbital analysis was performed using the NBO version 6.0.[4]

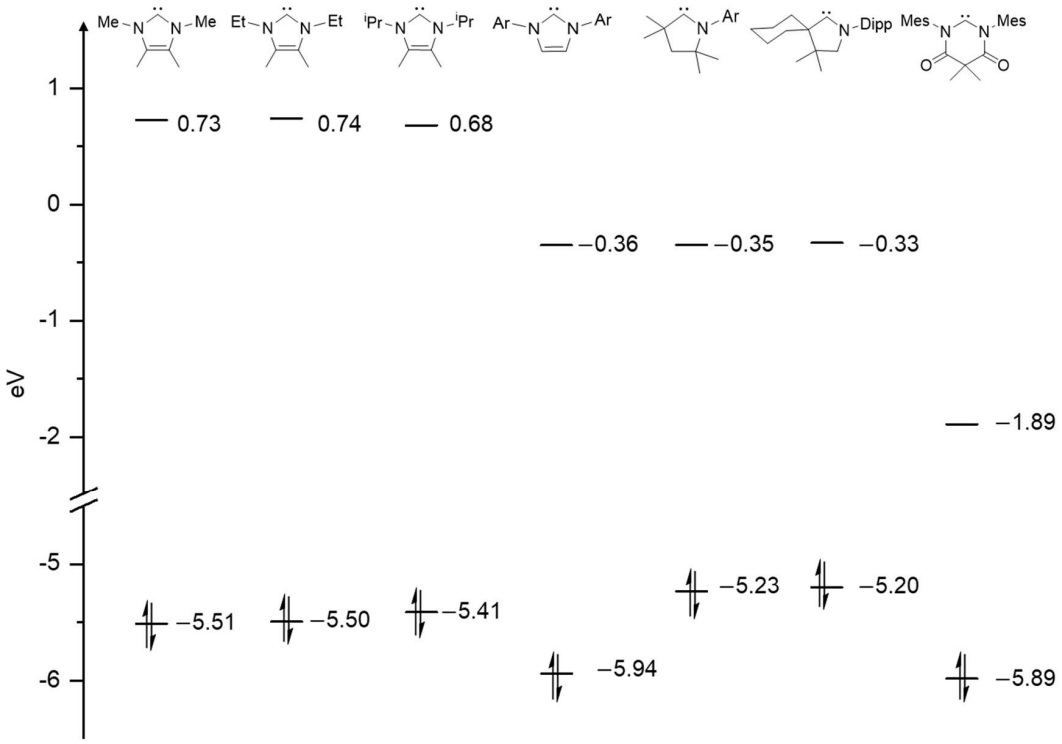

Figure S44. Energy of frontier orbitals (eV) of N-heterocyclic carbenes (^{Me}NHC^{Me}, ^{Et}NHC^{Me}, $^{i\text{Pr}}$NHC^{Me} and ^{Dipp}NHC^{H}), diamidocarbene (DAC) and cyclic alkyl amino carbene (^{Me}cAAC) at B3LYP-D3BJ/def2-TZVPP level of theory.

Table S15. Selected bond lengths [Å] and angles [°] of **1a-c** of the XRD structure and the optimized geometry (B3LYP-D3BJ/def2-TZVPP).

	1a(XRD)	1a(Opt)	1b (XRD)	1b (Opt)	1c (XRD)	1c (Opt)
Ga(1)-Sb(1)	2.5523(2)	2.572	2.5380(5)	2.594	2.5528(4)	2.604
Sb(1)-C(	2.184(2)	2.199	2.183(4)	2.168	2.194(3)	2.182
Ga(1)-Cl(1)	2.2773(5)	2.288	2.2700(10)	2.277	2.2561(8)	2.274
Ga(1)-Sb(1)-C	92.22(5)	87.2	90.73(10)	98.8	94.82(7)	104.6

Table S16. Selected bond lengths [Å] and angles [°] of **2a** and **b** of the XRD structure and the optimized geometry (B3LYP-D3BJ/def2-TZVPP).

	2a (XRD)	2a (Opt)	2b (XRD)	2b (Opt)
Ga(1)-Sb(1)	2.6093(9)	2.618	2.6103(4)	2.628
Ga(2)-Sb(2)	2.5457(9)	2.561	2.5541(4)	2.576
Sb(1)-C(	2.225(5)	2.250	2.245(3)	2.265
Sb(1)-Sb(2)	2.7461(8)	2.765	2.7385(4)	2.765
Ga(1)-Cl(1)	2.2353(15)	2.259	2.2426(7)	2.264
Ga(2)-Cl(2)	2.2656(15)	2.298	2.2599(8)	2.265
Ga(1)-Sb(1)-C	91.44(12)	97.0	90.85(7)	99.0

Table S17. Mayer bond order of **1a**-**2b** and **5** (B3LYP-D3BJ/def2-TZVPP).

X-Y	1a	1b	1c	2a	2b	5
Sb(1)-Ga(1)	1.08	1.06	1.08	0.88	0.91	0.92
Sb(1)-C	0.88	1.00	0.99	0.84	0.82	-
Ga(1)-Cl(1)	0.70	0.73	0.74	0.75	0.78	0.84
Sb(1)-Sb(2)	-	-	-	1.21	1.23	1.92
Sb(2)-Ga(2)	-	-	-	1.11	1.12	0.95
Ga(2)-Cl(2)	-	-	-	0.67	0.66	0.84

Table S18. Wiberg bond index of **1a**-**2b** and **5** (B3LYP-D3BJ/def2-TZVPP).

X-Y	1a	1b	1c	2a	2b	5
Sb(1)-Ga(1)	1.12	1.07	1.07	0.87	0.92	0.95
Sb(1)-C	0.84	0.98	0.69	0.67	0.56	-
Ga(1)-Cl(1)	0.58	0.60	0.60	0.62	0.62	0.65
Sb(1)-Sb(2)	-	-	-	1.08	1.11	1.87
Sb(2)-Ga(2)	-	-	-	1.06	1.12	0.94
Ga(2)-Cl(2)	-	-	-	0.57	0.57	0.66

Table S19. Natural Charge of **1a**-**2b** and **5** (B3LYP-D3BJ/def2-TZVPP).

X	1a	1b	1c	2a	2b	5
Sb(1)	-0.30	-0.23	-0.23	0.16	0.14	-0.06
Ga(1)	1.15	1.15	1.15	1.25	1.25	1.20
C	0.19	0.16	0.17	0.16	0.16	-
Cl(1)	-0.60	-0.58	-0.58	-0.58	-0.58	-0.56
Sb(2)	-	-	-	-0.58	-0.57	-0.13
Ga(2)	-	-	-	1.16	1.15	1.22
Cl(2)	-	-	-	-0.59	-0.59	-0.56

Table S20. Bond polarization P(X; Y) of **1a**-**2b** and **5** in % (B3LYP-D3BJ/def2-TZVPP).

X-Y	1a	1b	1c	2a	2b	5
Sb(1)-Ga(1)	55; 45	58; 42	57; 43	60; 40	60; 40	59; 41
Sb(1)-C	26; 74	26; 74	26; 74	26; 74	25; 75	-
Sb(1)-Sb(2)	-			56; 44	57; 43	50; 50
Sb(2)-Ga(2)	-			58; 42	58; 42	49; 51

Table S21. Summary of computed energy and free energy values of the compounds **1a-7**, the carbenes $^{Me}NHC^{Me}$, $^{Et}NHC^{Me}$, $^{iPr}NHC^{Me}$, $^{Dipp}NHC^{H}$ and $LGaCl_2$ in kJ/mol at different level of theories.

	B3LYP-D3/def2-SVP	B3LYP-D3/def2-SVP ZPV+Temp corrections	B3LYP-D3/def2-TZVPP	DLPNO-CCSD(T1)/cc-pVTZ energies on B3LYP-D3/def2-TZVPP geometries
1a	-4245.706627	0.74793781	-4247.889849	-4242.630253
1b	-4324.237254	0.80282689	-4326.504661	
1c	-4402.757145	0.85661891	-4405.113238	-4399.595877
1d	-5021.331591	1.11945932	-5024.341791	-5017.769291
2a	-8108.478893	1.35131679	-8112.419783	-8102.518092
2b	-8187.01115	1.40678541	-8191.037933	-8181.007342
2c	-8265.53141	1.46244435	-8269.643841	-8259.482948
2d	-8884.066066	1.72293307	-8888.845203	-8877.634856
3	-7945.234671	1.17950886	-7948.906196	-7939.995416
4a	-8328.22706	1.35810151	-8332.309796	
4b	-8406.738812	1.41393561	-8410.907525	
4c	-8485.232438	1.47017722	-8489.486449	
4d	-9103.809543	1.72160032	-9108.716534	
5	-7725.468466	1.17540822	-7728.988151	-7719.709917
6a	-8491.447217	1.52374529	-8495.793696	
6b	-8648.509532	1.6356609	-8653.044112	
6c	-8805.561731	1.7441704	-8810.268497	
6d	-10042.60288	2.259560362		
7	-3862.643707	0.57326041	-3864.407932	-3859.769029
$^{Me}NHC^{Me}$	-382.9426574	0.14723277	-383.368625	-382.7478731
$^{Et}NHC^{Me}$	-461.4708067	0.20126835	-461.9830253	-461.2334232
$^{iPr}NHC^{Me}$	-539.9980162	0.25370558	-540.5962611	-539.7187798
$^{Dipp}NHC^{H}$	-1158.573435	0.51377124	-1159.834562	-1157.90539
$LGaCl_2$	-4082.498997	0.57481469	-4084.411894	-4080.149647

Table S22. Energy values of the educts, products and the resulting reaction energies ΔG of all discussed reactions in kJ/mol at the B3LYP-D3BJ/def2-TZVPP level of theory.

Reaction	B3LYP-D3/def2-TZVPP + B3LYP-D3/def2-SVP free energy corection		
	Educts	Products	ΔG [kJ/mol]
3→4a	-8330.94808	-8330.95169	-9
3→4b	-8409.50844	-8409.49359	39
3→4c	-8488.06924	-8488.01627	139
3→4d	-9107.04748	-9106.99493	138
3→5	-15895.4534	-15895.4869	-88
4a→1a	-8330.95169	-8330.97899	-72
4b→1b	-8409.49359	-8409.53891	-119
4c→1c	-8488.01627	-8488.0937	-203
4d→1d	-9106.99493	-9107.05941	-169
4a→5	-16661.9034	-16661.9297	-69
4b→5	-16818.9872	-16819.0504	-166
4c→5	-16976.0325	-16976.172	-366
4d→5	-18213.9899	-18214.1285	-364
5→1a	-8494.25553	-8494.28382	-74
5→1b	-8651.37626	-8651.40367	-72
5→1c	-8808.49785	-8808.51324	-40
5→1d	-10046.4543	-10046.4447	25
5→2a	-8111.03414	-8111.06847	-90
5→2b	-8189.5945	-8189.63115	-96
5→2c	-8268.1553	-8268.1814	-69
5→2d	-8887.13353	-8887.12227	30
1a→2a	-8494.28382	-8494.28986	-16
1b→2b	-8651.40367	-8651.4129	-24
1c→2c	-8808.51324	-8808.52395	-28
1d→2d	-10046.4447	-10046.4431	4
2a→6a	-8494.28986	-8494.26995	52
2b→6b	-8651.4129	-8651.40845	12
2c→6c	-8808.52395	-8808.52433	-1
2d→6d	-	-	-
6a→1a	-8494.26995	-8494.28382	-36
6b→1b	-8651.40845	-8651.40367	13
6c→1c	-8808.52433	-8808.51324	29
6d→1d	-	-	-
3→7	-7947.72669	-7947.67175	144
7→5	-7727.66934	-7727.81274	-376
7→1a	-4247.05606	-4247.14191	-225
7→1b	-4325.61643	-4325.70183	-224
7→1c	-4404.17723	-4404.25662	-208
7→1d	-5023.15546	-5023.22233	-176

Table S23. Energy values of the educts, products and the resulting reaction energies ΔG of selected reactions in kJ/mol at the DLPNO-CCSD(T1)/cc-pVTZ level of theory.

Reaction	DLPNO-CCSD(T1)/cc-pVTZ energies on B3LYP-D3/def2-TZVPP geometries + B3LYP-D3/def2-SVP free energy corection		
	Educts	Products	ΔG [kJ/mol]
3→5	-15877.6318	-15877.6842	-137
5→1a	-8483.73579	-8483.76463	-76
5→1c	-8797.46	-8797.48	-36
5→1d	-10033.3177	-10033.2997	47
5→2a	-8101.13515	-8101.16678	-83
5→2b	-8179.56666	-8179.60056	-89
5→2c	-8257.99958	-8258.0205	-55
5→2d	-8875.92613	-8875.91192	37
1a→2a	-8483.76463	-8483.76742	-7
1c→2c	-8797.48	-8797.49	-19
1d→2d	-10033.2997	-10033.3035	-10
3→7	-7938.81591	-7938.77060	119
7→5	-7718.39154	-7718.53451	-375
7→1a	-4241.79641	-4241.88231	-226
7→1c	-4398.66084	-4398.73926	-206
7→1d	-5016.58739	-5016.64983	-164

In Table S22, we also report the DLPNO-CCSD(T1)/cc-pVTZ single point energies for the B3LYP-D3/def2-TZVPP geometries along with the B3LYP-D3 energies and enthalpies. While the agreement is not perfect, presumably because of subtle electron correlation effects and sizeable dispersion contribution, except for a few outliers the results agree within 10-20 kJ/mol. Furthermore, practically all trends are preserved at the higher level of theory, such that the conclusions are supported also by higher level methods.

Table S24. Compound **1a** – B3LYP-D3/def2-SVP
Electronic energy ... -4245.70662701 Eh
Final Gibbs free energy ... -4244.95868919 Eh
Gibbs free energy minus the electronic energy ... 0.74793781 Eh

Sb	9.59756652557791	0.83229243669902	4.28610361821223
Ga	11.63791247191916	2.38485424257423	4.52885813026563
Cl	13.54009793769461	1.98419265971191	3.31351926131084
N	10.84154702888384	0.24322860327421	1.36518797165725
N	9.25925440921666	1.69901224192789	1.19844658587314
N	12.36050341899545	2.49389702871826	6.37662993096709
N	11.58326910379082	4.38409768100061	4.28798314650130
C	11.68679324426144	0.02913871642583	-1.00703646334317
C	9.23461864743862	2.26592653979790	-1.25977693652997
C	11.80143722144496	-0.70871195340839	1.90272886950827
C	8.19634267118477	2.63450304869648	1.52271062756174
C	10.75823904081857	0.58259942610965	0.01709220084674
C	9.74992376611083	1.50398460220617	-0.08908799357053
C	9.93369952163701	0.93740967286018	2.10019962487598
C	10.30455232939839	3.62556889093034	9.33676821234740
C	8.56486123463472	2.37764061062668	7.98711495774014
C	10.05048174483358	2.74058669644861	8.10547967599240
C	15.39881820256707	-0.19708096746521	7.09566191120687
C	13.79396477285354	-0.97548497934354	5.29804593776483
C	14.08947036663124	0.10374632770310	6.35148164788153
C	10.94776110903403	1.50966444125253	8.11464430816339
C	10.66705743982185	0.44854220404955	8.98516995578453
C	11.47719467154858	-0.68475423969602	9.02433030504350
C	12.58161187626873	-0.77320142303821	8.17982842359552
C	12.90498281373563	0.26235224479062	7.29262592072599
C	12.08561461123256	1.41336292668682	7.27836701418262
C	7.37636661889219	4.65683500079869	5.19109159171437
C	9.28409618793605	5.98546578500514	6.17083955818890
C	8.88339655224263	4.92522507647546	5.13203216794046
C	12.42617306016805	3.67209844444435	0.53371375129647
C	13.26135667282187	6.03295073189264	0.85263387305714
C	12.51861586970604	4.85721653212272	1.50597975252540
C	9.37185267156994	5.27457509558577	3.73136693665773
C	8.52471400991652	5.91447688513500	2.81793035968185
C	8.95284046112754	6.22038378397601	1.52578446772491
C	10.23802425051020	5.86520430512051	1.12456803155856
C	11.13259828076380	5.23963228535269	2.00731678154775
C	10.69712906479859	4.97060191110736	3.32660131821484
C	13.95159916881723	3.38348382803417	8.01463649328079
C	12.58848455084091	6.61064264510636	4.56108645949275
C	13.14436386827686	3.50723045213680	6.74454468620957
C	13.25111695245619	4.70843505734180	6.01887349297837
C	12.45111790260822	5.15521091266262	4.94820993170913
H	12.73584335061017	0.25992071275817	-0.75776919414856
H	11.60121657735307	-1.06680939974748	-1.09537659760742
H	11.47112208605516	0.46275949515758	-1.99294555832824
H	8.15805723516021	2.09232764355817	-1.42320275826564
H	9.37597883966512	3.35094267113007	-1.11956251814639
H	9.76656414962642	1.97122586292084	-2.17440149815007
H	12.80138275592518	-0.25551091157492	1.94480907518175
H	11.48848915654999	-0.95112935262080	2.92735455067231
H	11.80972296945251	-1.61647234639547	1.28286765660150
H	7.25091018709715	2.31878270632071	1.05557115541303
H	8.08548656821575	2.64296437298067	2.61548111323761
H	8.46245391350576	3.64204634601494	1.17816984265016
H	9.66819941065118	4.52522350371451	9.30867159242097
H	10.08114869666947	3.08074942806371	10.26896836765444
H	11.35185487956237	3.95922410063502	9.38587457452604
H	8.36953656090738	1.78955564549428	7.07711447941512
H	8.21249565337721	1.79746729224599	8.85485859358443
H	7.95321970960472	3.29149828799019	7.93579230620259
H	10.31527416757083	3.33323287690566	7.21973467949823
H	16.24332522373041	-0.22111381731306	6.38792029089249
H	15.61944732307709	0.56471955707249	7.86053576617791
H	15.36604948892646	-1.17488733271811	7.60364252541216
H	14.59487984406338	-1.00518171576963	4.54237858969874
H	13.71549188743376	-1.97251333273164	5.76325061340974
H	12.84516143810380	-0.76359380737962	4.78501310730891
H	14.22045953014286	1.04841488347216	5.80773571681181
H	9.79702260556890	0.50984869783949	9.64279488004364
H	11.24134885459832	-1.50386389649434	9.70854268783067
H	13.20466217679349	-1.67052283393435	8.20234471303167

H	7.07820140076771	3.89700210179311	4.45311756935472
H	7.10333932319373	4.27558821630304	6.18553163871661
H	6.78186465266776	5.56879329028470	5.01748084529931
H	8.87450153444778	6.97386607705617	5.90318637300266
H	8.89038360609653	5.71468453950108	7.16376546900002
H	10.37428541947528	6.08053751959647	6.26639287525211
H	9.38185335199897	3.98287246546058	5.40230528696699
H	13.43194486860143	3.35236062714988	0.21815463597133
H	11.94679412222236	2.81241979766764	1.01512298956298
H	11.84899678677038	3.93902209974394	-0.36777727860295
H	12.78197584144574	6.34827075905839	-0.08851817426089
H	13.30327443426523	6.91457647296448	1.51126195357471
H	14.29599461061076	5.74071929448526	0.61132683237485
H	13.10934269687613	4.50913174187129	2.36311600129958
H	7.50837722697889	6.17221054849434	3.11797088052182
H	8.27776446559457	6.72350737125251	0.82849410168137
H	10.56425881850997	6.08719964323275	0.10569976452633
H	14.68575100388305	2.56951525242160	7.91335437560689
H	14.48398945070008	4.31566986374355	8.24079548082198
H	13.31106626813794	3.11916144984561	8.86790863075287
H	11.60458331662101	7.09459313473068	4.48301774420089
H	13.19898481375124	7.15601657703240	5.29132462795287
H	13.06292357854429	6.69946640382668	3.57311874338699
H	13.95293084284982	5.43893300305025	6.41765338166047

Table S25. Compound **1a** – B3LYP-D3/def2-TZVPP
final energy -4247.889848684893 Eh
DLPNO-CCSD(T)/cc-pVTZ single point energy -4242.630252612294 Eh

Sb	9.56573626872307	0.87244014727605	4.26627911284787
Ga	11.62029896713680	2.39998660411950	4.51712083913663
Cl	13.48201791893718	1.94961025942763	3.26494294183110
N	10.80861070745592	0.19818810789186	1.38200243245019
N	9.28050197193813	1.69203381096490	1.17875939513498
N	12.35122774073101	2.49226529902145	6.36212166606462
N	11.58080322604723	4.40001239333860	4.29083829246788
C	11.65054649851988	-0.09421377577172	-0.97598239508705
C	9.28388103460924	2.20066403644290	-1.28754998860817
C	11.72674951640174	-0.78253408847823	1.93793912547575
C	8.24775193714168	2.66860072897825	1.47769773362591
C	10.74240290645439	0.51289083841438	0.03021461252070
C	9.77105582375504	1.45587707393479	-0.09908742820497
C	9.92225491684307	0.93042617178883	2.09722445207672
C	10.32855452862932	3.60768138832719	9.31049918828284
C	8.56651755532813	2.35474633452421	8.00970159678598
C	10.05157073869824	2.71844199086738	8.09003090723453
C	15.39499871004805	-0.14788121978263	7.09862803024588
C	13.82921778045232	-0.98681563644794	5.30739224966057
C	14.08967836119749	0.11833483292662	6.33919447298336
C	10.94847439912403	1.49322565041814	8.08942330921156
C	10.67447041169226	0.43386393654656	8.95132486962766
C	11.48556992994733	-0.68941684177018	8.98626101368051
C	12.58391757322521	-0.76887166163981	8.14629040795422
C	12.90040792093422	0.26595502279571	7.26806500163102
C	12.07979723433439	1.40498674318576	7.25747379686955
C	7.39020485309388	4.65503440313172	5.18932072769717
C	9.26540051440532	6.01693438005114	6.16856758170068
C	8.89071258995734	4.94559001551794	5.13571563863464
C	12.40379079664032	3.75746196168369	0.50794712319501
C	13.25916169450725	6.08965889907040	0.90088323697923
C	12.50876951844317	4.90403335549552	1.52107138746530
C	9.37955019988839	5.30235309378017	3.74245884031528
C	8.53917413672089	5.95272116672687	2.84261089201640
C	8.96642126413480	6.27375925747792	1.56227445778139
C	10.24282994719042	5.92153755032293	1.15905673085314
C	11.12969879040827	5.28376495783659	2.02848568785105
C	10.69636283862647	5.00149965173859	3.33624455919124
C	13.94471899618908	3.37435538374486	7.99613088970881
C	12.59216630618358	6.61450879445035	4.59626732995055
C	13.12775381557145	3.50039835613455	6.73604196290948
C	13.23295277548362	4.70143049951285	6.02462260660049
C	12.44274428550580	5.15778207242252	4.96092492583360
H	12.69597648931610	0.10929421362123	-0.73548436401760
H	11.53044337113525	-1.17800701480304	-1.03277664443878
H	11.44750368080861	0.31590188522298	-1.96284047808891
H	8.21281420474800	2.05835487013258	-1.44458346118837
H	9.46100652190991	3.27315368173174	-1.18099350522344
H	9.80100046407163	1.86286359764525	-2.18289406581850
H	12.74449332616988	-0.40034197326935	1.91051397318080
H	11.44156271650769	-0.94823119578502	2.97357923552946

H	11.65193329741815	-1.71234030486233	1.37609352494563
H	7.31505089932386	2.39248971476005	0.98639903933467
H	8.10636180659365	2.67723260955186	2.55514252085966
H	8.56086192920349	3.65564367688618	1.14726332276893
H	9.69061426731412	4.49309871498923	9.29262429853535
H	10.13161915403454	3.06664346977194	10.23799768839479
H	11.36466473825986	3.94392939617378	9.33289376699693
H	8.35457457078927	1.75471520781075	7.12475513863341
H	8.23726067268926	1.79728157596013	8.88743350094409
H	7.96317687821171	3.26106759994887	7.95472132895882
H	10.29357161301277	3.30257185092946	7.20517088277147
H	16.23716743777938	-0.15720868523229	6.40468506081279
H	15.58665598627541	0.61532804115170	7.85385493285863
H	15.37371071850773	-1.11398874042552	7.60581503544134
H	14.63581050299742	-1.01710723068675	4.57376171594682
H	13.76389584866279	-1.96372172226069	5.79101834190790
H	12.89405721713227	-0.80597956582026	4.78071856147581
H	14.20678447027950	1.04785348872191	5.78736704835128
H	9.81367062618052	0.48743598797311	9.60358600629534
H	11.25623280858535	-1.50386536897966	9.66071990218069
H	13.20557728990778	-1.65397456702985	8.16685615248187
H	7.11117302284227	3.89073098957031	4.46462585015040
H	7.12400900192753	4.28290333464275	6.17747234873417
H	6.79017563229649	5.54816343718390	5.00658037554428
H	8.82746539806170	6.98136832430274	5.90274412957738
H	8.88990308843126	5.73699884237717	7.15408959576842
H	10.34288374609141	6.14368426916668	6.25081036317887
H	9.39751077112962	4.02222784219104	5.41151223575591
H	13.39728634305217	3.43667216761387	0.19232105060496
H	11.90581291971575	2.89793054232174	0.94638159564589
H	11.84659717976224	4.07121160618707	-0.37786028339134
H	12.78549281727370	6.42481161947567	-0.02333353923709
H	13.30277724216183	6.94514365380958	1.57502845073353
H	14.28188970661734	5.79712354150834	0.65861160490812
H	13.09111474307031	4.53077817559030	2.35965539157308
H	7.53290430582381	6.20620847835690	3.14186682162454
H	8.30001542344820	6.78372650170521	0.87880154378118
H	10.56651931280451	6.15459183227861	0.15345662374894
H	14.78091202672808	2.69616064108443	7.81774245570536
H	14.34110722209920	4.33841540249222	8.30264285064526
H	13.36187522517826	2.94880982553713	8.80965836068060
H	11.62465809737374	7.08647153511013	4.43845408597360
H	13.12745155886998	7.15206443320035	5.37390034998583
H	13.15072521612656	6.71036014894161	3.66561451299218
H	13.92386859002745	5.42248769512405	6.43065454989965

Table S26. Compound **1b** B3LYP-D3/def2-SVP

Electronic energy ... -4324.23725388 Eh

Final Gibbs free energy ... -4323.43442698 Eh

Gibbs free energy minus the electronic energy ... 0.80282689 Eh

Sb	6.63379460475540	12.29007807620315	1.26491985233481
Ga	6.47206370849812	13.08669714955781	3.70387671933588
Cl	5.66464450571803	15.19082974511257	4.13352722767435
N	8.01223474923358	13.11392395277580	4.99619789007046
N	5.33470188809197	11.95475808133811	4.87312729287422
N	6.85632711560358	15.44231165746168	0.57405217996609
N	8.81832081156088	14.54532261613915	0.57963720373658
C	7.77803672265645	13.01458039858777	6.30662430056727
C	6.54559930014687	12.60964665050581	6.85827897719361
H	6.48755349161150	12.62965927687216	7.94523819689978
C	5.44748506143355	12.02470818483943	6.20019759741545
C	8.89065925820451	13.32653719679227	7.28140291572913
H	9.82404160318162	12.82178951067679	6.99427995056869
H	8.61828667572817	13.02493233840774	8.30037141650950
H	9.10258778348214	14.40593925270225	7.28110677347899
C	4.36108339468773	11.41759243606515	7.05563000255771
H	3.38842123265170	11.87041511938574	6.81210694431221
H	4.56798498197873	11.56100341130520	8.12343669451260
H	4.25956551661704	10.34131956830870	6.85371268281339
C	9.34111347112566	13.36066017375119	4.51995406924305
C	10.11325246975986	12.25472920021262	4.07921454521335
C	11.43495670349288	12.48233377927028	3.67479852882173
H	12.04933238611968	11.64200664412322	3.35018643193216
C	11.97775826684153	13.76703116173843	3.66502774411870
H	13.01235510353499	13.92343402761350	3.34817168307085
C	11.18864570933213	14.84961548931996	4.04232159908603
H	11.60888730568053	15.85779678529039	4.01153512559180
C	9.86538003412991	14.67396390612659	4.47665566417935
C	9.52198686167326	10.85011475710569	4.04304460002551

H	8.46191905954146	10.96978325000397	3.77329570246101
C	10.15261669359218	9.96732325901635	2.96085012785362
H	10.11026706494674	10.45483778534554	1.97487497296149
H	9.60282322392759	9.01880642347354	2.88380197763598
H	11.20231490759154	9.71676025748834	3.18504051630181
C	9.58252411625143	10.15769902464058	5.41432290728622
H	9.16325523277439	9.14061644593387	5.34926307945130
H	9.00595222568832	10.70165634091718	6.17505736531680
H	10.62392636725723	10.07252479133202	5.76721433804877
C	9.04817957640976	15.90083210067959	4.85883615531653
H	8.09655464535259	15.56165371504810	5.28787702578399
C	8.69412332378564	16.71757488570902	3.60731344122967
H	9.60178566096384	17.09293093804476	3.10554457689443
H	8.06417707785539	17.58070753347228	3.87481477397509
H	8.12640786609749	16.10803212284610	2.89570849849150
C	9.75697243347030	16.78318970538810	5.89786408454014
H	10.66286941357863	17.25634374645383	5.48479956961938
H	10.06283534842999	16.20927173357906	6.78661038189673
H	9.08732201679338	17.59259333536628	6.23034120093684
C	4.33625795088069	11.12062897924177	4.26932820902536
C	4.65121022429140	9.76549710589354	4.01110179158962
C	3.67941652112346	8.95653833481844	3.40699697894919
H	3.90678853671045	7.90703078881305	3.20511522860104
C	2.43152113052772	9.46735169642279	3.05650531015721
H	1.68626835700758	8.82128169096154	2.58547821560128
C	2.14331909458769	10.80850839544300	3.29960788795728
H	1.17043737975344	11.21162823139210	3.00842430137063
C	3.08150194247852	11.65783507515041	3.90107622751313
C	6.00245705676858	9.16395144789676	4.37642238186169
H	6.63595467004314	9.97325771896764	4.76380951757426
C	6.70917964024190	8.57275448247902	3.14838749498676
H	6.11208968838346	7.77163663842283	2.68441443320134
H	7.67749860256627	8.13554186626171	3.43775390839145
H	6.89950414703606	9.34284257105729	2.38463309793691
C	5.87119508711445	8.11120951755632	5.48929203139285
H	5.27386992976247	7.24765887964966	5.15350464176063
H	5.38413714718800	8.52548804602841	6.38526045955117
H	6.86399034324638	7.73669119717828	5.78811970985860
C	2.74322547503602	13.12690267639995	4.10026594301099
H	3.57803920636988	13.59935620084950	4.63256829263700
C	2.62386998845470	13.83556963188326	2.74090139929717
H	3.49934447314131	13.61187302057326	2.11315679321297
H	2.56259843659752	14.92658963509320	2.87928605954370
H	1.72521453108316	13.50232836323681	2.19469598918249
C	1.47857795774012	13.33310256302228	4.94620397733113
H	1.30592807503479	14.40784157794129	5.11896203814505
H	1.56128591992866	12.84262052145461	5.92956763282384
H	0.58139504931954	12.92880401408920	4.44913011623456
C	7.50578975362250	14.27076470027108	0.79469106798120
C	7.75125043356986	16.44814861414529	0.21678479898362
C	8.99803041552337	15.87828100846914	0.22028703871964
C	5.40565906391594	15.61865913114958	0.66091118214570
H	5.21736426164365	16.63270326457321	1.03925867003927
H	5.04768601706084	14.92446111878163	1.42787139106252
C	4.71046545325919	15.36541764858969	-0.66990615477247
H	5.08009740082514	16.03390733318868	-1.46415527590391
H	3.62675052649679	15.52689694967351	-0.56010748140578
H	4.87055879277719	14.32198846307578	-0.98245460614490
C	9.89685310588077	13.57124603134964	0.73044814794299
H	9.55231579525317	12.85244167175125	1.48533566876447
H	10.76783616611965	14.09562417927836	1.14391161453379
C	10.23201752257012	12.85037200992112	-0.56798980569177
H	10.53391079118177	13.55016283769365	-1.36379096512085
H	9.36159235283323	12.27412984857536	-0.91798366948448
H	11.06162880396959	12.14630843957160	-0.39716693290942
C	7.33270380467827	17.85812935306704	-0.02108395386275
H	6.55977068682639	17.93392326205009	-0.80245588538393
H	8.19328835445119	18.46146163426150	-0.34036717670832
H	6.92506866594295	18.31541632972337	0.89629759274200
C	10.34229917388928	16.47886569381586	-0.00540537601881
H	10.90602124866852	15.94963591883639	-0.79046122693742
H	10.95075038293491	16.45275377347528	0.91468466600951
H	10.24471749184731	17.52928197420440	-0.31125890311410

Table S27. Compound **1b** B3LYP-D3/def2-TZVPP
final energy -4326.504660978677 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy

Sb	6.75995870270831	12.29160923293306	1.27164973756429
Ga	6.49267510676103	13.09142534026581	3.69756245244384

Cl	5.69550117597701	15.19940971801258	4.09751291837382
N	8.02195324594150	13.09176048153851	5.00407720481161
N	5.33321896168553	11.97398526390968	4.85499664311187
N	6.84655624281601	15.42238806456883	0.54976810227204
N	8.83786730705297	14.61785806042456	0.56440875839924
C	7.77634302745651	12.98626844031463	6.30374266348681
C	6.53717036288965	12.60407988397676	6.83949551212242
H	6.47102250258388	12.62444556903323	7.91554271214868
C	5.43831963069946	12.04564847618771	6.17688784710796
C	8.87549415254541	13.27500060898723	7.29595821525468
H	9.82637964661745	12.85728074698903	6.97230710428261
H	8.62543133586929	12.87619725668731	8.27528688848431
H	9.01378890753293	14.35246772959240	7.38927604544335
C	4.32862559387497	11.48703208317921	7.02946719249133
H	3.42050239166571	12.07155012976079	6.87481494781650
H	4.59124445089590	11.51835512555011	8.08336428626222
H	4.09239962947225	10.46178238837091	6.75071172555435
C	9.35791035259725	13.31944578397617	4.53842673477331
C	10.11165466816609	12.21078418755581	4.10052694778989
C	11.42887860650466	12.42094807997127	3.70083468606636
H	12.02667297066793	11.58250600047317	3.37552207243922
C	11.98583014215661	13.69113795839403	3.69729487055122
H	13.01296086747953	13.83354139000604	3.38712352340226
C	11.21573238027118	14.77626634279934	4.07618622187579
H	11.64797161995136	15.76826531077380	4.05328487543373
C	9.89578416630175	14.61727877689995	4.50210966943696
C	9.51323659662881	10.81486931397834	4.07502794397567
H	8.45428403558334	10.93668627500853	3.85259051111039
C	10.09903216341747	9.93709234528333	2.96840059715505
H	9.99687417710319	10.41764906847826	1.99538008893130
H	9.56431094307492	8.98993715358017	2.92656148787033
H	11.15144781891416	9.70557757409183	3.14050472669201
C	9.63124886969598	10.11775357991985	5.43743778243563
H	9.19842884148118	9.11734488293502	5.38840562489942
H	9.10782335428183	10.66629442880380	6.21819558002919
H	10.67785365970616	10.01905146730734	5.73290670221436
C	9.09649048958733	15.84737896304046	4.88990418823092
H	8.14471156942128	15.52128066982895	5.30131478331117
C	8.77622949265897	16.68873525079492	3.64878258878968
H	9.69224022881937	17.05208436340655	3.17695526250462
H	8.16496678605866	17.55044424682557	3.92064432100671
H	8.21667657922081	16.10706101146585	2.92258848518302
C	9.80994727726504	16.70274302816036	5.94416976522149
H	10.71038806958660	17.16878241585561	5.54044913501409
H	10.10800002773488	16.11481752111786	6.81215356472523
H	9.15180136599560	17.50319793297150	6.28598022122456
C	4.33221425234818	11.14179054671370	4.25225671229506
C	4.64910747443448	9.79555141276826	3.99532046607890
C	3.67993869751483	8.98531566656158	3.40747642618056
H	3.90373053843051	7.94562256880832	3.21052686171982
C	2.43494865415334	9.48895865258224	3.06630565448301
H	1.69481341928583	8.84538363373460	2.60896780417332
C	2.14699961468019	10.82281812672310	3.30384856240526
H	1.18080734363998	11.21728153840150	3.01912943391739
C	3.08114490778725	11.67114623543132	3.89524317496719
C	6.00177172621848	9.20400051157585	4.35233383633802
H	6.65046184962740	10.01929314158271	4.66527824737901
C	6.65962248293804	8.52292644541086	3.14797339086375
H	6.05219564688058	7.69771454927260	2.77350199286427
H	7.62804180973300	8.11272873698149	3.43287568190304
H	6.81744520821591	9.22733926431412	2.33140170335874
C	5.89667784679400	8.22849548867489	5.53259129035756
H	5.25271622035680	7.38219419817401	5.28685023432809
H	5.48630924716725	8.71323228170153	6.41806375682878
H	6.88210562767381	7.83751021720487	5.79277376712685
C	2.73640976519003	13.13327052911787	4.09871526551825
H	3.56142491600106	13.60587512016004	4.62505604348348
C	2.60066825219193	13.83902032206330	2.74266684557118
H	3.47235521950068	13.64015322303676	2.12111473645974
H	2.50958990509855	14.91708222987981	2.88175338711701
H	1.71884485386660	13.48283288816019	2.20461199774329
C	1.47193074325736	13.32891657159431	4.94317176785191
H	1.30183704028395	14.39167415397142	5.12336998283830
H	1.55177758529233	12.83118157159744	5.91019184397094
H	0.58786155075548	12.93173772774500	4.44147276305707
C	7.54378415387658	14.28661210903791	0.78365163959471
C	7.69420534750692	16.46159114017439	0.18696133580621
C	8.95575647143605	15.95098839427334	0.19144914305917
C	5.39026020391117	15.52890136279976	0.61574885736769

H	5.14723636562870	16.51260406841263	1.01182930714688
H	5.05940431284201	14.79740410328831	1.34333647490704
C	4.73634203984736	15.27826794320950	-0.73390682630708
H	5.08549246475560	15.97875800776777	-1.49366832438420
H	3.65470349750687	15.38309012153397	-0.64218817034834
H	4.95333871199096	14.26341857943541	-1.06721902967930
C	9.96077711116775	13.69863043830870	0.72423823022466
H	9.67860132555398	13.00330867464937	1.51022155781009
H	10.81175281468489	14.27480109949128	1.07774369818165
C	10.28467183330738	12.94782238338806	-0.55727881314421
H	10.51455762365701	13.62984063471059	-1.37693009618637
H	9.44030840409432	12.32316814599345	-0.84857903037847
H	11.14783531235098	12.30051688970173	-0.39683181865739
C	7.21563584128250	17.84757758268242	-0.05525245953755
H	6.44509109118525	17.88549735724827	-0.82663826936753
H	8.04172587000974	18.47862332704499	-0.37661398500800
H	6.79746755682758	18.28546272968625	0.85368066227969
C	10.26581343297070	16.60701234455093	-0.05407011567868
H	10.84669614644854	16.08304723397185	-0.81482197667031
H	10.86967680185858	16.64507936363331	0.85558950985810
H	10.11566237060202	17.62959848707407	-0.39385905179407

Table S28. Compound **1c** B3LYP-D3/def2-SVP
Electronic energy ... -4402.75714475 Eh
Final Gibbs free energy ... -4401.90052584 Eh
Gibbs free energy minus the electronic energy ... 0.85661891 Eh

Sb	5.64569314130529	2.57988321187346	1.96384950231169
Ga	3.79720749382051	4.05697938283716	2.96542553780024
Cl	4.21595829285569	5.56165020346698	4.64121804599112
N	2.49076122925416	5.16766184933838	1.92786905506478
N	2.38565584085537	2.93445998900679	3.81219047924123
N	7.72951778965204	4.93884574295970	2.73940604968376
N	7.43946118476971	4.85022888783877	0.58773391599494
C	1.27948633064744	5.39701324772299	2.44733663539402
C	0.72467487161646	4.66270511985102	3.51175417609137
H	-0.25245062962239	4.99761097997802	3.85585299253723
C	1.18793404976542	3.45590358275765	4.07454726146672
C	0.42488863040434	6.49303429242484	1.85195184404104
H	0.26210346963054	6.32828641296866	0.77702003152597
H	0.93322334985529	7.46461294188498	1.94305740961095
H	-0.54855880097664	6.55162007549198	2.35424893789380
C	0.25359556125070	2.72272172911201	5.00808875606195
H	-0.73704266219717	3.19373185805836	5.02853667734534
H	0.66559290194402	2.72050578026579	6.02828399325855
H	0.14651294291775	1.66912106192798	4.71259949204926
C	2.84157730374440	5.79048661568565	0.68526746500193
C	3.43610763724817	7.07406733303940	0.66094348213908
C	3.66370194053556	7.68196748209286	-0.58185169126262
H	4.10937330257831	8.67884609802732	-0.61311422963837
C	3.33251559698034	7.04102735511450	-1.77391441189524
H	3.51113516449066	7.53506829606852	-2.73241336827809
C	2.79563141722678	5.75627342772017	-1.73659664833253
H	2.55466136457529	5.24601354313220	-2.67215644718075
C	2.54718314584904	5.10805062951395	-0.51890742287261
C	3.86243597772488	7.78733817573369	1.93402236836991
H	3.43155974824317	7.24883023255305	2.78743192200000
C	5.38978119024847	7.70439093898935	2.09047194727002
H	5.90312942947552	8.23063290479455	1.26777534659623
H	5.72503607177674	6.65899606199684	2.09004726415752
H	5.70735955080541	8.15555638282421	3.04375458462945
C	3.37614582559957	9.24093316530872	2.00468939401436
H	3.84631775480834	9.87532105879519	1.23545452822138
H	3.62525220471766	9.67557903990271	2.98598380806849
H	2.28474079408674	9.31134302747756	1.87108819249243
C	1.93146323296876	3.71620739382335	-0.52168287855763
H	1.93957533768202	3.35232689078156	0.51388482602752
C	0.46532526429708	3.75225039338801	-0.98162038310939
H	0.37823704440436	4.11902461618276	-2.01786482452350
H	-0.14266683034138	4.40920371145377	-0.34086779503824
H	0.02183695674335	2.74408897712777	-0.94310720500330
C	2.75892138364637	2.73198960930266	-1.35894096752702
H	2.28900304746251	1.73626434766936	-1.35365047624688
H	3.77369545072668	2.63012396347910	-0.94338174133485
H	2.83515921682779	3.05079767335040	-2.41126640643019
C	2.72684060365337	1.62034996793493	4.27541601761835
C	3.21596732466551	1.42675912024951	5.58662230269876
C	3.50552515246962	0.11984941414100	6.00310330887459
H	3.88067035738283	-0.04631194564576	7.01562806726960
C	3.34006119734628	-0.96474883920505	5.14698650900870

H	3.56878433308767	-1.97683958447854	5.49072523154972
C	2.90843485167349	-0.75241956948148	3.83820935550003
H	2.81331237898954	-1.60443323840582	3.16413194445124
C	2.60642252395136	0.53407481944058	3.37376070510408
C	3.51392205328271	2.58970006292289	6.52128911280697
H	3.12304941342279	3.50828106929511	6.06516831445865
C	5.03608909667300	2.77504556911946	6.64735366128051
H	5.50027656531369	2.84870644122933	5.65343141198186
H	5.49554272362939	1.92133893904559	7.17339260485167
H	5.26771524678458	3.69569398725721	7.20594776806148
C	2.86475854366319	2.43482584373247	7.90412060103053
H	1.77531813288061	2.28703755186902	7.83230203898925
H	3.04502161183331	3.33604586969051	8.51203967953801
H	3.27850001547167	1.57632394723192	8.45787188915658
C	2.16647218184221	0.75550317791088	1.93046703092416
H	2.56777100936749	1.73362666884611	1.62433272333387
C	2.74411921333400	-0.28345256794146	0.96303785994894
H	2.51614854048431	0.00079740851665	-0.07464292381058
H	2.31438190821746	-1.28499633228878	1.12670020436902
H	3.83821582275175	-0.35642734869672	1.05932372626449
C	0.63675242329649	0.83004584988003	1.79543379409990
H	0.34817224655206	0.96261963201467	0.74009891246783
H	0.21482541549245	1.67317506637346	2.35948159150029
H	0.16741998151016	-0.09819770180492	2.16178490298424
C	7.01340956968695	4.31474878523574	1.76469932110188
C	8.61660774000026	5.85535629306122	2.17722855273605
C	8.43431634827470	5.79961429789553	0.81758461722183
C	7.63920819302940	4.54296441831192	4.16544978227912
H	6.67533614280285	4.02202699580580	4.21859483813777
C	7.57734726847653	5.72165287249615	5.13272193413873
H	6.88865558164782	6.49440841558685	4.76748024827870
H	8.56223488632126	6.16315607140151	5.33986962101438
H	7.16841460241370	5.35639332767313	6.08600922947900
C	8.73693329111788	3.53421198911100	4.49678501484000
H	8.65624161480014	2.65708330967841	3.83693761056609
H	8.62042178045547	3.19015938923646	5.53613732920259
H	9.74366793874787	3.97047315553632	4.39211983476803
C	9.55020292515080	6.73005741438326	2.94559762995734
H	10.24254477687061	7.22912994301656	2.25446564183141
H	10.15376640747153	6.15984793398601	3.66717297971549
H	9.01463524648203	7.51297150848493	3.50416399996154
C	9.11897014261509	6.59744009938128	-0.24186671509912
H	9.47009618390132	5.96752469803080	-1.07216735562259
H	9.99594912721333	7.10409288903861	0.18291537456763
H	8.46213364469831	7.37285718044492	-0.66714262037887
C	6.91828103562878	4.39884010544942	-0.71951334146438
H	6.01104682117315	3.83961772030200	-0.43682852520791
C	7.88220340050972	3.41344398208201	-1.37705110498810
H	7.43397261634814	3.01925051951596	-2.30252612807296
H	8.07981867545423	2.56325916103052	-0.70652824860446
H	8.84354571656091	3.88323604317956	-1.64045774084070
C	6.49024057106500	5.54851048013744	-1.62567760235443
H	7.33118451715198	6.04009310434202	-2.13507459448771
H	5.91987066528726	6.29872604256692	-1.06226581019667
H	5.81974718673840	5.15156587974980	-2.40191514391382

Table S29. Compound **1c** B3LYP-D3/def2-TZVPP
final energy -4405.113237554055 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -4399.59587741948

Sb	5.64049076361881	2.60659610775484	1.98868324745323
Ga	3.78693519573093	4.08008625605344	2.98053190484416
Cl	4.19437023750008	5.57473057305659	4.66257783340905
N	2.48183622629192	5.17853713463104	1.93370979497510
N	2.37984235164759	2.93697066515204	3.80782707860101
N	7.75014193998123	4.92872741770336	2.72690431741179
N	7.44857616968232	4.82808704280057	0.58692617865531
C	1.26697969347295	5.38469897151554	2.43995961160249
C	0.71013251610575	4.63497941046171	3.48137696886452
H	-0.26745978650423	4.95005358570782	3.80898253782596
C	1.17727161441637	3.43808670338920	4.04618985871724
C	0.41049202857729	6.48466716744152	1.86321233534466
H	0.32454755807284	6.39778696733668	0.78176908800580
H	0.86885901732580	7.45380743403596	2.06476756443181
H	-0.58387246480092	6.47095772093884	2.30020345261903
C	0.23510609580195	2.70825552946574	4.96940451600894
H	-0.78672916505959	3.05123087082851	4.83125864589276
H	0.52385153753957	2.89721094272924	6.00464758882263
H	0.27902204674685	1.63239657517130	4.81793650039461
C	2.83074893297071	5.80919438931496	0.69395867076227

C	3.42473406465621	7.08358101675884	0.67488980584701
C	3.65209592870423	7.69308275683032	-0.55824840920618
H	4.09521500834541	8.67943511752672	-0.58601845651749
C	3.31832378363425	7.06290163779979	-1.74600351122667
H	3.49445036149235	7.55636577416205	-2.69286396824159
C	2.77928335453064	5.78740148429393	-1.71397188144727
H	2.53565309803624	5.28925422953408	-2.64278727891618
C	2.53401805394654	5.13709539603795	-0.50591604530982
C	3.84886420804165	7.79041626244908	1.94607432290034
H	3.42212820865570	7.25514922694029	2.78982776819125
C	5.37478813001033	7.71540681963489	2.09670755934677
H	5.87325091999744	8.25189873225330	1.28600620457304
H	5.71369190150884	6.68190320314991	2.08028975448829
H	5.68561527692332	8.15395519711215	3.04565678676607
C	3.36390132901635	9.24166660343824	2.02045225831850
H	3.83106423535784	9.86901803788854	1.25937665714571
H	3.61283805463871	9.66600420392935	2.99416781521268
H	2.28329714752743	9.31070246950128	1.88832984908736
C	1.91701562961783	3.75076762048368	-0.51655811721782
H	1.92526216310925	3.38126634292968	0.50564489166504
C	0.45334780581849	3.79182317212457	-0.97565504258214
H	0.37089123431663	4.15761811799296	-2.00094897189498
H	-0.14570894385959	4.44273830104151	-0.33902074026405
H	0.01492018792350	2.79324904221644	-0.93870847824566
C	2.73685876074735	2.77433804507753	-1.36545870400904
H	2.26138782757404	1.79314290082187	-1.37550608865052
H	3.74000344859632	2.65918698408342	-0.95402168743888
H	2.81689216352246	3.10830235936393	-2.40103595908965
C	2.74017440333941	1.62776793053007	4.27119306352604
C	3.23079373940687	1.44251812867469	5.57363982754018
C	3.55843519433267	0.14994263007782	5.98048788638276
H	3.93548075584672	-0.00896621310589	6.98176616556784
C	3.42391214140035	-0.92865689001576	5.12447816880534
H	3.68267266727599	-1.92486738320704	5.45843802997269
C	2.98028157056008	-0.72403098158040	3.82673571554820
H	2.90683592087352	-1.56732231595431	3.15615406863188
C	2.64241179457689	0.54807830334819	3.37184829677843
C	3.47778966776244	2.59974300759471	6.52208500573894
H	3.08777012802594	3.50644231368501	6.06706028269578
C	4.98791715158492	2.80845037687421	6.70873805783745
H	5.48332244819984	2.90455278458792	5.74416690644070
H	5.43483890724199	1.96306902019124	7.23617444581257
H	5.17639878319810	3.71559646352982	7.28421692804489
C	2.78625371310484	2.41548231654152	7.87797746137372
H	1.71548253349554	2.24164978160579	7.76567684210917
H	2.92280189566815	3.30720525799872	8.49182077249980
H	3.20090372053288	1.56942515018013	8.42844834289992
C	2.17544427246157	0.75450511724575	1.94036580963328
H	2.49977972266495	1.74993776430674	1.63827700755630
C	2.80248502236989	-0.23667169895104	0.95762730964089
H	2.53976861138070	0.03845087822878	-0.06295851892752
H	2.44385595085686	-1.25418063026156	1.12057786428986
H	3.88956782558429	-0.23714394380508	1.03483653535443
C	0.64446802504192	0.72065879363980	1.83174020237989
H	0.33320937543172	0.85240066082178	0.79388261892311
H	0.17971283403378	1.51037673282618	2.41891117137598
H	0.25573888203282	-0.23776200887186	2.18197065605944
C	7.01630306908323	4.31406111752023	1.76600720115532
C	8.65595687455328	5.81447656974086	2.15229126221688
C	8.46772316353793	5.75061084322908	0.80382177918722
C	7.64803890973020	4.55871939263636	4.15718648471596
H	6.68725676881483	4.05467529114237	4.21513872362426
C	7.60211522631387	5.75523735190713	5.09830428101512
H	6.94004824451807	6.52851071885078	4.71670746709244
H	8.58594797902308	6.17721159425645	5.29386194375030
H	7.18780735022918	5.42007394153039	6.04803982560824
C	8.73317713092818	3.54851469200168	4.51049710948642
H	8.64532236858536	2.66817903124258	3.87441636425427
H	8.61337263381566	3.23194691572357	5.54682302707046
H	9.73288484703968	3.97041916155849	4.39758118310077
C	9.61390642573693	6.66857078290703	2.90648416888730
H	10.31405823611327	7.13053639852479	2.21406799475824
H	10.19423450473345	6.09565518525097	3.62860219460866
H	9.10777235545238	7.46818768619021	3.44746547243225
C	9.17320881939281	6.51173971762052	-0.26355868259828
H	9.50629858055781	5.86593623903122	-1.07491859262913
H	10.05429225322398	6.99448225929035	0.15318657438171
H	8.54468944239064	7.29081916418766	-0.69639706911419
C	6.90047773006156	4.38944555111306	-0.71191252540418

H	5.99072970649935	3.86003473873664	-0.42407605572192
C	7.83155860861943	3.38512998221064	-1.38038121852782
H	7.37040391015986	3.01446261046303	-2.29637267044006
H	8.00859398358854	2.53476640909454	-0.72235945974105
H	8.79254007252342	3.82905988372837	-1.64315333341434
C	6.49944878740151	5.54933744103200	-1.61226978046332
H	7.34564760844406	6.01275475033653	-2.11588730276666
H	5.95797957474386	6.30690188239458	-1.05080419157179
H	5.82437732439048	5.17242182894623	-2.37937112737185

Table S30. Compound **1d** B3LYP-D3/def2-SVP

Electronic energy ... -5021.33159139 Eh

Final Gibbs free energy ... -5020.21213208 Eh

Gibbs free energy minus the electronic energy ... 1.11945932 Eh

Sb	6.42308953602760	10.27412657953024	3.79141961095739
Ga	6.06600237889035	12.50503390552742	5.09032146263720
Cl	7.49475186664992	13.40691245562818	6.59632238256277
N	7.30148312743059	8.27076607858556	6.32523164837880
N	7.23774247311920	7.42830374472214	4.32683697960632
N	6.21365006711947	13.76361200350542	3.50841111481561
N	4.32663770826645	13.34039857807269	5.69538187155839
C	10.51873000943521	11.23734988575377	6.89980063602389
C	10.48118516928896	8.75222769108689	6.60127261190344
C	9.61344551889142	10.02303546721378	6.67209215981883
C	4.17173996729383	8.97030887256800	7.22405268819370
C	4.32034445017499	7.66988707871686	9.37949818343624
C	5.08669828624867	8.14135095810972	8.13982040488668
C	8.50548939745847	9.89968933299848	7.71437014441197
C	8.60632408541280	10.54095534786290	8.95763718498942
C	7.63832959811545	10.36358130216379	9.94157793636900
C	6.51484206338631	9.57600318765762	9.69587544174138
C	6.34477037608880	8.93876098176717	8.46209701314933
C	7.36302852934114	9.10279560536475	7.49722630017456
C	10.20304163053067	9.39770218327835	2.22908376576269
C	10.68979473831898	7.00883739126351	2.95821531258356
C	9.63803960962361	8.12639914990918	2.87692821182756
C	4.63196547234341	5.10702689227114	3.36629961715147
C	3.49489413416329	7.16267836735656	2.41348606487788
C	4.76102465070242	6.61242764415986	3.07927044469989
C	8.37838207790228	7.63733111943220	2.17827938723965
C	8.34052893723666	7.49378461257951	0.78584068081749
C	7.18159178670144	7.06040590835001	0.14225096624909
C	6.02971838826764	6.77542849067460	0.87574065467048
C	6.01488625584206	6.90681629866482	2.27048256465381
C	7.20895775235715	7.31352057978942	2.89567846278415
C	7.63650068346332	6.91650222153921	6.42847284987859
C	7.60078056157659	6.39616866215740	5.17882524405003
C	7.02807487126720	8.60255299177697	5.02344960574521
C	4.04768172295761	11.33629739742997	0.77484749933027
C	3.91637145716804	13.85617747069709	0.78429744533976
C	4.60610135022603	12.62367602762017	1.39362617647103
C	10.00220726588758	15.21499884423953	2.80678695310525
C	10.01686770953549	12.97480040767461	3.98101715690093
C	9.14486375770365	14.04569388130175	3.31496872462367
C	6.12388712171023	12.72875826605277	1.29159801698034
C	6.79017870007633	12.24008385644047	0.16172597329364
C	8.17625190977728	12.33412213637268	0.04442256742524
C	8.91661922698784	12.92873405698789	1.06273105891270
C	8.29534407559904	13.43423493765621	2.21292348033742
C	6.89305815641040	13.32514760979768	2.32320581410843
C	2.00980570488672	10.15549102834543	3.97469291120408
C	1.64391118312105	12.63939263664994	3.68818228928390
C	2.46822932383902	11.55332386091364	4.39889285443069
C	5.47986715097072	12.76594599326816	9.34657715073373
C	3.82726713873553	14.65105113044778	9.62754167240342
C	4.45287942210406	13.65578331472197	8.63815670259823
C	2.47077626398769	11.75180729902886	5.90786539273507
C	1.51884791310362	11.11207470643140	6.71132848873603
C	1.49900032849492	11.29786637504292	8.09263082034060
C	2.45315760881928	12.11579534314276	8.69185303737917
C	3.41918548910962	12.79017768770957	7.93012453944738
C	3.40800373393966	12.61438812894690	6.52658809806098
C	6.24349714452779	16.05119972275885	2.60602421349671
C	2.85710610434461	15.28406156855377	6.05925223166092
C	5.75248019062403	15.01202207642425	3.58761277895874
C	4.81067300292717	15.42577841521934	4.54355733447714
C	4.05972541415258	14.62218448011427	5.42176770869249
H	9.93471884958101	12.16456127630803	6.97231746023505
H	11.12409715437749	11.12212185172475	7.81403824118285

H	11.21997182605084	11.33621781143587	6.05832553161124
H	11.26305655970468	8.87384379179500	5.83431798010143
H	10.98191268947757	8.57279356131939	7.56715077847196
H	9.90703791342522	7.85242124393278	6.34599983747733
H	9.12210132209714	10.15693858265125	5.69337067696618
H	3.24822075373657	8.41743199689559	6.98851478018248
H	3.88602053232191	9.90697130945312	7.72200914933486
H	4.66011039649254	9.23628637472544	6.27571491360153
H	4.96636037747723	7.11802081931852	10.08073375841219
H	3.86945703507771	8.51600514530671	9.92259474256337
H	3.49647177370216	7.00413409979488	9.07821582387631
H	5.38917180179648	7.23893027810852	7.58373548821403
H	9.46135234381400	11.18307349042888	9.16306056291126
H	7.74756554404693	10.86673487510695	10.90525282677629
H	5.75254379708843	9.47492967934934	10.46807067489740
H	9.42949506268149	10.17690169210436	2.16236425036142
H	11.03408932396313	9.79141831910199	2.83619517662612
H	10.59626814216430	9.20511971016857	1.21734470697243
H	11.58150581162782	7.35562659137276	3.50521897733820
H	10.29407733845285	6.12378198332136	3.48154386675179
H	11.01043338506970	6.68915765550214	1.95289007662141
H	9.36389485250526	8.39271421509100	3.90574966367026
H	5.51315926666150	4.71948797911155	3.90050540731461
H	3.74394497452209	4.90431308648667	3.98714486020216
H	4.52984007536841	4.53466984010236	2.42942835908909
H	3.25452179980571	6.63074223271801	1.47873558322512
H	2.63090234662056	7.04816095711403	3.08670710407547
H	3.60989531788977	8.23238025344395	2.18709164981396
H	4.86597886324648	7.13105116536632	4.04407678958539
H	9.22830032622509	7.73326117827678	0.19720219144656
H	7.17147981476385	6.95510506687812	-0.94567678777720
H	5.12522582323716	6.45679246900676	0.35480996316980
H	7.88785492663306	6.47351602478843	7.38673506872366
H	7.81438693636083	5.39923384383108	4.80706952525193
H	4.14677372724419	11.33015782877697	-0.32262760969357
H	4.55892166042114	10.44737477072696	1.17408915097723
H	2.97368297454284	11.24520872849910	1.00033817837156
H	2.82070006078019	13.75494362037124	0.84312500407127
H	4.19154919379190	14.78067041748136	1.31005783777941
H	4.19192124384169	13.97269744679505	-0.27702580306467
H	4.35520981043046	12.61146794450653	2.46329904041187
H	9.39026162404444	15.98645013217293	2.31317305465045
H	10.53903689041593	15.68884564456194	3.64455596707394
H	10.75792999742338	14.87844780572617	2.07809707733161
H	10.75129913520018	12.55773055196924	3.27200412439103
H	10.56486138391747	13.40233915662025	4.83363918381063
H	9.39595181866024	12.14827213993408	4.35223289517081
H	8.47057452187313	14.43218197710188	4.09137468427740
H	6.21709140092833	11.76793343705971	-0.63759398710608
H	8.67899342532663	11.93861078339627	-0.84185139146625
H	10.00312785638587	12.99592317486418	0.97000171297524
H	2.58768535789803	9.37526991957267	4.49105969035894
H	0.93838953196077	9.98837891285843	4.17250662604593
H	2.16575971375377	10.02472069907555	2.89408097924370
H	0.60519541457816	12.64750676489182	4.05812750829034
H	2.06869437874455	13.64179567564066	3.83924063737885
H	1.61505415187262	12.45375873093435	2.60283195868555
H	3.51059028215808	11.65168359266928	4.06385891264916
H	6.28703407697807	13.37186997633878	9.78784506039406
H	5.00602158826519	12.17969708330381	10.15113001827725
H	5.94445583683515	12.06807507416073	8.64220774329501
H	3.37073072298573	14.13764405074412	10.48920270208400
H	4.60097725831458	15.32812311988337	10.02349035561093
H	3.04326496388432	15.26763784757789	9.16059427668135
H	5.00369122976974	14.22643152397171	7.87836801030877
H	0.78178187449548	10.45383039730414	6.24948882610300
H	0.74829428696257	10.79023476332979	8.70371494002773
H	2.44759394812631	12.24169661027483	9.77680115117811
H	5.61050911549014	16.94742297082985	2.62402462308978
H	7.27024103366899	16.34569368958627	2.87675655091851
H	6.28721622008394	15.65854893141958	1.58169240526439
H	1.96888469162571	14.64071632145380	5.99573829754879
H	3.03636891058754	15.46924585165840	7.12748080142844
H	2.64086219467282	16.24315306732503	5.57281110378850
H	4.51663970202744	16.47287818325888	4.49611934193368

Table S31. Compound **1d** B3LYP-D3/def2-TZVPP
final energy -5024.341790630281 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -5017.769290515395 Eh

Sb	6.51079465424082	10.30715939380610	3.70326206820362
Ga	6.15206420833858	12.53411258611423	5.06109774894476
Cl	7.51123642085935	13.39460170994104	6.66636820127194
N	7.36241835027935	8.32231797128876	6.27952266529160
N	7.31608400156191	7.46156114620940	4.28016623998730
N	6.20747944140152	13.79103569386098	3.48789351146832
N	4.36808373018740	13.37831660758917	5.77049862481093
C	10.47206587413151	11.38508319270349	7.22770317310289
C	10.41533689773181	9.01732962647641	6.38987673289457
C	9.54102635118169	10.23976711368992	6.77450388378059
C	4.20926603691177	8.78844591083284	7.02678713567666
C	4.28584284729370	7.44430747379340	9.15794300768541
C	5.10440973860707	7.98062945534778	7.98191506047064
C	8.45961695212240	9.91737922449178	7.80452828536898
C	8.50938528874106	10.43370353877862	9.09777506004661
C	7.52835227681882	10.14585075153446	10.03960518388100
C	6.42601220787771	9.36122661925977	9.68775569498399
C	6.31658463464953	8.82659992501077	8.41052885559380
C	7.34888928336640	9.09778593891629	7.48904597956201
C	10.35045176985321	9.05894989301258	1.71565857973763
C	10.58000340160229	7.02317376004319	3.21608635159434
C	9.62340058944982	8.11534922565280	2.68467382421934
C	4.63939258989016	5.39252196504235	3.94016808803958
C	3.44926604020415	7.00231284671269	2.39073791363847
C	4.73614018927970	6.73825344091353	3.19279456979211
C	8.35477497964300	7.51358638738704	2.06809815746528
C	8.27049167397935	7.21704350467142	0.71289274912572
C	7.08773685473780	6.72314098470322	0.15598620593061
C	5.95775891900583	6.55328182676295	0.95706872439967
C	5.98723411331308	6.83784687580017	2.31781358551839
C	7.21480397533733	7.27800383373690	2.86477369033402
C	7.73652559892389	6.94686381538050	6.38747378782207
C	7.70405063107978	6.43966335416012	5.14901182353351
C	7.09465591278138	8.64564708613972	4.99014835950968
C	4.04154854754453	11.41784164841077	0.76922282224652
C	3.96338546332771	13.93168724210498	0.47650833033343
C	4.58786835842059	12.77049550454461	1.28286094121019
C	10.00792578471234	15.23774499376274	2.75161151642539
C	10.00066526543212	13.03377880304345	4.02006444291112
C	9.13246003680513	14.08595984122294	3.30475453785603
C	6.12602403281492	12.83956798641761	1.23060536526637
C	6.79147804545095	12.38226879155916	0.09471235129883
C	8.18535902409442	12.43784606479010	0.00469834997770
C	8.91603672095790	12.97491298115336	1.05504449806846
C	8.29493526246884	13.46514249932116	2.20130379675684
C	6.88014948788995	13.38267057005668	2.29154257658893
C	2.09006653158251	10.23962080335301	3.92905745993460
C	1.69827081087938	12.73967343268160	3.73976397849163
C	2.54160890235878	11.63358242154199	4.42058935935865
C	5.45469945432566	12.74356376043382	9.53499641708050
C	3.75772342311966	14.60396751863259	9.68949317902745
C	4.46391963526141	13.61481748380410	8.74253256095556
C	2.53208677562936	11.77137733706873	5.92671804618241
C	1.59341539884663	11.08723320178821	6.70728909266823
C	1.58200156069231	11.20085319152426	8.08808939420975
C	2.52587565824625	12.00066022535629	8.72859661142230
C	3.47151204306888	12.73250224897043	7.98738976664634
C	3.45640239213285	12.62154976536118	6.59271890906516
C	6.15886339752836	16.08759922375475	2.58097976644783
C	2.96253803105430	15.37550821164558	6.20697738775689
C	5.71020621016349	15.04924260895408	3.58286849689591
C	4.80992221599474	15.44847906616156	4.56692216210857
C	4.09876623685841	14.66049465818899	5.49308592149235
H	9.90417438654379	12.26896754719595	7.50978692976669
H	11.09698024535185	11.07463481200397	8.06716835379405
H	11.13161812245549	11.65757275333235	6.40481339290572
H	11.17007887075935	9.33507868571865	5.66999290865914
H	10.92714571372387	8.61907871062862	7.26810414600008
H	9.84274657052947	8.21551327143600	5.93591505310735
H	9.02474186608938	10.57399814091946	5.87196333610266
H	3.39144802600831	8.16658025328833	6.65623456164752
H	3.77394506208342	9.63790196011745	7.54971606867491
H	4.75861506001040	9.16881247014133	6.16883628521683
H	4.89726465705388	6.87225900511491	9.85688135994548
H	3.79934915393656	8.25061778814314	9.70894130212877
H	3.49820944712200	6.78855016464880	8.78275715935769
H	5.48903105609016	7.12026470958752	7.43262896044267
H	9.33008866854969	11.07548248659060	9.38612054841096
H	7.59850037207074	10.55820106773585	11.03653507688799

H	5.65467516987797	9.17834647054143	10.42177951863645
H	9.66339885208441	9.79558754862208	1.29907205635533
H	11.13449956996499	9.59725162990722	2.25102057840745
H	10.82374892275164	8.51668232318590	0.89588610260898
H	11.43846560080463	7.48620397367338	3.70442167182604
H	10.08711749442983	6.38351132344019	3.94563357372842
H	10.94394997137186	6.39728774562909	2.39908958776064
H	9.29957712041932	8.72361226801852	3.52688157665933
H	5.50091476776295	5.22685800574788	4.58323543169633
H	3.74716658621207	5.38001135154895	4.56800785728514
H	4.57295535197963	4.56168228426208	3.23488765978089
H	3.23418975201503	6.19198347997935	1.69303632033655
H	2.60117225662781	7.08592631337646	3.07094338991282
H	3.52496521939388	7.93226596871498	1.82840194434902
H	4.81269958276133	7.53339053990616	3.93448012374012
H	9.12348580445397	7.38628320488491	0.06882160715692
H	7.04170520018971	6.49497749593353	-0.89999214189367
H	5.03914591313731	6.21366159549854	0.49594152830554
H	7.99950022885202	6.52728522552451	7.33914506017897
H	7.92679171343824	5.45603429163410	4.77298619016757
H	4.26190335585053	11.26886268225067	-0.28749398075273
H	4.46337075142446	10.58751299986337	1.33613510923134
H	2.95571141375137	11.39619838083838	0.88320039653017
H	2.87480316985227	13.83964731431998	0.46020845992924
H	4.20924145547475	14.89994469764564	0.91176263958141
H	4.32199370890198	13.91963794593891	-0.55373625362792
H	4.28654035761441	12.88055254819223	2.32168759455105
H	9.40244329247979	15.96111680212408	2.20454236945241
H	10.51215966815168	15.75509977909842	3.56932315042103
H	10.77082208579223	14.86057267158894	2.06978599399023
H	10.70272750737193	12.56883574214697	3.32433319666389
H	10.56402267968793	13.50023570460698	4.82744403137324
H	9.37629423825158	12.25149718790042	4.44518743571057
H	8.46155129878245	14.51056367177850	4.04809096223091
H	6.22835207464185	11.96266871271368	-0.72693960894294
H	8.68570769475568	12.06210938701594	-0.87762985484705
H	9.99741648215249	13.01838106064172	0.97908417584844
H	2.63191945892611	9.45218290403660	4.45221448981941
H	1.01898038680294	10.08489504171959	4.07884312800209
H	2.29570901588060	10.14319169410876	2.86474839852010
H	0.66080992712042	12.68896547580771	4.07911552548713
H	2.08162690321606	13.73290854198702	3.97349584121416
H	1.71310135820963	12.61771440085981	2.65643509365886
H	3.57274039584060	11.75536358781743	4.09067031784193
H	6.17668848660085	13.37247170472878	10.05822767726873
H	4.93181440270968	12.13404385991267	10.27361859494470
H	6.00559575383298	12.08586793202943	8.87046079457584
H	3.21708330021223	14.07966796734708	10.47817357960252
H	4.49430746822916	15.25064836559850	10.16916835911128
H	3.04285947172152	15.23459070627303	9.16022704883235
H	5.04634548079002	14.18062067840371	8.01969858231877
H	0.87182867510616	10.44565799396460	6.21711413623417
H	0.85150185364475	10.65768181949628	8.67734445384743
H	2.52327066897029	12.07296867734587	9.80679917675900
H	5.46847442972276	16.92822261577700	2.55139107201128
H	7.14210836749935	16.46122209052202	2.87987640888200
H	6.26519770997631	15.67170867296180	1.58340012023287
H	2.23465659822538	14.68535460119238	6.61923215658085
H	3.38083001483578	15.95812865622201	7.02866346814385
H	2.46482025827569	16.06395668222537	5.52679806822781
H	4.51081487845799	16.48654640908731	4.52903104802022

Table S32. Compound **2a** B3LYP-D3/def2-SVP

Electronic energy ... -8108.47889312 Eh

Final Gibbs free energy ... -8107.12757633 Eh

Gibbs free energy minus the electronic energy ... 1.35131679 Eh

Sb	10.03021937078583	1.43116371242676	3.66778767062819
Sb	11.20521571827188	-0.91819907125490	4.55983999678594
Ga	11.97292564250877	3.02913484886173	4.39059659740670
Ga	9.26989394852234	-2.12011231849807	3.37688492948501
Cl	13.89923171418907	3.25903616933526	3.21487191874928
Cl	7.69024012517590	-0.93603142956849	2.18076336616316
N	11.38092140872305	4.92535567390849	4.48542464266197
N	12.62858921808319	2.93899526760053	6.25267066084958
N	8.10247463647006	-3.27492891209015	4.51862841948174
N	9.64442328260296	-3.58602396779983	2.04418778541050
N	9.85475905833237	2.21782535055221	0.59338588129045
N	11.73321317534357	1.17573013884045	0.80330995749244
C	12.01248893134406	5.77018722203703	5.30442648949594

C	12.86767844779650	5.35284702150633	6.34116068994583
H	13.34058844403829	6.15254150347177	6.90883862540528
C	13.07299280098757	4.05005967898098	6.84453951990456
C	11.81782982755944	7.25672597374343	5.12059765117519
H	12.39332238712873	7.59345286820857	4.24341436520685
H	12.16616659839485	7.81597151907489	5.99795546432704
H	10.76656487499522	7.50756579034114	4.92470700928324
C	13.83032342360163	3.92741502803179	8.14548056199686
H	13.26575069334232	3.32583693737717	8.87203498744313
H	14.03918334813785	4.91389626761136	8.57742416419554
H	14.78212920560445	3.40172310443148	7.97961127697613
C	10.33863688717588	5.36771514012569	3.60696881561420
C	10.63206883317903	5.84582083012970	2.30914006831118
C	9.56596770247049	6.25200957475235	1.49128736262829
H	9.78018452674246	6.63061562854172	0.48899653456709
C	8.24744525847397	6.18902649752190	1.93326349218293
H	7.43260847549354	6.51771553539255	1.28300159894799
C	7.96945742136050	5.69045116704456	3.20616868503002
H	6.93353245097889	5.62789477554869	3.54348686795294
C	8.99688094131057	5.26517177530152	4.05792612410429
C	12.05192204535750	5.92908212387723	1.76838773684126
H	12.74098540470322	5.64728160108712	2.57503726535132
C	12.41337102136219	7.34932397080172	1.30625328719622
H	13.47699893590112	7.39913000979108	1.02260194487081
H	12.23577744647630	8.09435767174693	2.09761501680228
H	11.82338201120729	7.65634089196550	0.42700188926402
C	12.26555896776333	4.91452316097240	0.63495212265304
H	11.60132277949374	5.12111244973478	-0.22071440567482
H	12.07323898482832	3.89341854451958	0.98501801187305
H	13.30714110000894	4.94850159401976	0.27868194669181
C	8.67333870669804	4.74849183579028	5.45326227159630
H	9.51046073102224	4.10508376510753	5.75560243542922
C	8.59882299763072	5.90028724376529	6.46930845588242
H	9.55144279436970	6.44346791713935	6.54337518642650
H	8.35663585492036	5.51457896122916	7.47224031214969
H	7.81635394169218	6.62246066176732	6.18307721758245
C	7.39899532897023	3.89735624719597	5.50254043999151
H	6.49212926665745	4.49844199770582	5.32740298674304
H	7.29320809769811	3.43731845376268	6.49667962048184
H	7.43003322164849	3.08697853072549	4.75925700740666
C	12.72414503021079	1.67155178269519	6.93052671742206
C	13.90742988829567	0.90496063916590	6.85435349993599
C	13.96092118803015	-0.30301309005793	7.56444489609582
H	14.86687922364133	-0.91104341254797	7.51356259503152
C	12.87790902041565	-0.74769407890895	8.31649505224250
H	12.93859874770231	-1.69313943838411	8.86066247791863
C	11.69776061396177	-0.00692970062563	8.33674119267081
H	10.83348863018102	-0.39546389839942	8.87526469209778
C	11.59119977687567	1.20021279500768	7.63704692640728
C	15.08765683924454	1.30644350025784	5.98175773514572
H	14.89965010583437	2.31552501112204	5.59184773238291
C	15.18544211072598	0.36885151878977	4.76650577422976
H	14.23338140245998	0.33008459958794	4.21923405413539
H	15.42777903566728	-0.66027962532329	5.07979094616015
H	15.96775813335544	0.71503939910047	4.07240895910160
C	16.41537304604888	1.34132387900939	6.75355873668935
H	16.70720372626917	0.34074839018658	7.11188684740331
H	16.36211777124659	2.00341090980569	7.63271603799876
H	17.22571416063488	1.70776697072162	6.10276233862714
C	10.27335206906157	1.96375450515445	7.61068659740157
H	10.20859148131350	2.43973811124035	6.61976673944142
C	9.05466681462756	1.04675659413895	7.74381498692944
H	8.13194467108934	1.61635826678726	7.55696002085734
H	8.96849885409993	0.61573077385125	8.75326216032005
H	9.10145774344844	0.21796125589994	7.02307934043048
C	10.22630186649859	3.09315705826147	8.65222290659557
H	10.98232016133715	3.86766741330548	8.46076535767750
H	10.39088563815406	2.69279089928448	9.66615321243402
H	9.23996708036322	3.58458143293216	8.64065377789042
C	7.45923234214130	-4.33304363013611	4.02528118691674
C	7.75790224594605	-4.91534335938329	2.77984939254610
H	7.14822610278934	-5.77502186179213	2.50438764552252
C	8.83134790657928	-4.63225141102060	1.91011093165882
C	6.35292148877839	-4.96432025541217	4.83881281396671
H	5.48258477277993	-4.28929714803684	4.85897806864963
H	6.65745911433559	-5.11356456773169	5.88397147235193
H	6.04036625824252	-5.92556697369036	4.41149954101234
C	9.03612203476439	-5.60270019189025	0.76762583708714
H	8.68082619440658	-6.60516506981019	1.04053705705043

H	10.08861930696138	-5.66013388328482	0.46235375962677
H	8.45824064748017	-5.26765798162383	-0.10750459593167
C	7.96929241323174	-2.90778800835957	5.89742249490561
C	8.92080933603131	-3.41807074335070	6.81435774556758
C	8.80532137042483	-3.06517430511093	8.16417631512929
H	9.52680544342324	-3.45509040524861	8.88481529079973
C	7.78767756272889	-2.21793425079399	8.60167078244053
H	7.71116829261527	-1.95268437786456	9.65939051323262
C	6.88447955842706	-1.69237027936117	7.68171141721725
H	6.10963777681407	-1.00168933469668	8.02249285589913
C	6.96234023794530	-2.01266327970234	6.31883115496753
C	10.03601201497926	-4.34727133988056	6.35273070132526
H	10.16287449272978	-4.17995202695341	5.27437087815673
C	9.65171817442675	-5.82464912406287	6.53477814506125
H	8.74165418208540	-6.08172134900478	5.97337345980480
H	9.46942582545913	-6.05404213783923	7.59799927257860
H	10.46101448513990	-6.48316589241292	6.17862748032132
C	11.38187097613342	-4.04343719602916	7.02122703418698
H	12.17438286507717	-4.66320839007236	6.57274808304424
H	11.36795824350163	-4.26938808427103	8.10000335007761
H	11.65759205027988	-2.98579178266982	6.89390909565157
C	6.00584375643678	-1.35277135591920	5.33707470758608
H	6.18552575275535	-1.78868830080405	4.34530744747124
C	4.53193426189985	-1.58549946013671	5.69971769749523
H	3.87468987416855	-1.15352370444091	4.92756581284338
H	4.26831335163926	-1.11152641577756	6.65956416401093
H	4.29620376079743	-2.65832051570176	5.78533997422294
C	6.31218447387701	0.14898745739326	5.22035661818102
H	7.36818891072118	0.31719684061515	4.96875779693699
H	6.09910763578154	0.67539018662495	6.16559169998445
H	5.70446269362847	0.60654333370928	4.42384591181673
C	10.77172469042226	-3.38752929853966	1.18402458282124
C	12.06361075000687	-3.69176074188459	1.68789371925900
C	13.17407468872453	-3.45948880725943	0.86852401562015
H	14.17301805273221	-3.69006859347533	1.24007658229984
C	13.02694151796914	-2.93821570951542	-0.41752053397447
H	13.90614802660622	-2.77166952619364	-1.04587061421125
C	11.75574007228803	-2.63179742749762	-0.89397771681952
H	11.64200358053523	-2.22539548923113	-1.90208745739639
C	10.60985828821336	-2.83995187199914	-0.11014515710034
C	12.23706902603171	-4.30369817617374	3.07193058653313
H	11.46143443708745	-3.85852818190589	3.71088452050721
C	11.99175882239980	-5.82169601157083	3.05170729301327
H	10.98080564511962	-6.07005025554000	2.70039196932951
H	12.10369137911590	-6.24285993781925	4.06422238654228
H	12.71582462061096	-6.32668749419944	2.39087216062223
C	13.58662646421500	-3.98047341253305	3.72005206283707
H	14.42290179321437	-4.48954892563257	3.21314039299598
H	13.58767058583676	-4.31912795800291	4.76731185820565
H	13.77599762915771	-2.89651158761340	3.71821988487971
C	9.25135487318662	-2.46320427021408	-0.68779539517148
H	8.48184146941450	-2.71761257151494	0.05311037535312
C	8.94840179014386	-3.21942080522337	-1.99239867695753
H	7.91756743748652	-3.01407390946219	-2.32418506909254
H	9.06028972844454	-4.30781121617788	-1.87763228148465
H	9.62417178279664	-2.90555568414140	-2.80495788368867
C	9.15640173853802	-0.94864596063245	-0.91909995774538
H	9.88423399947022	-0.61471945571283	-1.67577319867682
H	9.33840133735788	-0.40400324277492	0.01444800903743
H	8.14809741289010	-0.67607080116420	-1.27117730820557
C	10.66562261761794	1.62169201050510	1.50218297481882
C	10.41959339921978	2.17166754742508	-0.67733214050029
C	11.61481826655878	1.51394848200158	-0.54189033990972
C	8.52885730719972	2.73720580393368	0.90984229331903
H	8.12772804736566	3.25911248283902	0.03438793832858
H	8.58810644503332	3.44882769810755	1.74115658429230
H	7.86421623372741	1.90498394553720	1.18636240990388
C	12.87105924861897	0.45285541087013	1.35881327580964
H	13.19527985987909	-0.31124953348172	0.64236870348376
H	12.54906032237970	-0.05371544231356	2.28168140862095
H	13.68540452428496	1.15172265397004	1.59067867026867
C	9.76244125304939	2.73884728199265	-1.88662055143449
H	10.41434018112349	2.61512619415087	-2.76176859229260
H	9.55664506514681	3.81633172194093	-1.77358249757053
H	8.80808200252138	2.23251900137987	-2.10807501997195
C	12.65308687958333	1.15994897650612	-1.54785243474290
H	12.38013640533513	1.55618460906491	-2.53511806003240
H	12.76514995808182	0.06716005233483	-1.63845716111752
H	13.63734090655805	1.57418560652338	-1.27480586431441

Table S33. Compound **2a** B3LYP/def2-TZVPP
final energy -8112.419783337860
DLPNO-CCSD(T1)/cc-pVTZ single point energy -8102.518091824143

Sb	10.03378002509996	1.42247897920141	3.63285571062070
Sb	11.19908139491998	-0.92227688423927	4.52077324675714
Ga	11.96144712508704	3.03527934394766	4.36443462800854
Ga	9.25924523839918	-2.12622114249517	3.36074169246618
Cl	13.84083072263239	3.23409769277904	3.12625270218729
Cl	7.71185161610980	-0.94052780072799	2.14391098824048
N	11.36909994344057	4.93111781015822	4.48343126119696
N	12.64817325065346	2.93657699616455	6.21333572312832
N	8.08591181608962	-3.26855834771445	4.50674794993040
N	9.64528522753806	-3.60734078477067	2.05240959398659
N	9.87291467032456	2.25462876708016	0.58936744519436
N	11.72445613702702	1.18287228912434	0.77705489950576
C	11.99807660437692	5.76232256957592	5.30766796031226
C	12.86478213721996	5.33999241076233	6.32195771895935
H	13.32965262153560	6.12934475369343	6.89017518174037
C	13.08692991158387	4.04138680965796	6.80637326179856
C	11.78713669455373	7.24786393679725	5.16442075556341
H	12.38365749199004	7.61680541828957	4.32844656334200
H	12.09710536729655	7.77356184322297	6.06333387501908
H	10.74929963646690	7.48854735320730	4.94701118309078
C	13.86257190593638	3.92189695812293	8.09314948623431
H	13.35548473901192	3.26484531723864	8.79691381077729
H	14.00661491240865	4.89648208600484	8.55076460819828
H	14.83889113027612	3.47914460767160	7.89681937737225
C	10.31779813548985	5.39139129006745	3.62483357258429
C	10.59928712002026	5.90266221251325	2.34627244631097
C	9.53272495308518	6.33275906730550	1.55511516696895
H	9.73563121241601	6.73561566213003	0.57184356879499
C	8.22598585454348	6.26246125494414	2.00569382643132
H	7.41430558722731	6.60959573044986	1.37977951911442
C	7.96015542860682	5.73157267233524	3.25938163241789
H	6.93705941457420	5.66329954115803	3.60024483704532
C	8.98836307583148	5.28047952334348	4.08356681798268
C	12.00924581234418	6.00149648776404	1.79524066589288
H	12.70178454915453	5.69113848105536	2.57375477317079
C	12.36747326406126	7.43442828997314	1.37936125384638
H	13.41903825732591	7.48943795898311	1.09389516214405
H	12.19664906837141	8.14545217199137	2.18781476647377
H	11.77579062178589	7.76331942231447	0.52323007177946
C	12.20198601192459	5.03894160006368	0.61710664064222
H	11.53071724618983	5.28825729701698	-0.20729626959292
H	12.01125188154700	4.01312791364720	0.91899587921005
H	13.22774651841614	5.08897147720438	0.25003444796871
C	8.67305352926778	4.72680892562390	5.46159682865426
H	9.50356619372989	4.08405749576393	5.74533309459345
C	8.58969521344181	5.85006236702507	6.50512762218466
H	9.53134693380111	6.38855887856732	6.59627503750911
H	8.34539758826004	5.43867144906132	7.48527678462693
H	7.81276423005413	6.56763883040179	6.23441212107305
C	7.40258984085658	3.87362114711626	5.49057438860821
H	6.50439130853895	4.47433133224587	5.33962852201555
H	7.30594272127179	3.38917136057731	6.46186727869333
H	7.43134862702908	3.09526099521435	4.72943798569724
C	12.76044293798604	1.66754399222064	6.88635948362138
C	13.93737614223391	0.91058297359334	6.78650718288354
C	14.00888055838556	-0.29153027606909	7.49001958206825
H	14.90593404657885	-0.89129112056915	7.41888248969970
C	12.95040374430397	-0.73649345622227	8.26154153668995
H	13.02433942152109	-1.67347381627422	8.79703026126758
C	11.77640908277958	-0.00159100056308	8.30892864070594
H	10.93343536488318	-0.38757540315814	8.86194233317404
C	11.65093027700668	1.19677270563960	7.61336258511578
C	15.09892978409690	1.31818774038790	5.90009941987208
H	14.89969838943924	2.31351651044238	5.50993834399829
C	15.19739928383226	0.37053529361648	4.69624932386204
H	14.24952809677799	0.31263809993898	4.16513787754125
H	15.45650898775064	-0.64005583504706	5.01819237040091
H	15.96137461970992	0.71779216329219	3.99930040912806
C	16.43272021647025	1.36803008620892	6.65581956348767
H	16.73279950636339	0.37892910409388	7.00522103324020
H	16.38130529335461	2.02211209926011	7.52717117752197
H	17.22132463617286	1.74049089640812	6.00000978621121
C	10.33404068411698	1.95307954060598	7.62024291513261
H	10.25996677528232	2.46123724801196	6.65826319997104
C	9.12169336465029	1.02847444920897	7.73061490319666

H	8.20620504549049	1.59861811290907	7.57269920769173
H	9.04732638391627	0.56754361165819	8.71561805294828
H	9.16573944754301	0.23469737986771	6.98683785120152
C	10.28926857503999	3.03485831357346	8.70737015198332
H	11.05118112369070	3.79805600985136	8.55930103385110
H	10.43858415174553	2.58974167764066	9.69294005585234
H	9.31769266402163	3.53174697721755	8.70729211598305
C	7.45239161983408	-4.32661133011965	4.01819758757952
C	7.75677084234257	-4.91381693172713	2.78463091254046
H	7.15392338570893	-5.76666080874331	2.51542775042029
C	8.83216802562826	-4.64594580428484	1.92473936188045
C	6.34488826244249	-4.96034046167617	4.82226203885971
H	5.46356765901114	-4.31757876083568	4.79150455058006
H	6.62083580291327	-5.06744359296008	5.86895429799326
H	6.07722472727952	-5.93340862589776	4.41931599683298
C	9.04199864020558	-5.63204991162639	0.80142338903622
H	8.65847276297597	-6.61159507076973	1.07592270434758
H	10.09098418177390	-5.71888979596640	0.53100564289744
H	8.50263692230321	-5.29554866300899	-0.08421494033297
C	7.93592987161888	-2.89776418660840	5.88343059307906
C	8.85883903510235	-3.41510387968470	6.81224727403442
C	8.71783268530214	-3.06823432806730	8.15313129141138
H	9.41320749914428	-3.46306312854779	8.88069976418526
C	7.70560373294466	-2.21774911608689	8.57041111366079
H	7.61079472645688	-1.95782402358304	9.61666626000577
C	6.83168712752649	-1.68444313297021	7.63879635014066
H	6.06249541053701	-0.99646255334352	7.96297390172310
C	6.93319638096689	-2.00182866127939	6.28485404148625
C	9.97498022288402	-4.35080820656856	6.38213386632961
H	10.09962887384415	-4.22985007409244	5.30830893899003
C	9.60151806754889	-5.81849901592972	6.63100479482780
H	8.70159542428544	-6.10100442057693	6.08613023922720
H	9.42138402519597	-5.99569618774057	7.69326426199582
H	10.40877900849376	-6.47909378064274	6.30924939698267
C	11.31572812303802	-4.01113599725859	7.03770731107213
H	12.10259653181001	-4.64302245046153	6.62390410127867
H	11.29669620862895	-4.18346639450523	8.11511773428788
H	11.58407857339920	-2.96989715180476	6.86212474225870
C	5.99663873227250	-1.33957183875683	5.29308325098223
H	6.18898010477777	-1.76438102929874	4.31062996883996
C	4.51945879439057	-1.57260254298115	5.63091867366877
H	3.88433271485566	-1.13757578921752	4.85733977657828
H	4.24777495950725	-1.10864188818344	6.58069689917789
H	4.28477033591494	-2.63525644101933	5.70424005113134
C	6.29941704295817	0.16176189768338	5.19883674848854
H	7.34769464098127	0.33454233972320	4.96368855867835
H	6.07516058890350	0.66641166359748	6.14072805489358
H	5.70145445430004	0.62106042327547	4.41074493046524
C	10.78793307240672	-3.43784884799244	1.20649565506696
C	12.05882325273578	-3.75858100762104	1.72929478628720
C	13.17788532899375	-3.56120796934569	0.92616029607664
H	14.15792959007493	-3.80259229635580	1.30988743365788
C	13.05933227101062	-3.05177217809213	-0.35921862998758
H	13.94150485369955	-2.91053272817807	-0.97045722680636
C	11.80866614604430	-2.72474616214759	-0.85243671478826
H	11.71864369021593	-2.32799048259861	-1.85521056535212
C	10.65484080364785	-2.90403099609059	-0.08726967047122
C	12.20604806439558	-4.34813217926111	3.12162469164652
H	11.42741529036861	-3.90093538548084	3.73738168442536
C	11.96729365004119	-5.86494911384711	3.11736777100132
H	10.97352855913829	-6.11727115041656	2.75302128222757
H	12.06218117541907	-6.26531159247615	4.12821387420824
H	12.69964317189498	-6.36852309141903	2.48309009031952
C	13.54374219648415	-4.01718464799437	3.78458969574730
H	14.37813793914303	-4.52604254409313	3.29852960636513
H	13.52773229129066	-4.34294090543882	4.82446971615952
H	13.72916937009978	-2.94366613667803	3.77332774101959
C	9.31585268756304	-2.51123117866223	-0.68691861950964
H	8.53652134225722	-2.74848463426664	0.03349097959556
C	9.02483162950499	-3.26796770697702	-1.99101504334359
H	8.01176108749832	-3.05050765210191	-2.33368486945082
H	9.11986952311806	-4.34639395852930	-1.87036965633195
H	9.71230443800984	-2.96716637111777	-2.78360826897071
C	9.25102325589146	-1.00055193508967	-0.93659539074049
H	9.99194726206536	-0.69661230361064	-1.67759824830466
H	9.42532920022347	-0.45125243960537	-0.01647615486677
H	8.26384077661539	-0.72096131216375	-1.30872872231070
C	10.67060085449542	1.63223216940580	1.48556129914413
C	10.43166996746823	2.21607675936986	-0.68134342533204

C	11.60682580428085	1.54061108951252	-0.56005447141527
C	8.56513401243340	2.81082397511398	0.91622917208222
H	8.17331586804626	3.32690746242520	0.04646518362142
H	8.65221188294282	3.52160212521742	1.73118309555463
H	7.88849347682580	2.00736736782803	1.20344747890553
C	12.84608426104140	0.41641388133765	1.30360588138967
H	13.05330458263690	-0.41300766233715	0.63261634645728
H	12.56532695592478	0.00800543583415	2.27178232497139
H	13.71684456166962	1.05779721782366	1.41235666058136
C	9.78290966648052	2.81333291967945	-1.87566239439910
H	10.42402392249081	2.69090015632321	-2.74573567276530
H	9.60113530568446	3.88208164551546	-1.74564215986221
H	8.82725322694131	2.33393520811314	-2.09773510653597
C	12.63244672357534	1.17850410126832	-1.56994146162934
H	12.36273258754542	1.58217670304035	-2.54323017787522
H	12.72753559460752	0.09531550365869	-1.66725160658517
H	13.61388497075097	1.57310260471272	-1.30076462617183

Table S34. Compound **2b** B3LYP-D3/def2-SVP

Electronic energy ... -8187.01114953 Eh

Final Gibbs free energy ... -8185.60436412 Eh

Gibbs free energy minus the electronic energy ... 1.40678541 Eh

Sb	7.16928615900190	12.12623634492173	1.34066645104330
Sb	4.60792675515768	11.72068419332749	0.34536221970275
Ga	6.51933889701778	13.04568271734368	3.71591612655768
Ga	5.68648810252729	10.92335138421392	-1.85599956806422
Cl	5.82865792120101	15.18818521105678	3.99301963003860
Cl	7.95578804757401	11.07530619537862	-2.19170648163696
N	8.01160989453384	12.98787904140000	5.03103521781961
N	5.24419202361845	12.03348412820125	4.83224842663426
N	5.40695188554376	9.02044345795190	-2.43613101936110
N	5.06707836628482	11.68101498903897	-3.61418024672859
N	7.02885196196144	15.34576218368522	0.43514022913909
N	9.04988791605264	14.58998498646467	0.48777939967906
C	7.73786731971283	12.91928482008916	6.33667565782692
C	6.47189942931394	12.58367478589283	6.85013989669011
H	6.38718588930255	12.59924773572373	7.93546767140814
C	5.34855335539080	12.07887674480605	6.16217385137533
C	8.82843444721912	13.22227760816942	7.33750362594584
H	9.79680129450258	12.80918091960764	7.02565386157131
H	8.57260264063767	12.83561079138648	8.33198434811500
H	8.95646185104932	14.31386650600561	7.41493128047963
C	4.21447874802508	11.53986328589105	7.00129799143472
H	3.31710075678948	12.16211064208953	6.86961985181649
H	4.48214248770953	11.52371827345523	8.06495736054632
H	3.93871984648726	10.52477479082816	6.68164840236143
C	9.35963501108468	13.09890266422313	4.55847235547271
C	10.03685502482168	11.90685614845490	4.19583010855917
C	11.35626233352226	11.99941217640993	3.73406933776978
H	11.89284821307496	11.08951169068756	3.45995308221262
C	11.99678475704149	13.23339872081082	3.62643845701032
H	13.02933366140162	13.28607081862427	3.27155814914576
C	11.31128069351764	14.39757005732515	3.96334919071263
H	11.81306411600176	15.36352053871166	3.86846771189882
C	9.98714341331557	14.35941228278889	4.42670798083419
C	9.37781168745773	10.54491666844551	4.36568376960156
H	8.29171719626152	10.70701191932017	4.35246928356011
C	9.71125178466200	9.56581083132896	3.23512835664358
H	9.48443733459247	9.99949918562099	2.25026184319237
H	9.11354742391313	8.64824394678813	3.34414534443126
H	10.77087152442206	9.26359550869910	3.24712808184797
C	9.72361632847124	9.93816610546394	5.73630420580774
H	9.24587800257360	8.95275397211807	5.85517622803358
H	9.38028968912851	10.57611078983545	6.56316055806734
H	10.81303958661267	9.80401298538767	5.84099038137892
C	9.28477536092879	15.66551427201955	4.77113338235430
H	8.30147163188017	15.42176930677549	5.19453398074412
C	9.02346315728813	16.50008650200833	3.50819046117832
H	9.96700130319244	16.77854628583696	3.00948691626882
H	8.48674208483851	17.42696800203334	3.76516321292601
H	8.39896194882150	15.94870249605012	2.79580438990057
C	10.06640580437084	16.48441637455126	5.81063860644233
H	11.02236156918956	16.85368050725376	5.40442830818352
H	10.29859836165636	15.89188125343257	6.70909668640658
H	9.48070577180627	17.36383810149094	6.12317529063640
C	4.14036434382370	11.34079950941591	4.21993558188476
C	4.34666844984491	10.01324257399170	3.77578439488322
C	3.26185205090905	9.31895288659877	3.22862039180348
H	3.40148945324949	8.30153665011761	2.86306221158946

C	2.01302087221208	9.92451012569935	3.10121393711025
H	1.17823008595488	9.36835545285025	2.66873898275289
C	1.84418665533154	11.25216128247965	3.48242427639792
H	0.87580740750783	11.73534318831919	3.33447839519609
C	2.89949390057154	11.98905120164885	4.03848446448074
C	5.72236469846479	9.36488431993581	3.85880824419017
H	6.45701995066720	10.17052464644556	3.70262516609575
C	5.95425507451689	8.32764069481889	2.75876361741848
H	5.34910448778373	7.42204711845348	2.91359052931114
H	7.00812947058895	8.01261290462526	2.74895889273134
H	5.70895338170552	8.73413305806610	1.76686059610363
C	6.00739660980964	8.76279032427526	5.24451379870002
H	5.24619067223006	8.00817421248739	5.50240628418811
H	6.01799116026952	9.52494496333602	6.03630770603078
H	6.99064264888345	8.26506058384504	5.25152467825782
C	2.69604890728251	13.46374831906694	4.35401759465186
H	3.58989835398366	13.83035698465523	4.87570349868432
C	2.58309071719856	14.26617210502759	3.04675130197400
H	3.42969583409737	14.05288106345947	2.37998101792377
H	2.57443284018549	15.34770492745206	3.25521713666548
H	1.66100526986047	14.00588182670020	2.50098419053882
C	1.48327861853255	13.72445350903803	5.25893888557446
H	1.42481378671310	14.79357778253475	5.51972861705238
H	1.53823018640658	13.15023928377856	6.19775656311207
H	0.53700038062997	13.45473684210427	4.76264361540920
C	5.46484725430849	8.67074043895793	-3.72099301935032
C	5.43355909291709	9.59196353431116	-4.78525461163783
H	5.51457000431166	9.16091222868726	-5.78164943812114
C	5.15112492605788	10.97028949008635	-4.74110663654022
C	5.54871316726946	7.20536059071772	-4.08337839669946
H	5.45967170933210	7.05947538147433	-5.16710798445234
H	4.76719353834659	6.62288870406060	-3.57528381412597
H	6.51156062624900	6.79138487127710	-3.74836274840059
C	4.90719935469404	11.65633837223013	-6.06695688893308
H	4.86247594110035	10.92665517968909	-6.88497866931597
H	5.71144345390527	12.37527851635983	-6.28086307517530
H	3.97101373434230	12.23274944003947	-6.04812550986850
C	5.21008447025958	8.01599422561605	-1.43285518134752
C	3.88907608175682	7.76474387195047	-0.99179827455979
C	3.67925965968919	6.75122487230185	-0.04841666559983
H	2.66379414247122	6.53637710005019	0.29128033869838
C	4.74486989456119	6.00769882837944	0.45680863193943
H	4.56348895611563	5.21489553387998	1.18721267023065
C	6.04345057806169	6.29482693538164	0.04391160035405
H	6.87848216079055	5.73167263545743	0.46679766930639
C	6.30497462828480	7.30455039177126	-0.89279520189281
C	2.70868950880350	8.54017957696295	-1.56030904374029
H	3.11608632380289	9.44581039621210	-2.02934154968598
C	1.72273711645029	8.99316391527141	-0.47812329551199
H	0.93439502679788	9.62221579509666	-0.92098593560041
H	2.23607643324053	9.57913169229057	0.29837785162364
H	1.22061810188882	8.14052471229466	0.00764521815058
C	1.99718546411588	7.74322456288990	-2.66601468502449
H	1.15206297847037	8.31921934642253	-3.07688490176258
H	1.60128879801193	6.79171257265061	-2.27351719080670
H	2.67754040730522	7.50952230265471	-3.49827835749177
C	7.74528076488216	7.62961889057351	-1.26336565772434
H	7.73023757008893	8.35102889793936	-2.09075076675755
C	8.53623105662978	6.39534001184156	-1.72136338900453
H	8.03651078881726	5.86915719252003	-2.55039038276842
H	8.67092611580760	5.66853835517643	-0.90338880562303
H	9.54040761115467	6.69203251626706	-2.06517723826092
C	8.45518897510274	8.32228607094251	-0.08939048901106
H	9.46053718088213	8.65803288366004	-0.38876501271439
H	8.55854911688159	7.63848135335225	0.76921153943912
H	7.89822040423271	9.20815162267142	0.24434652538496
C	4.61928650296820	13.04077911917484	-3.67307233162569
C	5.50589827535453	14.08162562474824	-4.03416669281975
C	4.98827808625166	15.37758876170292	-4.17334765876845
H	5.65768574258576	16.18984549397489	-4.46640405980258
C	3.64547165622377	15.65140837820433	-3.92994873552095
H	3.26085683842817	16.66780723886360	-4.04781368008864
C	2.79974615620071	14.62901395995022	-3.50133204779113
H	1.75695226159486	14.85594891788844	-3.27441795328357
C	3.26654662858284	13.31677874240893	-3.35717643190314
C	7.00228213394745	13.85683553909624	-4.20492149343826
H	7.19115977456466	12.77534978435816	-4.19973380138081
C	7.75661561622537	14.43943987953445	-2.99771209819277
H	8.83405860311782	14.22477720744809	-3.07409633967535

H	7.39820099241425	13.99525670881093	-2.06013679334346
H	7.62359459838965	15.53243557711070	-2.93839807649488
C	7.55546852895461	14.43364934584014	-5.51592581943774
H	7.00934702981124	14.05685121488237	-6.39511930273180
H	8.61637805124668	14.16001824392083	-5.63415373896671
H	7.49657700496097	15.53427505480434	-5.53877850750442
C	2.33303863586641	12.20909451627335	-2.88886506717611
H	2.96017860843383	11.46952549375919	-2.37132866131478
C	1.29092627582132	12.69247621732318	-1.87436842390780
H	0.53727393937890	13.35314268002011	-2.33346818901890
H	1.77082901142899	13.23026576636049	-1.04233156323847
H	0.75218262552399	11.83094887718587	-1.45095455312971
C	1.66492392131981	11.48862285446561	-4.07096422551229
H	1.08354953945497	12.19782564593056	-4.68343348827238
H	0.97576050361732	10.70812308437165	-3.70991939585775
H	2.40412157847220	11.00002933418210	-4.72212038752227
C	7.76284996446410	14.25099506169352	0.73867275587188
C	7.85067328977144	16.37950385900689	-0.01040595959158
C	9.13393112890835	15.89763203275216	0.02054134918664
C	5.57502686450040	15.46134057206233	0.60448019674166
H	5.38736092716889	16.34139471956149	1.23599978073754
H	5.26255839854812	14.58634206400911	1.18109897270649
C	4.80991489741261	15.50615948887300	-0.70533289987912
H	5.07462334970122	16.36867019999221	-1.33149376467703
H	3.73326347323541	15.56182684891978	-0.48706047835140
H	4.97325162646386	14.58397606929699	-1.27767874238222
C	10.20564966082137	13.71342718247534	0.69710478199216
H	9.93463492903734	13.00767146875078	1.49177553851110
H	11.01653715697342	14.33380803558094	1.09977408812080
C	10.63167133339480	12.97069967424347	-0.56119107818655
H	10.92723300137231	13.66519674057328	-1.36332230327262
H	9.81676268996177	12.33705527747410	-0.93953098121272
H	11.49571534803536	12.32805530678379	-0.33084230803278
C	7.34311468423013	17.72299278586703	-0.40631284090707
H	6.84428902509102	17.70050164656283	-1.38891866953589
H	8.17377065558002	18.43917628285683	-0.46637577141454
H	6.61629617937447	18.11017472158422	0.32432244756219
C	10.42588518402916	16.55967773420922	-0.31086163159482
H	10.96262550700457	16.03363208518129	-1.11652321158897
H	11.09615555676501	16.59952549459255	0.56411602366460
H	10.24977588713678	17.59104838346961	-0.64413542069442

Table S35. Compound **2b** B3LYP-D3/def2-TZVPP
final energy -8191.037933160827 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -8181.007341632433

Sb	7.20400704405332	12.18780984409457	1.32096984407372
Sb	4.66920281250607	11.72711273610562	0.31751563742890
Ga	6.54669063051214	13.07225450066547	3.70626337543969
Ga	5.73625477542906	10.89211480659368	-1.87298073925970
Cl	5.89867442665915	15.22246474038649	3.99004006466725
Cl	7.99202476792940	11.04395002897404	-2.24325338099435
N	8.03248664879071	12.96691788508868	5.02400585400204
N	5.24629220371398	12.07749485205015	4.80531477019015
N	5.43211031550310	8.99231323088966	-2.44524080386554
N	5.07251905198308	11.64647591065390	-3.61524995714035
N	7.02503024512121	15.39176927050963	0.44985504100724
N	9.04520026588855	14.65982598050616	0.49567861169251
C	7.74859204330340	12.88490685665046	6.31966707103605
C	6.47739124503744	12.57952491388598	6.81927298925330
H	6.39087539709030	12.58575624122069	7.89390331051873
C	5.34769866048198	12.11542412094539	6.12929485811083
C	8.83291536926965	13.13640756155007	7.33656166353035
H	9.79813775573976	12.76534456066607	7.00217429359237
H	8.58245089104207	12.68060823338941	8.29071128863771
H	8.93611257901962	14.21189670874561	7.48979945926953
C	4.19624448860475	11.62450866699764	6.96840125635735
H	3.38383639290782	12.35103408748364	6.93320615102716
H	4.49912794078651	11.49316025213464	8.00338946490436
H	3.79737262582578	10.68705454463980	6.58718241839596
C	9.38597265442844	13.07506089510608	4.56548296142952
C	10.04933169827619	11.89385690826007	4.17516938262535
C	11.36666154513181	11.98585084061337	3.73215241478534
H	11.89204877425419	11.08879703634475	3.43786120063901
C	12.01772210375361	13.20863687618621	3.66791190150851
H	13.04428397252827	13.25951887509169	3.32920912791951
C	11.34496811173830	14.36285285173065	4.02961434733133
H	11.85292415486428	15.31611774957366	3.96933599650945
C	10.02344584993564	14.32480306270443	4.47672183561362
C	9.37558091933620	10.53891869257258	4.29106783415599

H	8.30185848401125	10.70636547574350	4.23896105107357
C	9.74430344454295	9.57930959093870	3.15911860138237
H	9.56280927905635	10.02711195349889	2.18345674013450
H	9.13821769001394	8.67650167949940	3.23113204718949
H	10.78927545820917	9.26973685388066	3.20944158175082
C	9.66614315382886	9.89875540882468	5.65640960925420
H	9.17257504356496	8.92922322812660	5.73273883471114
H	9.30970381431972	10.51888097302870	6.47694811567576
H	10.73901693214487	9.74550051170764	5.78843065334883
C	9.33425488291496	15.62600773935890	4.84430932580324
H	8.34943634286805	15.38971248019446	5.23964169310998
C	9.11830344293235	16.49895257538858	3.60160590201532
H	10.07198202915272	16.77753963558056	3.14792356878377
H	8.58959988863640	17.41432032407049	3.87024417520386
H	8.51842562929221	15.98016308232691	2.85963017165640
C	10.10649744607535	16.40635542839199	5.91631189482725
H	11.06501717588402	16.76557671675338	5.53785524455750
H	10.30969374272708	15.79489029776144	6.79537331042300
H	9.53046722609065	17.27701316068588	6.23316870630223
C	4.13568503954623	11.40223526633367	4.18490376484722
C	4.31975663646174	10.07226102930862	3.76473306456660
C	3.23865274464424	9.39977970021768	3.20417480773941
H	3.36311913517215	8.38498924510105	2.85736727025633
C	2.01533482177971	10.02948173670908	3.03733053563505
H	1.18834701843824	9.49534069659222	2.58962236509978
C	1.86815920119908	11.35573195791591	3.40207003476390
H	0.92377316048797	11.85339526912055	3.22839484545627
C	2.91973971367854	12.06962335300772	3.97610783905398
C	5.66925373834449	9.38953737788473	3.89450377001750
H	6.42608773386239	10.16743907258389	3.78844288002707
C	5.92112324796872	8.36159442370989	2.79306414888996
H	5.29835966651565	7.47579414707681	2.91469810899256
H	6.95897850601805	8.03054159349693	2.82343729999906
H	5.72465096665161	8.78086200328631	1.80763496993085
C	5.86689388537879	8.75547789829632	5.27852028377213
H	5.08502399777047	8.01948747571510	5.47526583794701
H	5.84622332451957	9.49596846134405	6.07609972603586
H	6.82967657208216	8.24372897470695	5.32648132428050
C	2.73072202412022	13.54041413981232	4.29387960991231
H	3.61704501101820	13.89511856430844	4.81438784925250
C	2.61764444792453	14.34794806286401	2.99314208768555
H	3.44573772041332	14.12625139163963	2.32372197285819
H	2.62506372244759	15.41749875585777	3.20662307001673
H	1.69425456922155	14.10512955126612	2.46367067537863
C	1.51807492360681	13.80416177733437	5.19428048052158
H	1.47240169520553	14.86126455735278	5.46134564757920
H	1.56230145746215	13.22409363122470	6.11684782437453
H	0.58347718480109	13.55034517039343	4.69180645160301
C	5.47573605243950	8.64931000504513	-3.72602660458642
C	5.43320012307673	9.56789748716674	-4.78200012010083
H	5.50586902179663	9.14242647674896	-5.76965729411358
C	5.14381438457476	10.93747565869014	-4.73605429930720
C	5.55549064304652	7.18942291815888	-4.09713322522018
H	5.44937596696019	7.05564006662189	-5.16997113838886
H	4.79041460060501	6.60758806207671	-3.58656076353697
H	6.51755769336351	6.78219529332371	-3.78582494213363
C	4.87576223059405	11.61263228656139	-6.05897470984762
H	4.80846495692968	10.87996404749095	-6.85824916729388
H	5.67629912010223	12.31308190906772	-6.29478326015234
H	3.95318589143915	12.19002122792092	-6.02615455589149
C	5.23155118336740	7.98108708197887	-1.44897976659047
C	3.91590179095882	7.70835681085934	-1.03378734947909
C	3.70929077879882	6.69774025742550	-0.09774296843808
H	2.70203000981055	6.46663495629707	0.22149158775605
C	4.77215067657809	5.97972775881149	0.42697653031546
H	4.59402746715516	5.19523222077519	1.15085175011819
C	6.06467625916147	6.28403947072871	0.03422510504792
H	6.89331030352165	5.73910225628433	0.46575440236093
C	6.32200522808571	7.28751653886567	-0.89833376907102
C	2.72819286081926	8.45934415563045	-1.60849963212985
H	3.11825341769629	9.31683833697885	-2.15214197918166
C	1.79877199988884	8.98950504129605	-0.51404047522014
H	0.99158912379460	9.57485364669979	-0.95576296457621
H	2.34322223992521	9.62425645769225	0.18364755894404
H	1.33899237703515	8.17768153980993	0.05183944220099
C	1.95387988962919	7.59760487760960	-2.61479301491635
H	1.11735785140249	8.15964528477781	-3.03365556911107
H	1.55316682341522	6.70322829831652	-2.13357091990779
H	2.58808940228811	7.27737192711241	-3.44122346549954

C	7.75778984646020	7.61888821937708	-1.25950456396789
H	7.74683855952779	8.32845882341393	-2.08294496990960
C	8.55777084681564	6.38838556077143	-1.70404213335218
H	8.07108679430121	5.86086805078997	-2.52544042185039
H	8.68778705011071	5.67640349706066	-0.88713544177959
H	9.55162792650418	6.69060526653221	-2.03823274583087
C	8.45569129375721	8.31127720622117	-0.08238161380425
H	9.45755750088948	8.63242748732603	-0.36983636951773
H	8.54137682182164	7.63398011440277	0.76938804609878
H	7.90551355374617	9.19329545777977	0.23862368353120
C	4.60602731313202	13.00006715103681	-3.67258322337601
C	5.47185030087502	14.04377084219260	-4.04223174638835
C	4.93998410208702	15.32529693850806	-4.18324046100721
H	5.58982705734998	16.13724738657042	-4.48103214805999
C	3.60262397443272	15.58087885215899	-3.93557237468492
H	3.20761411727189	16.58120928702825	-4.05598534656839
C	2.77853501407246	14.55577555951550	-3.49652895178786
H	1.74563938565814	14.76997696223017	-3.26354081123503
C	3.26098647027633	13.25822759398048	-3.34660455301878
C	6.96486953175485	13.83792224649795	-4.22238654860184
H	7.16709886792644	12.76964544301900	-4.22476336334915
C	7.71650854614296	14.43101173343095	-3.02156316366954
H	8.78597136865255	14.23640314052744	-3.10869984109284
H	7.37466050681817	13.98572238675452	-2.09034768221062
H	7.56411475745909	15.51080334391676	-2.96445671476849
C	7.50354188606662	14.42828419026759	-5.53036314611245
H	6.95779378916130	14.05874868444750	-6.39909860828527
H	8.55440982579714	14.16196847978823	-5.65403187604262
H	7.43795186240695	15.51765933586257	-5.54010712037191
C	2.34688389333756	12.14950663051472	-2.85608619958937
H	2.97965682614546	11.42036167621580	-2.35239750402350
C	1.32350899254128	12.63510470060222	-1.82700569194838
H	0.57160264153451	13.28842489061354	-2.27282777622587
H	1.81340999720041	13.16925012928428	-1.01316471682568
H	0.79769154695072	11.78239795614599	-1.39815105427197
C	1.65415529844185	11.42544170257722	-4.01826843639766
H	1.05441466597617	12.12414076626241	-4.60503250636828
H	0.99115220361708	10.64586559933785	-3.63951775483995
H	2.37430365657164	10.95204558646869	-4.68414741144781
C	7.76590732384421	14.30356030732198	0.73861634937972
C	7.83631131086991	16.43846358412331	0.02507105273747
C	9.11532413133240	15.97281089484901	0.05051634376042
C	5.57084121530895	15.48784319731523	0.61495662349568
H	5.37006116860593	16.35651486638285	1.23903480270217
H	5.27092791863245	14.61270437641788	1.17760654494331
C	4.81575356483897	15.53262865104253	-0.69795517279641
H	5.08043373736322	16.39224359753286	-1.30926925341359
H	3.74796346114991	15.58291512105304	-0.48764455770517
H	4.98938226423536	14.62378857792499	-1.26752483113732
C	10.20893496030029	13.79291973573492	0.69474917523986
H	9.95203111451682	13.08783536506037	1.47962576138417
H	11.01290572385163	14.41331490895966	1.08270507561082
C	10.61993291101528	13.06160103521815	-0.57218265247251
H	10.88452234690255	13.75881475873165	-1.36757374041103
H	9.81354274379738	12.42470225112744	-0.93094132443943
H	11.48882963613852	12.43611978057671	-0.36485556919199
C	7.31790572712833	17.78438408682319	-0.33151635154275
H	6.80455390416154	17.78282766154745	-1.29419283619373
H	8.13879639951168	18.49569381207951	-0.39032847074758
H	6.61382457779462	18.14900655268774	0.41716588524405
C	10.39689254435385	16.65071021828842	-0.27070415451998
H	10.92672233430266	16.15298433175155	-1.08445211721913
H	11.06454986766612	16.67564366126678	0.59312673574122
H	10.20985881606384	17.67765770668086	-0.57583979563565

Table S36. Compound **2c** B3LYP-D3/def2-TZVPP

Electronic energy ... -8265.53141030 Eh

Final Gibbs free energy ... -8264.06896595 Eh

Gibbs free energy minus the electronic energy ... 1.46244435 Eh

Sb	7.34626388320602	12.32544196236396	1.37801414569257
Sb	4.82579930540438	11.68373116812682	0.44237145046372
Ga	6.56126595723511	13.03941827610181	3.78640242173909
Ga	5.80683076652886	10.90919820545822	-1.82124734675445
Cl	5.86443884143869	15.14987776354219	4.23625744475094
Cl	8.05433568972436	11.03324048064331	-2.25134299882845
N	8.01115061637384	12.85599451106175	5.13400792851947
N	5.22003048901099	12.00663402172397	4.81660347939272
N	5.46067523057769	9.01568105672625	-2.38887820466615
N	5.10286229084538	11.66426107926046	-3.55488675767172

N	7.06757018911641	15.52116486298936	0.28494465267781
N	9.11422107582901	14.80804344905931	0.24519233033119
C	7.69301555717472	12.74571049397986	6.42712846437553
C	6.39455935336479	12.46281454459558	6.88919305820861
H	6.27346229384007	12.45542618947645	7.97099911290674
C	5.27311584770357	12.03316186148085	6.15106062213948
C	8.77194428688125	12.92478323559235	7.46932959569624
H	9.67004481968405	12.34252445051556	7.21949445458776
H	8.41464695509239	12.62658159138266	8.46272231962119
H	9.08238358363882	13.97975026952910	7.51079025287518
C	4.06996820043144	11.57179368196675	6.93957686846644
H	3.24795222125458	12.29294918926063	6.81190444231712
H	4.30433601242805	11.49101840134269	8.00819323576289
H	3.69568497705301	10.60494148366082	6.57605746071777
C	9.38098995037700	12.98346930217823	4.73272485071849
C	10.06384486732776	11.82178633415178	4.29619332581892
C	11.42046495590665	11.92942825812648	3.96290424972609
H	11.96554633589228	11.04190326981369	3.63872557418681
C	12.08828759196889	13.14988682099905	4.05246348191634
H	13.15230752029851	13.21148064687629	3.80958709734893
C	11.38993392391025	14.29354551390391	4.43078724349747
H	11.90924821948323	15.25386998330762	4.46295695902163
C	10.02831945486253	14.24114393347965	4.76000151868889
C	9.35725202452502	10.47532684548633	4.23081942183035
H	8.29882354664800	10.68235090017956	4.01843888610737
C	9.87492874484782	9.57487000655842	3.10537463107804
H	9.86086888826626	10.09512148032791	2.13600857001212
H	9.23497162243509	8.68529685371776	3.01567933227991
H	10.90019452478162	9.21911853718308	3.29690968213604
C	9.40966005353189	9.74470113644750	5.58275807825493
H	8.92853939215126	8.75699475347776	5.50529392404635
H	8.88835366526718	10.30495576645566	6.37137384902818
H	10.45342129388727	9.58996884740588	5.90273929319826
C	9.28845303767418	15.53170684811702	5.08289911091623
H	8.28718626477224	15.27077798670979	5.44883639732537
C	9.08662641741947	16.35884371115847	3.80181725053515
H	10.05190376900976	16.72062723222268	3.40930124750044
H	8.44829718580014	17.23315581094044	4.00284537258749
H	8.59666111150790	15.76279866771341	3.01932098388361
C	9.98665810567512	16.36831641393580	6.16452802947635
H	10.96272906082859	16.74993289322551	5.82302806116846
H	10.16346889070198	15.78648816471407	7.08283002826516
H	9.36867869645177	17.24101498685717	6.42996058007774
C	4.13401057406776	11.32566197721330	4.16183904651377
C	4.33042186449292	9.97520591051665	3.78873734226694
C	3.27035152967883	9.28643235041738	3.18952958497689
H	3.40791870887335	8.25019166603707	2.87851321829287
C	2.05168879328241	9.91854780695959	2.94899394113101
H	1.23412680154395	9.36836312785308	2.47849394933058
C	1.88906984483706	11.26068805441113	3.27966625910362
H	0.94324846143628	11.75848696670806	3.05440821621879
C	2.92013671802108	11.99134497721567	3.88728788767923
C	5.66383833803205	9.28388704082163	4.03099109305275
H	6.43308454240313	10.06960948137788	4.02885704781399
C	6.02235667427241	8.28893590211364	2.92539334021332
H	5.38589491882590	7.39209518229560	2.95504917171558
H	7.06251470144012	7.94770786796406	3.04318750740860
H	5.91729039568957	8.74330573141068	1.92991653414817
C	5.71464839860564	8.60850356680493	5.41195528954098
H	4.90095841900776	7.87133502845421	5.51317017410018
H	5.62213762323686	9.33399396920474	6.23254345677227
H	6.67016039803937	8.07631688987737	5.54610704019377
C	2.71354617717039	13.46930872791187	4.18254784022239
H	3.57568627782771	13.82789768391810	4.75985631537400
C	2.69007869545006	14.27471963199312	2.87363232099261
H	3.58755697951502	14.07425303295607	2.27263707723705
H	2.64701929689492	15.35499379832236	3.08528224193133
H	1.81707140687415	14.00448071392687	2.25664079142770
C	1.44883482131915	13.74031957067530	5.01069326242684
H	1.39121877299722	14.80728087641030	5.28057786189273
H	1.43496737073433	13.15338299757716	5.94296382960225
H	0.53212256436819	13.49218963552868	4.45153762286218
C	5.48963590750101	8.65859257154624	-3.67340720920332
C	5.42597823209911	9.57478788201721	-4.73825243681185
H	5.47461043976584	9.14266795035268	-5.73626228790851
C	5.13339632660772	10.95088519941525	-4.68281530385519
C	5.56363249619172	7.19095968068943	-4.02722444866847
H	5.49769706861340	7.04031931080765	-5.11194686930834
H	4.76246895836576	6.62130431694239	-3.53532472879044

H	6.51228584560108	6.76622815082605	-3.66572227138147
C	4.81152135583849	11.62640537901880	-5.99769898974291
H	4.70951489456493	10.88790420483089	-6.80251320359467
H	5.60470580394144	12.33634270257259	-6.27231324352566
H	3.88221607507849	12.20946045180416	-5.92513285223067
C	5.23214550445403	8.01897993414422	-1.38578842412275
C	3.89782994489564	7.76868464355856	-0.98878411428262
C	3.65992069525478	6.77029580821540	-0.03536666785491
H	2.63412488602235	6.55660749598649	0.27401626123889
C	4.71083514658422	6.04045953440794	0.51795877360253
H	4.50796351036550	5.26046671346045	1.25647149057948
C	6.02185474443348	6.31970968155973	0.13787511638991
H	6.84373523765917	5.76210882052572	0.59274477796571
C	6.31026268390670	7.31232788944948	-0.80824030948314
C	2.73150362967992	8.52949400538625	-1.60617767845652
H	3.15328440914901	9.37482438778673	-2.16584091665871
C	1.79100756902997	9.10850924733404	-0.54372869350071
H	0.99314204605071	9.70054877794944	-1.01862173103416
H	2.33708928109568	9.76118875454004	0.15276226691045
H	1.30168583645123	8.31638692853891	0.04580462854297
C	1.96382033065993	7.65968793802382	-2.61426170931691
H	1.14759278057336	8.23462340104437	-3.08135895524120
H	1.51898768484598	6.77911443783484	-2.12137157524296
H	2.62058883253688	7.29720641050940	-3.41930826395746
C	7.75708445835380	7.62362364985781	-1.16272178015950
H	7.75641827674891	8.32382139766868	-2.00818588353014
C	8.54691874088320	6.37510606724748	-1.58256372166324
H	8.05628337227114	5.83743729222901	-2.40978025525404
H	8.66201920876486	5.66390889115260	-0.74812933628518
H	9.55883819712346	6.65794893525994	-1.91503478153238
C	8.45365762562473	8.34109015834888	0.00309235445917
H	9.46076082201504	8.67380509663654	-0.29316614104484
H	8.55098973963139	7.67259225635612	0.87409737058278
H	7.89009394961991	9.23048550077047	0.31816254055351
C	4.67336570322842	13.03001592022633	-3.60454167534794
C	5.55821798432132	14.04534498608163	-4.03629474384321
C	5.06288485899912	15.35158500265820	-4.16095506961999
H	5.73019500955860	16.14438214501693	-4.50746995742163
C	3.74108917008411	15.65654213615487	-3.84768797947613
H	3.37039538410002	16.67869974699792	-3.96075016548506
C	2.89991890742310	14.65831695195802	-3.35738807073390
H	1.87652586018515	14.91137576176507	-3.07692781726102
C	3.34699415836998	13.33875013572812	-3.21596176304891
C	7.03222081184224	13.77624991968302	-4.30653774895268
H	7.19249295987679	12.69054283365816	-4.29564167304801
C	7.87743264293504	14.35907986154120	-3.16468916072334
H	8.93816381754988	14.09063165166555	-3.28815513889945
H	7.54939137432832	13.96762780157025	-2.19300770147260
H	7.79707048312918	15.45715657471777	-3.14264307625603
C	7.51352821916562	14.31974883061352	-5.65964181268606
H	6.90489704891255	13.94561020734151	-6.49774712556264
H	8.55790544576652	14.01774235454161	-5.83945708514872
H	7.48034354276494	15.42113554011006	-5.69496442107888
C	2.41891718850937	12.25834473303681	-2.67650728642938
H	3.05902692201163	11.52023550754679	-2.17219867276456
C	1.43921316079595	12.78431390120774	-1.62156471843435
H	0.68459186632964	13.46220986013777	-2.05281903068953
H	1.97495436820741	13.31432793056493	-0.81958382489854
H	0.89684088721332	11.94522880304483	-1.16104276540337
C	1.67973336397930	11.52494020656091	-3.80699621514008
H	1.06510662189914	12.22774573781770	-4.39383254543634
H	1.01187902359137	10.75193835088461	-3.39403936613608
H	2.37777473122644	11.02537240244186	-4.49424997963430
C	7.87051481243335	14.51571011773720	0.70867868455650
C	7.79431492084076	16.43892855525693	-0.47046339606385
C	9.08954273077990	15.98515663177105	-0.50137572081843
C	5.63393225072875	15.61825722303225	0.65103528844690
C	5.33323760134791	16.90495313598234	1.41784735174921
H	5.49056376876831	14.77632047789483	1.33724238793955
C	4.71784032075547	15.41004412879581	-0.54818696206301
H	4.71124757445794	16.27036245543076	-1.23046367979522
H	3.68988514691422	15.26140308578878	-0.18728776324058
H	4.99333422224783	14.50882212064273	-1.10926531424983
C	10.29888920001177	13.96249314891557	0.53087160844072
H	9.97779387940038	13.33117120682459	1.37152050271050
C	11.49656012749064	14.78037245329658	1.01165087626209
C	10.63464406785899	13.04969852705130	-0.64528172280220
H	10.98475722833769	13.62287484630973	-1.51818354744990
H	9.76665892769030	12.44982181643350	-0.95143110873120

H	11.44151200449975	12.36127828391383	-0.34926359117526
C	7.22632813712673	17.64490894688252	-1.14050874876995
H	6.32816735584591	17.39964261560063	-1.72441150270059
H	7.96713311877545	18.06577697393006	-1.83346187600062
H	6.95849412990627	18.43639660378502	-0.42387935870691
C	10.25063311056062	16.57284037716594	-1.23218914030320
H	10.81599323224377	15.80543085107002	-1.77946844855630
H	10.95150464745653	17.09880514196723	-0.56531781085166
H	9.88925128653662	17.30114639195612	-1.97067646804114
H	12.01705854893784	15.29034166645650	0.19033418893829
H	12.21318586564573	14.09787838815349	1.48708554100474
H	11.19601993730266	15.52102636942300	1.76489595223023
H	5.28612501229246	17.78258696510641	0.75679440357346
H	6.07355910697036	17.07593064849808	2.21001281735489
H	4.35337603168124	16.79903789063779	1.90447762256648

Table S37. Compound **2c** B3LYP-D3/def2-TZVPP
final energy -8269.643840829443
DLPNO-CCSD(T1)/cc-pVTZ single point energy -8259.482948055793

Sb	7.36417046134869	12.35343522477324	1.36575051540512
Sb	4.86408072989586	11.66743435281699	0.43119412547243
Ga	6.56824833773139	13.05236516520156	3.77559753772830
Ga	5.83025806846783	10.89689923634034	-1.83452581455706
Cl	5.87276417618955	15.16357543453673	4.18309138095727
Cl	8.06723606234502	11.00576652056533	-2.28471236046602
N	8.01488940946556	12.86413184732295	5.12566302851646
N	5.22630855713617	12.02788505133527	4.80862052797429
N	5.44794728004639	9.00902392542166	-2.39165551483296
N	5.10782746004033	11.65668497674178	-3.55825909616483
N	7.07319337564526	15.52984763902938	0.28739104602807
N	9.11397332546424	14.82542346936924	0.25232512552526
C	7.69388602881128	12.75048058711410	6.41086497897158
C	6.39975458491305	12.47793618357643	6.86828241319574
H	6.28108483535080	12.46830151223973	7.93963488436521
C	5.28166436098235	12.05631844327549	6.13638143129445
C	8.76268722384409	12.91255005661224	7.46179910573719
H	9.68857887320548	12.42175216116528	7.17060102703816
H	8.42922043078571	12.51144538366262	8.41485292937417
H	8.98977087163096	13.97082112444414	7.59592843668988
C	4.08169938388156	11.61104598210551	6.93285918136437
H	3.31538082472535	12.38652495916914	6.88627893268527
H	4.34546627846434	11.44878640603732	7.97419589628254
H	3.63943297116407	10.70465882606252	6.52716058076982
C	9.38690286979985	12.99128170613834	4.73211946530473
C	10.06565442839606	11.83951418546357	4.28933458860051
C	11.41691604486542	11.94898352619864	3.96841732077535
H	11.95820807691621	11.07442742028272	3.63878209772899
C	12.08204263822604	13.16090678872136	4.07365351263378
H	13.13646260713280	13.22291917337912	3.83795243602411
C	11.38717737248672	14.29472892394262	4.45738738326628
H	11.90267551223735	15.24438140414460	4.50275931455523
C	10.03137764760723	14.23993357488728	4.77747788169911
C	9.36023120706741	10.49834726221266	4.20081596665161
H	8.31696932674874	10.70307931543967	3.96422693308165
C	9.90415975550991	9.60237829337311	3.08812308102392
H	9.90681325875241	10.11867101513754	2.12883969580869
H	9.27431925155191	8.72011379290181	2.98839071998121
H	10.91668453313428	9.25548154297030	3.29997221493832
C	9.38284241649643	9.76200375667813	5.54762859232245
H	8.89412515413541	8.79118990092200	5.45722521892816
H	8.86329673412397	10.32246248881872	6.32222696395091
H	10.41016554163002	9.59429643939549	5.87691724405297
C	9.29609131237401	15.52377091366986	5.11491539821008
H	8.29955741419117	15.26599549666943	5.46398896139618
C	9.11949549811812	16.37535834922970	3.84928831244437
H	10.08617474449876	16.72297582577044	3.47852428069531
H	8.50031900940533	17.24758535503057	4.06079461344361
H	8.63212548526339	15.80685699884035	3.05953152623780
C	9.98835090405099	16.33709672721746	6.21456838011384
H	10.95527843401745	16.72099112765764	5.88523167146846
H	10.15999519310998	15.74148405843420	7.11144904412126
H	9.37212372560281	17.19407086277159	6.49038686763449
C	4.15050003564975	11.32801894320334	4.15710812188634
C	4.35325268486486	9.97573454601502	3.82927248386969
C	3.31092162686217	9.27473795035792	3.23130261736246
H	3.45197372817692	8.23954548660278	2.95615718477323
C	2.10545646688486	9.89663378928160	2.94791654996108
H	1.30716864934381	9.34038657822873	2.47665405004021
C	1.93586747367587	11.23856991848628	3.24079759761458

H	1.00284219715895	11.72372666491694	2.98798614582217
C	2.94752958160891	11.98025926160500	3.84947130416933
C	5.67262401393322	9.28608848297339	4.12204446986855
H	6.42354990510881	10.06750971965183	4.22311470810014
C	6.11177782663211	8.36592377591987	2.98448239324281
H	5.46643876839022	7.49334171238182	2.89572750876623
H	7.12389259554634	8.00191785215249	3.16462737758636
H	6.09508569765932	8.88958679559293	2.02999147511948
C	5.62872876892342	8.52714428286484	5.45592219084781
H	4.84458666909279	7.76792291588250	5.43766915548880
H	5.43336651453679	9.19289728152114	6.29558146712256
H	6.58036214096347	8.02654053503312	5.64150258185477
C	2.72401346335695	13.45392379523311	4.12877925680684
H	3.57366849503019	13.82615460779401	4.69566101728305
C	2.67752049243564	14.24799748069959	2.81691121570874
H	3.56205597615110	14.05545545465505	2.21353371383231
H	2.62426019134327	15.31781586473567	3.02347320817856
H	1.80799343999016	13.96678364253306	2.21946549589802
C	1.45920311845887	13.71053033410807	4.95708757504690
H	1.38991302955304	14.76801456513339	5.21759310814336
H	1.45718292930659	13.13289781010119	5.88222568592888
H	0.55678230412663	13.44684416155439	4.40335338096956
C	5.46530696976758	8.65525510313080	-3.67040682561416
C	5.40516329221538	9.56834702369952	-4.72830888767077
H	5.44521227712468	9.13956652353257	-5.71645070222171
C	5.12629694191102	10.94028411524983	-4.67671211291689
C	5.52971443217523	7.19236138109689	-4.03138850181765
H	5.41322104007996	7.05098694927957	-5.10221305723011
H	4.76573991590384	6.61901105008295	-3.50993787105110
H	6.49234093923411	6.78195551513006	-3.72519383125677
C	4.81033978019662	11.60535571666425	-5.99474135686109
H	4.62798904097581	10.86094731214518	-6.76475969423830
H	5.64473627382463	12.23050844948959	-6.31145508078646
H	3.94134949017335	12.25518265677053	-5.91222753651093
C	5.21577220902123	8.01515464704639	-1.38633283247124
C	3.88897527259964	7.77291386101422	-0.98844241409673
C	3.65186245697515	6.79069073385719	-0.02948550035134
H	2.63648975070754	6.58354477651200	0.28071665162010
C	4.69515371512219	6.06909087457259	0.52861668867244
H	4.49315112174233	5.30623057743753	1.26927662730483
C	5.99848196595525	6.33769247283708	0.14408022336218
H	6.81097437325796	5.78631275296766	0.59759140088720
C	6.28592203743940	7.31295677662281	-0.80874675576986
C	2.72282143204011	8.52398618731178	-1.60769401891407
H	3.13348693922954	9.35503510373468	-2.17633155006712
C	1.78763741643621	9.10890877285823	-0.54765306861043
H	0.99343514082999	9.68680602592128	-1.02143110385911
H	2.32949423420259	9.76319750928099	0.13335046248726
H	1.31133726831707	8.32582826238091	0.04413511918243
C	1.94674015351957	7.63913771043757	-2.59234609166607
H	1.13086145445449	8.20159865843514	-3.04967071437765
H	1.51729725899644	6.77414764379664	-2.08305444456610
H	2.58817443918453	7.27154570718587	-3.39280744782203
C	7.72956985248681	7.60367725480899	-1.17265111433155
H	7.73550734073336	8.29250574448331	-2.01365920293251
C	8.49918122142305	6.34372567753574	-1.58782267176725
H	7.99972804472422	5.81104508567040	-2.39823524121607
H	8.60877992807379	5.64764200280642	-0.75450424664220
H	9.50108336435955	6.61275736655137	-1.92620525421556
C	8.44333690282421	8.30758924696799	-0.01265429490547
H	9.45167865554166	8.59962484669211	-0.30800155002544
H	8.51585071140743	7.64745035159782	0.85360272591978
H	7.91188110275612	9.20769187451743	0.29035990147307
C	4.67634746232556	13.02213399660309	-3.61300961881455
C	5.55218723344032	14.03129578959615	-4.04987848892294
C	5.05614935441638	15.32846396993537	-4.17907376436747
H	5.71365579119351	16.11400129392892	-4.52689565314302
C	3.74111501323818	15.62940890539770	-3.86960609054347
H	3.37082819576441	16.63955279937635	-3.98737855012968
C	2.90822677593105	14.63678171347441	-3.37601604142747
H	1.89494338128603	14.88726893194436	-3.09786996047115
C	3.35757785505976	13.32746670841379	-3.22572799237447
C	7.02017805401729	13.76685473639124	-4.32845353857959
H	7.18215390896057	12.69196493131434	-4.32609323465972
C	7.87118337538013	14.35057475824189	-3.19459830849083
H	8.92211179056859	14.09673083550994	-3.33743652437130
H	7.56250740674926	13.95243593755217	-2.23104288505434
H	7.77819566666260	15.43722435630207	-3.16638954815061
C	7.49083030726935	14.32028985266811	-5.67857906618939

H	6.87247407141273	13.96730085073427	-6.50413227132313
H	8.51909673706401	14.00931523554924	-5.86925881305812
H	7.46965961458128	15.41139715589926	-5.69625413912723
C	2.43342424812839	12.25410490853699	-2.67784895361865
H	3.06691897140053	11.51327046810871	-2.19258144964241
C	1.47790696162758	12.78238294572839	-1.60576888109720
H	0.74406012911098	13.47964183094479	-2.01296788415609
H	2.03080346878562	13.27780235794616	-0.80831689598935
H	0.92643898499536	11.95414515615910	-1.16208263500323
C	1.66649632612890	11.54135264240194	-3.79932825569310
H	1.04439438208833	12.24887915836336	-4.35130105638671
H	1.01577001259967	10.77017921808805	-3.38424170800290
H	2.34216697143769	11.06052705536134	-4.50547057015824
C	7.87144635938588	14.52228409135753	0.70062260597028
C	7.80321088437466	16.45841912386240	-0.44630607977536
C	9.09048029556593	16.01201922151245	-0.47362816158880
C	5.63732882222354	15.61720632215352	0.64120586359862
C	5.31510166048815	16.91293620308178	1.37870789546294
H	5.49734331144756	14.79165896639815	1.33136170042021
C	4.73870645969982	15.39093091409046	-0.56290608891139
H	4.74765132703843	16.23261000100650	-1.25100938758493
H	3.71532879262979	15.25603595912827	-0.21547614551439
H	5.01768552256796	14.48873641632811	-1.09828669439828
C	10.29796651173404	13.97921432908924	0.53291908995454
H	9.98131430176737	13.34846279321402	1.36153601279747
C	11.49681523805593	14.79110669353363	1.01120361506195
C	10.63129832105646	13.08059861212411	-0.65031925465932
H	10.97457286074729	13.65885374193756	-1.50870778001527
H	9.77114992925840	12.48903087365596	-0.95500017347243
H	11.43197163670954	12.39713668261436	-0.36552369388699
C	7.23951919579323	17.67153360119026	-1.09794571396559
H	6.34163975028872	17.44198843257280	-1.66851522166998
H	7.97017481641898	18.08693652441218	-1.78855697625603
H	6.99091856780266	18.44999878726160	-0.37685078414941
C	10.25190440424763	16.61115966976029	-1.18643942890815
H	10.82031751792225	15.85952557767223	-1.73106539078819
H	10.93576773387595	17.12849160476073	-0.51306586965988
H	9.89540167120932	17.33753997169996	-1.91336014149742
H	12.00829095823964	15.29577754277608	0.19549296989686
H	12.20524861299734	14.10912672704182	1.47564538454009
H	11.20593557270817	15.52470782474192	1.75982347017068
H	5.22878709581407	17.75897875991814	0.69908398234811
H	6.06020435124745	17.13074337017893	2.13960701420896
H	4.35843011335511	16.79194695388254	1.88346830934971

Table S38. Compound **2d** B3LYP-D3/def2-SVP

Electronic energy ... -8884.06606622 Eh

Final Gibbs free energy ... -8882.34313314 Eh

Gibbs free energy minus the electronic energy ... 1.72293307

Sb	5.47149625783816	13.95478272800644	0.10152376921661
Sb	7.04208242206256	12.00753074426007	0.96442177953823
Ga	5.66180413382387	13.32941869413821	-2.43881601684075
Ga	6.62992356322607	12.66544478003152	3.48865609501428
Cl	5.65283429210319	15.13478767383776	-3.80137906937673
Cl	6.10276195967732	14.81190666168394	3.97751732342198
N	7.26472995083447	19.10020826559201	-0.97139240785424
N	5.15924704546126	19.39047824894746	-0.96325966673534
N	4.06149332155293	12.37093076517139	-3.10158597557290
N	6.92698595480565	12.12461622046383	-3.37567252564919
N	5.31255276089606	11.57513569450072	4.47856356669175
N	8.12989491851213	12.35542805359853	4.77437300331868
C	7.94786089060129	18.80519276638163	-4.33804074306574
C	9.55647497700419	20.75879805530084	-4.15948283478450
C	8.63346506424442	19.80802509609353	-3.39078739287021
C	9.32723088693885	19.04512391525398	-2.26960089563202
C	10.67628065044201	18.67637008383388	-2.36148446872278
C	11.26505358527857	17.88150760894913	-1.37898658992475
C	10.50061411091789	17.39051000256066	-0.32165215710245
C	8.84897785136645	15.78470337868500	1.43490190288724
C	7.95622016645064	18.07700631831734	2.02646205361067
C	8.27011281873819	17.09176805085271	0.88747144213473
C	9.14197813761971	17.71292633202443	-0.19682411086038
C	8.59515465365692	18.59084720142661	-1.15334242966861
C	6.10094038349159	18.43633546905689	-1.24986480245652
C	3.55509607428312	20.95288201359688	-4.43234641538163
C	4.19501839819008	18.49172091097109	-4.49203826898740
C	4.05850800635096	19.75095687856374	-3.62190283085242
C	3.18843638934963	19.45570206250403	-2.40948446682704
C	4.13078935827262	17.16175252630908	1.32738358865426

C	2.70869804550667	18.86899912153846	2.53866119932218
C	3.61134550438295	18.60762825103926	1.32960601146345
C	1.79616999756652	19.34518053939321	-2.54257550257334
C	0.99518191459619	19.03358283788831	-1.44675557392175
C	1.57011744365401	18.81619018418478	-0.19328921206543
C	2.95535380095136	18.91048997980374	-0.01109029058325
C	3.74401480467704	19.23078052504396	-1.13646126336520
C	5.71365957238463	20.59548836330464	-0.52793177860168
C	7.05674113515555	20.41007025881108	-0.53037394508102
C	3.65537323877977	9.02208876439452	-2.46333259424607
C	3.93047331518872	9.46279736102750	0.00501391668010
C	3.81547311517371	10.10082619371416	-1.38003187050704
C	0.96896443704465	15.04000383424300	-3.92863640015517
C	2.52180276106298	15.76167687560308	-2.06923349519619
C	2.16202484427246	14.63632715409487	-3.05145386008600
C	2.72694665800818	11.16082621678859	-1.45512189477317
C	1.56233081395283	11.05425370943508	-0.68589609028029
C	0.58765748650555	12.05182264765304	-0.71927412330174
C	0.78555556687347	13.18883665411813	-1.49835811046091
C	1.93339214839335	13.33924870285225	-2.29128332540680
C	2.88094464977769	12.29248562626115	-2.29301216920154
C	8.86782959462514	15.24354013579810	-2.41786728111822
C	10.11469846282593	14.57520995714149	-4.50937455921597
C	9.01660078947411	14.18112699816636	-3.51160902212624
C	7.44178073392554	8.60322709382596	-3.56226632313134
C	7.47180885101813	8.55851269109763	-1.05330194214023
C	7.40544818129191	9.46603186888559	-2.28801703718253
C	9.24765853813155	12.81321047905259	-2.89230833027207
C	10.48840700701572	12.51557186398236	-2.31040814911471
C	10.73900020199966	11.26851164889395	-1.74592702668995
C	9.74212714907356	10.29331779032362	-1.75397800186005
C	8.47666688103383	10.55071034863353	-2.29607385041506
C	8.23567310958195	11.82867748430527	-2.86332489950862
C	2.76776350987274	11.59218124185162	-5.03137443563016
C	7.68389664491621	11.48266201635541	-5.62240397540319
C	4.07510226754404	11.93446467696632	-4.36024688374172
C	5.26407669679793	11.78999106789740	-5.10782156905525
C	6.58804240638578	11.80159015187730	-4.63358192758634
C	2.71794918972860	13.67497033330979	4.68726108632818
C	2.13215618442790	13.63634586663413	2.23176039443272
C	3.06140516895445	13.07801955468297	3.31361043074314
C	5.40550633254864	7.48019834924577	4.98093700477848
C	6.33666760124963	8.31427567197973	2.78240347632267
C	5.61928491238305	8.70764334399720	4.08478498830639
C	3.11377478751405	11.55655507942749	3.33765579318329
C	2.02768852233776	10.79744276688149	2.87979859471223
C	2.06198021318804	9.40424724008873	2.88398106376024
C	3.21832984331070	8.74147690795877	3.28758246741957
C	4.33051375773425	9.45355220976449	3.75386806556812
C	4.24397239714487	10.86478535025271	3.83586307151836
C	10.49026072400640	15.06235226607989	6.73618129765339
C	9.19834012555394	16.27441161452915	4.95414689491779
C	9.50642213530380	14.90030632847056	5.56137091295723
C	9.77541014576560	9.43136406875879	4.45784229268298
C	9.89385016478094	9.60940178490343	1.94796655431925
C	9.45818467825485	10.31168198027838	3.23671340206669
C	10.04903655565909	13.90270921434074	4.54206711001535
C	11.24928352285106	14.20311296723872	3.87975733387869
C	11.83028114537169	13.31013010623156	2.98533652753867
C	11.23810589595532	12.06687077777118	2.76218504710319
C	10.04637533793859	11.70953366860332	3.40303739901499
C	9.43772366560420	12.65501347665361	4.26999964962033
C	4.27447116805224	10.87520213031984	6.60246289988244
C	9.00823933006303	11.94381516360680	7.04390871116988
C	5.42928798382652	11.44985342334528	5.81198635751260
C	6.59160952328052	11.75107156012175	6.53408384278859
C	7.88308459957935	12.03989339001769	6.03996408915584
H	8.69929408600854	18.16352816197144	-4.82786852789117
H	7.24742054532413	18.15312248859653	-3.79584362905922
H	7.38691199196834	19.33492846679808	-5.12555664182000
H	10.31207819899603	20.21444622013259	-4.74907960523792
H	8.96936390554148	21.36301702068731	-4.86936277451131
H	10.08712071936333	21.44724610847554	-3.48241615974784
H	7.84012490007584	20.42244818417591	-2.93914817908040
H	12.32270104758332	17.61528261874858	-1.45482577224506
H	11.27276204138712	19.01195576899615	-3.21108254807112
H	10.96223544354810	16.72340457482188	0.40657679688614
H	9.77305789177821	15.94633346761852	2.00961843514071
H	9.07054936647410	15.06877639258730	0.63033732832047

H	8.12593123866085	15.31504826628739	2.11380219964236
H	8.87663120857790	18.36639053013484	2.55972657820468
H	7.47638236211119	18.99234017829216	1.65244230048930
H	7.27318316974431	17.60923902234933	2.75166362042954
H	7.31158678936654	16.84935970193802	0.39882538546262
H	7.87649537323660	21.07040752170209	-0.26163937492458
H	5.06465136083064	20.00061054895459	-3.25604496192668
H	4.26490312814389	21.18831960974365	-5.24189506372944
H	3.44666117623737	21.84911004555545	-3.80055902133803
H	2.57863530032398	20.75306455525472	-4.90307314818443
H	4.85087229008718	18.68389948525973	-5.35646480444649
H	4.62373142974437	17.65926413563021	-3.91728405478263
H	3.21236103530662	18.17170226073389	-4.87825628936501
H	4.81952604430975	16.99888988668526	0.48717759486751
H	4.65657832891986	16.91212909897064	2.26223137470663
H	3.29379075678697	16.45547333038337	1.20971440775880
H	4.48732009345025	19.26885351184865	1.42537477235804
H	3.28516057765357	18.74486615418281	3.46876882063612
H	1.86824055941136	18.15696827475924	2.58485556213327
H	2.28945864825336	19.88797363457060	2.52751781866566
H	1.33579499806408	19.50236408551146	-3.52025757633934
H	-0.08814098503687	18.95276608148914	-1.56911760829852
H	0.92956316548970	18.56686839534759	0.65377796091399
H	5.10450211416387	21.45482795783511	-0.26216217882414
H	3.72676157424424	9.43880285272129	-3.47752254466523
H	4.44199684880440	8.25695997038069	-2.36506569259309
H	2.67960358759523	8.51805174970832	-2.36622435971866
H	4.84185852328179	8.85238436809448	0.06733662275534
H	3.97734646172133	10.22263917848490	0.79674715591942
H	3.07969363267189	8.80134141320832	0.22735049882897
H	4.76238108615049	10.62447229422061	-1.57499266196452
H	0.07818575879148	15.28287703674190	-3.32664747067004
H	1.22151906743996	15.93768367413410	-4.51533702826058
H	0.68828809265018	14.23952728127191	-4.63232982880740
H	1.68678109792264	15.97784231744520	-1.38425566330915
H	3.39610459880370	15.50014973532072	-1.45774720688078
H	2.76883430100183	16.68654145442850	-2.60581723488947
H	3.02887983794872	14.50149179165738	-3.71146382263523
H	1.42533108932919	10.18912463172768	-0.03708320293464
H	-0.31516605022920	11.95474694581522	-0.11073838086413
H	0.04012275844113	13.98700861104533	-1.48686497513355
H	8.07399210059052	14.98064490455848	-1.70417972628415
H	9.80283958211075	15.35215964100710	-1.85112377768844
H	8.60850379294064	16.22092000624241	-2.84558854242443
H	9.84555601401464	15.52140081641357	-5.00573954608281
H	11.08693346493637	14.73232283793843	-4.01447442947936
H	10.25412218918478	13.80661092797921	-5.28711325236022
H	8.07126416299325	14.15154252968472	-4.06666878987026
H	7.23932833120994	9.18788467965021	-4.46816369946926
H	8.42713566312875	8.12229172749050	-3.67916828399965
H	6.68002177334738	7.80891670870602	-3.50626047554006
H	8.37237780148483	7.92366694157012	-1.05644428930471
H	7.46955285846293	9.14188763219974	-0.12221480386644
H	6.60373513537561	7.88159367495626	-1.03733425945154
H	6.43708774003230	9.98373856947561	-2.27258472206362
H	11.27137611587521	13.27700111364126	-2.30930678453290
H	11.71288625171169	11.05166512760534	-1.29939198383196
H	9.94985640051444	9.31564763472203	-1.31778454527945
H	2.16268472610081	10.92188123414969	-4.40438679761399
H	2.17541898278508	12.51050687519422	-5.17133197573814
H	2.93148400557094	11.12230742880331	-6.00918794804403
H	8.13050791169861	12.43531190674253	-5.95551882157578
H	8.49318298304152	10.89433084336966	-5.17285250785030
H	7.29325810883391	10.95649812057869	-6.50272290990924
H	5.13805554954548	11.53476675579877	-6.15896016100983
H	1.72916429824322	13.32719785607191	5.03135347530827
H	3.46753437546096	13.40932275405119	5.44426879041220
H	2.69767444150780	14.77409324284248	4.62561609966957
H	1.06864935349213	13.45944640334267	2.46227157505761
H	2.27249647647780	14.72449882251524	2.15282134339693
H	2.33935258785868	13.19789606791057	1.24466295186998
H	4.07134237306107	13.43336704241501	3.06702759040556
H	6.37493508877413	7.03557885610832	5.25783709754419
H	4.87554324854691	7.74048507045682	5.91055986894302
H	4.82091442188518	6.69717550829702	4.47188669573417
H	6.51677807905865	9.19389494979128	2.14714542197739
H	7.30828381349723	7.84192703523881	2.99750814767541
H	5.73267249552227	7.60339199572496	2.19596363463335
H	6.28656879343063	9.39326466229162	4.62451789910911

H	1.13891416172336	11.30810016283622	2.50995182345616
H	1.19695561745318	8.83476133176372	2.53444462255297
H	3.26320971042210	7.65182765361388	3.22831311589239
H	10.03865213287747	15.67534614536356	7.53322035901876
H	10.79034294848334	14.09880014166210	7.17180966150131
H	11.40981386145613	15.57398138543039	6.40837760164817
H	8.43319561330075	16.19727800964143	4.17682435111031
H	8.81809801637086	16.95321931087907	5.73461273403866
H	10.09850804485396	16.73875294469692	4.52004786376641
H	8.55539062676254	14.51144345536534	5.94968904157311
H	10.86452506968864	9.31845085701790	4.58495687422481
H	9.36842358969207	9.85436555317391	5.38562541604422
H	9.34133232313479	8.42617249360511	4.33064765624645
H	10.95846032736811	9.32571268821643	1.97881819497565
H	9.31484074355677	8.68436174488792	1.80752178638418
H	9.73352325114967	10.24337868872626	1.06483369491645
H	8.36310609770529	10.41671252075362	3.20123085923978
H	11.73392340081933	15.16354808096056	4.06962723721102
H	12.75584892958118	13.57544962619591	2.46835065340529
H	11.71439750605504	11.36540204935059	2.07708128188122
H	4.27482881331435	9.77624330544368	6.54432555879427
H	4.35881215061519	11.15951601113840	7.65979209055332
H	3.30811337084538	11.21427331468720	6.20781798282159
H	9.99335539549521	11.95363836650223	6.56439243129439
H	8.95510817918957	12.79278890787562	7.74269463659200
H	8.90311781206432	11.02409992512176	7.63710463544776
H	6.52871561323320	11.59936529166247	7.61145814023070

Table S39. Compound **2d** B3LYP-D3/def2-TZVPP
final energy -8888.845202521998 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -8877.634856272080 Eh

Sb	5.47140118596178	13.92582181766286	0.08932000336977
Sb	7.05363905385140	12.00833622525422	0.96439854305998
Ga	5.66183783296393	13.29716391238572	-2.44972833471115
Ga	6.64752646513547	12.66316590536621	3.48801690630989
Cl	5.64347158998698	15.12398198692128	-3.77135457368086
Cl	6.17202866707571	14.81302872476892	3.96218027160429
N	7.23404063803588	19.21679824925828	-0.96480564519900
N	5.13006479726590	19.46571844391844	-0.96355107634829
N	4.08163773190639	12.31274637898975	-3.12114079128054
N	6.94409950256909	12.10971875699138	-3.37517398902705
N	5.31367033764496	11.60405752314723	4.48853273685245
N	8.14281022100034	12.31614770155578	4.76773776610730
C	7.93972339381455	18.96373137207578	-4.35300117445291
C	9.49481580120233	20.94481024328353	-4.11201749861256
C	8.58636852567912	19.95942941989615	-3.37548521135521
C	9.28498353566643	19.18901328491874	-2.26914726899601
C	10.62684898018561	18.82662532435344	-2.37437580353872
C	11.22406210072662	18.03301166323505	-1.40707126991961
C	10.47602721848208	17.53994490744619	-0.34921365080599
C	8.81866136580344	15.89534122081924	1.36810805154260
C	8.06129199609460	18.20261680550086	2.06019434560827
C	8.27375344548066	17.23946388586096	0.88347992921657
C	9.12553557474768	17.85678820868389	-0.21175362570775
C	8.56952069899025	18.72933598337813	-1.15525926333868
C	6.08783734685269	18.53905247326607	-1.26460636497918
C	3.45910473143732	21.04167560620013	-4.36589652371246
C	4.14159759249210	18.60534028429030	-4.51645028343845
C	4.00047916859238	19.82883724516980	-3.60175423565364
C	3.15469791395452	19.48292989882480	-2.39112649703983
C	4.15556023299129	17.18168857533737	1.31883503228704
C	2.73072954686873	18.87367171492559	2.53458167716901
C	3.62550019320812	18.62102239309739	1.32060559332474
C	1.77343374160443	19.32917405303946	-2.51558287650350
C	0.99450294790101	18.98321163986056	-1.42443827981376
C	1.58096687291520	18.77492229177691	-0.18334745149810
C	2.95561281303304	18.91257361195463	-0.01021106580566
C	3.72067066498533	19.26895192607969	-1.13069149356298
C	5.65937611563456	20.66752657006700	-0.50223493211175
C	6.99730773187749	20.50877164688164	-0.50026932141030
C	3.66134026385868	8.97798059164961	-2.45391970958323
C	3.92868695109513	9.42888111854377	0.00511759536212
C	3.83038320674130	10.06205401747200	-1.38060510425833
C	0.95961937747507	14.86052809899178	-4.05296090363269
C	2.45389877165175	15.71128367480004	-2.20821954686495
C	2.15094906328026	14.53544450901188	-3.14508897972410
C	2.74797057592354	11.12164586109946	-1.46913325470800
C	1.58954488682324	11.02484902992689	-0.70360726817053
C	0.61620944891487	12.01205485845655	-0.75291565514442

C	0.80591746168327	13.12735358335200	-1.55027388308850
C	1.94642649785160	13.26622314234456	-2.34248972084107
C	2.89594236542795	12.23360043897789	-2.32063223747038
C	8.88570284740722	15.26030747451182	-2.41258125975267
C	10.13612200513028	14.52080951548953	-4.46997054605240
C	9.02369135261444	14.16934609823525	-3.47534190026046
C	7.63226691769175	8.53252583148780	-3.55652225413795
C	7.42499446759884	8.58192079169068	-1.06328984152960
C	7.44401567038820	9.44015681998270	-2.33088742207240
C	9.23747896542585	12.81372305061216	-2.83236818724100
C	10.45367950659131	12.53168827809663	-2.21095674779533
C	10.70175616584187	11.29094793122212	-1.65064450899892
C	9.72864042107749	10.30492526926768	-1.70736374733795
C	8.48531438701446	10.54747625890211	-2.28555746441474
C	8.24455538397426	11.82146446910018	-2.84118520108757
C	2.82717156048882	11.49645378524313	-5.05671272992279
C	7.71817161769077	11.45900099872866	-5.60634491387758
C	4.11424555536392	11.86625569700279	-4.36830047769426
C	5.30500253351929	11.73676597529160	-5.10285904910114
C	6.61852472327223	11.77254434750632	-4.62574574565267
C	2.73356726414497	13.72076042821806	4.68065311940662
C	2.15431866109195	13.66822843647501	2.23375257783388
C	3.08177787822886	13.11318419646616	3.31543227596420
C	5.32713348520730	7.54741595897055	5.08824475072073
C	6.25096938365445	8.25268729916408	2.85307673655942
C	5.56820846549681	8.72907971778565	4.14275639308466
C	3.11987618882806	11.59595831950000	3.35398246538418
C	2.03250223489475	10.85042079356781	2.90205853993325
C	2.04761267805705	9.46462606023585	2.92145855305629
C	3.18615323214965	8.79582005145138	3.33629011766044
C	4.30028702967978	9.49451343158707	3.79594137201856
C	4.23366022785209	10.89907684054576	3.85982275995510
C	10.63441839683927	14.94282603451478	6.66717828800577
C	9.36767704398773	16.17191722127280	4.88878061253870
C	9.62841286675211	14.79854854245958	5.51219303672049
C	9.68757784054083	9.32965970699097	4.49080815697548
C	9.77407940839149	9.46716364481984	1.98532294759975
C	9.38018321170242	10.20317173116709	3.26513240888019
C	10.11967142220073	13.76956799993121	4.50499128768793
C	11.31640060371841	14.01315941665642	3.82940777754231
C	11.85098659273478	13.09001354512906	2.94920569372561
C	11.21313882407973	11.87335231119082	2.75369867951287
C	10.02065770449834	11.57541620136142	3.40552354213151
C	9.45960033457763	12.55248535673779	4.25564985535657
C	4.27475133720959	10.96384560306002	6.62470422746093
C	9.00893874339969	11.90326810776144	7.03364801861395
C	5.43341798484362	11.49711070195361	5.81701582151148
C	6.59695845942989	11.78590570179949	6.52752086506689
C	7.88968148897283	12.02681851840977	6.03081538268810
H	8.70678157099861	18.36338178184823	-4.84680912029711
H	7.26062602992547	18.28773422114084	-3.83495466831403
H	7.37675527798698	19.49414671509062	-5.12339877402999
H	10.26302947970943	20.43395676971093	-4.69467513745645
H	8.90521580978058	21.54101362379474	-4.80992261581328
H	9.99304383602746	21.62572127085913	-3.42031674313119
H	7.78141756027939	20.53938801458886	-2.92523274989597
H	12.27081228270605	17.77193355876662	-1.49472145430511
H	11.20911016188301	19.16474074178129	-3.21917643113980
H	10.94174051952023	16.87754668082767	0.36513515287502
H	9.75350360503402	16.00239343641423	1.91805610869725
H	8.98947948131798	15.21252521692139	0.53827668789563
H	8.09872099454484	15.43232593982247	2.03833856194968
H	9.01247885324024	18.44304517011554	2.53940370260785
H	7.60002811560382	19.13394241260223	1.73566007213336
H	7.41096349209695	17.74540201077648	2.80638581003043
H	7.29510388012574	17.05005179422980	0.43909014792275
H	7.79134550486877	21.17548177374036	-0.21829150247101
H	4.99801459417257	20.08424942256533	-3.24859435180649
H	4.13998057808998	21.30709053099957	-5.17638867066894
H	3.35299885069273	21.90851683323681	-3.71200958492194
H	2.48412821790310	20.83767640463299	-4.81118475121927
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H	4.58931566426359	17.76878433196426	-3.98309976896840
H	3.16634441608200	18.28882578501567	-4.89297252099098
H	4.82346004415579	17.01969676206064	0.47532007746535
H	4.69606945941399	16.95355420155190	2.23813019144744
H	3.32973188356150	16.47510275950132	1.22668117415341
H	4.48732546455461	19.28376437407750	1.41009419278536
H	3.31228570399508	18.75567414986558	3.44948835512918

H	1.90448386681607	18.16237828953053	2.58555942209437
H	2.30966366560598	19.88020020417022	2.52516337992776
H	1.30575613321119	19.47850017696337	-3.47903956637338
H	-0.07537537963701	18.86807978844232	-1.54031378512195
H	0.96041961732919	18.49984084835533	0.65697910870565
H	5.04229747065319	21.50179154985410	-0.22352671602223
H	3.71267000086762	9.38700271124795	-3.46088397544615
H	4.44592255841547	8.22534719523752	-2.36192920846120
H	2.69848430540010	8.47621349220833	-2.33943687675387
H	4.81885236646429	8.80674111944141	0.06872950021900
H	3.98659270691700	10.18448262102565	0.78554252053290
H	3.07224386400146	8.79099306733339	0.22198741467802
H	4.77543717018331	10.56958553164641	-1.57107887335106
H	0.06640592953678	15.10514599193779	-3.47585627556998
H	1.19505568129150	15.72419285047140	-4.67639035452689
H	0.71255650644668	14.02398469015939	-4.70854525899439
H	1.61442486131945	15.91052372386267	-1.54097871765969
H	3.33238945548052	15.51861851510791	-1.59513991678126
H	2.65218734942829	16.61461636347411	-2.78011279027007
H	3.02298750240160	14.40352479361812	-3.78052822187282
H	1.45647268489840	10.18014709142359	-0.04487585206595
H	-0.27646826240861	11.92269790876707	-0.14775129016703
H	0.06263545970713	13.91282944880303	-1.55520222127408
H	8.07915587068992	15.03622270205300	-1.71634177783758
H	9.80616040228486	15.35879488752039	-1.83939185128291
H	8.66322245123640	16.22268338008322	-2.86871669199340
H	9.89472419030401	15.45555564515090	-4.97793996916688
H	11.09711351706739	14.65754109490690	-3.97158400959085
H	10.26004930035676	13.74293329067386	-5.22526018994675
H	8.09189673886103	14.13943513909392	-4.03281846497185
H	7.52310933263409	9.07606163562311	-4.49129227694952
H	8.62368267094483	8.07534210477556	-3.54521266828853
H	6.89044401600293	7.73214701211635	-3.54995470473349
H	8.33757417992231	7.99386876150459	-0.95860286694286
H	7.31228311630529	9.19344595373444	-0.17029727253310
H	6.59327987161741	7.87800253870249	-1.10381361473421
H	6.47139454685571	9.91762797096850	-2.42513837204594
H	11.21776704407790	13.29615435546920	-2.17728352311292
H	11.65192185522595	11.08827396421908	-1.17406195660059
H	9.93572062312179	9.33504692301116	-1.27931606358254
H	2.15253650779778	10.97059604787810	-4.38510521552623
H	2.31662563960182	12.40856586386866	-5.37294886117030
H	3.01422531698576	10.88424635989423	-5.93485877297299
H	8.12711340749605	12.40586869200176	-5.96824329458357
H	8.53824152115823	10.91444087302273	-5.14754455887450
H	7.34205939687375	10.89936405673823	-6.45863473938273
H	5.18926127571750	11.47195888054900	-6.14187963152772
H	1.75308399203421	13.37674503209474	5.01777239577667
H	3.47271038997007	13.46337092740633	5.43527741148698
H	2.71058121865571	14.80834276245849	4.60768541946153
H	1.10153869690473	13.50288522455207	2.47060188687549
H	2.30372981945197	14.74378322300926	2.15118906716259
H	2.35293791099540	13.22520298172977	1.25877952334426
H	4.08394591120306	13.45995655802057	3.06935207417381
H	6.27738104404940	7.08848967192700	5.36551851427118
H	4.82450774765972	7.85879827168109	6.00390513295710
H	4.71500116420994	6.77507828863286	4.62068666114480
H	6.47235841320979	9.08989948314123	2.19197999131841
H	7.18652479658206	7.73978830343912	3.08025353902785
H	5.60887694306537	7.56194925272129	2.30488674711658
H	6.25622117102403	9.40860840273592	4.64112702031935
H	1.16143068343621	11.36315755875698	2.52402120882901
H	1.18550539957195	8.90842937274185	2.57709863486431
H	3.21600196016766	7.71565439811645	3.29084765867955
H	10.21668791233536	15.57411191799704	7.45338711105758
H	10.90483887038267	13.98361853073351	7.10554985583931
H	11.55447981437077	15.41500257594973	6.31905020207872
H	8.58812745615946	16.11712746055537	4.13857787683838
H	9.04324015356696	16.87306227478735	5.65962110636855
H	10.26875201502791	16.57921390284945	4.42795889353287
H	8.67950343154083	14.45507030015420	5.91825639566672
H	10.76419031881684	9.18597398177759	4.59831475386809
H	9.31324765905681	9.77503161506874	5.40941162828268
H	9.22366467203022	8.34780988468913	4.38240241434333
H	10.81849304223811	9.15112273118232	2.00806703434828
H	9.16455764684945	8.57114829466060	1.87357358156735
H	9.62285798109462	10.08732186975401	1.10423221712656
H	8.29894111604528	10.34222560154350	3.24091712863319
H	11.83404423034516	14.94783137192042	3.99766703389378

H	12.77059400927040	13.30980701709967	2.42327694480391
H	11.65059586735175	11.14971692384095	2.08273238835297
H	4.28513016902002	9.87425171278920	6.63620221481905
H	4.35070015142099	11.31054878497818	7.65278398851866
H	3.31958758408350	11.27153924656331	6.20804831492020
H	9.98264070868374	11.86740116381017	6.55640431167147
H	8.99031408164003	12.75623060033095	7.71265179685212
H	8.86989453608411	11.00489739669296	7.63265618210170
H	6.53262217011914	11.65830970886533	7.59723251143024

Table S40. Table S Compound **3** – B3YLP-D3/def2-SVP

Electronic energy ... -7945.23467148 Eh

Final Gibbs free energy ... -7944.05516263 Eh

Gibbs free energy minus the electronic energy 1.17950886 Eh 740.15 kcal/mol

Cl	4.37898275277206	11.37176718631362	6.94107412558526
Ga	3.51181988373766	12.36232560751784	5.12419168000236
Ga	2.91401697846143	15.76353832590720	7.55030240737391
N	4.79713986267866	11.87772927569659	3.68009415314853
N	2.11691968547016	11.09047183704906	4.54328770003215
N	4.30888510447261	16.82019693266837	8.49505354845830
N	1.57188635330420	17.20723396029891	7.57833118527626
C	4.85736764782441	10.61543584649714	3.26252146383965
C	3.81623873174941	9.69499073352670	3.48208077213790
H	3.99063222882846	8.68727047459328	3.10908603418378
C	2.51774614595936	9.94578486199559	3.96448942512630
C	6.08751480924229	10.12750446732177	2.53807721488339
H	5.87154188711626	9.23711942099356	1.93382464259938
H	6.85104988976194	9.86081213183560	3.28679506592080
H	6.52211513163576	10.90796335932935	1.90029261746446
C	1.51475175854500	8.82868444821882	3.78831437426325
H	0.58943480288824	9.19668673684567	3.32583716873140
H	1.23051425579742	8.41046507331210	4.76404220207606
H	1.93172386112472	8.02530635682603	3.16874924503471
C	5.71263252138161	12.88311704143788	3.22845681499247
C	5.32044975464815	13.69538619630722	2.13341413796632
C	6.14735082604388	14.76630673969848	1.77499937118259
H	5.86306658770667	15.41138500339553	0.94257378801030
C	7.32191381196837	15.03802880433682	2.47770078847057
H	7.94654642468207	15.88783401079093	2.19098717612826
C	7.69220021012335	14.22970333606754	3.54789931039303
H	8.60861729744486	14.45214686605751	4.09995959354016
C	6.90154820062421	13.14055453350625	3.94335681205407
C	4.03559832387536	13.40801274831589	1.36577727106420
H	3.31647290316755	12.99802811126558	2.09044652991481
C	4.25812066003147	12.33048015936795	0.28982232769174
H	5.03002696608069	12.65380009205052	-0.42796667818887
H	3.32682749634366	12.14560836970631	-0.26877344085283
H	4.57865519159384	11.37456098302629	0.72265242862401
C	3.39931150499895	14.65416573895628	0.74118266290505
H	4.00639982406693	15.05060658039661	-0.08886099478036
H	3.24854792923361	15.44781620497148	1.48569225490054
H	2.41291205123165	14.39672541091151	0.32563282397653
C	7.32792142406117	12.30063082755773	5.13640844162993
C	8.69257168376313	11.63238458426087	4.90221202256499
H	8.69707820235256	11.02844836056583	3.98110340281926
H	8.94562458431186	10.96983074293147	5.74606295053625
H	9.49877598541743	12.37897585328223	4.81155180390335
C	7.34799058669724	13.13846549738315	6.42055270332905
H	8.12387581692606	13.91663193718337	6.37985463855677
H	7.54010842133527	12.50373739547403	7.29869366679624
H	6.38595554846376	13.64139355233496	6.59494887418457
C	0.71746902398847	11.23435879192880	4.86088894074873
C	-0.11705661241417	11.91301690452303	3.93954895629087
C	-1.49608641423122	11.92975078525862	4.18439443432266
H	-2.15938005668643	12.43610641058018	3.48268470778724
C	-2.03593507642600	11.31925470349140	5.31585608721754
H	-3.11517941056594	11.34384062345038	5.48853582561496
C	-1.19438643072469	10.70620579925037	6.23874664882208
H	-1.61913051963855	10.26000652288695	7.14039286672188
C	0.19231933563188	10.64887644102945	6.03592996698835
C	0.45778857367027	12.59624788572454	2.70428948412685
H	1.42320416035691	13.02972242552866	3.00468167747038
C	-0.40506025695133	13.75956645188796	2.20267523494164

H	0.14733716979957	14.32536937733813	1.43702445104337
H	-0.65641973190790	14.45811980995700	3.01397755454105
H	-1.33991634342253	13.40500376436605	1.73821422534545
C	0.72534863697020	11.60411301863927	1.55868901093468
H	1.06510726498934	12.14196651965330	0.65967802816549
H	-0.19421279964357	11.05660933900927	1.29330822011547
H	1.50202629645611	10.87174793146355	1.81515896119623
C	1.07182245005596	9.98807948299156	7.08956358203193
H	2.08070871549798	9.87358911471706	6.67245106630735
C	1.20363559818103	10.89186569962282	8.32490569492458
H	1.60734845375138	11.87963026909179	8.07042530436543
H	1.88963443738437	10.43940241564624	9.05857403972338
H	0.22562703608273	11.03893796015336	8.81343546817214
C	0.57325164471882	8.59167040166922	7.49458672281926
H	0.43246194795173	7.93111832628923	6.62414496738923
H	-0.38825912937688	8.63749511341612	8.03118098213091
H	1.30046154146679	8.11336574771036	8.17023392861099
C	3.92308914211916	17.71306258052521	9.40898494429677
C	2.58905795288434	18.14535495196968	9.56393288822032
H	2.40044934380597	18.79785111870307	10.41475569395147
C	1.51841455378900	17.98339405610354	8.66965417947568
C	4.94890278480996	18.31192479550869	10.34108179977354
H	5.87053544289448	18.57810370337701	9.80530921925878
H	5.23032201541078	17.57628249640056	11.10942355738165
H	4.55100289262573	19.20357977621161	10.84112343113032
C	0.24506638131105	18.74243855827903	8.95444975314052
H	-0.02986982298173	19.39953196708792	8.11830256680491
H	0.33867433314988	19.34328039711472	9.86760439750152
H	-0.58657239939023	18.03061730020844	9.07546895055984
C	5.70245291541132	16.51890547263705	8.31923288974289
C	6.40235450960054	17.14617257052463	7.25748468294524
C	7.77513434819646	16.89822678620028	7.12885064841207
H	8.33424640958787	17.37725201571687	6.32447863983588
C	8.44071490788205	16.05120417790208	8.01355067611302
H	9.51398762462493	15.87568382356899	7.90123122297030
C	7.72937829030393	15.40583651935511	9.02036278511289
H	8.24868364144573	14.71347763358323	9.68648664719495
C	6.35374134975201	15.61456856230154	9.19154578031575
C	5.70366647488988	18.10492875605010	6.30062372924581
H	4.66370968590213	17.76026924398059	6.20167508944979
C	6.31531154057751	18.09888724435130	4.89396753236806
H	5.67485121867981	18.66569739683048	4.20223595492701
H	6.41163381074191	17.07553270111616	4.50123188468271
H	7.30986583715186	18.57303843048575	4.87809862827929
C	5.64725918651015	19.53289213347887	6.86847579719416
H	5.16895165248020	20.21567272689199	6.14868336250076
H	6.66153526633371	19.91173689588974	7.07423622919585
H	5.06968123971935	19.57879830945578	7.80199841944264
C	5.61663929968905	14.83838938993122	10.27442377595666
H	4.58799138190425	15.21696612962296	10.32904197535955
C	5.52435242634404	13.35151945413814	9.89664748209474
H	5.06268444535976	13.20484839960827	8.91216476959540
H	4.90702845445694	12.80707371350842	10.62826607310002
H	6.52346475372357	12.88475084966230	9.87614448825102
C	6.25913941284915	15.00261320190396	11.66084960178988
H	7.26335671518776	14.55086811368083	11.69922450611095
H	5.64550298983316	14.50010534923899	12.42537898173510
H	6.36514738681447	16.06003183780361	11.94973853802452
C	0.59390286994553	17.38376224008994	6.53933168414557
C	0.82151418490130	18.38033892519471	5.56251664684778
C	-0.13175827180778	18.54949530403455	4.55177312473900
H	0.02429415487147	19.31540583963269	3.78898699757976
C	-1.26282593706392	17.73771319753852	4.48540806761969
H	-1.98846121440547	17.87438415895967	3.67911518388024
C	-1.45983759342931	16.74481318611162	5.44283475021597
H	-2.33949585511351	16.10066883707162	5.37987447708610
C	-0.54663868972171	16.55657730978327	6.48874290372885
C	2.07743156781033	19.24306759232999	5.57284399227564
H	2.77823962818301	18.79026428219294	6.28763280416935
C	2.76696395323911	19.26605282723435	4.20082183847668
H	2.96253049977784	18.24699689932521	3.83905933211820
H	3.72204598003153	19.81022488491029	4.26059336434419
H	2.14918771458855	19.77711302832946	3.44506009989277
C	1.78850440865329	20.67210412148309	6.06046297991222
H	1.06333232494063	21.17525249267175	5.39948284571517
H	2.71222418850768	21.27293631973758	6.07134851382886
H	1.37438159863153	20.67808285474244	7.07920557164032
C	-0.75893287892009	15.43993534474326	7.49533766556034
H	-0.07957397228301	15.60865691189491	8.34155383581215

C	-0.37631773990852	14.09564584269689	6.86427114166952
H	-1.04542920921739	13.85129299395524	6.02775190200947
H	-0.43135249298786	13.28488918532265	7.60349973701081
H	0.64666737034645	14.11302147428541	6.46332954471889
C	-2.18625149419954	15.39750666564210	8.05706638650629
H	-2.92678676569416	15.13725484824890	7.28349538378525
H	-2.48214752383810	16.36785910984210	8.48824857258726
H	-2.25852509455887	14.63517685435203	8.84972888186897
Sb	3.85694446036621	14.99539433432433	5.20037820313762
Cl	1.86213419558872	15.61589851729933	3.90605535300058
Cl	2.24177113704790	14.34743480225145	9.14187743323848
H	6.58488268442517	11.50539851729162	5.27762506011290

Table S41. Compound **3** – B3LYP-D3/def2-TZVPP
B3LYP-D3/def2-TZVPP final energy -7948.906196075955 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -7939.995416282133 Eh

Cl	4.53212222875283	11.35340141483402	6.86878161179947
Ga	3.58369022870418	12.35371218082365	5.10599774545232
Ga	2.84566671379596	15.77043374751697	7.55433438169893
N	4.83915901034940	11.92111054636400	3.62339625319796
N	2.19976922688315	11.06869100165698	4.53758911127784
N	4.24560223014479	16.78835332463204	8.52819501817277
N	1.53444550302398	17.24307585856221	7.56575734754562
C	4.90673707989904	10.67006602905782	3.19381946762128
C	3.89798604876396	9.72980364830754	3.43542037849539
H	4.08696278856021	8.73884466318986	3.05567829267537
C	2.61422508710185	9.94046046031716	3.95211203738293
C	6.11366760365107	10.20669964649242	2.42135858424755
H	5.87134392953663	9.36024192330481	1.78402141601682
H	6.87912382593270	9.88975878101454	3.13272069092597
H	6.54057447916177	11.00490606638007	1.82047744636692
C	1.64530954636961	8.79417833686234	3.80800514903902
H	0.68855983496913	9.12975642104074	3.41462512834455
H	1.44660333240220	8.34843025776138	4.78155831041496
H	2.05270655503173	8.03033508564492	3.15220783362872
C	5.73598373982986	12.94010987656341	3.16334077153245
C	5.31633054786791	13.75548235380951	2.09148420406980
C	6.13021252062125	14.82073374936074	1.71785530179164
H	5.82605184490543	15.46619611450702	0.90720211093739
C	7.31873709495050	15.08456931758408	2.38407618295698
H	7.92919892962712	15.92730074527107	2.08779955875936
C	7.71536685024765	14.27353747372844	3.43196634487499
H	8.63935628824284	14.48762643906312	3.95187564554039
C	6.93859094311085	13.18910448504531	3.84111450129418
C	4.01538555429584	13.47633834336979	1.35662425640386
H	3.31287433938337	13.08127489067450	2.08969892978119
C	4.20520840464646	12.39859588718181	0.27779551758893
H	4.96927716291890	12.70831041547296	-0.43785675719146
H	3.27399705025865	12.24065849460492	-0.26732780089702
H	4.50491498821369	11.44322061524160	0.70094417728809
C	3.38003194703985	14.72212908640184	0.73811071678981
H	3.96348669676539	15.09493162646608	-0.10545777056409
H	3.26709202285449	15.52102944458877	1.46789769027193
H	2.38765633277865	14.47476187432667	0.35996504972530
C	7.40657352887956	12.33788274861505	5.00521182994550
C	8.76340406523661	11.68117836119380	4.71648471505594
H	8.74266316638925	11.10549836350178	3.79079005070833
H	9.03593895350999	11.00800318063081	5.53092387085670
H	9.55462506304100	12.42698977577936	4.62354987634970
C	7.47438594571550	13.15869798153635	6.29615749743742
H	8.24063162199725	13.92994456612893	6.23239037820147
H	7.70454153475018	12.51699528407562	7.14648502411380
H	6.52814298238365	13.65189432875233	6.51189095569443
C	0.80341350161019	11.18906080565111	4.87945085473472
C	-0.05563168171336	11.84070730593887	3.97253564226384
C	-1.41884141787953	11.85747210336276	4.25533940045774
H	-2.09829922028070	12.34301655129241	3.57103368622705
C	-1.92154671540022	11.27100782829907	5.40651963273534
H	-2.98413029452494	11.29895496910031	5.60918495221240
C	-1.05793379999663	10.67654428976151	6.30780928060801
H	-1.45185676024122	10.24675935084711	7.21832905382799
C	0.31466585519840	10.61773348403297	6.06629405379483
C	0.47286722057904	12.49478598100031	2.70689979263400
H	1.43954021356525	12.92821900473737	2.95812141746476
C	-0.41294177178342	13.63777692110527	2.20576889559089
H	0.11140933115531	14.19179146434598	1.42715265949511
H	-0.65762240332043	14.33743612461627	3.00288443455101
H	-1.34297869245481	13.26563155894403	1.77157483980366
C	0.69783239270891	11.48208295187519	1.57408241761326
H	1.01285419781586	12.00012400425824	0.66721728626848

H	-0.22578047217323	10.94480182982892	1.35035936715246
H	1.46785106539484	10.75486386398412	1.81941661016018
C	1.21481273852968	9.96328326204796	7.09842232804707
H	2.20912615669787	9.85755113824876	6.67138932256494
C	1.34774339391596	10.86403462965626	8.33122747987716
H	1.72700739871655	11.84779044340058	8.07151038242267
H	2.04018008028945	10.42476540782468	9.05041737567767
H	0.38091363082601	10.99657649656960	8.82129136778038
C	0.73026719827087	8.56717266884637	7.51141447581434
H	0.57670879250059	7.91232621845198	6.65288125829210
H	-0.21130066735519	8.61389340149502	8.06041968621833
H	1.46736849595362	8.09977221181516	8.16583342265298
C	3.86855091004136	17.69892214550352	9.41950192155870
C	2.55691060568814	18.18172774128908	9.53472696262942
H	2.38146801238940	18.85484931079393	10.35817563960119
C	1.50076440973464	18.04427422574567	8.63000985606475
C	4.88466801189365	18.27379274313720	10.37254670095232
H	5.82513781379720	18.48972286938791	9.87094606954465
H	5.10178204131383	17.55085100818020	11.15866883935761
H	4.50711315539302	19.18174197573876	10.83424910616215
C	0.26171846409896	18.86200294235516	8.88790327829432
H	-0.07732435005794	19.37545550255145	7.99152736168522
H	0.43195724855391	19.58981153471746	9.67611550386977
H	-0.54736012705550	18.19621827887792	9.19453283422693
C	5.63745463899251	16.45892032670139	8.38642316298410
C	6.37418033590516	17.07883038147377	7.35691959774660
C	7.73883004259002	16.81377741764629	7.27109320547256
H	8.32459416646272	17.28452304159980	6.49557297451399
C	8.35962599754232	15.95242902893982	8.16184953398210
H	9.42186026888262	15.76286177313585	8.08135223461439
C	7.61199220243827	15.31316479598479	9.13418423336292
H	8.09522039777614	14.61584703562409	9.80441022516414
C	6.24332861491981	15.54529451672869	9.26666761122161
C	5.72320470854235	18.04455765434322	6.38066041265340
H	4.68670452720810	17.73085920701843	6.26200699143172
C	6.36642671197765	18.00915121990863	4.99187837192557
H	5.76477354558711	18.58510705988142	4.28989979817711
H	6.43912994413624	16.99054243887114	4.61329815744617
H	7.36601684473265	18.44647071915601	4.99807093777746
C	5.69713191191323	19.47840019150317	6.92823751841983
H	5.24354118442958	20.15276555323449	6.20042573097686
H	6.70993427451667	19.83159414886920	7.13136914146460
H	5.12113718262595	19.55050753987040	7.84886416815653
C	5.46714841028890	14.78802994738917	10.32859326056364
H	4.45580641380212	15.18609983910554	10.36536734203409
C	5.35537574389124	13.30616217975268	9.94807505677505
H	4.90613627499550	13.17276182082685	8.96778579672944
H	4.73201222421617	12.77698874363798	10.66972377645898
H	6.33973036917538	12.83364820884567	9.93428447045909
C	6.08474423299730	14.93268789140363	11.72599418399126
H	7.06190005991287	14.45098373079112	11.78312737958428
H	5.44119597741577	14.45669606935023	12.46707725610564
H	6.21671037564597	15.97655917378275	12.01245122532179
C	0.56757321171361	17.41340512369899	6.51540263672242
C	0.84305938880707	18.34639716712186	5.49966693699832
C	-0.08908130838399	18.50264104238325	4.47824841251184
H	0.10106880749011	19.21457003563636	3.68698507412033
C	-1.24611048840395	17.73998084885516	4.44157391227109
H	-1.95109411520641	17.86387237885574	3.63010843948634
C	-1.49173479023333	16.81348105222825	5.44095834253933
H	-2.39098825115152	16.21366243186579	5.40313429279372
C	-0.60053998889433	16.63939174582079	6.49813328680993
C	2.12108852136407	19.16835332821064	5.49089634976648
H	2.80651960431651	18.71464993729622	6.20381366361661
C	2.80870516876403	19.16075333412751	4.12167089008616
H	2.99625937480401	18.14467325126774	3.77806880119520
H	3.75975109161230	19.69122594997766	4.17890690911537
H	2.20390678098559	19.66252994811619	3.36545558396970
C	1.87080590460266	20.60996341167632	5.95614649216735
H	1.15969243427002	21.11083334606523	5.29649168376656
H	2.80093353952182	21.18071472228096	5.94679181417218
H	1.47002116782945	20.64244255278972	6.96820384229320
C	-0.89735698916397	15.61132457143224	7.57059705924494
H	-0.15481279684240	15.71766165199840	8.35735462529752
C	-0.76612554540096	14.19402871542092	7.00552570242099
H	-1.52900527219657	14.00170599188793	6.25201805748819
H	-0.87245137997841	13.45339388400573	7.79704502759558
H	0.20388010334827	14.03884091799572	6.53556969087467
C	-2.27561489718454	15.81825100480527	8.21023742362269

H	-3.08220683507750	15.65409221157560	7.49387092009530
H	-2.38601689954006	16.82900688300288	8.60610298702644
H	-2.41516868277146	15.11435336070961	9.03217498037536
Sb	3.79136801377141	14.99779137025806	5.20582451545625
Cl	1.80666643644582	15.49985317676098	3.92270411015445
Cl	2.09184393359228	14.33698616223764	9.08123110660460
H	6.67938783777675	11.54546506739448	5.16138819331101

Table S42. Compound **4a**

B3YLP-D3/def2-SVP

Electronic energy ... -8328.22705940 Eh

Final Gibbs free energy ... -8326.86895790 Eh

Gibbs free energy minus the electronic energy ... 1.35810151 Eh

Sb	9.519151	1.001734	3.863650
Ga	12.037710	1.770453	4.681117
Ga	9.115841	-1.482303	3.050101
Cl	13.974979	1.398680	3.589217
Cl	7.146439	-1.197830	1.868817
N	12.046563	3.855450	4.208411
N	12.530063	2.208373	6.602938
N	8.510899	-2.822471	4.383190
N	9.959421	-2.821760	1.826569
N	7.885971	2.112153	1.284625
N	9.939206	1.718325	0.763564
C	12.790196	4.719716	4.892114
C	13.374423	4.439438	6.136658
H	13.948256	5.252686	6.577806
C	13.149207	3.337543	6.969579
C	13.038046	6.125860	4.380646
H	14.032708	6.168037	3.910736
H	13.040872	6.840528	5.214736
H	12.298059	6.445223	3.639229
C	13.629814	3.495690	8.397969
H	12.841706	3.226001	9.114078
H	13.946839	4.529254	8.584306
H	14.477455	2.829081	8.602554
C	11.315774	4.303887	3.070170
C	11.931740	4.468843	1.802519
C	11.124017	4.861343	0.724622
H	11.583791	5.007225	-0.255974
C	9.761896	5.102822	0.881130
H	9.156150	5.403980	0.023236
C	9.180024	4.987100	2.143139
H	8.120697	5.217634	2.267864
C	9.938948	4.603978	3.255451
C	13.445490	4.393564	1.591043
H	13.905923	4.142965	2.555655
C	13.982067	5.760007	1.116358
H	15.083163	5.773958	1.160355
H	13.603609	6.595876	1.720127
H	13.693357	5.953715	0.070279
C	13.905252	3.313634	0.599216
H	13.374013	3.392584	-0.364456
H	13.769920	2.307088	1.008661
H	14.980307	3.437823	0.392469
C	9.340579	4.639399	4.660351
H	9.860610	3.875933	5.255841
C	9.616137	5.997426	5.332165
H	10.688861	6.201063	5.429926
H	9.181905	6.016049	6.344305
H	9.164821	6.817776	4.749748
C	7.841637	4.335290	4.721414
H	7.239200	5.111984	4.222417
H	7.513286	4.295794	5.771485
H	7.608698	3.363862	4.268778
C	12.279874	1.245065	7.641262
C	13.307410	0.388352	8.092212
C	13.006124	-0.509612	9.125147
H	13.782780	-1.188304	9.484846
C	11.732782	-0.568291	9.687338
H	11.519802	-1.281150	10.488274
C	10.724537	0.269356	9.212211
H	9.722580	0.199336	9.636856
C	10.978149	1.182926	8.184210
C	14.699818	0.376006	7.469460
H	14.777450	1.240967	6.795302
C	14.910299	-0.875535	6.603461
H	14.155191	-0.929253	5.812239
H	14.834103	-1.792340	7.211865

H	15.908364	-0.854653	6.135900
C	15.818090	0.483932	8.519368
H	15.868616	-0.419620	9.148350
H	15.683339	1.344187	9.193840
H	16.796414	0.590992	8.023411
C	9.876863	2.086439	7.648899
H	10.126151	2.300941	6.599824
C	8.502035	1.418493	7.640119
H	7.781056	2.040745	7.087785
H	8.102549	1.270529	8.656400
H	8.545994	0.436718	7.151848
C	9.839640	3.440353	8.375407
H	10.780718	3.995419	8.251326
H	9.665457	3.299059	9.454983
H	9.025707	4.070697	7.980791
C	8.095832	-4.007681	3.913728
C	8.477729	-4.537820	2.672896
H	8.082596	-5.526140	2.441626
C	9.449343	-4.053414	1.779166
C	7.154535	-4.848189	4.744951
H	6.140495	-4.427802	4.652491
H	7.412365	-4.836344	5.810655
H	7.131161	-5.885307	4.387777
C	9.917862	-5.038822	0.730873
H	10.045114	-6.032240	1.182556
H	10.860279	-4.735674	0.262106
H	9.154802	-5.130349	-0.057341
C	8.347558	-2.545022	5.786274
C	9.372061	-2.968257	6.672981
C	9.189208	-2.744943	8.042684
H	9.969044	-3.045756	8.742018
C	8.032842	-2.137302	8.530539
H	7.913196	-1.974104	9.604771
C	7.038914	-1.730201	7.647039
H	6.138383	-1.247446	8.033629
C	7.173355	-1.921693	6.263796
C	10.620400	-3.695341	6.176008
H	10.852289	-3.283734	5.184235
C	10.386940	-5.208896	6.012016
H	9.651617	-5.446651	5.233667
H	10.043201	-5.657019	6.959384
H	11.329607	-5.703963	5.727833
C	11.847069	-3.470596	7.069054
H	12.749555	-3.836793	6.554086
H	11.767551	-4.026544	8.018522
H	11.995238	-2.407628	7.291558
C	6.039473	-1.488787	5.342844
H	6.293407	-1.794620	4.319729
C	4.707327	-2.160492	5.715832
H	3.934657	-1.920536	4.967249
H	4.338335	-1.813793	6.694970
H	4.799836	-3.255829	5.770412
C	5.874425	0.038247	5.324696
H	6.820050	0.533302	5.062270
H	5.557430	0.420127	6.309287
H	5.111773	0.330676	4.584517
C	10.959171	-2.400025	0.891555
C	12.300121	-2.293162	1.342313
C	13.254708	-1.788084	0.448672
H	14.287502	-1.675604	0.776110
C	12.906737	-1.421815	-0.852139
H	13.668520	-1.025875	-1.528774
C	11.593605	-1.573765	-1.289270
H	11.334273	-1.312102	-2.318219
C	10.595485	-2.069668	-0.436650
C	12.693744	-2.745236	2.744888
H	11.975455	-2.293315	3.447089
C	12.613069	-4.275422	2.906147
H	11.591150	-4.663087	2.819975
H	12.982621	-4.559679	3.903885
H	13.243189	-4.783077	2.156686
C	14.079265	-2.266161	3.179700
H	14.879816	-2.743108	2.588685
H	14.241517	-2.539505	4.231698
H	14.179205	-1.175494	3.106977
C	9.187532	-2.273249	-0.988662
H	8.570722	-2.723796	-0.200963
C	9.194414	-3.216170	-2.204825
H	8.162417	-3.461214	-2.504284

H	9.724346	-4.157230	-1.998216
H	9.685895	-2.746834	-3.072701
C	8.506949	-0.949000	-1.351685
H	9.053626	-0.420056	-2.149206
H	8.432075	-0.298012	-0.474448
H	7.481950	-1.133554	-1.711600
C	9.065814	1.689616	1.792536
C	8.016913	2.422347	-0.065906
C	9.323582	2.174419	-0.396680
C	6.623880	2.159484	1.999290
H	6.230209	3.186172	2.012154
H	6.788623	1.813578	3.024510
H	5.905088	1.478238	1.525084
C	11.304410	1.223279	0.853669
H	11.823864	1.417015	-0.086367
H	11.299109	0.145093	1.045615
H	11.833771	1.718963	1.669908
C	6.875721	2.915111	-0.883470
H	7.197275	3.101421	-1.916861
H	6.463645	3.857234	-0.483976
H	6.053313	2.181163	-0.915014
C	10.045523	2.336624	-1.686599
H	9.349690	2.655665	-2.474070
H	10.511923	1.393416	-2.010795
H	10.840570	3.095564	-1.604974
Cl	11.618758	-0.598794	5.409731

Table S43. Compound **4a** – B3LYP-D3/def2-TZVPP
final energy -8332.309796149853 Eh

Sb	9.50731718456526	0.99446748969623	3.83454768745315
Ga	12.02938466758143	1.75212362138397	4.66220483113031
Ga	9.11356702611839	-1.49160876351825	3.02518368756675
Cl	13.90898825232305	1.36783603985137	3.49783222636768
Cl	7.17286940456758	-1.20425921460686	1.80572359022977
N	12.03545806311547	3.85296203592925	4.19713277368732
N	12.55048806848934	2.19309380231370	6.57590075487820
N	8.49790052658405	-2.81920271383528	4.36421228172053
N	9.97016319282051	-2.84646707687486	1.82842567809187
N	7.87758178834773	2.12507278340056	1.29059848338803
N	9.91460444018891	1.72608972373857	0.75112055523676
C	12.78576750269631	4.70436668537849	4.87529598987276
C	13.38994021644607	4.41227668444603	6.09964484390944
H	13.96440260650857	5.21583356317374	6.53140733358874
C	13.17490353478690	3.31688335180150	6.92979577266672
C	13.01779478485714	6.11952631172792	4.38975823762943
H	14.00315135238684	6.18073361359120	3.92729636254849
H	13.00895346271158	6.80967267644270	5.23049524102505
H	12.28092631625714	6.44028157739267	3.66206135878982
C	13.67393931679198	3.48234210983798	8.34797190599525
H	12.91580879957674	3.18989758235435	9.07083579691968
H	13.95734262786831	4.51554168904698	8.52770056151142
H	14.54069526117522	2.85123857873055	8.52774998568733
C	11.29069965159194	4.32129966882721	3.07595553031225
C	11.88857086645575	4.50848802780307	1.81187666132761
C	11.07437028439779	4.92153882710947	0.75688265733549
H	11.51806505895155	5.08329898992010	-0.21670539977717
C	9.72355578340171	5.16548941549123	0.93349968735541
H	9.11518955755324	5.48312463082279	0.09714829834053
C	9.16047734843651	5.03161389230165	2.19372360710179
H	8.11503967379605	5.26622870761907	2.33470889768722
C	9.92639024053356	4.62544464714167	3.28285453752187
C	13.39456074464265	4.43477640573969	1.57866919894892
H	13.86684985408117	4.16049004468834	2.51883903618852
C	13.92788782735756	5.80925068401553	1.13052546457777
H	15.01867001760893	5.81442712652530	1.15956811445482
H	13.56483562113390	6.62269368563135	1.75433662452684
H	13.62556618770605	6.02324766002512	0.10397301805304
C	13.83048235621251	3.39038125042739	0.54375677757841
H	13.28874104234849	3.51197938730797	-0.39690178906640
H	13.68987480117490	2.38001870479677	0.91061577046415
H	14.89303728424203	3.51390795392075	0.32867705234670
C	9.34556127323488	4.64846764929483	4.69064323292105
H	9.87382488977712	3.89762775883357	5.27524378835750
C	9.61075399661415	6.00918409097840	5.35569077292504
H	10.67246452257643	6.21809795493452	5.44548319800001
H	9.18333872505024	6.02564557560967	6.35903666761012
H	9.15336036067682	6.81384331926030	4.77647327773985
C	7.85327070053927	4.33044773579469	4.76956824334979
H	7.24503526181268	5.08459122364995	4.26723645654255

H	7.54108238184754	4.30789989571742	5.81396297978468
H	7.63111193340457	3.35684865966553	4.34179285213663
C	12.30000917058637	1.24065219739974	7.62554596591260
C	13.31942436284461	0.38924512905266	8.07998695615927
C	13.01952147026745	-0.49411687127731	9.11564970669869
H	13.78629877239998	-1.16695370947000	9.47496441789919
C	11.75591774005383	-0.54074149505167	9.68108319301375
H	11.54419023059508	-1.23973217299080	10.47973638470125
C	10.75745674900220	0.29658029708761	9.20783677960126
H	9.76714124377580	0.23677188955832	9.63448077301287
C	11.00913544801531	1.19338548685807	8.17512387875100
C	14.71104003802642	0.37084224542053	7.46669649272789
H	14.79764104052535	1.22609761322259	6.79833343278912
C	14.92492140172155	-0.88483531087878	6.61264143871444
H	14.19204805470936	-0.93558252068085	5.81509403851639
H	14.83017089533269	-1.78699480659929	7.22068428252138
H	15.92251296506462	-0.87417781524176	6.16944656895366
C	15.82076926894077	0.47428908278211	8.52282103082295
H	15.87077203170406	-0.42790204880035	9.13443953376968
H	15.67673675216661	1.31757431192611	9.19866746376326
H	16.78971792320809	0.59151793132509	8.03480891826256
C	9.91215831504406	2.10210923922300	7.65196198257085
H	10.15053525357313	2.32184049098272	6.61231950585391
C	8.53493191490865	1.44509890006870	7.65452965181281
H	7.82087553455091	2.07349375257221	7.12153855345603
H	8.15206788087822	1.29570399047996	8.66526603411966
H	8.56437759591433	0.47657738434107	7.16255042966786
C	9.88697813747858	3.44535735211934	8.39376417780418
H	10.82406844441941	3.98742721425754	8.27540548753843
H	9.71541955788199	3.29082713992789	9.46084930454219
H	9.08409493117040	4.07862829969591	8.01170356992351
C	8.08436762455926	-3.99964603830792	3.89809269952552
C	8.47081065591741	-4.53331941165537	2.66935804264295
H	8.07348564583948	-5.50959064108047	2.44064893944636
C	9.44786612190464	-4.06594480748052	1.78422200244619
C	7.13838334424894	-4.83893757336393	4.71988461300832
H	6.12636978847013	-4.45917401781894	4.56983470098010
H	7.35137426562408	-4.78576769213338	5.78287045355986
H	7.16311078164828	-5.87682687614428	4.39915830005223
C	9.90945787029579	-5.06382529215619	0.74943942446994
H	10.01975265290954	-6.04431898254641	1.20774213996416
H	10.84996592323741	-4.77908554258759	0.29068390012485
H	9.15752584031241	-5.14956783006248	-0.03535072183691
C	8.32971803735578	-2.53892423862898	5.76652696888938
C	9.33973601917246	-2.96967085678891	6.65369502088778
C	9.15353145327675	-2.74643601246589	8.01467370487837
H	9.92048203113588	-3.05018812354954	8.71078498627376
C	8.00755553386247	-2.13032560681148	8.49430304678462
H	7.88531308661218	-1.96714943251872	9.55714165203833
C	7.02953794903198	-1.71362025355330	7.61041928631433
H	6.14112770199586	-1.22611957902907	7.98888663693067
C	7.16803208192642	-1.90517551222280	6.23534807971217
C	10.58193117555823	-3.70498519959794	6.16767419831923
H	10.81805272643418	-3.31275396060879	5.18052511291079
C	10.34011516278908	-5.21707046734581	6.02865396260218
H	9.59406554468575	-5.45827884435929	5.27722100040582
H	10.01555719991669	-5.64226995261865	6.98081573335329
H	11.26735060990875	-5.71338300302427	5.73735213781944
C	11.80653273825921	-3.48239409394258	7.05989123771002
H	12.69594884385260	-3.85875217594244	6.55229812572922
H	11.71879311147118	-4.02520522481164	8.00364334289158
H	11.96350853848347	-2.43008424414323	7.27322450738254
C	6.04330500798343	-1.46134592639194	5.31631378542114
H	6.30276969646894	-1.73998689781965	4.29803983751794
C	4.71548481759972	-2.14822542121491	5.66737484936976
H	3.95591327677963	-1.89996991134135	4.92401396958579
H	4.34585282189125	-1.82210083362263	6.64112235494009
H	4.81481450370352	-3.23246793260027	5.70240060721981
C	5.86095526289385	0.06128891744849	5.33926038851448
H	6.79131194711199	0.57002408709906	5.09269781611286
H	5.54129714508519	0.40586441893749	6.32444836969184
H	5.10060203776156	0.35800886925575	4.61426785285864
C	10.98927795559157	-2.44596842286930	0.90449988056110
C	12.31652834987250	-2.35414104859955	1.37340369784825
C	13.28518208894643	-1.86262543649082	0.50108737853921
H	14.30242739717479	-1.75607804764286	0.84421031117746
C	12.96537627593863	-1.50174914488545	-0.80050237192721
H	13.73412254756394	-1.11784044250267	-1.45837440338853
C	11.66727968903421	-1.64687608926419	-1.25761848598250

H	11.43131979610264	-1.39135502110284	-2.28223861927753
C	10.65467267341550	-2.12411678506797	-0.42407228177108
C	12.68542771288188	-2.82080909481863	2.77285718709302
H	11.94938364619600	-2.40464155147923	3.46123626746669
C	12.63216993980251	-4.35296563917633	2.89420679428407
H	11.63413395356977	-4.75268665056756	2.74331517936719
H	12.95483327669536	-4.65059693341042	3.89259347924212
H	13.30352280343622	-4.82044614087638	2.17075570192337
C	14.05132942056800	-2.33259423280753	3.24644003516898
H	14.86226521835388	-2.78554381926122	2.67088218747987
H	14.18980035652709	-2.62116554981146	4.28686455175885
H	14.13782748602477	-1.25058182863511	3.19178579271015
C	9.25842708482415	-2.30758691614875	-0.99984153210954
H	8.62202415073410	-2.73584114336036	-0.23001534268489
C	9.27176898493263	-3.25783172009819	-2.20691461140413
H	8.25048256662706	-3.47286457159048	-2.52580977392930
H	9.76500775676708	-4.20188747416380	-1.98121643513028
H	9.79412738217118	-2.81063717553506	-3.05428599965903
C	8.61818751733953	-0.97534535770730	-1.39483782934950
H	9.18381047409505	-0.48703553086282	-2.19032273157826
H	8.55713081723477	-0.30907463606166	-0.54121251625610
H	7.60212077361897	-1.13893904856926	-1.75720782207130
C	9.05342573145176	1.68949546613005	1.78425892222398
C	7.99902161365317	2.44712570318601	-0.05455254242848
C	9.29246488103909	2.19785659423044	-0.39589706203959
C	6.62653597666582	2.18636220687778	2.02173782293634
H	6.25698325761755	3.21025428239571	2.04950410956820
H	6.79979616640761	1.83209391562246	3.03098000180816
H	5.89578559372118	1.53267598046845	1.55154346842540
C	11.27624871777987	1.21794331164791	0.81802525478470
H	11.78811152628581	1.45273804383311	-0.10494278971785
H	11.26360127277284	0.14214789353016	0.95712921711948
H	11.80191487059238	1.66979394153118	1.64813090258183
C	6.85986249012785	2.95955608669175	-0.85536668301128
H	7.17365430832540	3.14588411044797	-1.87988276955770
H	6.46930071835604	3.89579387167221	-0.44982521774096
H	6.03625104942081	2.24324921823105	-0.88371946659904
C	10.00488899937925	2.38084697485824	-1.68359642155943
H	9.30842614681313	2.70446695355172	-2.45385752063628
H	10.46969206471484	1.45448600847598	-2.02150632655845
H	10.78805207438091	3.13628986848599	-1.59581350008416
Cl	11.63399809778254	-0.60042178351636	5.37815783651043

Table S44. Compound **4b** – B3LYP/def2-SVP

Electronic energy ... -8406.73881200 Eh
Final Gibbs free energy ... -8405.32487639 Eh
Gibbs free energy minus the electronic energy ... 1.41393561 Eh

Sb	9.62755440969851	0.97514682284423	3.72416598590931
Ga	12.17903417406638	1.82931047324355	4.74293838855519
Ga	9.18992352759343	-1.54788492058768	3.00901500671175
Cl	14.15437908451233	1.51175186437354	3.71651690083428
Cl	7.24885623452152	-1.33241933516451	1.78107186115098
N	12.15884016709815	3.92912336541242	4.38204040224176
N	12.63016868899980	2.19475148928667	6.70282200864686
N	8.55940162135421	-2.81287516648307	4.40571693174378
N	10.01148525937548	-2.97529142245912	1.84772284634396
N	7.78535396509502	2.30434932874555	1.36534068851187
N	9.62236655135819	1.55150299388440	0.52423553802309
C	12.86071625779356	4.77993971899220	5.12477174317393
C	13.44663384756579	4.45435754207474	6.35574335329909
H	13.99449374982347	5.26006019914155	6.84157125364539
C	13.23095815156736	3.31144458835255	7.13240754365020
C	13.05171769448604	6.22525039946931	4.70628957203117
H	14.07862382458916	6.36422503436482	4.33480215349074
H	12.92627065898629	6.88761097747654	5.57374467430400
H	12.35952504543533	6.53540620863160	3.91813333220132
C	13.68702365179647	3.41283963506897	8.57440832567543
H	12.87936796236631	3.13498354958450	9.26557391629333
H	14.01742929116276	4.43404484944094	8.80111874727069
H	14.51781355359325	2.72433911519815	8.77458717982118
C	11.43928374787559	4.39866766611628	3.24660324027900
C	12.08181431788673	4.62695607571995	2.00331387206696
C	11.27359775485316	4.94187229122096	0.89976804502275
H	11.74444262746780	5.10817440395159	-0.07267363039785
C	9.89392041375982	5.08609904542017	1.02496560680149
H	9.28757282867346	5.33309460826595	0.15067709723892
C	9.29467449825665	4.97255448935381	2.28117818407912
H	8.22636174087137	5.17046738240522	2.38685306485075
C	10.04864698800291	4.64148632985085	3.41176340482181

C	13.60445670641439	4.74418361045906	1.87464463895084
H	14.03363438874582	4.53039171068140	2.86151569808022
C	13.97093532878433	6.18836404006625	1.46980135510833
H	15.05459633677995	6.35437414124881	1.58348916147893
H	13.44307402782464	6.94490970383188	2.06594151986007
H	13.71950873267890	6.37105430700360	0.41222004657250
C	14.29396527626865	3.77895656163280	0.90175844047600
H	13.86621713105099	3.84058010273779	-0.11168257200360
H	14.24373455844860	2.74558427639375	1.25803711559142
H	15.35941157231895	4.04931533415438	0.82367067620467
C	9.45628134498542	4.73171637812231	4.81886843299681
H	10.07672582146701	4.10553574884269	5.47381866591967
C	9.56566739292214	6.18057651681574	5.33148345305409
H	10.59553826914930	6.55468019695927	5.30150182247569
H	9.21271009626658	6.24658357582480	6.37324478612434
H	8.94661910957944	6.85512020740866	4.71650384067696
C	8.01199806185663	4.25272303096159	4.96683872471679
H	7.31564731344187	4.81224900568118	4.32194885723419
H	7.67915380121802	4.40090561003635	6.00578832088568
H	7.92549881729454	3.18217605659077	4.74412614110010
C	12.35198732659956	1.20445843048606	7.70652976345403
C	13.36788946857777	0.34026962195109	8.16909895402488
C	13.04759056872570	-0.55521346648047	9.19840046515897
H	13.81519716917701	-1.23735614128005	9.57060652543008
C	11.76637629413735	-0.60478586218800	9.74396708627160
H	11.53941023971165	-1.31326016153144	10.54496922680142
C	10.76740312785781	0.23305491120153	9.24942819685121
H	9.75860339169941	0.16732669595618	9.65824011275383
C	11.04021523021521	1.14458986089930	8.22437160879027
C	14.76703001026050	0.32494383592133	7.56198147592223
H	14.86439847860168	1.20796609288673	6.91430249468450
C	14.96417175433218	-0.90333011884042	6.65975632957021
H	14.21162731045771	-0.92111065835239	5.86415663009426
H	14.87271920509884	-1.83654935384826	7.24038283016180
H	15.96370421554452	-0.88200635189032	6.19573634291440
C	15.87848725732544	0.38380610373614	8.62213197659791
H	15.91355131911390	-0.53931842214430	9.22324950587456
H	15.75164691031540	1.22501381237817	9.32198778188788
H	16.86135335925670	0.49247621377080	8.13574507496747
C	9.95282446457955	2.05486450513165	7.67147814440450
H	10.22666347599025	2.28319078278922	6.63092509606558
C	8.58053784093196	1.38525550755632	7.61809430591829
H	7.86742376391547	2.02353452116793	7.07526098485380
H	8.16377088289772	1.20154656216189	8.62117662384606
H	8.63782537048455	0.42184399902744	7.09647954773833
C	9.89863885800182	3.39801707988948	8.41741636841015
H	10.84683450729658	3.94822990809041	8.33309404845636
H	9.68837249073652	3.24109500016821	9.48835221522721
H	9.10228675185142	4.03966796284092	8.00601845310153
C	8.13597040266506	-4.02162883088982	4.00400251693715
C	8.52003237564954	-4.62849089958447	2.80211451648878
H	8.12603131925018	-5.62967572412410	2.63344588167882
C	9.50247108137648	-4.20743054016520	1.88777937424043
C	7.20304315265534	-4.81209395591744	4.89236427967138
H	6.22399350393164	-4.31148800386163	4.92244609550872
H	7.56269275054892	-4.86557185888305	5.92768201247644
H	7.06412217176572	-5.82959472685677	4.50658568465511
C	9.98333480704763	-5.27265664651102	0.92550927587444
H	10.06473971427363	-6.23522643616243	1.44866668158515
H	10.95063529299864	-5.02614297291575	0.47442758122826
H	9.25044260626921	-5.39964140458003	0.11428445725942
C	8.39275604707999	-2.48756371663628	5.79823208678234
C	9.40895850220275	-2.89761722310790	6.70028564083831
C	9.20283112411203	-2.67840445147392	8.06735113965713
H	9.97474693764780	-2.97209297741291	8.77834039657815
C	8.03004304924898	-2.08853962806831	8.53748703901134
H	7.88876964195358	-1.93305400797090	9.61027446851411
C	7.04937811998813	-1.68395341764983	7.63819669984812
H	6.14006401021746	-1.20728900678405	8.01124533521965
C	7.20891950681651	-1.86822573253328	6.25676110553218
C	10.67331241408412	-3.60987054468832	6.22101704191496
H	10.90518086770550	-3.20716439594259	5.22528187282674
C	10.47309048619929	-5.13033387700477	6.07580982688647
H	9.75370960571532	-5.39491798902564	5.29135751267525
H	10.12773500770640	-5.57143067690171	7.02592830811884
H	11.42981692361138	-5.60908881874570	5.81178713659681
C	11.88721512635193	-3.34847546378050	7.12044001304375
H	12.80214324154555	-3.70421583658724	6.62055721550552
H	11.80987116596270	-3.88991675235824	8.07830702410650

H	12.01276569897935	-2.28076063013196	7.32990431875048
C	6.09823214563055	-1.41547499281151	5.31701438961454
H	6.35486420408866	-1.74017611998671	4.29979687289993
C	4.73702807787363	-2.03377523991237	5.67621538410472
H	3.98641414795305	-1.77139179988324	4.91305329911477
H	4.36498637507832	-1.66423905167471	6.64571882028750
H	4.78405617650530	-3.13158281930270	5.74109026866787
C	5.98712433483261	0.11634232062911	5.28759862051700
H	6.94636036954408	0.57297866393844	5.00516163618366
H	5.69991321822251	0.51535781898062	6.27436742456948
H	5.22366211637184	0.42916741666776	4.55829430801778
C	10.99137054167666	-2.63928039175906	0.85836592789521
C	12.33418795420003	-2.46249309070475	1.27647941119088
C	13.28002639611097	-2.08193065931113	0.31549303610619
H	14.31572679316978	-1.92613785264872	0.61612536083724
C	12.92269693364246	-1.90837520127747	-1.02216385628067
H	13.67864966582614	-1.61709799369429	-1.75595976296972
C	11.60435715937646	-2.11304940672409	-1.41920112738279
H	11.33335358996071	-1.98280961402149	-2.46966170229278
C	10.61169777199012	-2.47454270322187	-0.49597012228785
C	12.74249856077900	-2.72704168830800	2.72048074246911
H	11.99619496057299	-2.24309482889525	3.37026279489961
C	12.73962056030208	-4.23248426627887	3.04478548877222
H	11.74451387552945	-4.68740669189053	2.96078758276251
H	13.08340889908747	-4.38989541497485	4.07896136091334
H	13.42580963961006	-4.77633467036774	2.37418078983825
C	14.09699568153122	-2.12709390729123	3.09740249918052
H	14.92620472502620	-2.62740660950915	2.56897178857866
H	14.26566787902846	-2.26241033569244	4.17431692731488
H	14.14373561209076	-1.04833606177125	2.89796216934855
C	9.18194377601739	-2.66507810240354	-0.99514458845482
H	8.56900525543265	-3.02542075988461	-0.15935502768374
C	9.10886479949001	-3.69532590590569	-2.13550525789136
H	8.05840590080835	-3.92753972898851	-2.37440163322719
H	9.61881613923023	-4.63551826015132	-1.87904603040922
H	9.57639952672951	-3.30999308765420	-3.05624880325540
C	8.54826582618987	-1.34058300023197	-1.44754549118398
H	9.10978656482519	-0.89959525931709	-2.28826789150670
H	8.49986809005861	-0.62117598593094	-0.62179096765529
H	7.51457731233585	-1.51169345331640	-1.78801923302265
C	8.92670661382470	1.64182598874418	1.67925632653060
C	7.78654178809549	2.67513247803957	0.02211578940417
C	8.95451479904870	2.19631707276111	-0.51019649263282
C	6.66525526811213	2.52914283422845	2.27883962141618
H	7.01994076839135	2.22513376289352	3.26895256337794
C	5.40944376964614	1.74391860348472	1.91942614224863
H	6.46430910037840	3.61083194116961	2.31745303931231
C	10.84213978237258	0.76327754204683	0.33849661864848
H	10.77722511695768	0.29842786018207	-0.65029818652736
H	10.80920745786595	-0.04739612322025	1.07279450180372
C	12.11755323041576	1.55256010779943	0.49213392350415
C	6.71719338131784	3.49458801322293	-0.61576464231352
H	7.08841670285740	3.92789082194199	-1.55481331066369
H	6.40518474178005	4.32732540731692	0.03434039326568
H	5.81731169002391	2.90553983934075	-0.85513908049962
C	9.50917280367799	2.30924750672798	-1.88708737550040
H	8.85443471651885	2.93213639474931	-2.51127712093063
H	9.59475045335854	1.32470576820269	-2.37336798276169
H	10.51062325208526	2.76758503248893	-1.87996371115172
Cl	11.69013375832222	-0.50331552105004	5.38623785179145
H	4.98888256327211	2.04456431430387	0.94927905341469
H	4.64182801209635	1.92997775082222	2.68636226538301
H	5.63067536229468	0.66866736448597	1.89355239154719
H	12.16509847839433	2.38639224959219	-0.21926241045981
H	12.97678801227346	0.89004488596605	0.31899358781658
H	12.20150274259664	1.95774339639006	1.50627376133593

Table S45. Compound **4b** B3LYP-D3/def2-TZVPP
final energy -8410.907524731201 Eh

Sb	9.59169340838927	0.97443182865683	3.73006890440192
Ga	12.15827215356526	1.81671063083695	4.72094911273057
Ga	9.17174581633687	-1.54744473332017	2.99472131191723
Cl	14.06167453552670	1.48719996374992	3.59157250597634
Cl	7.25909150493839	-1.33000581958127	1.73488113834401
N	12.15517144727868	3.93448686300668	4.36821842958077
N	12.65474705463571	2.18027984157674	6.67128837311051
N	8.53318102665936	-2.80947645067522	4.38771814812655
N	10.01643752587927	-2.97841963840946	1.85357931370094
N	7.77429720273486	2.29820891937501	1.38138764469019

N	9.60927379075076	1.55087539329731	0.55303710913209
C	12.87042482922563	4.76668323285613	5.10555595525215
C	13.47587431207812	4.42558941887757	6.31516941328458
H	14.02906423133556	5.21868253694680	6.79167231037502
C	13.26756218387836	3.28902811272089	7.08774554640791
C	13.05414970095013	6.21797780629306	4.71569840640210
H	14.06657512855467	6.36632004545673	4.33960437519097
H	12.93553104580719	6.85259722804817	5.59144882712510
H	12.35765283955925	6.53865535957801	3.95087248849195
C	13.74771099419486	3.39276901590371	8.51880024510154
H	12.96726541514201	3.10153209849277	9.21858797225192
H	14.05763651865494	4.41081906317625	8.73683828590087
H	14.59105343209791	2.72986499270405	8.69474051518520
C	11.42509521415101	4.42682523009523	3.24926154623308
C	12.04978102075062	4.67876342633289	2.01031243423093
C	11.23374970409023	5.00699146407737	0.92648493707714
H	11.68920228052156	5.18860059664703	-0.03845912491532
C	9.86339570889254	5.14499332836794	1.06722825350635
H	9.25318026471863	5.39871441719046	0.21085102329847
C	9.28227897610641	5.01458917988740	2.32163845619246
H	8.22554882327967	5.20863046252084	2.43993082199098
C	10.04484762838850	4.66992165127774	3.43222501582402
C	13.56558567338271	4.80243471414570	1.85948246157827
H	14.01287882123554	4.56427046610243	2.82105066592015
C	13.92077280500962	6.25617925762119	1.48707881329538
H	14.99621227531138	6.41503684295291	1.58237240257908
H	13.41000881424518	6.98752784320523	2.10878070185974
H	13.64819314042362	6.46044834430010	0.45036397013475
C	14.23083724091457	3.87802544427108	0.83579242403758
H	13.77379688571200	3.97323526975463	-0.15033406500216
H	14.19545235074938	2.84127244576405	1.14886684420352
H	15.28126857338327	4.15726281653370	0.73711351307537
C	9.46689411860651	4.74549559783646	4.84173330839316
H	10.08446811420987	4.12017105250057	5.48217783762046
C	9.57804983784105	6.18853954457060	5.36376080547191
H	10.59972459621204	6.55461383611423	5.33957494194043
H	9.22532199068906	6.24385660096993	6.39477204803191
H	8.96682549529868	6.86062326168653	4.75771990248608
C	8.02472528731034	4.27087308656342	4.99570896226437
H	7.33513906724624	4.82638646497083	4.35872611993827
H	7.70176532480718	4.42084267472983	6.02645554144041
H	7.93595351554893	3.21048986342552	4.77692989115452
C	12.37830878861844	1.19822357791258	7.68504013587563
C	13.38674137321447	0.33697375155309	8.14565395985991
C	13.06854604546195	-0.55024450577925	9.17239906084243
H	13.82667915148708	-1.22814545048534	9.54010712122029
C	11.79741620717568	-0.59152806724319	9.72168345341391
H	11.57259093960237	-1.29095890782124	10.51639484907217
C	10.80803197313819	0.24951511345970	9.23590290866971
H	9.81153018967600	0.19178167288296	9.64794760286078
C	11.07800989987871	1.15050185420989	8.21145692610819
C	14.78541434917695	0.32057070993994	7.54884217187039
H	14.89671838123067	1.20537681914879	6.92410203351587
C	14.98183497041332	-0.89502225766533	6.63426494339426
H	14.25154660587240	-0.89137734827637	5.83276816797204
H	14.86881040321459	-1.82393250353754	7.19738960228607
H	15.98088589997553	-0.87970908172132	6.19487627654109
C	15.88731493514011	0.34888868675181	8.61692879925054
H	15.91889000472923	-0.58514234892162	9.18001173523059
H	15.75308843288587	1.15823531505452	9.33553874578705
H	16.86159541920831	0.47472916039505	8.14199784264281
C	9.99387072362883	2.06828848122413	7.67633665346495
H	10.25237878883834	2.30000221798301	6.64365827013970
C	8.61683429183883	1.41306822115853	7.64117959046193
H	7.90893838562615	2.05965771197647	7.12272397596397
H	8.22196841341749	1.22781771865929	8.64098744579252
H	8.65342280261077	0.46323877666316	7.11495068427137
C	9.95807805855376	3.40147022860339	8.43621459101224
H	10.90293376099702	3.93634248222170	8.35239294626775
H	9.75491337792722	3.23326486781562	9.49562194758313
H	9.17211286061911	4.04706180568711	8.04005207932966
C	8.11394605690195	-4.01063101826512	3.97894235499027
C	8.50939010861353	-4.61201519563173	2.78758537759506
H	8.11633578167542	-5.60098884724182	2.61236329474922
C	9.49911090955736	-4.19985085126979	1.88882755628801
C	7.15889713506920	-4.80266987302232	4.83708584742118
H	6.15509510280814	-4.39864333364981	4.69895441787278
H	7.39334823563470	-4.73332845274672	5.89482109206670
H	7.14960263353641	-5.84754716565046	4.53943523837181

C	9.98258532512651	-5.27390627573805	0.94241673521029
H	10.09990831327324	-6.20947528908014	1.48548071678775
H	10.92372349662172	-5.01944203396650	0.46812302823554
H	9.23836066666974	-5.43781174104416	0.16304760642681
C	8.36360063498655	-2.48267424198446	5.77964943287777
C	9.36714488662939	-2.89914906526026	6.68038167329573
C	9.16420322391356	-2.67145763343964	8.03819775601577
H	9.92458861933819	-2.96818951523874	8.74443515663488
C	8.00651894209174	-2.06490778007401	8.50140545921395
H	7.86777172845965	-1.90221351309726	9.56231390297434
C	7.03920657007382	-1.65326869201797	7.60347109319130
H	6.14486789900378	-1.16710760213815	7.96932075462403
C	7.19642091041381	-1.84664488347323	6.23080648401069
C	10.61638912932530	-3.63369843539511	6.21166910403121
H	10.84937968153816	-3.26468773831570	5.21444563348113
C	10.38871782795879	-5.15122694150521	6.11123002489075
H	9.63999046410207	-5.41791413199678	5.37106669863994
H	10.07452325750767	-5.55509762111583	7.07603672029846
H	11.31901132790090	-5.64569227679009	5.82669654912585
C	11.83726378555096	-3.37585991070847	7.09829572757140
H	12.73136377506560	-3.75894358356092	6.60421225809264
H	11.75281109908847	-3.89042197208163	8.05790619829025
H	11.98444001887625	-2.31734079786175	7.28250176790558
C	6.08723730651544	-1.39660358621515	5.29610234012031
H	6.35133290881186	-1.69088835327760	4.28298248523114
C	4.74197621054159	-2.05230738159233	5.64008443334002
H	3.99822108994348	-1.80198369907330	4.88165588744896
H	4.36415400996453	-1.70288884267836	6.60253127895488
H	4.81857507180408	-3.13752758265284	5.69449701916088
C	5.93563401024998	0.12939205405482	5.30494248111568
H	6.86965423822188	0.61381303925960	5.02454437514924
H	5.65187580915377	0.49134757814084	6.29478807074557
H	5.16115776652349	0.43203476635539	4.59919328062453
C	11.01785761132336	-2.65450396428416	0.88144234865337
C	12.34826626693997	-2.49941140325235	1.32021657092636
C	13.30770016224507	-2.11905054232185	0.38502521916632
H	14.32910577505233	-1.97443566470393	0.70169442101767
C	12.97631611807832	-1.93033156955660	-0.94933437186027
H	13.73862916815768	-1.63892455389043	-1.65994220705632
C	11.67234502164656	-2.12591245709963	-1.36896856508533
H	11.42475993434409	-1.99216414168606	-2.41364747727984
C	10.66672466910465	-2.48626428628672	-0.47104598682662
C	12.73283242531515	-2.79449389374132	2.75993855063677
H	11.98530507505102	-2.33080144317521	3.40454877214756
C	12.72568140608875	-4.30552420746533	3.04585326861986
H	11.74134711183655	-4.75184107471234	2.93534509931556
H	13.05279695131325	-4.48401846036375	4.07070125993645
H	13.41516121713311	-4.82521416900153	2.37720825467064
C	14.08347255673007	-2.21431172792156	3.16925095983920
H	14.90746788711619	-2.70295398737883	2.64402957822974
H	14.23225786852862	-2.37981250377269	4.23410770933562
H	14.13823999846818	-1.14211535072464	2.99683189927514
C	9.25450306301234	-2.68558225019635	-1.00280161898562
H	8.62477846543969	-3.03649605716012	-0.18956401009915
C	9.21836206081079	-3.72730412538427	-2.13152096927049
H	8.18509078010679	-3.95761701783104	-2.39603783779998
H	9.71432429722942	-4.65487582058057	-1.85008546907965
H	9.71141992726342	-3.35261399019829	-3.02989675880971
C	8.63332154137677	-1.37376136790296	-1.49781724081006
H	9.21893267982596	-0.95246930808610	-2.31762473451354
H	8.55782886234858	-0.64628203122185	-0.69548648487398
H	7.62316268715007	-1.55487699881337	-1.86769595994395
C	8.91285464406096	1.64386442965714	1.70248769202830
C	7.77603682507772	2.65492347675249	0.03775824417838
C	8.93860960759092	2.18063117798501	-0.48533283654026
C	6.66180891286902	2.54490766099251	2.29555080563912
H	7.01568597152345	2.26035609623413	3.27994040937441
C	5.40432640749488	1.75987525320181	1.95267395882359
H	6.46542785684056	3.61699419607743	2.31081315170478
C	10.83476122818445	0.77075700451284	0.37910435765762
H	10.74786825875668	0.24280209236933	-0.56336236955997
H	10.84541936520444	0.02650641936219	1.16725929982534
C	12.09082169001187	1.59807860781329	0.43603898287657
C	6.70816853570931	3.46457725662036	-0.60608593850680
H	7.08220170974496	3.89901481815986	-1.53099620024788
H	6.38852917095218	4.28574800376820	0.03708873885331
H	5.82497773776635	2.87312892689608	-0.85087878996770
C	9.49077171285444	2.29166938980122	-1.85893310683874
H	8.78300601326475	2.80393311443448	-2.50664356626443

H	9.68657350177408	1.31117251769351	-2.29335121854880
H	10.42713387159824	2.85187057032628	-1.86796394487049
Cl	11.70257303343985	-0.50679405645739	5.35325204932166
H	5.00072934247007	2.03113482248731	0.97924976020409
H	4.64110444203425	1.97659405330958	2.70055246823153
H	5.61198314900052	0.69289334953738	1.96094662651763
H	12.10260374191494	2.36543986035402	-0.33411304541818
H	12.95408513758228	0.95006032653462	0.29843432571940
H	12.18027549276852	2.07762382549611	1.40401730599360

Table S46. Compound 4**c** B3LYP-D3/def2-SVP
Electronic energy ... -8485.23243856 Eh
Final Gibbs free energy ... -8483.76226134 Eh
Gibbs free energy minus the electronic energy ... 1.47017722 Eh

Sb	9.423021	0.950410	3.594865
Ga	11.905073	1.807565	4.725427
Ga	9.139515	-1.682474	3.147736
Cl	13.935564	1.316570	3.876826
Cl	7.057977	-1.802912	2.128516
N	11.996906	3.877495	4.254661
N	12.345773	2.216196	6.678809
N	8.694699	-2.974546	4.623836
N	10.028651	-3.055739	1.988602
N	7.686135	2.357326	1.146861
N	9.713957	2.136872	0.399577
C	12.660488	4.747954	5.018595
C	13.171041	4.465158	6.290988
H	13.692265	5.287172	6.777735
C	12.941924	3.340043	7.089607
C	12.891145	6.181391	4.571022
H	13.894914	6.266415	4.129751
H	12.857939	6.852598	5.439304
H	12.165424	6.527185	3.827991
C	13.392962	3.472136	8.531110
H	12.598269	3.179078	9.229921
H	13.697000	4.504504	8.743881
H	14.244445	2.809871	8.734119
C	11.449643	4.390224	3.039737
C	12.275257	4.623038	1.910535
C	11.705446	5.262163	0.798258
H	12.332981	5.473975	-0.070924
C	10.378488	5.677613	0.798890
H	9.969101	6.206048	-0.064567
C	9.575493	5.433442	1.911232
H	8.540026	5.774111	1.903089
C	10.088959	4.796548	3.046744
C	13.779629	4.349357	1.897022
H	14.066925	4.002106	2.898236
C	14.579038	5.623917	1.561055
H	15.649814	5.464177	1.765580
H	14.245618	6.497712	2.137635
H	14.487640	5.883275	0.493498
C	14.188620	3.238191	0.919822
H	13.867335	3.468289	-0.110574
H	13.777374	2.272113	1.223921
H	15.285465	3.135988	0.909762
C	9.233337	4.659526	4.304131
H	9.483325	3.690859	4.763320
C	9.537500	5.752005	5.346487
H	10.541870	5.656920	5.775068
H	8.821171	5.681957	6.180248
H	9.440557	6.754894	4.899089
C	7.730725	4.656843	4.007413
H	7.365612	5.664824	3.750101
H	7.172694	4.325031	4.896232
H	7.485926	3.983451	3.178243
C	12.095460	1.240522	7.703480
C	13.126649	0.388757	8.152752
C	12.838057	-0.482865	9.212052
H	13.617316	-1.155978	9.576697
C	11.575321	-0.514492	9.799983
H	11.372566	-1.202389	10.624894
C	10.562140	0.316020	9.321046
H	9.568208	0.262918	9.766420
C	10.802061	1.200347	8.265479
C	14.508936	0.372683	7.507544
H	14.570714	1.231519	6.825085
C	14.711259	-0.883295	6.645594

H	13.898952	-0.991241	5.917434
H	14.741370	-1.789660	7.272268
H	15.662945	-0.814997	6.094489
C	15.647795	0.490302	8.533241
H	15.701968	-0.400351	9.180161
H	15.535745	1.366432	9.191073
H	16.617076	0.577559	8.016012
C	9.702767	2.104985	7.725214
H	9.955472	2.324983	6.676577
C	8.332887	1.429078	7.712261
H	7.604044	2.055980	7.174837
H	7.938491	1.263971	8.728041
H	8.386796	0.455091	7.210720
C	9.655004	3.454249	8.460286
H	10.593885	4.014885	8.347086
H	9.473783	3.305052	9.537742
H	8.841468	4.083424	8.063212
C	8.339094	-4.209472	4.241983
C	8.706898	-4.801665	3.024321
H	8.366830	-5.825269	2.880839
C	9.604152	-4.323707	2.059275
C	7.483488	-5.060304	5.153580
H	6.446397	-4.695955	5.085805
H	7.782335	-4.992033	6.205865
H	7.499043	-6.111142	4.839177
C	10.117838	-5.342265	1.065611
H	9.844117	-6.356464	1.380964
H	11.210167	-5.279226	0.968270
H	9.702439	-5.164428	0.064881
C	8.589823	-2.682396	6.032298
C	9.665192	-3.083003	6.867602
C	9.537880	-2.896792	8.247168
H	10.358659	-3.184934	8.903529
C	8.385166	-2.340865	8.800048
H	8.307453	-2.204745	9.881800
C	7.339853	-1.956733	7.969339
H	6.436955	-1.523257	8.405515
C	7.415239	-2.122155	6.576968
C	10.917821	-3.750426	6.306488
H	11.053698	-3.364408	5.287660
C	10.777546	-5.281650	6.218737
H	10.010013	-5.599079	5.502277
H	10.525808	-5.706996	7.204603
H	11.730756	-5.728606	5.892588
C	12.178604	-3.402265	7.104228
H	13.073747	-3.725381	6.549893
H	12.200542	-3.916726	8.079428
H	12.251728	-2.323093	7.276049
C	6.205655	-1.742874	5.732757
H	6.422565	-1.994340	4.686134
C	4.945585	-2.520556	6.151276
H	4.121568	-2.319549	5.447266
H	4.603420	-2.222746	7.155992
H	5.115673	-3.607052	6.173056
C	5.927045	-0.235566	5.798918
H	6.789837	0.343737	5.445065
H	5.706242	0.084157	6.830090
H	5.057214	0.020245	5.175182
C	10.948974	-2.728075	0.939331
C	12.323996	-2.604304	1.252921
C	13.219969	-2.378233	0.199060
H	14.284233	-2.279213	0.411931
C	12.776661	-2.282193	-1.119432
H	13.495079	-2.116802	-1.926613
C	11.417548	-2.384643	-1.405072
H	11.077586	-2.291657	-2.438877
C	10.475125	-2.596514	-0.389439
C	12.818012	-2.725845	2.691499
H	12.116117	-2.160770	3.327535
C	12.824318	-4.184393	3.184236
H	11.820995	-4.626200	3.220789
H	13.237860	-4.230170	4.203092
H	13.457972	-4.811014	2.534401
C	14.203138	-2.112308	2.911162
H	14.992608	-2.700642	2.413627
H	14.430465	-2.096660	3.986013
H	14.255580	-1.073359	2.560309
C	8.991042	-2.667968	-0.742263
H	8.451195	-3.061627	0.127808

C	8.703101	-3.588456	-1.938449
H	7.615780	-3.707461	-2.070385
H	9.139576	-4.591089	-1.809294
H	9.102689	-3.175261	-2.878911
C	8.401071	-1.273238	-1.007305
H	8.827165	-0.825944	-1.920009
H	8.582004	-0.593391	-0.164261
H	7.310787	-1.345473	-1.141338
C	8.882051	1.740124	1.411177
C	7.798144	3.182820	0.028686
C	9.066339	3.040069	-0.448027
C	6.295549	2.053039	1.604623
H	5.789113	3.027088	1.549148
C	6.114969	1.533425	3.017307
C	5.648660	1.092400	0.597800
C	11.103165	1.704643	0.063729
H	11.678271	2.639316	0.023832
C	11.146370	1.018581	-1.305032
C	11.748290	0.787338	1.076603
C	6.724117	4.102960	-0.446779
H	7.094446	4.703846	-1.287492
H	6.415568	4.799326	0.350651
H	5.822881	3.573588	-0.791371
C	9.670195	3.730874	-1.627874
H	9.197825	4.713506	-1.758226
H	9.517234	3.169480	-2.563206
H	10.746102	3.899732	-1.503212
Cl	11.256147	-0.525036	5.486110
H	6.488561	0.510587	3.117527
H	5.031570	1.508895	3.213764
H	6.584061	2.166875	3.775280
H	11.926885	1.270377	2.036370
H	12.717188	0.462387	0.677667
H	11.150600	-0.113577	1.243295
H	5.744696	1.445527	-0.438710
H	4.577641	0.985552	0.828711
H	6.115016	0.101622	0.680059
H	10.653558	1.575313	-2.107589
H	10.693942	0.025600	-1.240301
H	12.199476	0.878956	-1.589081

Table S47. Compound **4c** B3LYP-D3/def2-TZVPP
final energy -8489.486449261107 Eh

Sb	9.42321488310344	0.94442938580217	3.51421315779140
Ga	11.91731052894613	1.81137413794691	4.76945348581653
Ga	9.10245318222981	-1.68648759852535	3.08646212736411
Cl	13.93402416740086	1.35756427041797	3.89113998854693
Cl	7.03565086516411	-1.82313544520850	2.06183789573458
N	11.96494703549238	3.88659191557538	4.30515594949114
N	12.39150745497771	2.23280857589610	6.71548549167156
N	8.67280002520092	-2.95414764916181	4.58480573274070
N	9.99174751569592	-3.08794502392449	1.95783541390095
N	7.70539981048061	2.31801175833560	1.06918928771575
N	9.73537697399862	2.09546753715742	0.35375098891329
C	12.64136011264363	4.75172810338409	5.05249047034503
C	13.20013038748775	4.46630980591455	6.29581123335864
H	13.72947448390726	5.28350389695135	6.75802657672423
C	13.00352035326966	3.34908415159379	7.10025849588298
C	12.83132355082930	6.19566403320384	4.62625287039580
H	13.84357181531616	6.32786312943403	4.24608800819870
H	12.72165480568141	6.84519498230283	5.49179998377848
H	12.13513917084573	6.51479633065474	3.85987404352154
C	13.50951940913123	3.48494937588864	8.51937277744413
H	12.75766632601875	3.18054946122037	9.24352967377093
H	13.79983025957196	4.51290625702132	8.71756930005187
H	14.37524693390391	2.84597456709796	8.67747833319983
C	11.38660225588175	4.39819212664621	3.10444491634108
C	12.18342471518671	4.64726768539047	1.96856426637351
C	11.58407149042113	5.26637972014426	0.87058251239872
H	12.18619326736155	5.49071325740771	0.00002020363063
C	10.25543832655240	5.64809386956564	0.89239971933053
H	9.82221168176188	6.15674861301662	0.04204566072031
C	9.48284455806456	5.39312231218187	2.01414949307022
H	8.44989353222953	5.70736977721462	2.02374421161618
C	10.02647383948612	4.77219637991742	3.13445362825423
C	13.68984846147074	4.41458971450669	1.93243503461472
H	14.00030258822687	4.06991991741905	2.91562489003905
C	14.44647068081414	5.71269872210020	1.59803977549668
H	15.51434460487578	5.57611682669207	1.77475415318303

H	14.10676487347107	6.55912148472800	2.19060910161209
H	14.32162390537408	5.97939829782476	0.54700682337850
C	14.11495696283509	3.33345326743149	0.93342460375868
H	13.78094934652949	3.57577094699646	-0.07844180948027
H	13.73063255649391	2.36142181646852	1.21739740161218
H	15.20329613845924	3.26033895540113	0.91299466283406
C	9.19549765702771	4.61246063784411	4.39931103483133
H	9.47572709174204	3.66166552221744	4.85355225090794
C	9.48068602802698	5.71742936603506	5.42918035243825
H	10.49206774270481	5.66844547072679	5.81985337907518
H	8.79903089374824	5.61732013540603	6.27465437522369
H	9.32704538322754	6.70273804832000	4.98487088725123
C	7.69261206770035	4.57065552397580	4.12279137397922
H	7.30094384299489	5.56289473166333	3.88991004654796
H	7.16363983279883	4.21031367826712	5.00508381116638
H	7.46007092441786	3.91064356835701	3.29282628382733
C	12.14675973343599	1.26713051916657	7.75089708541465
C	13.16411163739092	0.40186260883994	8.18000793592534
C	12.87625052727236	-0.47174276975004	9.22795325883211
H	13.64074361045512	-1.15480847162818	9.57268436253570
C	11.62799997276955	-0.48860592554024	9.82830441891663
H	11.42559901318957	-1.17650723330124	10.63886160346837
C	10.63078050592957	0.36319982569322	9.37677831991203
H	9.65215901981107	0.32389424240421	9.83200765419286
C	10.86914563702398	1.24667662185081	8.33060997489564
C	14.53854342157182	0.37397158778961	7.52966339304633
H	14.61663265801080	1.23725089534290	6.87149391921102
C	14.71296510789191	-0.86899669614441	6.64822383962164
H	13.92022900777174	-0.93077841996781	5.90928883185991
H	14.69596550475568	-1.77780060656437	7.25222833574749
H	15.66799190930380	-0.82378092341079	6.12242061538213
C	15.68080242723600	0.44576537919832	8.55181530054456
H	15.72675799238329	-0.45831830510911	9.16108460563553
H	15.58037556228282	1.29224624397348	9.23184894436885
H	16.63701278169385	0.53913013550241	8.03425298796031
C	9.77922269952048	2.17501031734624	7.82466583626628
H	10.01641608512389	2.41303852876669	6.78746285496088
C	8.39917004752191	1.52493265515061	7.82295375212492
H	7.68268749093294	2.17032140092380	7.31254122955612
H	8.02336205068172	1.35443809274390	8.83326885317755
H	8.42419239199975	0.56811601460661	7.30938959365368
C	9.76416370918865	3.50194276657007	8.59568558279807
H	10.70245489096444	4.04307156282560	8.48421939553780
H	9.59813686279595	3.32421932451898	9.66012972823037
H	8.96222794912861	4.14684774529515	8.23185311676308
C	8.30599015284884	-4.18579938400930	4.22240292438591
C	8.65496041791806	-4.79099974405081	3.01540572323618
H	8.30212171087817	-5.80085967542613	2.88445026540654
C	9.54897542059610	-4.34062729810132	2.04432459219098
C	7.45600031820733	-5.02410912420826	5.14649305037782
H	6.41933160139815	-4.70176101087014	5.03617610026183
H	7.72432693573914	-4.90760752998360	6.19122402189831
H	7.51423827384982	-6.07482155190900	4.87615956112496
C	10.02482857155571	-5.37976659244852	1.05792805967186
H	9.84361227685344	-6.37661218858234	1.44996481153674
H	11.08385352970555	-5.26980418803437	0.83956300234777
H	9.48902974644553	-5.28211290473800	0.11497564638630
C	8.58841846424341	-2.64607281803341	5.99097263796025
C	9.65600426972446	-3.06052240717638	6.81507066411528
C	9.54175696456100	-2.87042882649016	8.18728998498962
H	10.35433951011659	-3.16638452315908	8.83320408179505
C	8.41049842128259	-2.29264063031044	8.74227948033670
H	8.34234756479282	-2.15376700327377	9.81322706026798
C	7.37780873613662	-1.88408889858202	7.92060831282803
H	6.49832502621357	-1.42965483964902	8.35644943771874
C	7.44177787872487	-2.05115480117155	6.53597085371777
C	10.89371454235819	-3.74333074256999	6.25136754204951
H	11.02072995539811	-3.38679209344358	5.23110516950538
C	10.74084649203231	-5.27261686507939	6.20315511800476
H	9.96629347476235	-5.59406910609415	5.51266762783833
H	10.50035566106562	-5.66345704518390	7.19397535936862
H	11.67732418871517	-5.73015148938400	5.87952762977265
C	12.16458697861287	-3.39218464217429	7.02755050836735
H	13.04070554659132	-3.72497489821220	6.46951191380756
H	12.19301638739985	-3.89144036658346	7.99819858155725
H	12.24656770262711	-2.32259213548222	7.18653808824049
C	6.24695197018629	-1.63162854940266	5.69895303044302
H	6.46070156842063	-1.85865726871685	4.65733779374056
C	4.97399922336643	-2.39566781493849	6.09173593481855

H	4.16383387150147	-2.15284835909459	5.40195242963418
H	4.64669763983484	-2.12659506480696	7.09772168990217
H	5.12183428957262	-3.47420188127714	6.07351015250127
C	5.99296720450690	-0.12477715529869	5.80722580836225
H	6.85708206519494	0.44399325917927	5.46970040442157
H	5.77957982092511	0.16515418272624	6.83702954965842
H	5.13477667864899	0.15598370051021	5.19665331534763
C	10.93255084860022	-2.78287767599358	0.92121609615478
C	12.29385344469244	-2.67639826594807	1.26108131538170
C	13.21095349018386	-2.46293554023470	0.23446949369535
H	14.26120016235125	-2.37768730706789	0.46930617537371
C	12.79921014974939	-2.35967803924559	-1.08567645775400
H	13.52867496095701	-2.20243581905278	-1.86948883414520
C	11.45287256443815	-2.44577255191810	-1.39798949019627
H	11.13983406250618	-2.35063737793001	-2.42890872471525
C	10.49132104169862	-2.64797638557499	-0.40898099998607
C	12.75449094654168	-2.82443056961860	2.70257307671968
H	12.01451040191562	-2.33077074931273	3.33595596481612
C	12.82268215154469	-4.30606667314211	3.12390564098641
H	11.85248496155256	-4.78970594607809	3.09289974851515
H	13.19712354164287	-4.37772675142745	4.14473171118927
H	13.50507974449484	-4.85034843659348	2.47223910238829
C	14.09837790103021	-2.15419143589985	2.98268455845386
H	14.92079490155645	-2.67855710429462	2.49122959828227
H	14.29446324953956	-2.17100006753367	4.05299112335684
H	14.10754139587315	-1.11261202276012	2.67108954526621
C	9.02086606538297	-2.71690929268265	-0.79401966892255
H	8.46569676027788	-3.10377402309406	0.05588442633132
C	8.76395086105541	-3.63995044713423	-1.99244007814455
H	7.69057263721355	-3.77086056872529	-2.13677509972611
H	9.21047144700669	-4.62488135366363	-1.85630682396543
H	9.16908805481643	-3.22204744956983	-2.91550446907428
C	8.44183237021977	-1.32590255852354	-1.08514833309162
H	8.89242815949967	-0.89171816443040	-1.97952868670388
H	8.59623579035925	-0.64512647154807	-0.25086527483886
H	7.36660840634262	-1.40133711948371	-1.25001869685913
C	8.89297586839257	1.70058914693615	1.35106818398997
C	7.83423911080938	3.13738358380010	-0.04805576915976
C	9.10022219656919	2.99601195833962	-0.50187877821619
C	6.30796137250763	2.02658861755407	1.51279430464343
H	5.81597729514927	2.99622378272711	1.45170474281510
C	6.10344375075372	1.50735395813957	2.91945141211581
C	5.66697739724492	1.07432929630876	0.49880748207299
C	11.13060103937392	1.67289750457883	0.03709521050376
H	11.69367345606000	2.60231303826791	0.00367499519632
C	11.18900056908997	0.98898543498872	-1.32941425602534
C	11.77373726677170	0.75592272053535	1.04801113271051
C	6.77479905794033	4.06074958718113	-0.53803088741941
H	7.15349014880473	4.63655992467940	-1.37885729261344
H	6.47739208302905	4.76624582223367	0.24096939858721
H	5.87702583823003	3.54273458952198	-0.87407526037463
C	9.73142164527285	3.70482503429857	-1.65214148732809
H	9.27716066177452	4.68668194448524	-1.76451034274812
H	9.59387384110862	3.17218336983660	-2.59372589590415
H	10.79620337946729	3.85666056984097	-1.50178872301961
Cl	11.23517355729321	-0.43157771847690	5.50938651709556
H	6.46985167409428	0.49429980287834	3.03034707200538
H	5.02574980907769	1.48826126684664	3.09189739062544
H	6.55514579672034	2.13355493565762	3.67802331201123
H	11.93235680345815	1.22408129070488	2.00754281197371
H	12.74272373526334	0.45448637379193	0.65594925996354
H	11.19037779293638	-0.14590086646636	1.19363450897525
H	5.77849853346715	1.42689484337336	-0.52478770801584
H	4.60275272843389	0.97840826965340	0.71536804813698
H	6.11988522584121	0.08969678684784	0.58123729608269
H	10.67154953074219	1.52209995552710	-2.11803560965781
H	10.77729194666548	-0.01026877095606	-1.26009502576234
H	12.23533985183179	0.89246694044102	-1.61775956289353

Table S48. Compound **4d** B3LYP-D3/def2-SVP

Electronic energy ... -9103.80954302 Eh

Final Gibbs free energy ... -9102.08794270 Eh

Gibbs free energy minus the electronic energy ... 1.72160032 Eh

Sb	5.47216973148500	13.55122758887958	0.81921439932987
Ga	6.39022909982443	12.87921884947076	-1.61906742812485
Ga	5.78634761124589	12.59587850514269	3.30712340643871
Cl	7.41761617628693	14.95889194093535	1.27188676047931
Cl	6.87936006297758	14.96052041850031	-2.33793971064680
Cl	4.84247715219160	14.42501215055246	4.26816350428043

N	7.27614300946170	19.28852569122138	-1.24983224076607
N	5.25824465847986	19.68991931629873	-0.70380243430137
N	4.74508213202487	12.44684416222762	-2.66919648940939
N	7.59369869725271	11.77818321942347	-2.75380372370708
N	4.83252007815220	11.10990361370887	4.19114372961406
N	7.43929433262625	12.47150929866707	4.39911447247117
C	7.29766981052045	17.36334501536407	-5.15568170714465
C	7.20798445781151	19.80439500253147	-4.50013670428910
C	7.31702086213532	18.35634803907438	-3.99096178754023
C	8.52021432070093	18.20542550976363	-3.06974252772785
C	9.72696138095267	17.66731890430180	-3.53024011799026
C	10.84154804281386	17.57169324692116	-2.69533280072187
C	10.75233037714190	17.97037283907506	-1.36563043785403
C	9.88465332977222	17.69321182345656	1.52488694542643
C	10.31655850925175	20.11755834190270	0.94144858088902
C	9.47781857479952	18.86863959903351	0.62548225314638
C	9.55880843337519	18.49602294811309	-0.84866775405064
C	8.46695903015124	18.64222598181330	-1.72564916547367
C	6.05689458699252	18.67563102078766	-1.15209076613043
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C	3.58150101497666	20.32634411947980	-2.97257735199441
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C	3.63880275339728	19.02503921181610	3.21078311366762
C	4.25795808762507	18.73866135020254	1.83742243760652
C	1.63647155710374	19.60342060336124	-1.51163901709547
C	1.10823037499771	19.12397982644580	-0.31428039247859
C	1.94690937944042	18.86544263621379	0.77061302752676
C	3.33022346758781	19.06897615932814	0.67802475977471
C	3.84044541164814	19.53623125506277	-0.54939841899908
C	5.94430415802906	20.89373319089836	-0.53762941552914
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C	2.80024428740035	8.76880435399243	-1.70087470950565
C	4.55387860987747	9.89030615014446	-0.27957350982257
C	3.68554028396192	10.01068684136894	-1.54012336074388
C	2.36472294790308	15.55371829042743	-3.71389653850093
C	3.50140841812832	16.08485954364009	-1.52110468083922
C	3.27999385126546	15.01661950077888	-2.60130419547265
C	2.90526952043673	11.31661376188949	-1.50607758749080
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C	0.93868601817730	12.57667377727578	-0.83183788819736
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C	2.73909609394017	13.72638142471711	-2.00332139758119
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C	9.98237261407858	9.09254654814963	-1.78535993818059
C	8.78411632780872	9.73705535148357	-2.11661541454774
C	8.80910260606226	11.13861775479555	-2.32614983503077
C	3.59766982891069	12.05911966125052	-4.79996687940031
C	8.47432060509363	11.53655547257901	-5.03919075137062
C	4.85030935233482	12.22378197050188	-3.97636870488754
C	6.08763676259357	12.08529696439056	-4.63967977071419
C	7.34205966207011	11.81429385335339	-4.07704623622450
C	0.94492773803791	12.15214417676823	4.66316064822499
C	1.84991765793315	13.17813091007599	2.53736010579076
C	2.14499898449056	12.22930336994300	3.70518881052184
C	5.42888566331596	6.98193109351317	4.18045617898645
C	6.40874422364241	8.32689067523766	2.27763049272467
C	5.52495777574887	8.36902548189648	3.53027234731488
C	2.56661504178373	10.84555120604974	3.23582171997998
C	1.64931796759359	10.03813253583643	2.54639412665773
C	1.95841628552974	8.72567799318812	2.19886550466292
C	3.20286208021992	8.19478871072845	2.53943057064850
C	4.16167684247915	8.96844218790232	3.20348394539782
C	3.84050424363843	10.30999660291244	3.53281435328091
C	9.06615833290921	15.59156411896671	6.49915110428390
C	7.64121554402230	16.47145160595194	4.61451859079772
C	8.22135998487074	15.20976817057588	5.27167834932686
C	10.07775952061135	9.90727432585589	3.12205238823381
C	8.84870673211755	10.74866812907870	1.07410119687851

C	9.03897654292622	10.90340146300188	2.58311967416471
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C	10.16579314418041	14.92579043758449	3.69162731363935
C	10.91477544309803	14.22089054909109	2.75255158574285
C	10.53647132125950	12.92974498518886	2.39387203868808
C	9.40475775908809	12.33033044834004	2.95882594352482
C	8.64582122694220	13.06715925261288	3.89153756496675
C	4.09141065679429	10.07695791398565	6.29206062002150
C	8.60045019915818	11.97549037511044	6.51122648777643
C	5.08217140906003	10.89288825656102	5.49627349204563
C	6.22915163241952	11.33523628702509	6.16120464883589
C	7.38403543054066	11.94572643826769	5.61686428939797
H	8.09842450705509	17.55972806871761	-5.88878575270071
H	7.39192896970017	16.32782451013262	-4.79623676930249
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H	8.42723016169853	19.09736478653273	0.85514072634661
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H	4.64837697486573	20.53850454085377	-2.82195511055316
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H	3.91985864945971	19.60575749876044	-5.00588275755782
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H	3.88135065566629	16.58802657046250	1.77904316933259
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H	4.39967790114725	18.89823778034131	3.99688615670462
H	2.82218848655154	18.32290393641423	3.44455993725262
H	3.23880614491600	20.04975846403779	3.27740303783629
H	0.97026436724996	19.80516724530344	-2.35368217856993
H	0.03213226444334	18.95369881454128	-0.22289462360743
H	1.51962661504379	18.49421239963965	1.70344429292503
H	5.45874866491320	21.80395580256918	-0.19654960866848
H	2.11381712005913	8.86437482444214	-2.55702705143637
H	3.42906152660171	7.87856236256049	-1.86235428950642
H	2.19799789927063	8.57904657336827	-0.79897051627481
H	5.05230941601107	8.91359197882446	-0.23194792816976
H	5.33647813424320	10.66254446985837	-0.25435114091191
H	3.94273158064231	10.00349318441449	0.62539298218195
H	4.36231431343035	10.04526336096448	-2.40762444097478
H	1.38816129203972	15.87102285420360	-3.31327309588755
H	2.82475116779513	16.43067820177072	-4.19174789455349
H	2.17446502197360	14.80370749584768	-4.49786600196910
H	2.54775993442010	16.48258784585651	-1.13725157953613
H	4.06168034018277	15.67715106165568	-0.67076854456821
H	4.09762377300760	16.92327701946821	-1.90469306903947
H	4.25982670240450	14.80132742869457	-3.04616593073526
H	1.21964835705686	10.47608405682035	-0.45504734438510
H	-0.04285961394546	12.60680750037837	-0.35241422650224
H	0.92778215055767	14.67328453779752	-1.32133703336321
H	9.30700602488814	13.81172633463121	-0.36326040995892
H	11.07258160457679	13.92009284736714	-0.52996122612477
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H	11.09520118170213	14.89213197774421	-3.53995484268207
H	12.18103221909415	13.67261057392648	-2.84551760519270
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H	7.63089052754532	8.04465490986877	-0.25886850234576
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H	6.67147477260032	9.63139969144697	-2.00030139930963

H	12.10377460950482	11.74753996692306	-1.71510625874811
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H	9.98792161990871	8.01356931173799	-1.62355873780092
H	3.04473961728481	11.16864240495444	-4.46058736781414
H	2.91831588385485	12.91197583397466	-4.67159504350931
H	3.83673829686831	11.94117418579452	-5.86397769207850
H	9.22233316496218	12.34034211748003	-4.95679277533186
H	8.99535707390316	10.59808466990340	-4.80785768774254
H	8.11012066905550	11.49958571121716	-6.07322648108537
H	6.03968981292611	12.04927059230269	-5.72634853987135
H	0.04127326774553	11.77189795881559	4.15876285958136
H	1.15017889157787	11.49013428525669	5.51966181361059
H	0.71068278744229	13.15341185844331	5.05887417320879
H	0.95647896132020	12.86539554989805	1.97540222340795
H	1.68573797728288	14.20135940450130	2.90894568801451
H	2.68439927103679	13.21984885773471	1.82234366016667
H	2.97848583532011	12.66346249908649	4.26899475062113
H	6.42784659883517	6.63918281016456	4.49471929581683
H	4.77814536735939	6.99109573406948	5.06910399226192
H	5.03005234951323	6.22787319725957	3.48317074796389
H	6.48668089155873	9.31925898896943	1.81442155620562
H	7.42599266213703	7.98352965207135	2.52498060080420
H	5.99115088808110	7.63898257298491	1.52642241314860
H	6.02539023474656	9.03051067653174	4.24907584284998
H	0.66603578045097	10.44524484648817	2.30063829201263
H	1.22569530597384	8.10947536461895	1.67154212542964
H	3.43713051145751	7.16266662772975	2.27031182513923
H	8.44312151489380	16.10729005661061	7.24799728847658
H	9.52461715922876	14.71434600449436	6.98034516746523
H	9.88361569654385	16.27736282901509	6.22248836832289
H	7.06519072303895	16.21747527082421	3.71740802653156
H	6.97331472828962	16.99354961851247	5.31827809995601
H	8.44109964909386	17.17112624476271	4.32276309146138
H	7.36560215507137	14.61153023178295	5.61248269860505
H	11.06548723373249	10.07908272300764	2.66430489363784
H	10.19397964062261	9.99870461165342	4.21391489318541
H	9.77851748955866	8.87089116621988	2.89402749286255
H	9.76766936049552	10.97821660434817	0.51917291131275
H	8.56567386814343	9.71882098640638	0.82017622245227
H	8.06079725998751	11.42102318837389	0.70624561106044
H	8.08238545269176	10.66270392167265	3.06765397011348
H	10.46825502057907	15.93848959169925	3.96439379705709
H	11.79266955450347	14.68318890959592	2.29481830036483
H	11.12564501906181	12.37800158791459	1.65844916849272
H	4.09486196811492	9.02441345106235	5.97289220845887
H	4.32499260940832	10.11664196481551	7.36335131378577
H	3.07031558595712	10.45091648712674	6.12929947779180
H	9.52813891269851	12.09918042061032	5.94010880066719
H	8.52203589677198	12.82299115853582	7.21033275606390
H	8.65502415095876	11.05565532444275	7.10941646864840
H	6.29893284445411	11.06389864979264	7.21393380567986

Table S49. Compound **4d** – B3LYP-D3/def2-TZVPP
final energy -9108.716534191015 Eh

Sb	5.16713341433985	13.31440958832126	0.89433307259075
Ga	6.39759172275371	12.90282489094513	-1.52069048499499
Ga	5.65736017563976	12.34585251727604	3.39614172772463
Cl	6.91174448073526	15.00055958100135	1.50278790595913
Cl	6.91452131630591	15.06344562231415	-2.16693611185020
Cl	4.58953061719173	14.11693498407579	4.46040284437488
N	7.27523072883934	19.54137198347703	-1.56953327642211
N	5.25120818405495	19.75082409809233	-0.92049525525504
N	4.80357689435383	12.57544497616153	-2.74628602604148
N	7.63539021106160	11.86128403615898	-2.74416974869101
N	4.80383901352902	10.81820941823724	4.42665367039294
N	7.33650315120386	12.31857401968437	4.52527248990611
C	6.93001748939794	17.91784531795592	-5.14670659415455
C	8.01724780180799	20.17881934659589	-5.54699866986366
C	7.52194289801938	19.18335887512622	-4.48507402527587
C	8.61724111637264	18.80827041630668	-3.49862515013680
C	9.81542698682965	18.25656882037294	-3.98976073904719
C	10.84480783264668	17.90456148324656	-3.12195474802696
C	10.69319406238230	18.07283243812352	-1.75663632994206
C	9.59849460060450	17.34905719791417	1.00167337197295
C	10.28768843017425	19.78632694849241	0.88522439619635
C	9.35725693087882	18.69761596609261	0.29094404090965
C	9.50775776609434	18.59227362007272	-1.21163478745369
C	8.49100427816247	18.97355008045712	-2.11621832749535

C	6.02931149891326	18.93850520258305	-1.69665683350564
C	2.54597170146409	21.73304949631806	-3.54762677113507
C	3.71016261877125	19.55977688531680	-4.10830615657344
C	3.46569016191413	20.61216191281230	-3.00974874419719
C	2.94856189399851	19.96733508215294	-1.73930294804962
C	3.90406721257164	17.06471481279806	2.14133740371300
C	4.61423498076726	19.43535745800611	2.58822430310921
C	4.36172169472404	18.38603814903959	1.48916770123784
C	1.57422446138427	19.74170685149269	-1.54450533202454
C	1.11223717897105	19.14070505785412	-0.38262334104783
C	1.99997047155453	18.72721802023977	0.60338757252215
C	3.38756453647945	18.90047284276021	0.44052689416696
C	3.82085456665745	19.53982460600419	-0.72610321594743
C	5.95943921122131	20.82122952028294	-0.34476180384177
C	7.23979873507659	20.68261681060407	-0.76652785439585
C	3.33854247375348	9.51106823164229	-2.72224801764542
C	3.75027251329056	9.31660779040124	-0.24509774066488
C	3.86224850095321	10.21920120141577	-1.46408447827747
C	2.22011069323507	15.58710980809239	-3.78462444874605
C	3.62593491488359	16.28793051782811	-1.80302619898573
C	3.28426293391421	15.14200443160780	-2.76772375118241
C	3.14560529857381	11.56702642722952	-1.27550454169787
C	2.09245598844413	11.71981654534432	-0.37327428815623
C	1.40385524826159	12.93771677340449	-0.28547977167917
C	1.76275947761338	13.99847532024126	-1.10398769280078
C	2.84481429678045	13.90893397565636	-1.98830379793562
C	3.53824232655716	12.67945444305360	-2.05656180998360
C	10.21823140317638	14.37918355220278	-0.96580585634686
C	11.18311069605454	13.67532496450728	-3.19682451871765
C	10.04542788314936	13.46949099883686	-2.18037620106034
C	8.21180258601636	7.99159755551354	-3.69636711532318
C	6.98917024547207	8.15038851409119	-1.48248211319445
C	7.69189477894360	8.93140227166369	-2.59764920631049
C	9.93168357527318	11.98928752372048	-1.80214212918661
C	10.98269859201634	11.35168314890547	-1.13314771042201
C	10.96276163348833	9.97493664586713	-0.90160438224238
C	9.90260086378220	9.20895252648242	-1.38496055188171
C	8.82080680455289	9.80543226041744	-2.04095017841474
C	8.81970873328863	11.21201237711759	-2.19699970714990
C	3.74684958529482	12.51874768044625	-4.96906820582067
C	8.52315323836292	11.48823686170596	-5.01751502271939
C	4.94620894415595	12.44875613376860	-4.04693714045678
C	6.19970085715672	12.24040253572365	-4.66918192576169
C	7.41429555725316	11.88165602600694	-4.05683833671986
C	0.88307351660549	11.38625824636146	5.37158597143490
C	1.48383502712745	12.67173977936638	3.27320421245435
C	1.97482630526394	11.67001089207137	4.32728048298216
C	5.84403087347175	7.34516585110129	4.66997067938542
C	6.26824902169770	7.56619384477739	2.19471683080868
C	5.70843770190338	8.25630662006994	3.44017497301974
C	2.47311477014056	10.37916387303389	3.67814175354196
C	1.57834625050274	9.54428388724202	2.99640326494517
C	1.98966713868882	8.32305064587466	2.46797634012935
C	3.31731310452929	7.91203448702456	2.61488779036582
C	4.25228317815353	8.72443432034732	3.26120791109432
C	3.82088594115177	9.96685341912796	3.78366791524619
C	9.09350376763823	15.51818024517987	6.48767677586186
C	7.48509677401422	16.33391641810273	4.72173177279464
C	8.15149239237363	15.08727365132267	5.35228880094652
C	10.22822236351321	9.87375779155586	2.81675660298524
C	8.25424609726185	10.52028182394170	1.36163879488483
C	8.93577507860031	10.72839742779290	2.71312120819719
C	8.88047024303884	14.26422869809092	4.29752841833658
C	9.94823458021959	14.84316512207096	3.60039160876158
C	10.60852826678143	14.16765485699949	2.58689627623610
C	10.25734250465508	12.85185299232391	2.28210716261744
C	9.23283866491965	12.21116636305559	2.98549297549685
C	8.52035729697928	12.94012174061180	3.94878441781350
C	4.13453444107364	9.89104444684591	6.61365808588367
C	8.55702380442749	11.96425518018755	6.63479909454786
C	5.08752197956061	10.66156753147188	5.71711118980423
C	6.22455580611821	11.18510520879319	6.34946088314083
C	7.32922329195592	11.83920067650604	5.75403550894553
H	7.68753431760558	17.40124227987979	-5.73909884245669
H	6.55502471215588	17.22980227101812	-4.39011732620751
H	6.11106714919961	18.19296383544948	-5.81305823573022
H	8.79176834398225	19.74239435298589	-6.17919749766847
H	7.19144647436358	20.47817028336941	-6.19468709989618
H	8.42885702550215	21.07666756374918	-5.08245168544698

H	6.71709912629904	19.65682354460016	-3.93134343221062
H	11.76341786253585	17.48800984736681	-3.52251975286947
H	9.93457898428404	18.11002893063194	-5.05386743174766
H	11.48978314629436	17.77715538404624	-1.08473631370425
H	10.63802465738618	17.02766018112823	0.90892326299321
H	8.96210898651503	16.57100754036637	0.58704834262352
H	9.36880322790787	17.44373522846085	2.06256701907470
H	11.33546285322856	19.50243264468923	0.76151283544896
H	10.14831174663908	20.74869186498450	0.38962657031221
H	10.09222656573003	19.91263121821899	1.95082396586494
H	8.33184108689879	18.98298959471437	0.51305746805434
H	8.10935133570178	21.28345710675184	-0.56654400982691
H	4.42756483763617	21.06847962357740	-2.77522150899769
H	3.05183262049143	22.25975715634938	-4.35727529394918
H	2.29248439671621	22.45433866560029	-2.76989437714371
H	1.61828153962944	21.32655174082116	-3.95388704105285
H	4.13861526464897	20.02987931599012	-4.99553681832222
H	4.39732515876953	18.79139743684775	-3.75856749009061
H	2.76970363893026	19.08424000063846	-4.39712571144439
H	3.65735579753671	16.31292782159190	1.39231973822856
H	4.70100857496369	16.66578442647079	2.76349230725051
H	3.03320008252672	17.21314106767041	2.78085305694301
H	5.30687097224960	18.18486459202182	0.98491243297339
H	5.35478651508948	19.06561931215629	3.29876855480889
H	3.69298980880175	19.64372845739619	3.13592990187249
H	4.98080332729767	20.37395181185259	2.17457159486668
H	0.87311853716542	20.04971931346995	-2.30751589218356
H	0.04718472709405	18.98522711355128	-0.24214318020390
H	1.62848079695618	18.23732694176923	1.49073045264999
H	5.49352535825355	21.56322917965811	0.27497560321855
H	3.43573682373510	10.13334758886101	-3.60926132279459
H	3.88992932283967	8.58435290444074	-2.89827710348282
H	2.28214083143014	9.25819923178186	-2.60235558278914
H	4.32834973672471	8.40516743804263	-0.39004497468684
H	4.11271174074361	9.80483890463184	0.65831636665795
H	2.72093571886000	9.01435369725765	-0.06049153664958
H	4.91820849782174	10.43689715025938	-1.63295890882471
H	1.31050692241180	15.91505258771199	-3.27775854937425
H	2.59382223263287	16.42869352360804	-4.36861278473929
H	1.94898474288847	14.78567920386847	-4.47165680723841
H	2.73777027905676	16.64287423931205	-1.28123841772316
H	4.36258588702062	15.97569067462607	-1.06687785877989
H	4.06559588576491	17.12239295772094	-2.34191118604245
H	4.19527584911900	14.89315527994330	-3.30628144888006
H	1.80599411620673	10.90426942400323	0.27371013935055
H	0.59885676789816	13.04875265257124	0.42590067109834
H	1.22942434074616	14.93797528440320	-1.02162025913486
H	9.40122552250030	14.26728161122599	-0.25625439857762
H	11.15365849362436	14.17734104738123	-0.43926041403912
H	10.23132838125481	15.41853696142172	-1.28972470830473
H	11.16377706758751	14.70103026015790	-3.56888408996944
H	12.15929668923554	13.50137382261912	-2.73808848356935
H	11.08704806503599	13.00143031265132	-4.04817366949227
H	9.11810792874809	13.75620538487656	-2.66545330215512
H	8.75103086536128	8.54167156564287	-4.46634130178002
H	8.89059951404555	7.24252479222208	-3.28372077662728
H	7.38202764501883	7.46408664931579	-4.17074953838913
H	7.67690283707721	7.47681038729220	-0.96958445825407
H	6.57472409731476	8.82916199907529	-0.74170795116490
H	6.17300379460843	7.55092656739456	-1.89092001853425
H	6.95453953936509	9.59158281488797	-3.04850207314190
H	11.83183166667554	11.93628787563902	-0.80266977741894
H	11.77683650149164	9.50141727741282	-0.36978285399979
H	9.90946929376989	8.13606717160883	-1.23546247926984
H	2.81156158251268	12.44420363327925	-4.42142449005151
H	3.75917101565890	13.47537511099037	-5.49298582143897
H	3.79559463404678	11.72782226609251	-5.71470014496128
H	8.75482945567503	12.34706723575920	-5.64828486061050
H	9.42826688022834	11.18168617288583	-4.50410061558094
H	8.19456025342945	10.67862483174754	-5.66727393630497
H	6.19532581905353	12.22573173717017	-5.74793461071406
H	-0.03142623511860	11.01678952728883	4.90284738265110
H	1.20834897378548	10.64209895628770	6.09818448904299
H	0.63450338822325	12.30227349472483	5.90956685813768
H	0.63513247839265	12.26938742557326	2.71698932353307
H	1.17078037841795	13.60013957225009	3.75290073668279
H	2.27075633448163	12.91798239409920	2.56336576914911
H	2.81548755979843	12.12862377492252	4.83945766890545
H	6.88884863310530	7.06478235801742	4.82309140180855

H	5.49162856283958	7.82988605828998	5.57747467323620
H	5.26574949787039	6.42824869514540	4.53147384219991
H	6.16031143823122	8.18996038332701	1.31193626089599
H	7.33082892052466	7.35583523392381	2.33304284148466
H	5.77302145264713	6.61312698138622	1.99753814234899
H	6.30548581795137	9.14865494784142	3.62399621246321
H	0.54389707497079	9.84942905754858	2.89266607406644
H	1.28455330832292	7.69259494633983	1.94262280211789
H	3.62728844410395	6.96441671409782	2.19654993512819
H	8.53423147117867	16.04719570630806	7.26077730361212
H	9.60041553192634	14.67152050706524	6.95041519438085
H	9.86433615364987	16.19616210592997	6.11585558324552
H	6.76017775943432	16.04089559998488	3.97053792866713
H	6.97501168706637	16.91407218835728	5.49252994376491
H	8.23211253326839	16.97362778226866	4.24932393138648
H	7.34934767021366	14.48246080585658	5.76938737663501
H	10.93021308924409	10.12315422188924	2.02249748955001
H	10.72211334505960	10.02500235886979	3.77673909277873
H	9.97462034496963	8.81574779856773	2.71762959071681
H	8.79882307897634	11.02099915703748	0.56583474137856
H	8.19750378277946	9.46141089618455	1.11480074509085
H	7.24128421507646	10.92021774176962	1.36322796440093
H	8.26675359972136	10.37594512853873	3.49702912197404
H	10.24020245261652	15.85769295446907	3.84084059336084
H	11.39500308621984	14.65711726138463	2.02835236801989
H	10.78622512248258	12.32065792930544	1.50611548411829
H	3.53511108385735	9.17181706919797	6.06356577904709
H	4.67585322081421	9.38178925881053	7.40640629843840
H	3.45253364727807	10.60801288227762	7.07565373248501
H	9.46054248862784	12.11497671890827	6.05073879361974
H	8.43924402884901	12.81889283322928	7.30061392940672
H	8.66337944251718	11.07322811690995	7.24878052882828
H	6.33439507034090	10.94478094962392	7.39446458500599

Table S50. Compound **5** – B3LYP-D3/def2-SVP

Electronic energy ... -7725.46846564

Final Gibbs free energy ... -7724.29305742 Eh

Gibbs free energy minus the electronic energy ... 1.17540822 Eh

Sb	1.40515285963876	2.05817032108000	5.02927498470370
Ga	1.16824712987168	4.35369115272883	3.78827583991779
Cl	-0.66201206850768	4.65261355048007	2.50885561461886
N	2.65081803151925	4.48913647480894	2.47055462685317
N	1.47343447440104	6.17059741087543	4.51545361407582
C	2.90407776197732	5.65932873714826	1.89644714245104
C	2.37427380855378	6.87983974517388	2.37873456970279
H	2.55555035112210	7.75368875663951	1.75406581931610
C	1.77838036647368	7.12962586769023	3.62449013355117
C	3.77303513960747	5.71827316568295	0.66394638223951
H	4.51752440572683	4.91176667332487	0.65735377799142
H	4.27996088046608	6.68876003626097	0.58194206339421
H	3.14051977765167	5.58801943771414	-0.22962764823074
C	1.43082601112324	8.55987927213180	3.96390510044878
H	0.33449728780750	8.67152871227234	3.91132600615248
H	1.88942635039569	9.26539178034128	3.25970470106517
H	1.72421160930215	8.82591003606236	4.98752912615622
C	3.27497604614808	3.25850779852555	2.07996649590490
C	2.75437469917753	2.50573292716307	1.00370198622269
C	3.34471348799865	1.26671320822859	0.71207616119514
H	2.95349173918592	0.67420310448950	-0.11812926884313
C	4.40016252025028	0.77158794571959	1.47093605261752
H	4.84086467557963	-0.19990148937748	1.23328129108218
C	4.88399183940567	1.51135949605076	2.54953349242234
H	5.69665809808547	1.10570615416422	3.15199820919195
C	4.33638427770566	2.75749037349645	2.87905497015212
C	1.55377271899264	2.96145602344608	0.18747898647230
H	1.24517221875878	3.95121094420667	0.54936488501827
C	1.88673140880111	3.08288189616358	-1.30797215424239
H	2.75098554341952	3.74307818434919	-1.48068007830972
H	1.02640152961762	3.49222973565323	-1.86173462520982
H	2.12834544601884	2.10260233970231	-1.75041031275068
C	0.35895963437965	2.01927764539550	0.40842660622174
H	0.57130828062954	1.00873341680947	0.02166250433113
H	-0.53484327512406	2.40533559172647	-0.10636512799331
H	0.11340918662867	1.93576318465906	1.47666701899908
C	4.88148020296864	3.55560508618525	4.05743796958330
H	4.02016122631946	4.05665651154104	4.52513357252532
C	5.84483339260535	4.65802315007414	3.58555059395812
H	6.69886108626714	4.22144123992249	3.04208536803805
H	6.24152925325760	5.21998824043343	4.44587297174872

H	5.35003055536290	5.37846868095240	2.91980380289937
C	5.53818560634383	2.68506074775849	5.13359583050348
H	4.88126469726269	1.86940788971109	5.46826774822747
H	5.77606234205197	3.29151065675414	6.01857584575276
H	6.48401907977461	2.24239021622847	4.78148198849161
C	1.25716437188464	6.50016460261446	5.89505879458003
C	-0.05241240836191	6.60226518296436	6.41343488066592
C	-0.21196903482232	6.83862891830712	7.78688909796754
H	-1.21998668636566	6.89961776269375	8.20356743922493
C	0.88770394670553	6.99872772305762	8.62552099096928
H	0.74582642971165	7.17167197988803	9.69457507907759
C	2.17516125503451	6.91718736472398	8.09841295965943
H	3.03131674071194	7.02144509482242	8.76645328663998
C	2.38804778524287	6.65158822676965	6.73987888226985
C	-1.28118755711462	6.44319177342850	5.53320538676875
H	-0.94691137960789	6.39400984196142	4.48923100945610
C	-2.23608423141551	7.64030661677050	5.64881375148953
H	-2.67846853672923	7.71986988711011	6.65533625148610
H	-3.06486301626104	7.53567282676387	4.93031620565425
H	-1.71786580543882	8.58940035159095	5.43690910935281
C	-2.00461849586378	5.12154040531554	5.83145700723963
H	-1.32088379750417	4.26650103550578	5.73086201788982
H	-2.83686984740518	4.96757882580648	5.12728973028229
H	-2.40616890152544	5.10620542133288	6.85862049110045
C	3.80925434654313	6.49782071766812	6.20968598268061
H	3.73954242204057	5.91371412754776	5.28207475920199
C	4.44712873650781	7.85051616405438	5.85126834318262
H	3.89469049677208	8.37096516787412	5.05734143084336
H	5.48013101273593	7.70494204499118	5.49555855470150
H	4.48143787646940	8.51239906022970	6.73256359206481
C	4.71734146046011	5.72723692938347	7.17680799129043
H	4.91491004193652	6.29305230002244	8.10088845678581
H	5.69224460585218	5.52836992136157	6.70659940001508
H	4.27303402412582	4.76217038204557	7.46221519910946
Sb	1.56759919367034	3.29353971816744	7.38259092515511
Ga	2.27775882207221	1.08185766279523	8.55372862298806
Cl	4.38363459434485	0.38616632464835	8.14915518203269
N	2.18214557219980	1.25229797414816	10.52000690158936
N	1.21420553230478	-0.57722096351115	8.44785307413940
C	2.04198650082001	0.16997235229084	11.28475928920363
C	1.65221598267045	-1.08648067788080	10.77985653179664
H	1.60365753014798	-1.89190658991062	11.51130014719765
C	1.17673666713954	-1.41010427274368	9.49098181808028
C	2.32368150640635	0.27443081026259	12.76436308562461
H	1.98652561376694	1.23508371804966	13.17574112105790
H	1.85631197429331	-0.54707314051651	13.32215872537969
H	3.41370880063218	0.22391942028201	12.92355065695543
C	0.58349569745018	-2.78600003018877	9.30449638842819
H	1.29416191379066	-3.42614214742321	8.75966786576783
H	0.36322532182480	-3.25678521326526	10.27068851640736
H	-0.33403666984831	-2.74640734375699	8.70159084092402
C	2.29872183415334	2.57764334879984	11.05486718740178
C	3.56695298897634	3.14899080763664	11.29913605091060
C	3.62389434293617	4.47929787090794	11.74157441944284
H	4.59836939022675	4.93350424900310	11.93538309339617
C	2.46714106655152	5.22976604666504	11.93159000272960
H	2.53341592855442	6.26490415019241	12.27632452780508
C	1.22236180070543	4.65808436820110	11.67018797991723
H	0.31885344954017	5.25419649517537	11.80877846426334
C	1.11214312266461	3.33694852706756	11.22109611998235
C	4.86260301290172	2.38151584713698	11.08422466460586
H	4.60619747790250	1.37322545251341	10.73291957165936
C	5.66255826987314	2.24022516986443	12.38902039986306
H	5.06054923636676	1.77584871236627	13.18594087787710
H	6.55537703481047	1.61501185343047	12.22667462491080
H	6.00545170182762	3.21906500012641	12.76270549450303
C	5.71312255331793	3.03355903190940	9.98300928211918
H	6.04423359992458	4.04422041227849	10.27445182451783
H	6.60780651698767	2.42517573066913	9.77787807521323
H	5.14826961365043	3.11220713817455	9.04379498015503
C	-0.25870553905649	2.73551844102498	10.94010230521267
H	-0.10718507258036	1.89963223422236	10.24286890231658
C	-0.88515478493296	2.14670768747460	12.21557163794638
H	-1.03110920884624	2.93017955767849	12.97764663424870
H	-1.86789745025267	1.69969631680053	11.99414761141013
H	-0.25337356183070	1.36246353545788	12.65591857189525
C	-1.22145697438150	3.72449234565955	10.27120358782452
H	-0.77865584722638	4.17361252723846	9.36876047696052
H	-2.14854077959502	3.20875375510931	9.97813342308976

H	-1.51048584873806	4.54250610396025	10.95043736388673
C	0.57716800301367	-0.89966117356713	7.20032450446181
C	1.24155314904894	-1.68484515376336	6.23080661093375
C	0.57831262162478	-1.95066307541915	5.02289640746868
H	1.07897946091360	-2.55585629218666	4.26407154821886
C	-0.68947103801179	-1.44270695969464	4.76487143508684
H	-1.18545358930618	-1.65594292040918	3.81485445216108
C	-1.31477028324150	-0.63267361937171	5.71262308624750
H	-2.29477853146130	-0.21223086393565	5.48809662455385
C	-0.69941230164568	-0.33865301392517	6.93579398731261
C	2.65958969795166	-2.20775163375372	6.41401943324362
H	3.00764996151883	-1.91809640942214	7.41443535266959
C	2.73521449515821	-3.73927031091484	6.30424105418398
H	2.48210082118703	-4.08500055528270	5.28873704371073
H	3.75626260383041	-4.08878608020908	6.52701603756576
H	2.04501351465253	-4.23939453846412	7.00142160127441
C	3.61170791704250	-1.55027701996820	5.40007635628374
H	3.56463291506784	-0.45484835735261	5.46249504794076
H	4.65205307837505	-1.85109192167616	5.60095034656806
H	3.36023266801831	-1.84361787349369	4.36757548968454
C	-1.37863098302201	0.58529709716552	7.93927982512319
H	-0.58076178564035	1.20297356505640	8.38185110178213
C	-2.04703279676855	-0.18180188071082	9.09201086799854
H	-1.32191021152348	-0.75186311699758	9.68809835474045
H	-2.55457495848466	0.51914363499660	9.77414135036005
H	-2.80406331644269	-0.88469472393954	8.70712539566873
C	-2.37465813536637	1.55074183793005	7.28918480307172
H	-3.27473045153301	1.03086135233783	6.92398426497642
H	-2.70751174537203	2.29952571684163	8.02269258932984
H	-1.91926675702524	2.08834128478139	6.44514345831457

Table S51. Compound **5** – B3LYP-D3/def2-TZVPP
final energy -7728.988151041533 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -7719.709916855060 Eh

Sb	1.70154224621831	2.06555635807039	4.90815695516504
Ga	1.30041746134922	4.32610659423278	3.64515555473423
Cl	-0.45814358990841	4.44310536808414	2.24676225549290
N	2.85153161861104	4.62862204371890	2.44962292300625
N	1.36770960820968	6.14218541441159	4.44856261141003
C	3.05998562900210	5.83805163722426	1.95172239802732
C	2.43558493720758	6.98923726696050	2.45379851246682
H	2.62817568531880	7.90061970632570	1.90828392375863
C	1.73851321201407	7.14809731442186	3.65659918613684
C	3.99588184573182	6.01579252430631	0.78498870615155
H	4.80873188605969	5.29478030014260	0.81088375300613
H	4.40360341347458	7.02321261089217	0.76234708364753
H	3.44370646358029	5.85104970078146	-0.14225648337688
C	1.41173500569052	8.57078556876664	4.04337968048634
H	0.80399595328096	9.01338299603818	3.25268617754128
H	2.31949311093128	9.16696600104773	4.12802085324097
H	0.86475624069936	8.63171362707509	4.97794924922038
C	3.62108156806219	3.48417740509166	2.05655265124155
C	3.26282178898659	2.74027282939761	0.92071085013335
C	4.00671729963387	1.59989876386710	0.61624191634185
H	3.74346704070091	1.01488100684323	-0.25464485529874
C	5.06143984258686	1.19546381981555	1.41422978441898
H	5.62194152706963	0.30406324192473	1.16542422004447
C	5.38739373669626	1.92563709541821	2.54740054259262
H	6.19700681229271	1.58748494488142	3.17605560346176
C	4.67799702031276	3.07174392754513	2.89558508488551
C	2.08012781361086	3.10322964691784	0.04298300135225
H	1.65063342699341	4.03137398077613	0.41220318693065
C	2.49143973015923	3.31787720625786	-1.41961419369753
H	3.28887126060547	4.05592986851166	-1.51041749894733
H	1.63727259536891	3.66479671494804	-2.00325740689161
H	2.84732787104657	2.39173004536192	-1.87395899040826
C	0.98568926192276	2.03179898906368	0.14190156238583
H	1.33241876435967	1.07989096737102	-0.26495558581416
H	0.10140620097247	2.34233339949950	-0.41557588781807
H	0.68419204662564	1.87314797804011	1.17560052004297
C	5.05160382486214	3.85914776627189	4.14152073895647
H	4.12693466147826	4.26544489792726	4.55416784112273
C	5.95427827938296	5.05290532100109	3.79614501626436
H	6.87589418080415	4.71086080001870	3.32142940893096
H	6.22345620954570	5.60044068798678	4.70084734682921
H	5.46314413423491	5.74931660456187	3.11959765289034
C	5.69730223966213	3.00045778687666	5.22985855423277
H	5.07741070131795	2.14588758283145	5.49897390059981
H	5.84656644387925	3.59638800994588	6.12755451292856

H	6.67739803569333	2.62973264662630	4.92617361391936
C	0.96271675061200	6.38581538891707	5.80474353668920
C	-0.40091798460937	6.38701883278550	6.14468250636769
C	-0.75329857155891	6.56382353228125	7.48162935003209
H	-1.79964096121937	6.55700409815045	7.75573558347446
C	0.20716489772155	6.75116308657170	8.46088691833898
H	-0.08526762845430	6.88120224360562	9.49373877787744
C	1.54619386656252	6.76032598989540	8.11188109530802
H	2.29257403688189	6.89033000666454	8.88260889699350
C	1.95096695512147	6.57461973287079	6.79113388192840
C	-1.49358038617212	6.21937142427070	5.10866735232123
H	-1.02861756865734	6.15823309215380	4.12971654000064
C	-2.43927704012629	7.42648096669629	5.08441083041283
H	-2.99014460167918	7.52778435811654	6.02119882584441
H	-3.16780746706166	7.31568454913116	4.27981182338544
H	-1.89015927887133	8.35457257562195	4.91887059763364
C	-2.26755355295159	4.91411237225267	5.32634567822722
H	-1.59790485897272	4.05471677440696	5.31270003601465
H	-3.00394508254326	4.77367239868591	4.53485231921455
H	-2.78822243331132	4.91954470886913	6.28604139933104
C	3.43671917371664	6.59159704292217	6.47710870104922
H	3.56721140854653	6.31605721684921	5.43261054212259
C	4.02439560419466	7.99757365413151	6.66736146910123
H	3.49890140849394	8.73823812083728	6.06638090048171
H	5.07775622430226	8.01174406333770	6.38254646254759
H	3.95380256401431	8.30732922318359	7.71142918715517
C	4.20718994730002	5.57622391030298	7.32700402632205
H	4.10726677141308	5.77934773596754	8.39303951343257
H	5.26931836425133	5.60513813251225	7.08278238571210
H	3.84674700454946	4.56397534559042	7.15225394797334
Sb	1.11637427464314	3.11017627799820	7.26661717561568
Ga	2.07870287966016	0.97842614117273	8.42921385478927
Cl	4.06788870057230	0.23974170785078	7.69945998623079
N	2.32179636876536	1.24462903530958	10.36976578443049
N	1.01058128280909	-0.67396773650308	8.58372794002513
C	2.27587780743690	0.21067337281861	11.20152010971005
C	1.77708969560176	-1.04643177527362	10.84180241459068
H	1.81374255410489	-1.79762838506885	11.61522417930178
C	1.10549478225463	-1.43036124251921	9.66808742597998
C	2.78901127798411	0.37292549510403	12.60916893767596
H	2.61515115405630	1.37689048164397	12.98708139764310
H	2.33306439411428	-0.35126215081430	13.27938473141142
H	3.86836464921985	0.20751895163064	12.61280740229940
C	0.46823966898447	-2.79658896866854	9.68408934046739
H	1.20411045678153	-3.53846511774206	9.37030016470048
H	0.14165825212269	-3.05495174032861	10.68858742065166
H	-0.37421434444062	-2.86031039007102	9.00137663773255
C	2.56613085788072	2.58739531914135	10.80803523002872
C	3.86908689932709	3.10914728735876	10.83617607013527
C	4.03605417355066	4.45040705637834	11.18421441063097
H	5.03355499499809	4.86780924410660	11.21110512550963
C	2.95324284270190	5.25508567076788	11.49161106678995
H	3.10526889194651	6.29302660088594	11.75757756648492
C	1.67077908126846	4.72796821033498	11.45239942895918
H	0.82961102592547	5.36440324397206	11.68542319022278
C	1.45034238814089	3.39811266101155	11.10724350104727
C	5.09124380034377	2.27537898515669	10.50067404808305
H	4.75849996448232	1.27086998122416	10.24912675619412
C	6.04940347286627	2.17449722659719	11.69546397168206
H	5.54619521877799	1.79535503281911	12.58517519418860
H	6.87704871536984	1.50366320509933	11.45967868890290
H	6.47290433150962	3.14841455615454	11.94708399653685
C	5.82058830819985	2.83027177654630	9.27131205593076
H	6.20883961555011	3.83239207409588	9.46211634727446
H	6.65860644461417	2.18495922530315	9.00552292218662
H	5.15743880482287	2.87545737142333	8.41142213848352
C	0.03931322171005	2.83442634968610	11.08146441174204
H	0.04081496346346	2.00085263738220	10.38127733477832
C	-0.36469681264482	2.27084711630561	12.45118714835955
H	-0.33914468934136	3.05441205857851	13.21095154016296
H	-1.37871725571493	1.86912208069707	12.41153461465016
H	0.29755907214025	1.46934835627861	12.77196538691113
C	-1.00644943562522	3.83920443279108	10.59362398412236
H	-0.73155524541779	4.26569592381951	9.63021825113424
H	-1.97092757888529	3.34251102612597	10.48501172241905
H	-1.14580848516490	4.65752488275118	11.30171418466788
C	0.21255260885509	-1.04486832921679	7.44812187319460
C	0.71891398111639	-1.91381594553447	6.46799715203306
C	-0.08464866766320	-2.19764049995729	5.36267294759462

H	0.28949277956522	-2.86416472012766	4.59765228529055
C	-1.33838640848276	-1.63300944099208	5.21777246675073
H	-1.94117952702430	-1.86112661497252	4.34884300282337
C	-1.81346987161311	-0.75585447929924	6.18169454279466
H	-2.78439270800234	-0.30214181593864	6.04952999329757
C	-1.05338579369960	-0.44117659495482	7.30344694475247
C	2.10275181278010	-2.53383964501091	6.54124586524480
H	2.58652575216233	-2.18260920573314	7.44993296729084
C	2.04099538371623	-4.06722867061900	6.58744853467036
H	1.64995443293895	-4.47399851465301	5.65337433681299
H	3.04069544038995	-4.47928653354783	6.73458572582680
H	1.40242671696208	-4.42736287813501	7.39353144193830
C	2.96940755018322	-2.07746969567269	5.35970762499605
H	3.01668014200842	-0.99271180043763	5.30101212708454
H	3.98796742382870	-2.45058275342263	5.47428157793238
H	2.57327253553904	-2.45505483828741	4.41536154982122
C	-1.58344708755548	0.52417727515782	8.34892746912438
H	-0.72222102813573	1.06202090465487	8.74521311722325
C	-2.23499294940332	-0.21128996609538	9.52819333913622
H	-1.54103854798542	-0.89359467897215	10.01528419421663
H	-2.57902034670460	0.50414613883233	10.27726582150824
H	-3.09658059476399	-0.78946038807779	9.18928305217798
C	-2.53833031218788	1.57448191046467	7.77874125439772
H	-3.49018048692037	1.13728778610422	7.47388714002634
H	-2.75448018692153	2.32666757751598	8.53692726542777
H	-2.10431209228102	2.08041332193237	6.91735667809552

Table S52. Compound **6a** B3LYP-D3/def2-SVP
Electronic energy ... -8491.44721668 Eh
Final Gibbs free energy ... -8489.92347139 Eh
Gibbs free energy minus the electronic energy ... 1.52374529 Eh

Sb	8.62685989219919	-1.70367061742880	3.01413361061841
Sb	10.74145489851728	1.18067419250402	4.67619612109240
Ga	8.08883068317725	-3.94442386763617	1.90683640850044
Ga	12.46242569432853	3.06375417991338	4.82974278220793
Cl	9.46307342618551	-5.19211990535805	0.55574146990136
Cl	14.34185997488977	3.34293715803608	3.53794656015429
N	11.15432136012846	-2.51446434322418	4.78796091970435
N	7.41028141881743	-5.44224203279838	3.05289435938369
N	11.70993983835189	-2.54915013999429	2.70146163290405
N	6.44510864141776	-3.85907902045809	0.78679178437801
N	11.63389501581379	0.93021027537034	1.59563907300560
N	9.60343958011976	1.65106673997398	1.73503064552306
N	13.25244410584327	3.19496437244283	6.65209414446149
N	11.84193529427343	4.96850422386208	4.79655593854867
C	8.85592993130688	-5.58619015308121	7.02864521000389
C	9.57736723603164	-6.20205408392235	6.01016700926873
C	7.66169789731756	-4.93034287314156	6.72843863395031
C	10.21981415714871	-8.34415216832836	3.91037572596329
C	13.34333312069988	-2.87741402435852	5.98567486376835
C	9.12117792487123	-6.19136951862190	4.68273783496929
C	7.17054557614294	-4.88321157939031	5.41882946128617
C	4.66222171248201	-5.13743412957222	5.25021878952640
C	10.39419550784944	-2.40232297308538	6.01877673022837
C	9.96140819438307	-6.86103617762756	3.60655818403141
C	7.90197503483902	-5.53881896549259	4.39516846188812
C	5.63939785542293	-2.91147126657694	5.94454161607079
C	5.85689459476265	-4.17799500125083	5.11127397072160
C	6.42516324730362	-7.68341965129442	3.21660955273458
C	11.27940357182153	-6.10006101709281	3.39712650873024
C	12.52317150971272	-2.75157667695483	4.75020182313875
C	6.59653242270248	-6.35213930653697	2.52245100253520
C	12.87537543380974	-2.79426084746571	3.42666990701233
C	10.65119510613868	-2.36411416974555	3.53528198590609
C	14.19387972063539	-3.04937424018950	2.78346268086938
C	5.88383968850190	-6.15396463461966	1.31962313947081
C	3.54873349742544	-2.65309834506286	2.25660575960714
C	5.73286223412212	-4.96844448146232	0.57252097273822
C	4.79074986433880	-0.58692480833490	3.01616857050350
C	4.87850940670123	-1.88422793533878	2.20404933037939
C	11.62733843028566	-2.51917279004936	1.25111954225300
C	4.69902745983147	-4.96784903208132	-0.52873835624813
C	5.35849238324194	-1.66120312542675	0.77655807996552
C	6.13893226545803	-2.63516859522925	0.10510423720412
C	5.04640688782885	-0.47265305569017	0.10363825422073
C	6.66446834223436	-2.37598103843633	-1.18120959440882
C	7.65904496990014	-3.30924397082083	-1.85296180330484
C	9.05911520061779	-2.67081719043589	-1.82230589646813
C	5.50532408643403	-0.23343954336187	-1.19124665702385

C	6.31901895901084	-1.17441208691749	-1.81639815443425
C	7.25758434015522	-3.69499845364924	-3.28296021119800
C	11.97083301199275	0.66848351407269	-0.90406952022899
C	8.81283700562986	1.65606770386088	-0.65885088028111
C	12.98274118078437	0.52528204670719	1.95198490670327
C	8.32837689173605	2.10941979837653	2.25221785395240
C	11.14803156311403	1.00437065004814	0.29069046479648
C	9.85354046791052	1.44338237528577	0.38391175615030
C	10.68256388550168	1.31543111484373	2.48839270242257
C	11.16016698742902	3.55214400462997	9.39651137794434
C	9.81223629762576	1.56024364180410	8.61618168474106
C	11.05417820857303	2.42116886357894	8.36065879677989
C	17.04308051427511	1.49479362805262	6.84274325566407
C	15.51251488153440	0.45625786870188	5.10720375367897
C	15.62572152851488	1.47523160747543	6.25514279008508
C	12.33584700365345	1.60298555660459	8.27580117132081
C	12.48470815866168	0.43958942698483	9.04226080093627
C	13.64291675037116	-0.33285511142107	8.96460186614000
C	14.65640655233061	0.03588801634191	8.08395951146762
C	14.55119955554281	1.18822804169056	7.29190650813023
C	13.39985278459535	1.99691220568884	7.42634527586106
C	8.03388546258636	4.08555397757467	6.39417705891556
C	9.28378166229322	6.22067812522909	6.91752213421240
C	9.26916264585677	4.93326111952007	6.07624425629119
C	12.30286090859087	4.44420284609181	0.91444902953877
C	12.47346058579149	6.95088422756432	1.23549542445675
C	12.19354256733850	5.60286096219937	1.91700558443169
C	9.42067517499254	5.23995591664163	4.59343851025549
C	8.29648944610831	5.51163382915607	3.80547059967159
C	8.42109868871463	5.81265729469665	2.44897083108146
C	9.68350217801213	5.83868698801923	1.86369474527708
C	10.84193814837621	5.58241675055795	2.61369726870241
C	10.70305262799593	5.29403964466258	3.98933636662149
C	14.66828451495096	4.36911596856011	8.27442569168791
C	12.33220906732462	7.35208761206108	5.10749346778303
C	13.75828916678420	4.35856947845773	7.06803234324391
C	13.49771064850937	5.59451276971159	6.44265455620150
C	12.54117603005640	5.89509447681566	5.44852386573570
H	9.22464996062769	-5.61076132130357	8.05762311707706
H	10.51765730451999	-6.70685386503536	6.24505642524640
H	7.10572323147164	-4.43816681718447	7.52798983438782
H	10.84199749828417	-8.47558145870739	4.81101073282229
H	12.99990877459291	-3.70900427545952	6.62343184996183
H	4.58999808449153	-5.52811848383705	6.27894794607676
H	9.27979116055803	-8.89404539129916	4.07523103327154
H	13.30170264909203	-1.95350197879152	6.58507595657763
H	10.58300019521681	-3.28053755406538	6.65066743780617
H	5.51284675462818	-3.13439129379156	7.01644510708632
H	6.43231580501971	-7.57837430422108	4.30925913237576
H	11.91484489196157	-6.13731786347134	4.29771912258309
H	14.39530274789819	-3.06073911072100	5.72891992485269
H	10.67255813290609	-1.47992380214388	6.55107933615037
H	10.75066293766005	-8.82018843972150	3.06993300601486
H	4.74656857934574	-5.99499396053220	4.56838167820943
H	7.27679165967258	-8.33227064980756	2.95141803274641
H	3.71931167889637	-4.61723029625690	5.01568063393635
H	9.32901654198869	-2.36814362940156	5.75551396995992
H	5.50084384676454	-8.18549772899213	2.90302054125869
H	6.48130393365712	-2.21301838401926	5.82230459565099
H	4.72121135447731	-2.40106660213470	5.61499220691489
H	11.84463667796828	-6.53198600275524	2.55615325018673
H	9.41126407603593	-6.80133269883421	2.65902271626344
H	11.08493719615303	-5.04655903220325	3.16126015169100
H	5.90675667465145	-3.86997308531732	4.05849601024011
H	14.94708056790627	-3.28567209195707	3.54698587515767
H	5.27933692710907	-6.99733573329935	0.98876312847994
H	14.14534602942052	-3.89844757267179	2.08200803968615
H	3.21639035096608	-2.77630250867532	3.30013567893851
H	4.60319711143396	-0.81839640796578	4.07442334460625
H	14.55705308939307	-2.17142010395127	2.22326401385148
H	5.63311029373450	-2.51539027376675	2.69524076637856
H	3.63782521655319	-3.65734417668606	1.81868333212683
H	5.73175216500471	-0.01871872306170	2.96300903785691
H	11.35619106615527	-3.50696876783449	0.85336518017980
H	2.75990354761594	-2.10879420110665	1.71115978330435
H	4.10792558137672	-5.89210029895714	-0.52226023089060
H	3.97132994481558	0.06576714874462	2.67354179878372
H	12.59114550840712	-2.20122343232668	0.83661537619288
H	10.83531756088823	-1.80915173311649	0.97126729612989

H	4.02106013355366	-4.10707703434479	-0.43371561935836
H	7.72093092417069	-4.23079817736018	-1.26039015669294
H	5.19146605153758	-4.86910881455375	-1.50816852468135
H	9.32257132978835	-2.36668506895682	-0.79900019191725
H	4.43600910107118	0.28183446283674	0.60172195244427
H	9.81935138194970	-3.38675643500932	-2.17159977366640
H	6.25267327156022	-4.14554914108420	-3.31706079673911
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H	9.09852959437695	-1.77469813290995	-2.46509737445526
H	5.24280732218546	0.69588669417896	-1.70357000068726
H	6.71188951120776	-0.96887701649812	-2.81483744489377
H	7.25250161214363	-2.82500944015560	-3.96009968006991
H	12.88227451324901	1.28690565568690	-0.95517143858441
H	12.28243341074081	-0.38920525892149	-0.90840757327350
H	11.39211522255215	0.84438466142370	-1.82070823771416
H	7.94442653705072	0.99857649182182	-0.48976603142503
H	8.45211563964804	2.69818323334225	-0.67147379414109
H	9.21459404721003	1.42425173698221	-1.65441923685749
H	13.65019515866619	1.39552744959013	2.02036164864599
H	12.94475073744370	0.04689830799340	2.94128115183024
H	13.36124114400520	-0.17936314452383	1.20280408803576
H	7.57064128006092	1.31887787502575	2.14082816654377
H	8.46012195626464	2.34295876023039	3.31690064209267
H	8.01576517130353	3.01572565518463	1.71691164596099
H	10.21376406829271	4.11430674046728	9.45318099011685
H	11.37450985631308	3.14643391596313	10.39927782435346
H	11.95425331082010	4.26729804416406	9.13981246557102
H	9.74018242072219	0.73620248440473	7.88960683216274
H	9.80580557468242	1.13035894168584	9.63094068947299
H	8.90365266454229	2.17097626308413	8.51576803967117
H	10.91847527433693	2.89614644274221	7.37898933227933
H	17.77279767415033	1.78335853587943	6.06911376029594
H	17.12879442200805	2.21309222674586	7.67390172438485
H	17.34458438803814	0.50665562370272	7.22737937633985
H	16.18084472083290	0.73188125927153	4.27656768818506
H	15.78070526333970	-0.55713601324230	5.45211068316298
H	14.48370807424442	0.42123156226173	4.71894561114906
H	15.42876836876884	2.46306587439078	5.81977867300427
H	11.67990116265779	0.13046205032041	9.71051557705071
H	13.74498855236130	-1.23267544281122	9.57688786578719
H	15.54723931079168	-0.59034268591333	7.99581245858292
H	8.05587778819514	3.14065947033350	5.82987552729781
H	8.01477716735056	3.84016106840052	7.46715496137764
H	7.09388917746116	4.61561808950372	6.17118681592970
H	8.44590005963238	6.88133839152624	6.63888466101420
H	9.18888768256256	5.98252789387102	7.98951362169517
H	10.21762821717678	6.78467857000400	6.78423673204071
H	10.14952898428074	4.34363238928786	6.36323658780898
H	13.31789262253301	4.39645268623104	0.48937403696715
H	12.10155332338453	3.48417334076252	1.40596472482056
H	11.58477106099228	4.56125529676340	0.08560775779572
H	11.77196806604447	7.14335543435356	0.40718194770981
H	12.38490407747069	7.78934214169935	1.94421414189096
H	13.49264283892242	6.96449088620112	0.81620074585295
H	12.96949929226480	5.43808844815869	2.67520371432525
H	7.30416855409195	5.48187237100953	4.25849192557582
H	7.53139069838024	6.02281316345023	1.84927263504994
H	9.77940844793313	6.06521212270690	0.79902432236419
H	15.62253430187039	3.87882426119386	8.02501383926688
H	14.87714591073786	5.39350722849308	8.60751856416519
H	14.23332252191378	3.79971420961249	9.10797523637016
H	11.27504586534175	7.57807299614175	4.91569427965703
H	12.70741492565022	8.00899337111946	5.90269419770547
H	12.88178779188864	7.58339818003200	4.17987198031511
H	14.02422786157394	6.45156115613853	6.86024820421975

Table S53. Compound **6a** B3LYP-D3/def2-TZVPP
final energy -8495.793696205532 Eh

Sb	8.22031280254482	-1.72651682628976	1.49564892493142
Sb	11.58327425743252	1.06483173080078	5.81687960211140
Ga	7.78583439335076	-4.27591650071328	1.24294373646987
Ga	13.03188818125495	3.22666383359154	5.46684493104012
Cl	9.41691194190062	-5.58772124766640	0.16631745464613
Cl	14.65012349079341	3.38301577866000	3.83818009217050
N	10.62772064624567	-2.33117719436280	3.59619612155085
N	7.19691092213586	-5.49076545314386	2.72603929389062
N	11.34620250599843	-2.54356980698905	1.56663363524241
N	6.21864002195511	-4.69615824944511	0.04807356800328
N	11.56031402411949	1.02215560016818	2.59549523865020

N	9.59596331919379	1.52452523544876	3.32619037660929
N	13.93333529962775	3.74695034674125	7.13818338135788
N	12.21451448675351	5.13108162711829	5.17102791014349
C	8.43582238517908	-5.01137012253147	6.74261529681103
C	9.18657027463069	-5.79319796545818	5.87080207994768
C	7.31203518121329	-4.33573356431859	6.25614345279467
C	10.07821699094168	-8.16045935635271	4.25988321516442
C	12.68677228599520	-2.87143627431530	4.99136114333210
C	8.81830613990844	-5.95994292427520	4.53769212109894
C	6.91355758670043	-4.45393164114606	4.92934364090185
C	4.43334337619331	-4.50438391732917	4.26820773978546
C	9.75913776826973	-2.18702913834960	4.75603246439230
C	9.68722344371966	-6.81006603199084	3.61687449285215
C	7.64854883127746	-5.30689002779179	4.06820188661836
C	5.43067021369962	-2.38984394786605	5.23081027157838
C	5.72078005101824	-3.64699458357247	4.39313482111426
C	6.25768097570394	-7.64459795584237	3.47446339832381
C	10.95522833185424	-6.02604667201323	3.20058405205605
C	12.00190211053335	-2.69489907395337	3.68849310979336
C	6.46092941568176	-6.58839725766362	2.41180947884481
C	12.43347464113383	-2.83051039974917	2.41141232660960
C	10.23644002121626	-2.24949385191994	2.31447597865395
C	13.76566093154227	-3.22307639007280	1.84927180265784
C	5.82075823239601	-6.78871803828877	1.18843860089243
C	2.65630383938297	-3.38061183533288	0.64912864012108
C	5.60565430101040	-5.88466445581675	0.13188748825383
C	4.11407183204151	-1.61948903322905	1.76946169557943
C	4.11086622735147	-2.89602338023227	0.91089892408247
C	11.38736622490242	-2.64768106829138	0.12041973886451
C	4.63665308283159	-6.31079445638096	-0.94433724712260
C	4.83050516399441	-2.73383360307379	-0.41269222632620
C	5.78948814640376	-3.67692520694983	-0.87224481522147
C	4.47884432119317	-1.68617678443730	-1.27013912515172
C	6.36650645761707	-3.56460429508860	-2.14159063528643
C	7.39156400407963	-4.56899322271300	-2.67211930173242
C	8.72187784935639	-3.86447218262154	-3.03779908019950
C	5.03763471668428	-1.56448524411574	-2.53096881922416
C	5.96913711657145	-2.50569085371904	-2.97016700925659
C	6.83795714983664	-5.33909266261559	-3.87954059341258
C	11.27807454162870	1.16569158999201	0.08394008766402
C	8.28348767221499	1.99339339846639	1.21693043691678
C	12.98530967722689	0.61834291917736	2.50792597293305
C	8.45138059703181	1.68345006423014	4.22256492008066
C	10.76921431306503	1.26622095684923	1.47238039311218
C	9.52261768775772	1.58794100592535	1.95103029915231
C	10.86925041355406	1.19468157265532	3.74694703355412
C	12.44875156728548	4.59371567281876	10.58149992363941
C	10.79941449110740	2.87601884350696	9.70723976069398
C	12.13400119673659	3.61475035906258	9.43873903458364
C	17.65149342828537	2.04510032073044	7.32465628682461
C	16.08424643054940	0.70032805644058	5.83568399514006
C	16.20236976477218	1.89609913032758	6.79539646634725
C	13.29275824752089	2.62706408895960	9.22417444881735
C	13.50893228829802	1.62056290608322	10.16926045703222
C	14.54711834792656	0.69918275211007	10.00948449291907
C	15.37934136480224	0.78904693454455	8.90482220725822
C	15.22247561198767	1.79586516402654	7.94913448552283
C	15.22247561198767	1.79586516402654	7.94913448552283
C	14.16509616310645	2.72645700599253	8.12602092378331
C	8.41994622515796	4.28398834621492	7.11890704443087
C	10.04189154368911	6.17653710077921	7.44083758366492
C	9.74541416500527	4.90091061978157	6.61620086300811
C	12.46784843029378	4.43407902421881	1.24827524686186
C	12.39297513770320	6.94709497456355	1.46908323669717
C	12.31864074622282	5.60632558664389	2.23201768673350
C	9.76945050372322	5.15489977650032	5.12244727410678
C	8.58205945210224	5.27967162932918	4.39046841070828
C	8.59175695692317	5.48640969214564	3.01951223672794
C	9.80152842634384	5.57307993077781	2.33783199669238
C	11.02370738769646	5.47952075764871	3.02922176118305
C	10.99780981264558	5.27597728455674	4.41285117528304
C	15.38010216484914	5.28221782778652	8.42353947688489
C	12.51383020800169	7.58392165149473	5.16478474011575
C	14.35656433101900	5.01732359628513	7.34658329749071
C	13.93058467521939	6.10902950600774	6.58029794086256
C	12.87633755221168	6.18575535681700	5.64817894299031
H	8.73092395510921	-4.90275334802216	7.77716752263262
H	10.07343647381819	-6.29242408241301	6.24476647009268
H	6.75734262232193	-3.69921015155221	6.93171757485947

H	10.78856176166513	-8.02285882663460	5.07558697903768
H	12.19041420438350	-3.62759464789077	5.60324964074316
H	4.14211376696615	-4.90355344673730	5.24146771554009
H	9.20747554336300	-8.67994521080309	4.66255398227294
H	12.70987996653084	-1.93474504798549	5.55435208436548
H	9.69874629638531	-3.13054980603356	5.29196825118236
H	5.00722576793381	-2.63926121572759	6.20480792522866
H	5.73560573923487	-7.22474892547982	4.33426156497614
H	11.57162751377828	-5.80172252300205	4.07334538900375
H	13.71496119607135	-3.19346270643425	4.82854612108419
H	10.13942514562451	-1.41112845790998	5.41656462902980
H	10.54700233224504	-8.80534884893118	3.51538399577545
H	4.56566431524610	-5.33257834986535	3.57689710946780
H	7.20995042447771	-8.02435860838693	3.83832019532499
H	3.61483814385808	-3.88729566271713	3.89420954872803
H	8.77089189103569	-1.91809962067911	4.39130806156875
H	5.67438847399516	-8.47324199203368	3.08016921156663
H	6.33480804302028	-1.80010989341555	5.38830923238716
H	4.71066870848369	-1.76006471032328	4.70857300534444
H	11.54173620875650	-6.61168487509831	2.49277485829313
H	9.12888541127401	-7.01632753104345	2.70749237220151
H	10.68554956150193	-5.09501368192215	2.71160906644265
H	6.00551209369216	-3.31070654314694	3.39593298872361
H	14.46994087279419	-3.43020719630597	2.65177264269329
H	5.30050957002109	-7.73176461540673	1.08958026962931
H	13.67392762255298	-4.11688742687051	1.23060636181384
H	2.13706858640750	-3.56901780303505	1.59010024868820
H	3.51585596913409	-1.77225873063261	2.66774234718890
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H	4.60866422307026	-3.67670645897614	1.48017148901409
H	2.65632213698847	-4.30006033894885	0.06403926891391
H	5.12803010527990	-1.35681341364497	2.07408063446286
H	11.40123827268494	-3.69274482735990	-0.18544459868192
H	2.09956024464916	-2.62745324471549	0.08930543461026
H	3.79631432652149	-6.85346335242845	-0.51359252398863
H	3.68973172716089	-0.77098428348083	1.23097776201526
H	12.26655653717367	-2.13153311890746	-0.26602674933881
H	10.48273931830451	-2.18773287853523	-0.27353739259098
H	4.26776825119639	-5.46667935121552	-1.51821218464441
H	7.62192694130569	-5.27880444267452	-1.88185455076445
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H	9.12050787807530	-3.33311896370581	-2.17501491828163
H	3.74448876705904	-0.96114034145930	-0.93769011623101
H	9.45568037028441	-4.60741176470853	-3.35466241602703
H	5.92479264478814	-5.87841885915502	-3.62282313135879
H	7.56984143394274	-6.06657956007192	-4.23656666111260
H	8.58040067293486	-3.15407766251169	-3.85379738340589
H	4.75087377439238	-0.74774447975714	-3.18248344431110
H	6.40191850157517	-2.40874647983052	-3.95543923702464
H	6.60375065322958	-4.66730119230355	-4.70698156147079
H	12.11537629028728	1.84558756192277	-0.08929517481526
H	11.61318787716615	0.15373982267304	-0.14998436045976
H	10.48948529164696	1.41555542842291	-0.62236089432241
H	7.42556507835789	1.40402346757289	1.54419066804028
H	8.06598334740017	3.05067096643638	1.39073279063239
H	8.40910009639176	1.82979108948190	0.15019007080823
H	13.59605319570185	1.47130711663056	2.22738659003254
H	13.28729333339906	0.27142814002563	3.49137997781805
H	13.07161107259886	-0.17935203522395	1.77656691559422
H	7.77520392094029	0.83578218629442	4.09884589338622
H	8.83304569471574	1.71536780229841	5.23974665269582
H	7.93245866814525	2.61077682552629	3.99189741093962
H	11.60848960070775	5.27188531017001	10.74764340431185
H	12.63989352609984	4.05936522126927	11.51354304479340
H	13.32656919724795	5.19984313265299	10.35649222769049
H	10.53783061921101	2.23117149411419	8.86786963390110
H	10.85546870906721	2.27008499130136	10.61144456043820
H	9.99982765261388	3.60509893339180	9.84980710206225
H	12.01033362176859	4.18935648994360	8.52410378713815
H	18.34441528131003	2.18520543954893	6.49361217192594
H	17.73335434108266	2.90275466161389	7.99308504447957
H	17.96278942058587	1.15900228376893	7.87934181302680
H	16.77415686068453	0.81961606704076	5.00000355615391
H	16.31762615989565	-0.23587403923568	6.34868879425633
H	15.07279761604890	0.62646836911312	5.43757715848492
H	15.97297751905779	2.79299655803923	6.22612683558266
H	12.85788674529775	1.54068766653274	11.02790443688183
H	14.69311778919479	-0.08102717081586	10.74520000064402
H	16.18017999252804	0.06816036782028	8.78165267848550

H	8.13579808428366	3.40925084640374	6.53631404134528
H	8.53429272593187	3.97492123633648	8.15568667314858
H	7.60248454041529	5.00780225847563	7.07711407129516
H	9.30522129471421	6.95274341701957	7.21873295637950
H	9.99161963178326	5.95338490583614	8.50718865753266
H	11.03096289915174	6.57666418861500	7.23149925820627
H	10.53207289436266	4.17318175728788	6.82529946669221
H	13.41578992728478	4.50672346823800	0.71363461630701
H	12.45256178805043	3.48824022412377	1.78247543434060
H	11.65878784667153	4.43278915466730	0.51601919758686
H	11.60161386980525	7.02013958290395	0.72232624021346
H	12.29795981721215	7.79921252952695	2.14237333911923
H	13.34905307573440	7.02563797890537	0.94939653737721
H	13.15663561264843	5.55876932321785	2.92201363366967
H	7.63563373516257	5.20577349222927	4.91034377880185
H	7.65917229497750	5.57774266160294	2.47292943797021
H	9.80581685983819	5.72892716594320	1.26847451244275
H	16.37555415951075	5.19779870133550	7.97763309801581
H	15.27616780111031	6.28620486561212	8.82880948483033
H	15.32239009345120	4.55816281498467	9.22949449009286
H	11.51167766751542	7.61761988729377	4.74959264694424
H	12.59816440431493	8.30758567881256	5.97298496783920
H	13.21770969422032	7.86717993341524	4.38036502189101
H	14.39697077192023	7.05283164372919	6.82533092903227

Table S54. Compound **6b** B3LYP-D3/def2-SVP

Electronic energy ... -8648.50953172 Eh

Final Gibbs free energy ... -8646.87387082 Eh

Gibbs free energy minus the electronic energy ... 1.63566090 Eh

Sb	10.94469524045337	1.41364646773671	4.38526245080484
Sb	8.76700320427718	-1.62098862734974	2.65238931220817
Ga	12.53151684431534	3.42756182562324	4.30510451133366
Ga	8.52104568056087	-4.11370179412022	2.09594248547726
Cl	13.72048369033300	4.17133983762505	2.50270130243187
Cl	10.39208216258299	-5.39758030847145	1.79473097158320
N	11.99412118881154	5.21524592796520	5.04105240269775
N	14.02223057538066	3.18922466955050	5.62808850364339
N	8.78965309314504	1.87290915635462	2.09294322582612
N	10.65571353817361	1.30691492864182	1.16080401997578
N	7.56485603000078	-4.39864165054310	0.37336706750700
N	11.32607132945709	-2.59307449352360	4.39784062603535
N	7.39964650816626	-5.46230385455148	3.08521042396113
N	9.61426984267596	-2.26345287111294	5.67552263500102
C	7.66746799991005	3.70418362343181	3.33192386561721
C	12.92500768981301	1.61317008576959	0.12248608469437
C	13.39408211789630	-1.73132153774171	3.28289387420447
C	8.17080630678990	-0.50593612548139	6.69674897410555
C	12.92567919330171	6.01975637513134	5.55928358470692
C	14.19542435291172	5.57907437545455	5.97686595411414
C	14.65922909218922	4.25559731204872	6.11584692145076
C	12.61048115644614	7.48797661811548	5.73582917008234
C	15.94624520617768	4.05851200120673	6.88408611830060
C	10.64471958128432	5.68706699992358	4.94192315981169
C	10.19553978601347	6.36722410069048	3.78713971824067
C	8.89764229648034	6.89733984315779	3.78864690935151
C	8.05385924365224	6.74206713750066	4.88623590576664
C	8.48815188896365	6.01336803614883	5.99233318096980
C	9.77703647457472	5.46647988794128	6.03801074101430
C	11.05665350939524	6.46875913549213	2.53832160569837
C	11.07669853370318	7.87408672754620	1.92414011229594
C	10.60121080424981	5.41907154785599	1.50897849372197
C	10.22827464351516	4.67607601031844	7.25887070334678
C	10.58416660101249	5.60507865532984	8.43036176353213
C	9.19949759209731	3.61686705233942	7.67413952802431
C	14.50375802488971	1.87195056292084	5.92495568846439
C	15.57268283838508	1.31440752974129	5.18670994588456
C	16.05029453633300	0.04896291499393	5.55648992292922
C	15.48156371649060	-0.65842945237361	6.61196040404288
C	14.38437873233624	-0.12554490788004	7.28815631103328
C	13.86958613180409	1.13276713931831	6.95286728227635
C	16.16563300689684	2.00717890677408	3.96868807745859
C	15.68705698570152	1.29702439964693	2.69180469171587
C	17.69763843790002	2.09627580508601	4.00752738822601
C	12.65647397981380	1.68924217658321	7.68550924155742
C	11.67594614761119	0.59646597152517	8.12528480611517
C	13.05704024616063	2.58066953960028	8.87151246665842
C	10.09855286820513	1.62613614038090	2.35952918594461
C	8.51570996096303	1.69411849656558	0.74124359864837
C	9.69797743346843	1.33177924939276	0.15037287747824

C	7.77668206365950	2.20782060186318	3.09406094777395
C	12.00663236707252	0.76961500907917	0.99517831122618
C	7.15375625868213	1.84716411894961	0.15778529412092
C	9.98330648094807	0.97831583930926	-1.26780041498725
C	10.18404587283012	-4.54542252079942	-2.80684723971050
C	8.44414003945275	-2.05594738609388	-2.40215900113691
C	7.31467519533364	-1.23969432371677	-2.42715094705255
C	11.01266874579047	-3.09441931175900	-0.89845059272353
C	9.84168030809124	-3.93078730123689	-1.44224265425161
C	8.56873720215352	-3.09920621040907	-1.47566743221050
C	6.29535790137710	-1.44232411842264	-1.49905955001330
C	7.50496020040631	-3.32402721633642	-0.57125249395262
C	6.37120081200888	-2.47621892642420	-0.55590192985010
C	6.68278003285397	-5.89051277310595	-1.36197272885796
C	12.18684010877096	-2.66013837057890	3.21177128546487
C	5.22830113940227	-2.68989232639371	0.42773151470858
C	4.86009857768392	-1.40416001626063	1.17999640828255
C	7.06306190661640	-5.59713211294526	0.07005131261035
C	3.99820456976087	-3.29675324419823	-0.26657038969597
C	6.84967310539589	-6.61100805824138	1.02188788192993
C	13.06835091383408	-3.47157521483580	6.02762120381674
C	10.02361907914342	-2.20338294067979	4.38271793948284
C	11.72795617034940	-2.91554016914768	5.69228781105889
C	6.90237228035427	-6.51217038501202	2.42771445071464
C	10.64355592497380	-2.70152417149985	6.50261301512066
C	10.64553817376866	-6.10067874973734	5.15558672701889
C	6.32829349305494	-7.66980689696035	3.21197626478064
C	5.27320137669548	-3.79852120485898	4.10360686267751
C	4.63844431388709	-2.57906461875004	4.78097963613432
C	7.25328050004495	-5.37369559030218	4.50842017810769
C	9.33769031335711	-6.84929858864008	4.86074708495438
C	8.27324786127972	-1.92052100658753	6.14184270894965
C	4.17981889057792	-4.68226864906077	3.47961504910944
C	6.19540435544385	-4.58478251976835	5.02970112214477
C	8.14717045086062	-6.04963979672806	5.37170002705261
C	10.45881468843192	-2.95260496756778	7.95892487302574
C	9.38747987157381	-8.27323018935226	5.43569593221490
C	6.01539990190395	-4.54414937726316	6.41784224667214
C	7.93717528068099	-5.95547882601633	6.75625818355714
C	6.87287440064033	-5.22767793226164	7.27999779896007
H	7.12704297335248	-0.29543419504106	6.97943889014466
H	8.80114075498588	-0.36267434246360	7.58698183692151
H	8.49035650361455	0.23220257652307	5.94565775310584
H	13.08234862215516	-0.72321413402614	3.59658558232550
H	14.16856821762526	-2.07947203761218	3.97986078178016
H	13.85521489174850	-1.66147087544906	2.28561610208725
H	13.03290859691591	2.62461481642941	0.53710533486853
H	13.92403394259775	1.15055588105540	0.10994580016941
H	12.57765619753742	1.67839498193400	-0.91829345245766
H	6.87499036903935	3.91779978380434	4.06455778360279
H	8.61199351775735	4.08917458331242	3.73727416575969
H	7.43844184363517	4.25244353474952	2.40505417726693
H	14.85928318247353	6.35185938959054	6.36048857063353
H	12.41296421598377	7.94738275941454	4.75480679613264
H	13.44273097961945	8.01779096443484	6.21583963834275
H	11.70009230591889	7.63284120302822	6.33483335149508
H	15.81163189619064	3.32510340876679	7.69266400690513
H	16.29770270596996	5.00445140093128	7.31449789924138
H	16.73035774973770	3.65574066558329	6.22682395429594
H	8.54031738750300	7.43479702872198	2.90758612085404
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H	7.81285838466809	5.86384825051772	6.83764610569424
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H	11.37848286695023	8.63452607507342	2.66250866153936
H	10.09187964744719	8.16890668715426	1.52594148578972
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H	10.60371042115516	4.40867133445297	1.94326766443044
H	11.27775436697084	5.40799106338862	0.64037064711541
H	11.14486574431394	4.14365041095344	6.97343258599869
H	11.39541192926498	6.29790432654838	8.16177384056060
H	10.91956169647685	5.02132884106218	9.30279398394286
H	9.71324743013673	6.20702638070872	8.73901569672984
H	8.24642082733479	4.06806515963353	7.99439654312214
H	9.58056006345462	3.02825778042607	8.52397316102387
H	9.00139048134240	2.92510103958252	6.84085024499099
H	16.88169659723506	-0.39017028312892	5.00059983990049
H	15.88391827994724	-1.63351614277605	6.89869549453093
H	13.91759664320408	-0.70084303242149	8.08897383249583

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H	16.07406271491395	0.26543206501793	2.64215743879114
H	16.02181725998095	1.84298225164539	1.79612074341821
H	18.17089817763436	1.10184154199888	3.96011350325391
H	18.05802668151376	2.58894125482646	4.92478374787987
H	18.06603586125514	2.67600324445981	3.14604329653520
H	12.11908790790302	2.33147638208510	6.97187428703886
H	10.73411190149570	1.05329247735612	8.46305602534647
H	12.07119754129782	-0.00232555072938	8.96232554367840
H	11.44408763363588	-0.08439450522129	7.29293891672372
H	13.61839390238865	3.46634714131034	8.54223467296687
H	13.68282427169383	2.02138938454758	9.58671882172741
H	12.16227763258204	2.93587479035338	9.40724328018253
H	8.06432959870594	1.69592223476825	4.02148245895343
H	6.82770724867384	1.76781217610345	2.75859573896735
H	11.90037002718418	-0.25634131194380	0.60556533753263
H	12.41038026860024	0.68833950684893	2.01285620392317
H	7.18932425858185	1.68558958432224	-0.92713972929895
H	6.73687637500704	2.85084624874832	0.34054499449509
H	6.45291941534293	1.10680045910229	0.57557812156842
H	9.04283308624362	0.84612961869939	-1.81474251954327
H	10.53185999659982	0.02691386415592	-1.33596839288824
H	10.57592566779145	1.75299904867637	-1.78016603860330
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H	9.25244523499403	-1.87667007981502	-3.11488697362276
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H	11.06343558447948	-5.20348266255001	-2.71868036423155
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H	13.85107671607924	-2.69971967045251	6.00418208159565
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H	11.50609860824103	-6.64543380577400	4.73637128034689
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H	10.19467883169917	-8.84842810460468	4.95451723796732
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H	10.80144005846961	-5.98179587032052	6.24091660523540
H	5.63716156483870	-7.31683524427089	3.99051565083221
H	3.90266736208138	-2.86908375944554	5.54862342378189
H	7.97507121504040	-2.67324808664101	6.88304758748058
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H	8.44270142365231	-8.81702928358467	5.27836639593115
H	3.57259111511524	-5.16579938679831	4.26304732862433
H	9.70488670298710	-3.73883265181867	8.13474534304943
H	9.58791930886615	-8.27127317043570	6.51955569494493
H	5.19891102714725	-3.95559481738307	6.83729246352984
H	8.61874886358831	-6.47527092802032	7.43364910562190
H	6.71552446118992	-5.18118729835082	8.36082401619010

Table S55. Compound **6b** B3LYP-D3/def2-TZVPP
final energy -8653.044112181955 Eh

Sb	10.91796468956774	1.41602361740500	4.40174374189484

Sb	8.81391848093794	-1.64710445390269	2.67665420907520
Ga	12.52315071825432	3.41241980791115	4.30748469951046
Ga	8.52932938533672	-4.12661260733230	2.09131863099880
Cl	13.68843432104296	4.06489837156027	2.46465190093006
Cl	10.39751329645036	-5.40589425091519	1.77554180930826
N	11.99541667447329	5.21139279173190	5.01733417542254
N	14.02540222081623	3.19371672410968	5.61970992229770
N	8.77929307506296	1.86803644388010	2.12095229448750
N	10.64373709075284	1.33306222875847	1.18762730539546
N	7.56327323094237	-4.38529026722581	0.37181399112572
N	11.34910440562573	-2.62924951495243	4.42104776163964
N	7.39761681099902	-5.47275427234390	3.06974071901021
N	9.64384026815226	-2.29060144149006	5.68826081784061
C	7.61492496761314	3.67383262783316	3.34279578215386
C	12.88252060704004	1.60268694532926	0.07889493149853
C	13.39210806106761	-1.74030414369915	3.30443581276266
C	8.19515292899659	-0.55375342572895	6.72585602248924
C	12.92366495451965	6.01211529333219	5.53126872157415
C	14.18583016087926	5.57594540832114	5.94927343010009
C	14.65282551967875	4.26189809107451	6.09592732215554
C	12.61594981394991	7.47889698498605	5.70462800615769
C	15.94236918347678	4.08787523483652	6.85882367375349
C	10.64819492546650	5.69099376514801	4.91487745295400
C	10.20511870081922	6.35049456654361	3.75606311571070
C	8.91762566982700	6.88535237906874	3.74887106792300
C	8.07919793410793	6.75689228060717	4.84403151581555
C	8.50861423069633	6.05088847862812	5.95678701846586
C	9.78643579979160	5.49846939176115	6.01041726112294
C	11.06476340792988	6.43851105807717	2.51089698911183
C	11.11369384814413	7.84569164600009	1.90796322079193
C	10.57724951097870	5.41535368792779	1.47353985403988
C	10.22544359766523	4.73010379279892	7.24430875090867
C	10.52254177989011	5.67233245267686	8.41839844281958
C	9.20733486224485	3.65666271414007	7.64147139683861
C	14.50984973738834	1.88075892250136	5.93223601667333
C	15.57356913031206	1.31734951773623	5.20783263638095
C	16.04264826287098	0.06035002098072	5.58936000363415
C	15.47151466000789	-0.63122277040965	6.64292445715739
C	14.38219648724346	-0.08980602395567	7.30904218167820
C	13.87584682432121	1.15948878435444	6.96214157815568
C	16.18496399207282	1.99591597673132	3.99678409370765
C	15.76337982868436	1.25402901564264	2.72055006188992
C	17.71239197114222	2.10214207768106	4.07612385259110
C	12.67036372584461	1.72661014122749	7.68988387446828
C	11.69260919589227	0.64365161780253	8.15015436004136
C	13.08078303168650	2.62418806185983	8.86477804032692
C	10.08473275867800	1.62904082787033	2.38700197438230
C	8.51003078945662	1.70456339880281	0.76980682542563
C	9.68715411495030	1.36241332905201	0.17972021568198
C	7.76163393425409	2.18043966383853	3.12248254837585
C	11.99868782513279	0.80597771147974	1.02490517599964
C	7.15284528017359	1.86526266951437	0.18790793802584
C	9.97254100405878	1.03360158026851	-1.23991916754296
C	10.13672064978641	-4.51286566620947	-2.82387429767103
C	8.43412814747970	-2.02285356064016	-2.37117843867296
C	7.31139485934170	-1.21127542185024	-2.38675552460215
C	11.00650371220372	-3.07875648052581	-0.93329565028867
C	9.82213398285904	-3.90721567449164	-1.45118856000159
C	8.55764264555383	-3.07118926814962	-1.46220291437785
C	6.29762948748239	-1.42410826318449	-1.46706795958275
C	7.50191278217082	-3.30249470950939	-0.56365845305392
C	6.37419696496582	-2.46094457475880	-0.53939900417562
C	6.67497076085237	-5.86407507734598	-1.36491399908244
C	12.21563412569662	-2.70431266328295	3.24195440585010
C	5.23193372874174	-2.68403679039057	0.43554142575104
C	4.85488064190569	-1.40503215020867	1.18928028922221
C	7.05504844603157	-5.57255388131265	0.06409883092474
C	4.00798471107474	-3.28461919703421	-0.26947303999244
C	6.84105926032921	-6.58770276914603	1.00329280008338
C	13.08376673409242	-3.49451396358493	6.05583761602794
C	10.05196778959672	-2.23920006388532	4.39901963870287
C	11.74766467389149	-2.94138466464644	5.71602573077059
C	6.89684871144496	-6.50652213917142	2.40253460589757
C	10.67006554643406	-2.72317491123417	6.51707292312906
C	10.62806853330498	-6.15693665966822	5.15148646472634
C	6.32352558198171	-7.67518686985001	3.16475086489428
C	5.27495054047714	-3.82869226620107	4.10327171675678
C	4.66264292290339	-2.60160446118343	4.78239854036966
C	7.24849909859604	-5.39935531705121	4.49390979863138

C	9.31568462794457	-6.88271343610218	4.83302752266104
C	8.30015357648556	-1.95722582164195	6.15020758837091
C	4.16278780238251	-4.70469072261168	3.50928153913484
C	6.19660920165026	-4.61921531529378	5.01819134607399
C	8.13489377991449	-6.07999289250989	5.34678510731322
C	10.48914737646390	-2.95690286173348	7.97261889103883
C	9.34668472346921	-8.31036241079828	5.39345244477176
C	6.01572391592398	-4.59098631226014	6.39834648286469
C	7.92687613888759	-5.99602180740163	6.72451161519122
C	6.86900266299072	-5.27644249971815	7.25071391662256
H	7.15937096115961	-0.35249575802328	7.00337493424446
H	8.81376631003644	-0.42870180515216	7.61364298701840
H	8.51369894844603	0.18845549630201	5.99492102648477
H	13.04901250571231	-0.74161101733756	3.57350972129655
H	14.14863532710204	-2.04264121085410	4.02503094439810
H	13.86887896409705	-1.69607261859463	2.32470598137367
H	12.89831402358890	2.65189253183974	0.36165409021233
H	13.90280384911027	1.22699053029705	0.15746635801974
H	12.57500927892414	1.51093882054706	-0.96015257891271
H	6.82740549264345	3.87170578522023	4.06953171978699
H	8.54297636028141	4.08333372842383	3.73222593067376
H	7.36811083220673	4.19629631797904	2.41845489190109
H	14.84060777171348	6.34387917250171	6.32793508120525
H	12.46135744792980	7.94018950859972	4.72829241909660
H	13.43144086132371	7.98971792719681	6.20886028106899
H	11.69817671844299	7.62933582767279	6.27017262106974
H	15.86614187514990	3.28255484627907	7.58699448741150
H	16.21481156295715	5.00699939205600	7.36993164982587
H	16.74753047454321	3.82022037140788	6.17492271792668
H	8.56577220883842	7.40485740581051	2.86802372011838
H	7.08570622025420	7.18534739349155	4.82188738768734
H	7.84002206421630	5.92508139634163	6.79758008003273
H	12.08020507769792	6.15969361844989	2.77911681733719
H	11.82115974523139	7.87029394330667	1.07788835593490
H	11.43072853431726	8.58573666332769	2.64427424980178
H	10.14241898311998	8.15823543037742	1.52070026772056
H	9.56933380756389	5.66237242590157	1.13236414712708
H	10.55333135366969	4.41044963428266	1.89265350226730
H	11.24336586886105	5.39937196908170	0.61051349356488
H	11.15219381158313	4.22010802201614	6.99301624437727
H	11.30859105099516	6.38388373926891	8.16774471997583
H	10.85198112046569	5.10490044128016	9.29032671375255
H	9.63241826248489	6.23838704474015	8.69989565361605
H	8.24741990829280	4.09193196376845	7.92335144039438
H	9.57332791363321	3.09300161246757	8.50103124510698
H	9.04875097571734	2.96009361129504	6.81825839499908
H	16.86620152722326	-0.38271769545230	5.04602042831009
H	15.86407683120490	-1.59646223738447	6.93552226950691
H	13.91630308278978	-0.65103162287503	8.10596154726119
H	15.77985295294459	3.00208855347914	3.92504556433122
H	14.67973039424618	1.19610404410543	2.65283994995438
H	16.16325709649660	0.23807998813186	2.71064675711487
H	16.12627104658349	1.78060026895027	1.83728537188953
H	18.18792404722051	1.12040035229817	4.04352911615094
H	18.03956429332723	2.59366835723833	4.99293686271481
H	18.09046091144639	2.67850326944971	3.23045432078214
H	12.13495555033256	2.35683170234033	6.97996529677551
H	10.76226916248172	1.10401467914786	8.48036704690414
H	12.09007772700407	0.06650977148700	8.98715048173780
H	11.46042675606197	-0.04333557827424	7.33723404819438
H	13.65274753019461	3.48698659716870	8.52871338866599
H	13.68947318060853	2.06696043236321	9.57963135040655
H	12.19748122452521	2.99459007614433	9.38733934012138
H	8.06678177581179	1.69183933734367	4.04389559137895
H	6.83246874039625	1.71823521492970	2.79606788418645
H	11.90283369792179	-0.23356864247461	0.70485770978729
H	12.42300500953917	0.80134779876173	2.02537501807770
H	7.18689222594953	1.69194004697879	-0.88456567513766
H	6.75357789674272	2.86697821513261	0.35692595773468
H	6.45059982804565	1.14687604903719	0.61295388907745
H	9.04019295202911	0.89833232118556	-1.77969720442952
H	10.53063270421090	0.10103616919213	-1.32212734376102
H	10.54544384198969	1.81835969167724	-1.73558451063960
H	10.36999696006062	-3.74324575404217	-3.56196745868075
H	9.23324326469914	-1.83837597188025	-3.07644076923936
H	7.22827658535447	-0.41164714219162	-3.11165020956897
H	11.25016734696255	-2.27202488533355	-1.62920353167031
H	11.00181968926498	-5.17371899080430	-2.75148461776294
H	9.29745040010542	-5.09423891374145	-3.20796716137237

H	11.88797014107945	-3.71020784095990	-0.81798262670037
H	5.42885380349352	-0.77990276901469	-1.47524821470279
H	10.77245642610468	-2.63904182027912	0.03618457491462
H	7.57973955323646	-5.98406760753461	-1.96377361307393
H	9.67937603864881	-4.72714616654225	-0.75220231849257
H	6.11337158322747	-5.04275290732082	-1.80443885055573
H	11.57044663043150	-2.47038108785077	2.39907769717192
H	4.51864976518629	-0.61959256942805	0.51077936601312
H	6.09045047166556	-6.77717174043976	-1.43591984013089
H	3.63015159211671	-2.61119125863123	-1.04116918611984
H	12.53387011875635	-3.73888226396932	3.11875352538728
H	5.70035507530290	-1.03014865513051	1.76786217025604
H	4.24872192215577	-4.23567671977527	-0.74340927309500
H	5.56957127043250	-3.40863180764805	1.17208131618937
H	13.85771363281199	-2.72861736670983	6.04565018401644
H	4.03642253938360	-1.60676944877102	1.88047474228560
H	3.20430341209211	-3.46242442652371	0.44692875542470
H	13.37303532748627	-4.27840702273514	5.35474351378086
H	6.45755297168905	-7.51422433817316	0.60772858542090
H	13.05978265608375	-3.93347446950157	7.05129027808003
H	5.89320666864176	-3.46126676628025	3.28358387998868
H	10.63029209092172	-5.16249037971759	4.71671086253016
H	9.24432883296699	-6.94386766266912	3.75000168576976
H	11.47568599286484	-6.70351149226414	4.73640781710040
H	4.13048291419190	-2.00046268917739	4.04698086762351
H	5.42643967773197	-1.97037319185477	5.23448416051661
H	5.73136218863670	-8.30893098725289	2.51053060971491
H	7.65812023160526	-2.05769185026542	5.27860749356530
H	3.50469421205434	-4.10574839341936	2.87786070589548
H	7.13071130092265	-8.27471546850299	3.58555628178276
H	4.55986247323635	-5.51093038956569	2.89731239120459
H	10.13948958222566	-8.88288022976105	4.90981791019354
H	11.42280118238879	-3.29767318239907	8.41449335789362
H	10.77034088489062	-6.06236445546146	6.23015806135997
H	5.70541084365768	-7.34265441752284	3.99603986200538
H	3.94321839073584	-2.87994327358849	5.55431790850209
H	8.00310922416841	-2.71244708909739	6.87362761788209
H	10.18813623337084	-2.04978038465171	8.49734068581876
H	8.40370344556933	-8.83343397722346	5.23274536797754
H	3.55635577932193	-5.14520321857581	4.30346706191897
H	9.72899700740895	-3.71908135485761	8.15918651213686
H	9.54489999889715	-8.31703300401916	6.46653036714052
H	5.20807657453227	-4.01025518941530	6.81850461113029
H	8.60112860193944	-6.51604227961982	7.39164321254809
H	6.71306872980856	-5.23878927710217	8.32110936867399

Table S56. Compound **6c** B3LYP-D3/def2-SVP

Electronic energy ... -8805.56173058 Eh

Final Gibbs free energy ... -8803.81756018 Eh

Gibbs free energy minus the electronic energy ... 1.74417040 Eh

Sb	11.10154966581211	1.20073302078389	4.14985855570429
Sb	9.15729165670779	-1.97338650705595	2.90191302893311
Ga	12.43406900521837	3.38175206121457	4.03535912956304
Ga	8.71146603962734	-4.40168528085710	2.23212135223478
Cl	13.28304199765904	4.23534839894790	2.09189609320029
Cl	10.34167588089263	-5.99981586316282	2.22328956066231
N	11.87925666458999	5.10798253225886	4.89757094739477
N	14.10589507029310	3.21618144082256	5.12030340361791
N	8.51578284901169	2.04164977928384	2.44655014401597
N	10.17459094834073	1.67052765503951	1.09203724430803
N	8.08692398845885	-4.52092462190472	0.33761061518738
N	11.63888221432371	-2.93059325001529	4.74498035873660
N	7.20268995034647	-5.51693228583031	2.94278384069130
N	9.97000289069747	-2.30009306092878	5.98624354414406
C	7.16193771123277	3.61968781872598	3.81253309741473
C	6.75853793106200	1.09786824079003	3.94780483912565
C	11.60224982401429	-0.15410479351190	0.20215477359983
C	12.06903110476228	2.27267901260504	-0.44280371971732
C	13.37810695675969	-2.04872552933585	3.20986588479258
C	13.15030347593974	-4.56508447153090	3.58590997387931
C	8.58875888353092	-0.43293555080818	6.90296148024748
C	7.92797105990775	-2.87582900721675	7.28548662389354
C	12.82465357278595	5.95203395008741	5.32371137725139
C	14.17667439947779	5.59940146304177	5.50691047918417
C	14.75279492040235	4.31476363418820	5.51189003165302
C	12.44076909793611	7.37358132385871	5.66911251210530
C	16.17943893884438	4.19629431050516	5.99505371499077
C	10.50956699470595	5.53152999029557	4.96208969581894
C	9.95339435982742	6.33447024439046	3.93980345710300

C	8.68170949737868	6.88885144195418	4.14605243827391
C	7.96294491697114	6.63494209459402	5.31182401229200
C	8.48052809637345	5.75572260077436	6.26198780464703
C	9.74441682086204	5.17377433762742	6.09806401951431
C	10.66410073591025	6.53742186110803	2.61121807369877
C	10.61560222724382	7.98114572461866	2.09651790176122
C	10.08251183712111	5.55906292513214	1.57388022252263
C	10.28540801849153	4.18428786881621	7.12018815448115
C	11.10143534586300	4.87661650156365	8.22263745577521
C	9.18867954219804	3.29822152953427	7.72184952517710
C	14.66741452620117	1.92044580378838	5.36628141127022
C	15.55041327835132	1.32671127374978	4.43500832568690
C	16.11419959718156	0.08315495567869	4.74958045764397
C	15.80272582635784	-0.57384981743554	5.93769283632433
C	14.88839610433693	-0.00331599377793	6.82128645080256
C	14.30450611183477	1.24180026608035	6.55450730638872
C	15.86024894050132	1.97070422902136	3.09323005329032
C	15.17074064340735	1.18307785076278	1.96700195166583
C	17.36576602211035	2.11166099122098	2.82931160970889
C	13.33220193548083	1.85282777602744	7.55400867343948
C	12.27048526447013	0.84914381074021	8.01987626503443
C	14.07745051941389	2.46428175058319	8.75126686675887
C	9.84223361204631	1.73707067970594	2.40876005333920
C	8.01075081906922	2.16219166724887	1.15279281369102
C	9.05792090413669	1.92021739712680	0.29889762676714
C	7.76313676753328	2.22280437822914	3.70697994890048
C	11.53419331993001	1.31279212244224	0.61835924958195
C	6.61338686607314	2.55261379385752	0.80416270381328
C	9.05425150518862	1.94436407345643	-1.19213396816823
C	11.20037762877688	-5.26269602949783	-2.30726532182381
C	9.89550517216694	-2.50601920238705	-2.24214748919072
C	8.97540769933165	-1.48622969232474	-2.47470539452727
C	11.87990930808403	-3.93517631095339	-0.25757378787114
C	10.70957500050690	-4.56506907622308	-1.03101662688957
C	9.64588091844761	-3.51284474829936	-1.30016640706756
C	7.79499406130455	-1.44192175137467	-1.73560906210401
C	8.42037451901666	-3.48483315523303	-0.59480803665459
C	7.49860936607825	-2.42812041225950	-0.78556889346801
C	7.32453542319750	-5.86412242791444	-1.56922494352258
C	12.44442825605077	-3.21230298251312	3.53200148397085
C	6.18792954108469	-2.36311804775862	-0.01283169915079
C	5.96183094708962	-0.98502778868174	0.62122901062725
C	7.46141804110061	-5.62161040330407	-0.08434794920277
C	4.99799390933288	-2.76819688347861	-0.89741198098261
C	6.90015665119116	-6.57771599893892	0.78258427665468
C	13.44663299988510	-3.39084797460800	6.49827617967328
C	10.34509897442075	-2.51476703082386	4.69467976845097
C	12.08462729868128	-2.96596096354590	6.06342247508907
C	6.68771911970023	-6.48001037002133	2.17228849227968
C	11.03024515613814	-2.57202833350625	6.84922580588865
C	9.77538222410690	-6.27460603679289	5.67554170650459
C	5.79572346307248	-7.52821853997921	2.79877598912530
C	5.19312560409809	-3.53213982159802	3.53708684345314
C	4.76459132269428	-2.18895069857031	4.13825067868777
C	6.74958569155053	-5.41017249266297	4.29960521581777
C	8.57307427095886	-7.03302894426511	5.08379439435310
C	8.61005486068569	-1.86433163633302	6.37093188058395
C	4.07060446394957	-4.13932887151860	2.68092044302222
C	5.69905579800595	-4.50782094274091	4.59093116803857
C	7.30599105489604	-6.22423486208194	5.31328209743024
C	10.97266347890175	-2.48851043013092	8.33809246621159
C	8.50025343398732	-8.46285385894959	5.63469652938079
C	5.12577625134128	-4.54150123203565	5.86914424025675
C	6.70063692134738	-6.21983983481493	6.57833799349432
C	5.59821559913058	-5.41318524308733	6.84907575787797
H	8.33010231592115	-2.86835572187971	8.30900227170763
H	6.85690185617724	-2.63637725879480	7.34892776462952
H	8.01132108014089	-3.89128047840033	6.87655161266319
H	14.06169803805122	-4.54664030668198	4.20011760813750
H	12.47346816748887	-5.35194857521722	3.94366147647956
H	13.44612175170826	-4.83769211071448	2.56236342500470
H	7.23992177852256	0.11293010287458	3.85156500734040
H	6.35410913256001	1.19031368189675	4.96787554341165
H	5.90668644682437	1.13235504846348	3.25155441001592
H	12.64214711280135	-0.40925565016357	-0.05510741158650
H	11.27182338800920	-0.80885170667689	1.02192030066585
H	10.97135383776892	-0.37231718589384	-0.67259270496736
H	7.54348446396015	-0.09699754536342	6.98804341128136
H	9.04574359182984	-0.34257042639642	7.90026029190357

H	9.11859350241185	0.24787705592548	6.21968425080379
H	12.82429795292314	-1.09833042025134	3.18189326880851
H	14.18973805785169	-1.94191913057320	3.94507317863449
H	13.83577374410632	-2.21551791566666	2.22226396942676
H	11.85831554079165	3.31711474892811	-0.17806761641552
H	13.16288079581658	2.16698296229059	-0.47932080078036
H	11.68016316263846	2.05553631961053	-1.44754366552722
H	6.82936820725796	3.79072655532441	4.84610069332849
H	7.91121486440435	4.38685717862488	3.57836457799052
H	6.29036616908075	3.76036447738681	3.15721769746385
H	14.83601811968288	6.41104800527218	5.80949806373918
H	12.06049009408840	7.89547267056669	4.77836988070251
H	13.29969291770868	7.92839933410897	6.06642601099062
H	11.62832557563707	7.39121512423213	6.41052144547598
H	16.28304418081277	3.40391599836504	6.74952982065976
H	16.53687714327370	5.14401090548178	6.41669395026858
H	16.83404009203356	3.91485169923828	5.15532682153371
H	8.24778315653469	7.52891419274329	3.37506885465465
H	6.98090904131378	7.09056720871993	5.46265340440136
H	7.88940715096327	5.51361396655267	7.14693055751987
H	11.71944773134247	6.26454074245205	2.73965672701371
H	11.23794061854222	8.08032445611843	1.19296451680835
H	10.99411151874363	8.69314892029078	2.84762207091262
H	9.59413261365329	8.29438860114468	1.82506281680944
H	9.01816577585928	5.77628996723895	1.38120540208673
H	10.15931332616980	4.51968156490867	1.92350023376995
H	10.63222886706455	5.63036850719522	0.62234699920828
H	10.95856325020061	3.51333857709745	6.56705180083938
H	11.98737242397032	5.38573172678963	7.81669922725003
H	11.45319464095943	4.14063489806466	8.96288120338745
H	10.48939705096893	5.62406740980889	8.75475545831940
H	8.51468414217281	3.85958129928846	8.38948484371219
H	9.64159882620890	2.49186908052582	8.31806325991715
H	8.58289451194237	2.82574340128079	6.93402732798066
H	16.80709840909272	-0.38103749516736	4.04419841910958
H	16.26570439900611	-1.53630488717733	6.17070626358578
H	14.62826378584167	-0.53136547058022	7.74109699007734
H	15.42203025559409	2.97657190834278	3.08955051387846
H	14.10166520413257	1.05403724426126	2.18713260370722
H	15.61463697717946	0.17978375669895	1.85256865985069
H	15.26497600605596	1.71749298659128	1.00881046712005
H	17.86174092548282	1.13131684578992	2.73961808776802
H	17.87168724367545	2.66615945008192	3.63600853531106
H	17.53698607858666	2.65468325278009	1.88598222624452
H	12.80967551657118	2.67068269089006	7.04049939685243
H	11.52629194113570	1.34932531390215	8.65907799801415
H	12.71183385560052	0.03253067607338	8.61269048892860
H	11.73975747061502	0.40554596019780	7.16427920447730
H	14.77356499092570	3.25457747336832	8.43345564778549
H	14.66109132711754	1.69639183947902	9.28596233789652
H	13.36926213224317	2.91112235609279	9.46727259720185
H	8.55185766658224	2.13942734002749	4.47252387765522
H	12.14670287600673	1.43776701113151	1.51975255524921
H	6.42230943688664	2.33344482861322	-0.25477106679597
H	6.43870281445437	3.63048292472495	0.95422597091103
H	5.86718760364205	2.00654996814136	1.39576299327150
H	8.01997413017782	1.90064405056845	-1.55887364035990
H	9.58794800443415	1.08152768323043	-1.60913322766758
H	9.51580700918097	2.86095114305726	-1.59189394850977
H	11.73181953642553	-4.56897366076784	-2.97910850620872
H	10.83440905698646	-2.52007665595536	-2.80004513333149
H	9.18312701133392	-0.72167868073797	-3.22766978146364
H	12.40870855911149	-3.18908828518719	-0.87411103586617
H	11.90157257933586	-6.07322844940458	-2.05130967621904
H	10.36741228319791	-5.70376240204140	-2.87815822458277
H	12.60049319842244	-4.70970534179653	0.04838813418612
H	7.08415524834710	-0.62995053982516	-1.90345870820589
H	11.51375353233241	-3.42683778116319	0.64545218885993
H	8.31998719207714	-5.97825267515337	-2.02430412028549
H	10.27548053423382	-5.33159684353797	-0.37641287446977
H	6.85193885832814	-5.00642353274703	-2.06922885446527
H	11.68471800303532	-3.26368885597281	2.74230726946140
H	5.86891416295770	-0.19557912326968	-0.14049983877916
H	6.73468301341325	-6.76649308813222	-1.77196256556492
H	4.89386634547695	-2.08601166115155	-1.75754172532730
H	6.78930234187435	-0.71479998625020	1.29419216645128
H	5.11658990120951	-3.78923365923784	-1.29004927557013
H	6.25412543466568	-3.09538575266220	0.80244067349332
H	14.23137433799135	-2.91311128326321	5.89829646917071

H	5.03159616445355	-0.98159473488016	1.21059656768155
H	4.05735081422680	-2.73714477017772	-0.32432362748256
H	13.57960679302645	-4.48212378815201	6.43140589596651
H	6.46003101939576	-7.44891033246401	0.30053911433862
H	13.60684179596563	-3.09853001402491	7.54469347171314
H	6.04643843005283	-3.31944841771998	2.87641824739021
H	9.85634567539215	-5.26360743299751	5.25097161350235
H	8.74774607470633	-7.10027262473009	4.00256427858757
H	10.71449983296022	-6.80464134165368	5.45221423198204
H	4.55473604692145	-1.46556694996973	3.33603537231889
H	5.56297903494226	-1.76563220058900	4.76618369475419
H	5.37925368072714	-8.19768272073355	2.03605627899604
H	8.07507208089193	-1.87257399159315	5.40772784850200
H	3.69822327127152	-3.40364691067892	1.95002354388071
H	6.36185815783256	-8.12811004582029	3.52708399173733
H	4.41824450266035	-5.01695824905282	2.11732257944660
H	9.40254882915465	-9.02533837554777	5.34620034003341
H	11.99093927937795	-2.50037220741104	8.74904919597429
H	9.68060487605845	-6.17949675940447	6.77068372188287
H	4.96977837235327	-7.06201190395611	3.35576189346430
H	3.84975234787443	-2.27542501512971	4.74665750480396
H	10.48865318050153	-1.56517248620874	8.68191314562965
H	7.62485634276954	-9.00578547523518	5.24345064410425
H	3.21983198273594	-4.45036559879283	3.30998541900984
H	10.42790303610431	-3.33905131837537	8.77898405082630
H	8.44071022583031	-8.48456266381195	6.73525010138205
H	4.29563155010947	-3.87289051670164	6.10286661546336
H	7.10577573548984	-6.85920717102530	7.36557699741641
H	5.12974775268739	-5.43494434186224	7.83636341221829

Table S57. Compound **6c** B3LYP-D3/def2-TZVPP
final energy -8810.268497346931 Eh

Sb	11.09299368202222	1.22820766483954	4.13475032774042
Sb	9.15007453363748	-2.01391646554347	2.93244339625004
Ga	12.43400243576553	3.40437291277132	4.03289034272672
Ga	8.71787723859286	-4.43568987802662	2.23129050583421
Cl	13.24945715958081	4.23958977254837	2.07298892728583
Cl	10.34763226794323	-6.02823168769972	2.23929327371519
N	11.90054607191301	5.13041420270318	4.90812036068144
N	14.11488668156013	3.23098275944417	5.09941133981015
N	8.50119584910979	2.04273443978331	2.45636500800195
N	10.14600219454584	1.68258851847834	1.09667101342409
N	8.10969360762704	-4.54897006606366	0.33349362141549
N	11.61779411476261	-2.94544751760479	4.77685256155713
N	7.19804485803831	-5.54676033441895	2.92315148679016
N	9.95929900009169	-2.29610353823823	6.00650865776347
C	7.15043956488847	3.61425767386147	3.82335840635004
C	6.75642500368682	1.10010353920224	3.96294114554782
C	11.57916184325187	-0.12859589019749	0.20903354243916
C	12.01169768571466	2.28680241785499	-0.46498875289298
C	13.33644071484211	-2.08432791656036	3.21743170492665
C	13.14514503721834	-4.58416541054099	3.65263573820711
C	8.59474245978804	-0.42034114798888	6.91750378699219
C	7.91672319720889	-2.84589894100361	7.30800598134982
C	12.85046464905179	5.96007190867131	5.33159507188864
C	14.19464861801295	5.60008492187805	5.49948661973536
C	14.76403493311562	4.32066088191912	5.48985519607726
C	12.48459114037106	7.37896594219325	5.69238245686492
C	16.19296285917627	4.20313752402515	5.95641584956103
C	10.53449251645785	5.56509759534553	4.98007299101461
C	9.98520954539636	6.37300195850113	3.96982592903657
C	8.71835732940307	6.91953336680006	4.17423902943699
C	7.99944138564510	6.65533773018658	5.32786234062940
C	8.51423851840790	5.77741425435234	6.26940789987591
C	9.77214530622033	5.20204127607439	6.10630234130243
C	10.70306593509935	6.60556265422242	2.65535777543525
C	10.68808512300724	8.06553559527064	2.19324651158172
C	10.09885463778970	5.68870073599955	1.57939443693402
C	10.30987019371450	4.21511710746689	7.12601731806489
C	11.10592861697052	4.91111014924098	8.23721906419689
C	9.21549667259798	3.32444082524099	7.71807424323906
C	14.67429729788288	1.93414696558396	5.34446956772789
C	15.53520244824083	1.33464253958876	4.40962331641386
C	16.09445923734005	0.09723879346312	4.72194201533751
C	15.80016722385194	-0.54562964538964	5.91281165456460
C	14.90836577971388	0.03261035320816	6.80197950971999
C	14.32796311022589	1.27056990806785	6.53605086209910
C	15.83468445905659	1.96954776315701	3.06663128523235
C	15.14918778112457	1.17098618047797	1.94920335400236

C	17.33652110682998	2.10928029214563	2.79527306936794
C	13.37231054270027	1.88783224395987	7.54118945082382
C	12.30979200765284	0.89278365598914	8.01462613776737
C	14.12989003004366	2.48623175352089	8.73396613412686
C	9.82639013896850	1.75302291151427	2.41185502182804
C	7.98658493475880	2.14831275918874	1.16760677291925
C	9.02190574944849	1.91452193254988	0.31347184081630
C	7.75782401078078	2.22316253530402	3.72021070253724
C	11.50385462445284	1.33735290110349	0.61442854931602
C	6.58527027366320	2.51445083340372	0.82503286817778
C	9.00359020122357	1.92011594933456	-1.17394308451530
C	11.23687520934415	-5.25027114101136	-2.28141191262108
C	9.90685995525178	-2.51827295654280	-2.22258843296819
C	8.97716215124850	-1.52146666587399	-2.46860241535148
C	11.89957522089681	-3.91117541958735	-0.24447299163594
C	10.73574604956584	-4.55656835150849	-1.00995271955695
C	9.66438273463955	-3.52088887848194	-1.28556253357633
C	7.79362555705822	-1.49656468345763	-1.74915542599731
C	8.43808917800057	-3.51078855660929	-0.59865678380781
C	7.50557159917124	-2.47778033790048	-0.80326446257824
C	7.36470523983240	-5.89367565054970	-1.57141582216460
C	12.41799522344120	-3.24754566490221	3.56704544284385
C	6.18873062409977	-2.42756781826024	-0.04903543841352
C	5.95726175491172	-1.06081521112231	0.60096121224060
C	7.48708183076823	-5.64327589713494	-0.08984879553851
C	5.01183924765357	-2.81228682315553	-0.95513278526149
C	6.91779444695382	-6.59297964056157	0.76675288790834
C	13.42879240672637	-3.36288309102583	6.52786558973736
C	10.32792811167851	-2.53241697103959	4.72118956622497
C	12.06564269661900	-2.95650718755766	6.09209543460102
C	6.69054090564296	-6.49953968858248	2.14721465904912
C	11.02117008753861	-2.55313140400801	6.86827491996586
C	9.74047160126579	-6.36983705176454	5.68359267536949
C	5.78919761025806	-7.54635315647362	2.75391419856863
C	5.18792149942919	-3.57008210104394	3.50655880205743
C	4.77599629637611	-2.22061300483869	4.09884613220209
C	6.73485449714489	-5.44150331836842	4.27674967393916
C	8.52888510492477	-7.08262875205136	5.06213252327630
C	8.60353985972765	-1.84880858348140	6.38625393973272
C	4.04767892014853	-4.17442419445847	2.67680725136869
C	5.69502433971214	-4.53719909651409	4.56133020249860
C	7.28276305697270	-6.24944726924642	5.28807115820632
C	10.96944884446936	-2.44331000106005	8.35153184150341
C	8.41334158499721	-8.51365661986828	5.59698631681795
C	5.12670753977054	-4.55890850037059	5.83312510361412
C	6.68481995475701	-6.23062552204632	6.54801221860340
C	5.59499309953403	-5.41934705717751	6.81397737615602
H	8.32762810296009	-2.83711947235256	8.31624098363808
H	6.86051452980608	-2.59039824287792	7.38013680253829
H	7.98210469238887	-3.85428739773620	6.90717209318508
H	14.05529544975271	-4.52685331512484	4.24664302188577
H	12.49753139116214	-5.36253686619371	4.04890228381308
H	13.42525438983759	-4.88171006712413	2.64316987731304
H	7.23099469845334	0.12486590122893	3.85935373037522
H	6.36524461001615	1.18897998798270	4.97712725107655
H	5.90818338019410	1.14156762559616	3.28053619178882
H	12.60754173438439	-0.37205231439492	-0.06055443677601
H	11.27093838239225	-0.77217960501746	1.03140331976666
H	10.94336033955496	-0.35340814347891	-0.64636130903069
H	7.56216179890458	-0.07569455574803	6.98497597832850
H	9.03061876227500	-0.34145280030190	7.91283677831548
H	9.13916110180677	0.24715333729437	6.25029674476211
H	12.77815321948439	-1.15067584625354	3.16585177799777
H	14.13642682617934	-1.95499491785844	3.94525733595837
H	13.79322091408060	-2.27083463825137	2.24477713417573
H	11.78685024908016	3.32208217993940	-0.22066038874883
H	13.09588269818264	2.19636882022280	-0.51139336770120
H	11.61574163220438	2.04873662819892	-1.45019417262498
H	6.81086285475545	3.77758971684004	4.84487684161578
H	7.89009379185657	4.37830012833226	3.59765156786421
H	6.29289065021594	3.74629131029662	3.16586215773031
H	14.85343915816854	6.39829412785735	5.80035473463149
H	12.13480360996193	7.91507087282134	4.81066190047394
H	13.34067261864922	7.90442425288701	6.10570036694071
H	11.67068339393023	7.40065407818522	6.41591468354261
H	16.31795504086378	3.38402173806316	6.66139216462928
H	16.52964154729180	5.12735371495127	6.41775360529712
H	16.83744269120911	3.98571875766429	5.10329789686305
H	8.29059010094058	7.56022439692846	3.41542270112563

H	7.02525458569672	7.10233982672701	5.47664170592593
H	7.92555195352411	5.53126922252587	7.14162355532798
H	11.74113985765408	6.30736246334269	2.77527274251167
H	11.30643386634393	8.17690971784656	1.30152307282946
H	11.08033638189197	8.73504489323255	2.96005371444852
H	9.68284157976439	8.40567719351090	1.93878445335523
H	9.05525069722269	5.95064636627779	1.39039811565029
H	10.13729733655544	4.64462926075813	1.88691957108927
H	10.65519137035320	5.77992870199728	0.64604387457680
H	10.98623516803398	3.55524783434254	6.58494646084231
H	11.97630680684292	5.43279833194212	7.84264713540932
H	11.46038350078587	4.18106962187324	8.96619899905659
H	10.48239437235069	5.63686026591478	8.76353249452271
H	8.53631911588754	3.87996786590847	8.36696999773617
H	9.66643944905572	2.53475585466414	8.31840641039274
H	8.63056588872821	2.84779925116358	6.93224394012905
H	16.76797484701948	-0.37102848712563	4.01708308183011
H	16.25699411187353	-1.49940425401991	6.14299072580078
H	14.66449301234977	-0.48271701223196	7.72084650138044
H	15.39996621192430	2.96529542789832	3.05902338276232
H	14.09169795824448	1.03809882296721	2.16961048929028
H	15.59764877660320	0.18068109486757	1.84407627786606
H	15.24048258836970	1.69540253387774	0.99750446736424
H	17.82357450727088	1.13654322113450	2.70846757034931
H	17.84005123730981	2.66087473347723	3.59039808034475
H	17.49797349832870	2.64421277192687	1.85820171114558
H	12.85580494911860	2.70332189767182	7.04035719931159
H	11.58751667109508	1.39468648211871	8.65930684288078
H	12.74943685182420	0.07798904764373	8.59094854985187
H	11.77069536580648	0.46380590223059	7.17072223023808
H	14.82491595329088	3.26268680328472	8.41649709733149
H	14.70215845819741	1.71633893622524	9.25552024974451
H	13.43511798488905	2.93247807835856	9.44697312634087
H	8.54166718988168	2.14451084619160	4.47547578382345
H	12.11969268135437	1.47713598389111	1.49838471099049
H	6.40117285670699	2.30001622060596	-0.22512796722510
H	6.39409146017973	3.57751456615923	0.97975222782840
H	5.85606693720730	1.95570282308544	1.40624860458537
H	7.97631836322141	1.84988194855222	-1.52428213877265
H	9.54563772122313	1.07198737343010	-1.58240191965127
H	9.43682382166085	2.83277794203164	-1.58491626999016
H	11.75737140323103	-4.55667471046227	-2.94391365030069
H	10.84282848271577	-2.51746139911599	-2.76444779602235
H	9.17896850596972	-0.76243100964995	-3.21306116943644
H	12.41063042064584	-3.17068926695936	-0.86325064516359
H	11.93796743968189	-6.04451717006273	-2.02064607611459
H	10.41745898434218	-5.69566522352689	-2.84726595479010
H	12.62201671404558	-4.67076738145579	0.05612154202673
H	7.07748380710056	-0.70643203611438	-1.92909239315985
H	11.53556988214748	-3.40737786478411	0.64911441746032
H	8.35347675974239	-6.06608228423238	-1.99788851498889
H	10.31331511381501	-5.31941642275457	-0.36114489711016
H	6.94826147061890	-5.03007758053350	-2.08688921730922
H	11.66298166236886	-3.32846936751544	2.79015971604598
H	5.89552723034859	-0.26759220179693	-0.14435124393955
H	6.74155706428447	-6.76110708549321	-1.76922131593695
H	4.92029363910296	-2.11905757908907	-1.79360095502817
H	6.76179077062162	-0.81334444526467	1.29330725485696
H	5.13583874064240	-3.81554846059205	-1.36192041458605
H	6.23985389773585	-3.16629380737564	0.74686871534265
H	14.20072075099409	-2.89680931543386	5.92127431840361
H	5.01954859426573	-1.06082033423449	1.15761949684669
H	4.07525863892719	-2.79189473574027	-0.39573332086123
H	13.56617980596477	-4.44379936520185	6.48338797773991
H	6.48611189013681	-7.45417048180588	0.28340614782776
H	13.58881203453753	-3.04992718351310	7.55713982142249
H	6.02414318557080	-3.37193066533337	2.83741464714325
H	9.85436890840752	-5.36258374780982	5.28510314023896
H	8.71221473553395	-7.14231655142266	3.99286260960514
H	10.65670122004825	-6.91897852352094	5.46385998361673
H	4.55277605264063	-1.51589973042801	3.29848609297391
H	5.58180966648674	-1.79723572410029	4.69748420931122
H	5.36426040048413	-8.18282480977054	1.98297057267291
H	8.07302943384153	-1.85665551729489	5.43324011489346
H	3.68380262788351	-3.45284154871755	1.94350154044769
H	6.34964830425959	-8.16768220783871	3.45240817344082
H	4.37327776309185	-5.06035227111538	2.13428188899389
H	9.29671676469334	-9.08764406052008	5.31368688500541
H	11.97910161773539	-2.47425909437146	8.75432884022227

H	9.63162005561229	-6.29821904679044	6.76830384276938
H	4.98109130742487	-7.08768300291742	3.32193292964665
H	3.88344019321094	-2.29860949832175	4.72142204122170
H	10.51580596230449	-1.51093492677558	8.67810338268411
H	7.53714832252094	-9.02456910538756	5.19545672502057
H	3.20898407463318	-4.45548353308586	3.31710587393208
H	10.41062665818333	-3.26515721738419	8.80160367922266
H	8.34200561418784	-8.54021287727292	6.68561659127367
H	4.30893067678122	-3.89089593259991	6.06231538749665
H	7.08226648522093	-6.86124956096946	7.33143130886764
H	5.13419166981056	-5.42954808592096	7.79302502501494

Table S58. Compound **7** B3LYP-D3/def2-SVP

Electronic energy ... -3862.64370660 Eh

Final Gibbs free energy ... -3862.07044619 Eh

Gibbs free energy minus the electronic energy ... 0.57326041 Eh

Sb	3.57202329188129	14.95397827337897	4.49913442398730
Ga	3.40031549554091	12.40659481936838	5.06890792122276
Cl	4.20324836019832	11.54393201167582	6.98094797324041
N	2.07898906084638	11.01618654948205	4.53820554969716
N	4.73865597736052	11.82806995651773	3.71412583786109
C	0.40378317528302	8.63820922021772	7.50032503604328
C	1.10215925289965	10.90218624557099	8.37105321692679
C	0.97227704562843	10.01576293997205	7.12120088785100
C	0.60453283402215	11.49448174281205	1.53539753385911
C	-0.22469602931589	13.78909317294201	2.17265412118058
C	0.50450544118522	12.53398082487023	2.66376643217944
C	0.13975641701158	10.71778594847873	6.05663069697152
C	-1.22767659649946	10.92316871297359	6.29494829342598
C	-2.02756790669564	11.60721737759229	5.38547125082902
C	-1.46207411203718	12.12442008393109	4.22033701373892
C	-0.10259465143589	11.94922367889275	3.93407372955484
C	0.68971525148035	11.21302588479801	4.85163799501376
C	7.43663245466961	12.94541171512087	6.43225873470342
C	8.70534500279936	11.62311900600704	4.68027597147786
C	7.34735926407239	12.22317953219854	5.07746537594070
C	3.18316809381899	14.53244293077271	0.75094124034317
C	4.68570278970213	12.57590150742329	0.26813448441997
C	3.99544048549763	13.39672057454262	1.37455466917148
C	6.80771385445535	13.15731936675864	4.00592481480467
C	7.50964651593897	14.32838509764875	3.69028310447339
C	6.97399905745543	15.29290040350290	2.83657071714022
C	5.75604093358896	15.06335980162456	2.20297323157596
C	5.04205463698654	13.85148774494632	2.39300183744246
C	5.57544685901621	12.91865871825981	3.35617676176066
C	1.52119748648119	8.72502955611436	3.86571199090317
C	6.09062150615689	10.09045966208078	2.61048233585294
C	2.50091905592245	9.86765976909250	4.00062582350203
C	3.81116527543591	9.63297188246265	3.52660881871597
C	4.84157329982003	10.56673848024155	3.31119524944339
H	6.62744251657243	11.40286161373945	5.20313941163799
H	1.08759586682645	8.12108969494331	8.19271684129159
H	-0.57148333451203	8.72503083796874	8.00665092790670
H	0.25762689234658	7.99391409259009	6.61923888465352
H	0.11918453665649	11.07076974701476	8.84117143501923
H	1.76261163107250	10.42574626785154	9.11294202007702
H	1.53983206049188	11.87881609583063	8.12217756242956
H	1.98657076043357	9.87051620792884	6.72674591157735
H	1.24732872399070	10.64670462054201	1.80863239995557
H	-0.39194271506327	11.10015307302055	1.27547823671062
H	1.03168034809685	11.95171546357959	0.62774909918524
H	-1.23566482817447	13.56145839638173	1.79741462174678
H	-0.31214186304990	14.53919733218204	2.97334233343870
H	0.33385351735635	14.24635845369657	1.34341078474513
H	1.52707184152085	12.84773066013524	2.92182360473045
H	-1.66862346618887	10.54301939009273	7.21894986987051
H	-3.09113691486228	11.75431824948328	5.59017689676067
H	-2.09066944532616	12.67978619827643	3.52342607914775
H	6.46856966541174	13.38692158168441	6.70596770160213
H	7.71601965486114	12.23149326027882	7.22330594605966
H	8.19581842211956	13.74533280718546	6.41095748382551
H	9.47788123063204	12.40461549225800	4.58974200368016
H	9.04625537863330	10.90813930784627	5.44656663684053
H	8.65513266706983	11.09267935464790	3.71661366340964
H	2.39720844069355	14.11524028094036	0.10285483786973
H	2.70196689495511	15.14756568955569	1.52618118886778
H	3.80748155384296	15.18473144076609	0.11829052050570
H	5.22578480175821	11.71047110010897	0.67273316002593
H	3.93812956148234	12.20090288344337	-0.44901501470179

H	5.40987198540901	13.19607124412013	-0.28580592796376
H	3.30116784953166	12.72588600584725	1.89772171248322
H	8.46746432228369	14.52143926288498	4.17824800740473
H	7.51209759473150	16.22656436894027	2.65806236262489
H	5.36552242889014	15.80257389029420	1.50193902775309
H	1.91968317765093	7.93766912932015	3.21369466483311
H	1.31273689832179	8.28786255641212	4.85331770586900
H	0.55957661803828	9.07315327921619	3.46510504148789
H	6.66644529368984	10.92252799738944	2.18694125625348
H	6.73666336372042	9.58079143559091	3.34429718288540
H	5.85067859268411	9.37069269760226	1.81617308476585
H	4.00943859652913	8.62141534623594	3.17375775727902

Table S59. Compound **7** B3LYP-D3/def2-TZVPP
final energy -3864.407931597702 Eh
DLPNO-CCSD(T1)/def2-TZVPP single point energy -3859.769028552560 Eh

Sb	3.57209015361520	14.90450414020573	4.52393877457012
Ga	3.37399201175756	12.36543099830857	5.10418969000077
Cl	4.20801413252219	11.49952725333543	6.99811100464140
N	2.05955160412877	10.97386554366515	4.56185270061497
N	4.71076934090392	11.82374005350731	3.73749600315884
C	0.37493914569197	8.74397546817842	7.57541977226476
C	1.06911890527071	11.02766441103274	8.38743113349963
C	0.94218209345154	10.10817098452994	7.16585139680887
C	0.75203950118984	11.40186275034025	1.54904668181384
C	-0.27084043862343	13.62926489684587	2.06325670626594
C	0.51120128823347	12.44798004075705	2.64301768697184
C	0.11868634528617	10.77635953341960	6.08353583625780
C	-1.24384750366052	10.99047937107370	6.30169481157376
C	-2.03555624436097	11.62309488692142	5.36107440503665
C	-1.46832635136192	12.07577182331812	4.17811560581049
C	-0.11576685398522	11.87958006626089	3.91172340791524
C	0.66071762510956	11.16573916451927	4.84791833048958
C	7.48267098720765	12.80630291000116	6.37337381758840
C	8.74919050791095	11.59818027636958	4.55337077431733
C	7.38361696451233	12.14029795778807	4.99226163656576
C	3.14817820326665	14.58343877766809	0.83437245402598
C	4.75091308728232	12.72811533684853	0.30095974574540
C	3.98351576582581	13.44852579999182	1.42395288475144
C	6.80565085396680	13.11403659333775	3.98043828280578
C	7.49946762835586	14.28845727233070	3.69069814158368
C	6.92698637027717	15.29522812754874	2.92496174995354
C	5.68314880495038	15.10898082246690	2.35063133504566
C	4.97758718354630	13.88747706044438	2.49410531229780
C	5.53614522152034	12.92767882809994	3.40610579777293
C	1.53287287245478	8.69507779071516	3.86242455684423
C	6.04408334974201	10.11026991790620	2.57401892896703
C	2.49232797006644	9.84685970540188	4.00760313005497
C	3.79141131523998	9.64365563991871	3.51005011352487
C	4.81269037375502	10.58000244631136	3.30481918471192
H	6.69463546111577	11.30472871706842	5.08923981846089
H	1.06983085404117	8.23550495297120	8.24599510743105
H	-0.57533839551828	8.84560860098325	8.10168960337264
H	0.20207125919205	8.10164374570978	6.71152137570250
H	0.09753099077631	11.19294316899012	8.85679472232408
H	1.73770275573958	10.58517204892920	9.12690755379520
H	1.48814943297712	11.99266832807471	8.10676990081002
H	1.94708280391498	9.95462650651485	6.78235086745948
H	1.47764399484924	10.64878817782080	1.84391240305323
H	-0.17931543281832	10.89576345625057	1.28763589945463
H	1.13094874115198	11.89110176393291	0.65005355849455
H	-1.21238151788342	13.31858062564885	1.60666903316298
H	-0.49105270854066	14.37251673366904	2.83001967183210
H	0.32151489977906	14.11383520314597	1.28955360763971
H	1.47868953764979	12.85808162362561	2.94308606940399
H	-1.68588574140846	10.66944832212980	7.23490882152312
H	-3.08884904781617	11.78036943215976	5.55298408726083
H	-2.08184667799569	12.60651837356698	3.46584153378188
H	6.51396975381149	13.17860188774089	6.69714082048936
H	7.82981649452554	12.08339021346093	7.11199285314439
H	8.18649413287340	13.64000456226863	6.35671477241638
H	9.49495471353924	12.39289370425044	4.50702483362814
H	9.10503182868502	10.85724597470118	5.27157465652867
H	8.70549584455997	11.12844437330642	3.57060693245013
H	2.40695922367387	14.17118113791511	0.15019797496142
H	2.62952424962611	15.13757494315207	1.61508997547557
H	3.76343010124991	15.27871455204618	0.25945622306214
H	5.28175791716029	11.85313793533898	0.66926379994329
H	4.05982729071552	12.39598762879458	-0.47488595764587

H	5.48110719133095	13.39823417289278	-0.15655901333070
H	3.31219388174340	12.72861593231117	1.88302163741786
H	8.47237968280164	14.45021139858002	4.13236327744004
H	7.45005036054195	16.23020212670892	2.77648128321023
H	5.26810766219479	15.87562054994984	1.71349448202696
H	1.95490782308358	7.91461268471191	3.23510483480311
H	1.30996480745666	8.26999333375539	4.84136897942101
H	0.58787538339412	9.02559110729150	3.43715186972970
H	6.60747749010163	10.93541277087430	2.14732897098716
H	6.69907029729197	9.59592319893981	3.28088459476463
H	5.78221601889131	9.40545516539678	1.78738246132537
H	3.99694442679133	8.64844421514987	3.14888430833618

Table S60. Compound ^{Me}NHC^{Me} B3LYP-D3/def2-SVP

Electronic energy ... -382.94265741 Eh
Final Gibbs free energy ... -382.79542463 Eh
Gibbs free energy minus the electronic energy ... 0.14723277 Eh

N	0.57223453118657	3.59779055620048	1.90050207550155
C	-0.18494579917287	4.45609078875789	2.64478780228978
C	0.30272101316808	2.25014622195092	2.16538127538177
C	1.55198850074442	4.05312784213338	0.93707200313284
C	1.00183222703566	1.12678282568907	1.47833051592569
H	1.54110850776965	5.14979810009502	0.94858306956265
H	1.31039979133658	3.70024480445867	-0.07945811583086
H	2.56414729802835	3.69928708850112	1.19504810107981
H	2.09187859940916	1.15221503581456	1.65116852132659
H	0.84708412651559	1.15144949530034	0.38554898909994
H	0.63100297546561	0.15845331693216	1.84367776277455
N	-0.94212019467408	3.59779060036397	3.38907961170409
C	-0.67260675362012	2.25014625740094	3.12420027295921
C	-1.37171645083669	1.12678271161413	3.81125230274386
H	-2.46176282811859	1.15221285361858	3.63841401728637
H	-1.21696848050980	1.15145081825820	4.90403382354037
H	-1.00088561540582	0.15845335562673	3.44590623941525
C	-1.92187030188164	4.05312777188320	4.35251370234064
H	-1.91099269429826	5.14979801327143	4.34100035773012
H	-1.68027590729834	3.70024725558248	5.36904340374874
H	-2.93402954484349	3.69928428654672	4.09454326828698

Table S61. Compound ^{Me}NHC^{Me} B3LYP-D3/def2-TZVPP

final energy -383.368625005640 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -382.747873077453 Eh

N	0.56951659852544	3.59379745999281	1.90316148540687
C	-0.18493817107835	4.44930254312544	2.64479560590030
C	0.29925484177410	2.24982500998296	2.16878138569179
C	1.54859565630564	4.05197211703634	0.94059039771255
C	0.99564291251350	1.12839816639316	1.48414070883241
H	1.53459235496309	5.13737562688188	0.95494881229385
H	1.30641864647803	3.70193067316443	-0.06449702344991
H	2.54929809548229	3.70123491814590	1.19934454323226
H	2.07451334862264	1.15354355736630	1.65717908499776
H	0.84025805833241	1.15303587125639	0.40257270189565
H	0.62560328711253	0.17157651560816	1.84855323109300
N	-0.93939832167309	3.59379731151624	3.38642401238542
C	-0.66913639251087	2.24982490889764	3.12080409400933
C	-1.36552598849978	1.12839808732296	3.80544328205692
H	-2.44439611374596	1.15354385226746	3.63240295726244
H	-1.21014321210447	1.15303573596373	4.88701162877568
H	-0.99548602702687	0.17157628704719	3.44103150239893
C	-1.91848055643919	4.05197174114806	4.34899196093883
H	-1.90447626339884	5.13737526677669	4.33463499877533
H	-1.67630743370278	3.70192873994969	5.35407966157000
H	-2.91918231992950	3.70123561015655	4.09023396822058

Table S62. Compound ^{Et}NHC^{Me}, B3LYP-D3/def2-SVP

Electronic energy ... -461.47080670 Eh
Final Gibbs free energy ... -461.26953835 Eh
Gibbs free energy minus the electronic energy ... 0.20126835 Eh

N	6.64501085153938	3.65053483746356	5.82970780666681
C	7.39892992758273	2.79539836175444	6.57823789962796
C	6.91048003698648	4.99911694032262	6.09933959194779
C	5.60637551425422	3.17482699072002	4.92747428423723
H	5.92668538394009	2.18282717681899	4.58004127596391
H	5.56424362202805	3.83775576254533	4.04801167277637
C	4.23838103217785	3.08090092874027	5.59917871079951
H	3.48467502653728	2.69500143887873	4.89391994904694
H	4.29197123875737	2.40026097418769	6.46267043667693
H	3.89563657256667	4.06388612241683	5.96040614825755
C	6.22584840322617	6.13103718097300	5.41053264780280

H	6.59988753983055	7.09358134743238	5.78744551660687
H	6.39831690254929	6.11350412595613	4.32030378016831
H	5.13372084651742	6.11520061156920	5.56621176318068
N	8.15285297942064	3.65053508834558	7.32676381762173
C	7.88738409278028	4.99911715164802	7.05713112041138
C	9.19148973296275	3.17482759881666	8.22899609554000
H	8.87118015359117	2.18282797705841	8.57642980142821
H	9.23362271202017	3.83775669034534	9.10845839269982
C	10.55948342241923	3.08090113266957	7.55728997181173
H	11.31319035992051	2.69500166159437	8.26254775286779
H	10.50589219318512	2.40026108702077	6.69379836419495
H	10.90222760974294	4.06388618643966	7.19606203282797
C	8.57201756047973	6.13103738413465	7.74593640128579
H	8.19797890203079	7.09358172220889	7.36902351323290
H	8.39955051108434	6.11350507929612	8.83616550745547
H	9.66414487186873	6.11519944064270	7.59025574486254

Table S63. Compound $^{Et}NHC^{Me}$, B3LYP-D3/def2-TZVPP
final energy -461.983025345654 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -461.233423231291

N	6.64316240743095	3.64578796044677	5.83655396045353
C	7.39893525213440	2.79334510398082	6.57823029094265
C	6.91167259821959	4.99057250270474	6.10494641467254
C	5.60802265216838	3.17014989602906	4.93210850195771
H	5.91879263575285	2.18042302873703	4.60516890530673
H	5.57946558392982	3.81860840999988	4.05497402312402
C	4.23671008387465	3.10023720616814	5.59509986142114
H	3.49115560336142	2.72811835510532	4.89070388132354
H	4.27302951146769	2.42726598649967	6.45132939291460
H	3.91219131197775	4.08063664708523	5.94574624763358
C	6.22753242975107	6.12005061057466	5.41976454236839
H	6.61425178380679	7.07138889411645	5.78082740111904
H	6.38350073595457	6.09122991012367	4.33855344128314
H	5.14904022915564	6.11499659468576	5.59268862149974
N	8.15470538083657	3.64578781794841	7.31990935967541
C	7.88619515626844	4.99057249005804	7.05151752158021
C	9.18984057479483	3.17015006002067	8.22435988816878
H	8.87906855768517	2.18042372371757	8.55129918776813
H	9.21839367120377	3.81860970502480	9.10149364397119
C	10.56115591269407	3.10023620358783	7.56137470077604
H	11.30670726022945	2.72811824202618	8.26577437600689
H	10.52484008749340	2.42726384910055	6.70514582825651
H	10.88567588659895	4.08063532570865	7.21072851032269
C	8.57033251116495	6.12004992498698	7.73670339723075
H	8.18361269563590	7.07138877691029	7.37564273658985
H	8.41436234364214	6.09122603851600	8.81791416085362
H	9.64882514276682	6.11499773613681	7.56378120277954

Table S64. Compound $^{iPr}NHC^{Me}$, B3LYP-D3/def2-SVP
Electronic energy ... -539.99801615 Eh
Final Gibbs free energy ... -539.74431057 Eh
Gibbs free energy minus the electronic energy ... 0.25370558 Eh

C	2.31836340438009	2.31814260376439	4.33553915038306
N	1.57811141268538	1.55531341972516	3.48551022633969
C	1.83767664628710	1.83134541175325	2.13667775501221
C	0.53564321327164	0.63250906032334	3.95598898133759
H	0.32758916052596	-0.05450283928645	3.12053435796387
C	1.15785233813320	1.14582897737686	0.99935066146652
H	1.52311046737154	1.54164094883688	0.04107822466542
H	1.34507799336023	0.05796260128875	0.99967784253600
H	0.06375827144728	1.28843887953323	1.02057160765401
C	1.03003037631555	-0.19266710226695	5.14214663545968
H	0.25048554933151	-0.90441940148528	5.45717142864698
H	1.28251657375628	0.46686320762032	5.98393823219690
H	1.93556755791181	-0.75855304534594	4.87456847254218
C	-0.74508991935182	1.40629326050094	4.28026957057071
H	-0.55204683571888	2.11397907898747	5.10141087085198
H	-1.55178103088172	0.72034216958900	4.58468423618820
H	-1.09129771188905	1.98213031761878	3.40719493000083
N	3.05847710783486	3.08110413656544	3.48550695217781
C	2.79883362175677	2.80514302616187	2.13667585212944
C	4.10090981913058	4.00394820779089	3.95598897094845
H	4.30899968454962	4.69091483853327	3.12050725334385
C	3.47857967401090	3.49073026927945	0.99934457537668
H	3.11326036193370	3.09497302363667	0.04107283190829
H	3.29135296849657	4.57859633095484	0.99974722153390
H	4.57267511814087	3.34811863172130	1.02048758196900
C	3.60644559032623	4.82918090049373	5.14207704219745
H	4.38597665202783	5.54092839481632	5.45714708073232

H	3.35387661406332	4.16968020716716	5.98386785230976
H	2.70094402217317	5.39507985075990	4.87440421422412
C	5.38162966825232	3.23018913730880	4.28037503964320
H	5.18854105552192	2.52254117489235	5.10153736656919
H	6.18829988558767	3.91616005032900	4.58479892916408
H	5.72788068925750	2.65431427105519	3.40734205195656

Table S65. Compound $^{i\text{Pr}}$NHC$^{\text{Me}}$ B3LYP-D3/def2-TZVPP
final energy -540.596261120698 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -539.718779760011 Eh

C	2.31829411946667	2.31820283420745	4.33728249069193
N	1.58212420658139	1.55677102077028	3.48868788787373
C	1.84192829457826	1.83417039476559	2.14347211393762
C	0.54093896409459	0.63192116682525	3.95214958167011
H	0.34842488482917	-0.05374552186720	3.12596595639730
C	1.16445131236790	1.14844819145263	1.00985321679140
H	1.52513091950703	1.54353794781098	0.06177472866664
H	1.35479444424920	0.07225715260475	1.01063868880816
H	0.08096748615760	1.28779988186297	1.03352005215603
C	1.02281971641262	-0.17951911913134	5.14838478649129
H	0.25029893878982	-0.88995879159003	5.44624799890472
H	1.24675690286766	0.47886258770399	5.98493625877312
H	1.92975751980279	-0.73201230771330	4.90288112868053
C	-0.74397182806234	1.39927705096590	4.26053466048944
H	-0.56722069671876	2.09599078321941	5.08014172325080
H	-1.54248779051862	0.71352730218918	4.54771547288773
H	-1.07672851195071	1.97068587343510	3.39302296749749
N	3.05440480295458	3.07969487105561	3.48868930771004
C	2.79458889680384	2.80230854799697	2.14347282291732
C	4.09556350540877	4.00457448997739	3.95215270384100
H	4.28806706851829	4.69023967941447	3.12596555767842
C	3.47204484061607	3.48805363556883	1.00985471155994
H	3.11135421005288	3.09297633469673	0.06177518740436
H	3.28169464631309	4.56424354918958	1.01066026988540
H	4.55552990264533	3.34870826809906	1.03350402467432
C	3.61365337517699	4.81601020187865	5.14837996536831
H	4.38615801549119	5.52646259992781	5.44625486972136
H	3.38971503073674	4.15762449292883	5.98492814121656
H	2.70671090786830	5.36848935578377	4.90286236601888
C	5.38048880215256	3.23724914459648	4.26055001855175
H	5.20374826738674	2.54053831534869	5.08016170861623
H	6.17898764448778	3.92301937154076	4.54772877970384
H	5.71326120093249	2.66584069448467	3.39304385116414

Table S66. Compound $^{\text{Dipp}}$NHC$^{\text{H}}$ B3LYP-D3/def2-SVP
Electronic energy ... -1158.57343538 Eh
Final Gibbs free energy ... -1158.05966415 Eh
Gibbs free energy minus the electronic energy ... 0.51377124 Eh

N	7.49273255791351	7.20254854088945	4.41746308201547
N	7.55210494971384	7.95555984423175	6.40525434937929
C	7.25501392612534	8.34827918663609	5.12793294925222
C	7.91693001291147	6.14095004612330	5.21807932103077
C	7.95900601750364	6.62303496225830	6.48663114948374
C	7.34325808139065	7.09401860144799	2.99474322929450
C	6.05737080586395	6.90115831473447	2.45613995002525
C	5.94529172231499	6.78580569126059	1.06289980460628
C	7.07146383101529	6.85074308035802	0.24506889372750
C	8.33605571119549	7.04274831211459	0.80337219532209
C	8.49816805573799	7.17188832903681	2.18847750884576
C	4.81805240507484	6.88484272160345	3.33836867234427
C	4.13431832874341	8.26172482385895	3.29832086465365
C	3.84178698221006	5.75726989940104	2.97943442562249
C	9.85801772638117	7.47678692283111	2.80337620169313
C	11.03176066491198	6.83984779859495	2.05190131362512
C	10.03531783606103	9.00002643090413	2.93390650134123
C	7.44444399646112	8.80745625892951	7.55474911426529
C	6.30463805585640	8.68761482688372	8.37755537145385
C	6.22807847716040	9.50992730880557	9.50858985280298
C	7.24494861920438	10.41928357135458	9.80324038690557
C	8.35586594650334	10.52526991467584	8.96904290002975
C	8.48144032537722	9.71883445202552	7.82849009368384
C	5.16043516182965	7.75868514430614	7.99306667330499
C	4.40602287649367	7.17857681742437	9.19400648854878
C	4.20516615169514	8.48573290758315	7.03014192015582
C	9.66642532173374	9.88320813038538	6.88880712468627
C	11.00927810412110	9.97333298394481	7.62506246674942
C	9.43791902627482	11.10000055590379	5.97607760770242
H	8.14578722698330	5.15915671241885	4.81283805257046
H	8.23487213752568	6.15343909797497	7.42680765074471

H	4.96060101792052	6.64369117412689	0.61297621111017
H	6.96427248687495	6.75493666875030	-0.83862114357818
H	9.20764841746713	7.10155047618163	0.14960069590238
H	5.14905883942575	6.71626729700836	4.37356457202954
H	4.83619435346644	9.04542685940744	3.61936732164069
H	3.25707124985184	8.28279187545073	3.96493171600312
H	3.79303181128161	8.49804441806096	2.27666157967127
H	3.39275334617706	5.90072134770274	1.98318212250657
H	3.01391017099330	5.72614590799751	3.70612493980402
H	4.33967274472800	4.77449770477511	2.98590039982442
H	9.86224709711564	7.06170384576168	3.82271559894887
H	11.17816983826259	7.28910652361116	1.05627188624247
H	10.88804876033761	5.75611285533967	1.91585129763168
H	11.96686593046873	6.99293825699323	2.61378458363969
H	10.04436485607734	9.47387279967248	1.93830398872611
H	10.98604268213875	9.24156396314579	3.43753459247510
H	9.21255396860569	9.44184351236348	3.51385834921198
H	5.35938552464568	9.44625261947410	10.16581576912432
H	7.16663089922583	11.05365150482140	10.69007287203347
H	9.13951752720620	11.24798241515287	9.20529124451578
H	5.59205162939654	6.91042272537820	7.44016243462780
H	3.67752844068308	6.42525595931830	8.85413228370463
H	3.83910443793841	7.95160117813750	9.73778364552642
H	5.08968166042675	6.69449592648347	9.90948548151776
H	4.74619786716791	8.86162095590307	6.15019767613875
H	3.72974748664889	9.34475122872933	7.53200477360327
H	3.40733818248210	7.80731950595908	6.68478122252646
H	9.70419574164788	8.99408323868119	6.24260247924533
H	11.16051087561300	9.11352317908130	8.29711135046531
H	11.08849731019536	10.89187534717352	8.22901652978804
H	11.83859292640892	9.99058888962522	6.89962921761855
H	10.26767125323154	11.21265662398944	5.25971913157285
H	9.37108316222230	12.02632070885605	6.57086926855635
H	8.50172846147612	10.98171731768348	5.41095779177681

Table S67. Compound $^{Dipp}NHC^{H}$ B3LYP-D3/def2-TZVPP
final energy -1159.834562338710 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -1157.905389737104 Eh

N	7.53464853164830	7.21992716511310	4.40259931799159
N	7.55391235036702	7.99965833173644	6.39259127373749
C	7.25063993450513	8.36759399584209	5.12372470240421
C	7.98836148384041	6.17617915493603	5.22787341934634
C	8.01089274437911	6.65149004003304	6.48539843603631
C	7.36358065759233	7.10518209755675	2.98971733471118
C	6.05912657650679	6.96958835537815	2.46693578692186
C	5.91140769836095	6.88659043477760	1.08456253027283
C	7.01328787788021	6.91923804154120	0.23588695001404
C	8.30019503212762	7.02960856332323	0.77642653761644
C	8.49986052167501	7.12458389343436	2.14813220052338
C	4.83799914253895	6.93294932798263	3.37794797250050
C	4.09600813955895	8.29502370767386	3.33488266188389
C	3.88479464042978	5.76353466443327	3.02582434389254
C	9.90689548685450	7.26595785123779	2.74786824766678
C	11.02353462327713	6.80557691002785	1.80005040823790
C	10.16162019658956	8.71934673938284	3.21795000258724
C	7.43027389480095	8.83993984472576	7.54985158952782
C	6.30157599516316	8.69202406075726	8.37920918348123
C	6.22517926943412	9.46920892583173	9.53090692487797
C	7.23616401720543	10.38294889194434	9.84725015741714
C	8.32792901999332	10.53221960355864	8.99791581893282
C	8.45731348878760	9.76507862116391	7.84125680978234
C	5.15384361760355	7.76146594707362	7.96098812824100
C	4.37439011913786	7.18099537393153	9.14328541628072
C	4.22136097015540	8.50701860900180	6.98771717154494
C	9.64087668502916	9.95367098097313	6.90000083499279
C	10.96246719329042	10.19981432175913	7.65459378679195
C	9.35535073092088	11.08921736247096	5.90099398564080
H	8.24051731321420	5.20804451349839	4.82736690970958
H	8.29072737975737	6.20708931141167	7.42268246893379
H	4.92063475235261	6.78814916349204	0.65543362992502
H	6.88063819049604	6.84935363988139	-0.83505766481221
H	9.14681782432873	7.04039263818930	0.10340157657661
H	5.18126476969850	6.77936309476062	4.39882774991547
H	4.76563414968501	9.09281489918186	3.65446926079782
H	3.23177647899478	8.27527720611203	4.00048692004995
H	3.75009737764523	8.51063141648670	2.32270609799264
H	3.40967007525650	5.90946534565804	2.05550983483688
H	3.09603860185359	5.68904807544373	3.77653175281497
H	4.42463562749353	4.81496371491674	2.99993525391582

H	9.94539383912048	6.62749962211042	3.63131735336930
H	11.13799135355907	7.48591372320357	0.95530145118659
H	10.83686772461870	5.80465100668189	1.40819877811053
H	11.97423138379207	6.78662052570628	2.33542770051180
H	10.20986943385641	9.39068020182033	2.35863727056319
H	11.11039562794669	8.77837778298355	3.75461961781185
H	9.36754031394729	9.06479498396633	3.87306765533928
H	5.37531631774757	9.37697347526971	10.19236424791072
H	7.15931728747526	10.98238544298951	10.74371695161492
H	9.09509050744191	11.25323517540121	9.25189668502896
H	5.59653703181203	6.92796366201232	7.41618207634894
H	3.63944461908862	6.45927923955036	8.78165031841613
H	3.82637994040382	7.95148330772088	9.68769211177542
H	5.03129918741400	6.67123841428648	9.84897123745665
H	4.78394738312980	8.93652757816217	6.16197944040023
H	3.69963234533574	9.31440885226831	7.50679065848357
H	3.47183605228208	7.82635217904703	6.57903242482416
H	9.75747193117226	9.03238453432609	6.33083145412275
H	11.15576297116878	9.41114325021863	8.38204960191718
H	10.95346234346075	11.15367834003264	8.18297290569215
H	11.79280945285146	10.22792911802331	6.94735300976352
H	10.19359877558869	11.21029023911122	5.21341385717391
H	9.20969356443385	12.03299937528153	6.43141988853235
H	8.45810943202069	10.87605213288916	5.32196557913199

Table S68. Compound $LGaCl_2$ B3LYP-D3/def2-SVP

Electronic energy ... -4082.49899693 Eh

Final Gibbs free energy ... -4081.92418224 Eh

Gibbs free energy minus the electronic energy ... 0.57481469 Eh

Ga	0.48129921539273	11.56005648722200	13.42196076226286
Cl	-1.09504998833544	10.40354949163211	14.38435660218510
Cl	1.53552237667454	12.93048798753822	14.78283150287011
N	1.81427613246541	10.46428164414879	12.51938026034667
N	-0.15909196809789	12.54441542379532	11.87687314886919
C	2.35533495935932	10.91077586778801	11.38211752200067
C	1.87305644426987	12.02664229841793	10.66520498269287
H	2.45493029390419	12.30387618330554	9.78783581158392
C	0.66648954096438	12.72778198022506	10.83814824710186
C	3.55978980447662	10.20268767849135	10.81283338688331
H	3.49715929662457	9.11615882119896	10.95429573074203
H	4.46437015802042	10.54346573916099	11.34087421569497
H	3.68062939060247	10.42773872281351	9.74586115027599
C	0.27740298284582	13.72823618894459	9.77862346703868
H	0.20507818885864	14.73246104354548	10.22310771435003
H	-0.71545037513009	13.50092920330716	9.36628642032034
H	1.00955894879575	13.74881257446635	8.96232246200811
C	2.25159159210908	9.23005416759557	13.11922284731763
C	1.50270853102655	8.05844175166078	12.85081635366168
C	1.93889696787789	6.85223925903366	13.41202828609086
H	1.38379054875054	5.93501334984654	13.21113622070750
C	3.06630889172588	6.80317655803066	14.23109521935875
H	3.38998991342705	5.85156834009525	14.66018503675979
C	3.76674512323198	7.97152593800165	14.51403511413619
H	4.63583537503342	7.93139688102690	15.17451407561165
C	3.37605720226126	9.20593035447768	13.97379996343102
C	4.15998387647723	10.45584529862387	14.35207163814368
H	3.72555053383649	11.30941120664447	13.81374788454341
C	5.64403479582692	10.35120262804037	13.96353455449954
H	5.77753046751195	10.11526240486185	12.89656113991623
H	6.15701745561350	9.56394861174793	14.53936652105163
H	6.16237258952339	11.30149049410334	14.16969919324080
C	4.01943337921079	10.75249569852558	15.85431915909966
H	2.96368491461355	10.84015016530669	16.14423687772454
H	4.51399728448299	11.70465686893702	16.10445975841073
H	4.48359020272796	9.95768680724621	16.46116912539009
C	0.26796240795684	8.09172378077848	11.95805979493628
H	-0.15820599604437	9.10061924850538	12.03382460265761
C	-0.82181106849977	7.11833479130652	12.42004961960327
H	-1.07768586039953	7.29003191926340	13.47602341409964
H	-0.51894146662644	6.06598569517937	12.29895433940519
H	-1.73380388445478	7.26248768295125	11.82286142978061
C	0.62613389876235	7.86196263155169	10.48083669479212
H	1.32790418751738	8.62212884513335	10.10769648591172
H	-0.27880185787077	7.90931877615529	9.85287898908740
H	1.09026862996752	6.87237247037883	10.33592958111590
C	-1.50110428343641	13.06383740262425	11.84024842378042
C	-1.79624923007344	14.32504719855477	12.40208230271854
C	-3.11838603233188	14.78714243966299	12.33371679614865
H	-3.36471674995112	15.76019844407191	12.76470707598121

C	-4.11957208197544	14.02992945989403	11.73107302834019
H	-5.14316378942723	14.41015297196852	11.68504560340741
C	-3.81340230458297	12.77961987077382	11.19653734358468
H	-4.60417383678236	12.18404888364866	10.73493305254911
C	-2.51021769240989	12.26904451644026	11.24645547511706
C	-2.21981604798148	10.89421853700700	10.65750491963111
H	-1.18982567179802	10.62497691130052	10.92765007542752
C	-3.14155867786057	9.81772940817151	11.24684794673841
H	-3.03329272338613	9.76702966389506	12.33940978302590
H	-2.88926600717357	8.83130254047353	10.82769689310303
H	-4.19942666694733	10.01276005435958	11.00917234220031
C	-2.29896120384459	10.90252624463096	9.12194389424423
H	-2.04802465438867	9.90798330131926	8.71806277903245
H	-1.60055504655232	11.62870690622195	8.67926446949530
H	-3.31379253136297	11.16005132613547	8.77669191204825
C	-0.74279796762328	15.18009524149953	13.09060570711537
H	0.22537054583231	14.67070920807583	12.99348757008462
C	-0.60806511998058	16.56774016274530	12.44400150897652
H	-0.39373375672180	16.49818525626747	11.36558145911852
H	0.21129544385001	17.13258147563641	12.91693677896739
H	-1.52959992006883	17.16084490757559	12.55980671445099
C	-1.04044643135722	15.30188902522978	14.59374334345912
H	-1.12827770101551	14.31132289453782	15.06206511041907
H	-1.98037171531366	15.85098368883433	14.76912137542509
H	-0.22727818260339	15.84088109743154	15.10493000769626

Table S69. Compound $LGaCl_2$ B3LYP-D3/def2-TZVPP
final energy -4084.411893960167 Eh
DLPNO-CCSD(T1)/cc-pVTZ single point energy -4080.149646978432 Eh

Ga	0.48000707278769	11.57882056459750	13.44281531024942
Cl	-1.11520853435243	10.49188308228679	14.44033979899532
Cl	1.54972109859018	12.94484866042959	14.78505694139652
N	1.79967425766308	10.46535677100492	12.53987638016852
N	-0.16184841665898	12.55089871568049	11.89096420417110
C	2.33675833536905	10.91273706842754	11.40807284001863
C	1.86472565538850	12.02844669541080	10.69890465608655
H	2.44557880073717	12.30047823185810	9.83245281652088
C	0.66639279266323	12.73052425042301	10.86295635411080
C	3.52835814185087	10.20170535414075	10.82316980208995
H	3.47621914528857	9.12840280861167	10.98323658472096
H	4.43572531205465	10.55732130410289	11.31280902032356
H	3.61389175441786	10.40648673562884	9.75959099696389
C	0.30260165651422	13.73843922139760	9.80619960275251
H	0.38799278317948	14.74365677342301	10.22192812743083
H	-0.72847074511006	13.62078789802814	9.48171215100887
H	0.96188244120575	13.65802684667997	8.94698912396320
C	2.24440763426393	9.22835020298335	13.12886193334375
C	1.49882337660635	8.06372102785062	12.86507441443988
C	1.94791657954357	6.86060361675204	13.40267735257077
H	1.39865762032824	5.95164109435747	13.20651965100643
C	3.08531791311684	6.80822744508754	14.19417054558117
H	3.41805031194531	5.86317935424697	14.60251865452577
C	3.78217416866426	7.96994949523517	14.47400015383881
H	4.65528915544780	7.92679512122335	15.11061265134433
C	3.37896317147786	9.20092275965397	13.95568777768761
C	4.16607704118592	10.44446137270375	14.32964838243678
H	3.73542325038237	11.29531345615042	13.80575696468120
C	5.64496158696169	10.33815977411436	13.93140157505828
H	5.76933075204312	10.10127957778643	12.87490560084714
H	6.15401332765043	9.56061297259451	14.50281510161290
H	6.15601757912023	11.28141284151811	14.12996683876037
C	4.04491150797119	10.72765450406128	15.83363677413315
H	3.00335083302899	10.80776966644023	16.13660627196277
H	4.53815670222147	11.66838680540383	16.08176751507334
H	4.51380821691257	9.93364340666738	16.41763743527525
C	0.25254189987486	8.09775145890037	11.99672878658721
H	-0.18376447806212	9.08943258484575	12.09374169941456
C	-0.81483419645960	7.10025464371038	12.45197312554060
H	-1.05075822951434	7.23533811188369	13.50688443253994
H	-0.50252200074350	6.06679032132830	12.29610865706692
H	-1.72922164244548	7.24989672984930	11.87984089656019
C	0.59167052602306	7.89073972442216	10.51394343947352
H	1.26819014281739	8.65945389097538	10.14313341911405
H	-0.31574009193336	7.92744398044136	9.90869284987908
H	1.06487110883777	6.91958553189735	10.35684593360387
C	-1.50615526889050	13.06196122877653	11.84449934813191
C	-1.81038902021348	14.31224689321077	12.40277263147488
C	-3.12906619849085	14.76037277356027	12.33264318436179
H	-3.38296178253984	15.72106640073181	12.75951812929649

C	-4.11630089113037	13.99951755811054	11.72990994187129
H	-5.13284846487710	14.36684094882723	11.68238429728603
C	-3.79955855015111	12.75976497191624	11.19677301432292
H	-4.57651136837663	12.16524544391870	10.73607610640983
C	-2.49964431502086	12.26324224418721	11.24961946128869
C	-2.19552492355793	10.89830225085660	10.65642855792416
H	-1.18085552489215	10.62795031988515	10.94034887454728
C	-3.12780826210567	9.81579691999374	11.20943043069774
H	-3.05559090870709	9.75828580529105	12.29416784678665
H	-2.85937920933854	8.84400475328746	10.79405827092215
H	-4.16792081624880	10.00734752043440	10.94358597495000
C	-2.24456313849459	10.92412676922363	9.12213854272742
H	-1.99356885612678	9.94167183419668	8.71839234999983
H	-1.53989479485650	11.64496814563966	8.70822153118292
H	-3.24207122754205	11.18902465498360	8.76718654733210
C	-0.76836596775708	15.17738913833413	13.08538450931359
H	0.19590531958237	14.68133959429565	12.99904748673601
C	-0.64416777003748	16.55711372574882	12.42556812944978
H	-0.42971535149382	16.47692770675727	11.35915675772459
H	0.16175934325980	17.12563056751810	12.89194332388102
H	-1.56352689761728	17.13441911015825	12.53384114224041
C	-1.07551572092779	15.31851036751203	14.58205311370074
H	-1.15387559583459	14.34411384859942	15.06105639797013
H	-2.01415698709331	15.85322314710649	14.73853041837242
H	-0.27977816937583	15.87236190172067	15.08138113416438

For reproducibility, below typical input files for geometry optimizations, frequency calculations and single point energy evaluation are listed as used in conjunction with the ORCA program package:

Optimization + frequency calculation at the B3LYP-D3/def2-SVP level of theory:

```
!B3LYP D3BJ def2-svp def2/J tightopt freq
```

Optimization at the B3LYP-D3/def2-TZVPP level of theory:

```
!B3LYP D3BJ def2-tzvpp def2/J tightopt
```

Single point energies at the DLPNO-CCSD(T1)/cc-pVTZ level of theory:

```
!DLPNO-CCSD(T1) tightscf cc-pVTZ cc-pVTZ/C
%basis
 AuxJ "def2/J"
 newgto    Sb "cc-pVTZ-PP" end
 newauxcgto Sb "cc-pVTZ-PP/C" end
 newecp       Sb "SK-MCDHF-RSC" end
end
```

D) References

[1] F. Neese, The ORCA program system. Wiley Interdisciplinary Reviews: Computational Molecular Science **2012**, *2*, 73.

[2] F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

[3] a) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456-1465; b) S. Grimme, J. Antony, S. Ehrlich; H. Krieg, *J. Chem. Phys.* **2010**, *132*, 15410.

[4] NBO 6.0: E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, F. Weinhold (Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, 2013); http://nbo6.chem.wisc.edu/

Supporting Information

Switching from Heteronuclear Allyl Cations to Vinyl Cations by Using a Chemical Charge Trap

Julia Krüger,[a] Christoph Wölper,[a] Gebhard Haberhauer[b] and Stephan Schulz*[a]*

[a] Institute of Inorganic Chemistry and Center for Nanointegration Duisburg-Essen (CENIDE, University of Duisburg-Essen, Universitätsstraße 5-7, 45141 Essen (Germany).

[b] Institute of Organic Chemistry, University Duisburg-Essen, Universitätsstraße 5-7, 45141 Essen (Germany).

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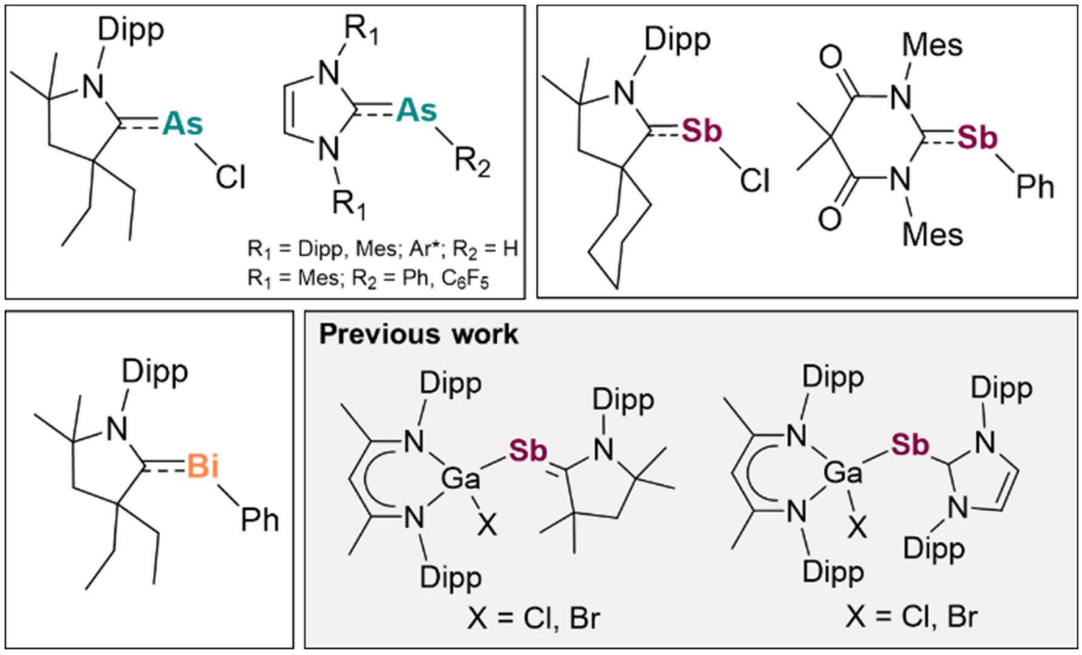
Additional Information to the article



Scheme S1 Structurally characterized carbene-coordinated arsinidenes (selected examples), stibinidenes and bismuthinidenes; Dipp = 2,6-i-$Pr_2C_6H_3$, Mes = 2,4,6-$Me_3C_6H_2$, Ar* = 2,6-Ph_2-4-Me-C_6H_2.[1-11]

General Synthetic methods

All manipulations were performed in an atmosphere of purified argon using standard Schlenk and glovebox techniques. Toluene and *n*-hexane were dried using an mBraun Solvent Purification System (SPS). Benzene was carefully dried over K, whereas dichloromethane (DCM) and fluorobenzene were dried over CaH_2. Deuterated solvents were dried over activated molecular sieves (4 Å) and degassed prior to use. The anhydrous nature of the solvents was verified by Karl Fischer titration. (^{Me}cAAC)ECl_3 (E = As,[12] Sb[7]) LGa,[13] Li[Al(OC(CF_3)$_3$)$_4$],[14] Na[B(C_6H_3(CF_3)$_2$)$_4$],[15] were prepared according to literature methods, whereas other chemicals were obtained from commercial sources and purified prior to use. Microanalyses were performed at the laboratory for microanalysis of the University of Duisburg-Essen. The melting points were measured using a Thermo Scientific 9300 apparatus. Cyclic voltammetry measurements were performed in a glovebox using a Metrohm Autolab PGSTAT 204 potentiostat with a three electrodes setup consisting of a Pt disc (*d* = 1 mm) working electrode, Pt wire counter electrode, and Ag wire pseudo-reference electrode using ferrocene as the internal standard.

Spectroscopic methods NMR Spectroscopy

^{1}H (300.1 MHz; 400 MHz) and ^{13}C{^{1}H} (75.5 MHz; 150 MHz) NMR spectra were recorded using a Bruker Avance DPX-300 spectrometer or Ascend™ 400 spectrometer. The spectra were referenced to internal C_6D_5H (^{1}H: δ = 7.16; ^{13}C: δ = 128.06), $CDHCl_2$ (^{1}H: δ = 5.32; ^{13}C: δ = 53.84) and C_4D_7HO (^{1}H: δ = 3.58, 1.72; ^{13}C: δ = 67.21, 25,31). IR spectra were recorded with an ALPHA-T FT-IR spectrometer equipped

with a single reflection ATR sampling module. The IR spectrometer was placed in a glovebox to guarantee measurements under inert gas conditions.

Synthesis (^{Me}cAAC)BiCl$_3$

^{Me}cAAC (200 mg; 0.7 mmol) and BiCl$_3$ (221 mg; 0.7 mmol) were weighed in a Schlenk flask, cooled to -78°C and 20 mL of Et$_2$O were added. The suspension was warmed to room temperature and stirred 30 minutes at ambient temperature, while a white precipitate was forming. The precipitate was separated from the solution and dried in vacuum to yield analytically pure (^{Me}cAAC)BiCl$_3$.

Yield 342 mg (0.57 mmol; 81 %). **^{1}H-NMR (THF-d$_8$, 400 MHz, 25 °C) δ [ppm]:** 7.31-7.47 (m, 3 H, C$_6$*H*$_3$), 3.06 (sept, 2 H, $^3J_{HH}$ = 6.5 Hz, C*H*(CH$_3$)$_2$), 2.20 (s, 2 H, C*H*$_2$), 1.91 (s, 6 H, C(C*H*$_3$)$_2$), 1.54 (s, 6 H, C(C*H*$_3$)$_2$), 1.43 (d, 6 H, $^3J_{HH}$ = 6.5 Hz, CH(C*H*$_3$)$_2$), 1.30 (d, 6 H, $^3J_{HH}$ = 6.5 Hz, CH(C*H*$_3$)$_2$). **^{13}C{^{1}H}-NMR (THF-d$_8$, 100 MHz, 25 °C) *δ* [ppm]:** 235.2 (C$_{q,Carbene}$), 147.1 (*C*$_6$H$_3$), 134.2 (*C*$_6$H$_3$), 131.0 (*C*$_6$H$_3$), 126.6 (*C*$_6$H$_3$), 88.2(*C*(CH$_3$)$_2$), 60.7 (*C*(CH$_3$)$_2$), 53.5 (*C*H$_2$), 30.9 (C(*C*H$_3$)$_2$), 30.1 (*C*H(CH$_3$)$_2$), 29.2 (C(*C*H$_3$)$_2$), 28.2 (*C*H$_3$), 26.1(*C*H$_3$).

Synthesis of (^{Me}cAAC)AsCl

(^{Me}cAAC)AsCl$_3$ (200 mg; 0.43 mmol) and two equivalents KC$_8$ (116 mg; 0.86 mmol) were weighed in a Schlenk flask, cooled to -78°C and 10 mL of toluene were added. The suspension was slowly warmed to room temperature and stirred for 2 days. The yellow solution was separated from the precipitate by filtration. The filtrate was concentrated and stored at -30 °C to yield light orange crystals of (^{Me}cAAC)AsCl after 24 h.

Yield 105 mg (0.27 mmol; 62 %). M.p.: 142 °C (dec.). Anal. Calcd. for C$_{20}$H$_{31}$NClAs: C, 60.69; H, 7.89; N, 3.54. Found: C, 62.2; H, 8.17; N, 3.86 %.**^{1}H-NMR (C$_6$D$_6$, 400 MHz, 25 °C) δ [ppm]:** 7.00-7.13 (m, 3 H, C$_6$*H*$_3$), 2.89 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH$_3$)$_2$), 1.80 (s, 6 H, C(C*H*$_3$)$_2$), 1.73 (s, 2 H, C*H*$_2$), 1.44 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, CH(C*H*$_3$)$_2$), 1.11 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, CH(C*H*$_3$)$_2$), 0.95 (s, 6 H, C(C*H*$_3$)$_2$). **^{13}C{^{1}H}-NMR (C$_6$D$_6$, 100 MHz, 25 °C) *δ* [ppm]:** 231.6 (C$_{q,Carbene}$), 148.0 (*C*$_6$H$_3$), 131.9 (*C*$_6$H$_3$), 130.3 (*C*$_6$H$_3$), 126.5 (*C*$_6$H$_3$), 70.3 (*C*(CH$_3$)$_2$), 56.4 (*C*H$_2$), 52.8 (*C*(CH$_3$)$_2$), 29.8 (C(*C*H$_3$)$_2$), 29.0 (C(*C*H$_3$)$_2$), 28.9 (*C*H(CH$_3$)$_2$), 27.8 (*C*H$_3$), 25.0 (*C*H$_3$). **IR *ν*[cm^{-1}]:**.3056, 2959, 2926, 2865, 1587, 1533, 1465, 1436, 1393, 1364, 1340, 1316, 1263, 1206, 1176, 1140, 1100, 1024, 944, 863, 797, 778, 760, 737, 702, 639, 608, 575, 531, 462.

Synthesis of (^{Me}cAAC)AsGa(Cl)L (1)

LGa (123 mg; 0.25 mmol) and (^{Me}cAAC)AsCl (100 mg; 0.25 mmol) were weighed in a Schlenk flask and 3 mL of benzene were added at ambient temperature. The solution was stirred for 1 h and the solvent was removed in vacuum. The residue was dissolved in 3 mL n-hexane and stored at room temperature to yield yellow crystals of **1** after 48 h.

1: Yield 152 mg (0.18 mmol; 72 %). M.p.: 262 °C (dec.). Anal. Calcd. for C$_{49}$H$_{72}$N$_3$ClGaAs: C, 66.63; H, 8.22; N, 4.76. Found: C, 66.5; H, 8.19; N, 4.32 %.**^{1}H-NMR (C$_6$D$_6$, 400 MHz, 25 °C) δ [ppm]:** 7.03-7.19 (m, 9 H, C$_6$*H*$_3$), 4.99 (s, 1 H, *γ*-C*H*), 4.00 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH$_3$)$_2$), 3.35 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH$_3$)$_2$), 2.67 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH$_3$)$_2$), 1.65 (s, 6 H, CC*H*$_3$), 1.62 (d, 6 H,

$^3J_{HH}$ = 6.6 Hz, CH(CH_3)$_2$), 1.54 (s, 2 H, CH_2), 1.36 (d, 6 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 1.32 (s, 6 H, C(CH_3)$_2$), 1.27 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$), 1.15 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$), 1.13 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$), 1.05 (d, 6 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 0.83 (s, 6 H, C(CH_3)$_2$). **^{13}C{^{1}H}-NMR (C_6D_6, 100 MHz, 25 °C) δ [ppm]:** 231.8 ($C_{q,Carbene}$), 168.2 (N*C*CH$_3$), 148.1 (*C*$_6$H$_3$), 145.6 (*C*$_6$H$_3$), 143.4 (*C*$_6$H$_3$), 142.9 (*C*$_6$H$_3$), 134.8 (*C*$_6$H$_3$), 128.8 (*C*$_6$H$_3$), 126.9 (*C*$_6$H$_3$), 125.1 (*C*$_6$H$_3$), 125.0 (*C*$_6$H$_3$), 123.7 (*C*$_6$H$_3$), 97.4 (*γ*-*C*H), 70.6 (*C*(CH$_3$)$_2$), 53.5 (*C*H$_2$), 51.4 (*C*(CH$_3$)$_2$), 33.0 (C(*C*H$_3$)$_2$), 29.8 (*C*H(CH$_3$)$_2$), 29.0 (C(*C*H$_3$)$_2$), 28.9 (*C*H(CH$_3$)$_2$), 28.8 (*C*H$_3$), 28.0 (*C*H(CH$_3$)$_2$), 26.9 (*C*H$_3$), 24.9 (*C*H$_3$), 24.9 (*C*H$_3$), 24.5 (*C*H$_3$), 24.4 (*C*H$_3$), 24.4 (C*C*H$_3$). **IR ν [cm^{-1}]:**.3056, 2960, 2926, 2865, 1696, 1531, 1465, 1436, 1392, 1364, 1340, 1316, 1260, 1206, 1176, 1139, 1096, 1018, 944, 863, 796, 758, 701, 639, 608, 575, 530, 462, 399.

Improved synthesis of (^{Me}cAAC)SbGa(Cl)L (2)

*Since the reduction of (^{Me}cAAC)SbCl$_3$ with two equivalents KC$_8$ gives stibinidene (^{Me}cAACSb)Cl in only low isolated yields (<30% as was also described by Bertrand and co-workers), the stibinidene (^{Me}cAAC)SbCl is prepared in situ according to literature[7] and reacted directly with LGa to increase the yield of **2**, whose full characterization was previously reported.[10]*

(^{Me}cAAC)SbCl$_3$ (200 mg; 0.39 mmol) and two equivalents KC$_8$ (105 mg; 0.78 mmol) were weighed in a Schlenk flask, cooled to -78°C and 10 mL of toluene were added. The suspension was slowly warmed to room temperature and stirred for 2 h. The red solution was separated from the precipitate by filtration and added to LGa (171 mg, 0.35 mmol) in 2 mL toluene, cooled to -78 C. The solution was warmed to room temperature over a period of 1 h and stirred for an additional 30 min. The solvent was removed in vacuum and 6 mL n-hexane were added to the residue. An orange precipitate formed immediately, which was separated from the mother liquor by filtration. The fine orange powder was dried in vacuum to yield analytically pure **2** (151 mg, 0.16 mmol; 47%).

Synthesis of (^{Me}cAAC)BiGa(Cl)L (3)

The reaction and purification were carried out in the absence of light due to the light sensitivity of the formed product.

(^{Me}cAAC)BiCl$_3$ (40 mg; 0.067 mmol) and two equivalents LGa (65 mg; 0.133 mmol) were weighed in a Schlenk flask, cooled to -100°C and 3 mL of toluene were added. The reaction mixture was warmed to -30 °C over a period of 3 h. The pink solution was separated from metallic bismuth particle, which were formed during the reaction, and concentrated. The toluene solution was overlayed with 5 mL of n-hexane and stored at -30 °C overnight to give colorless crystals of LGaCl$_2$. The mother liquor was stored again at -30 °C to yield pink crystals of **3** after 24 h.

3: Yield 16 mg (0.016 mmol; 24%). M.p.: 74 °C (dec). Anal. Calcd. for $C_{49}H_{72}N_3ClGaBi$: C, 57.85; H, 7.13; N, 4.13. Found: C, 56.1; H, 6.29; N, 4.18 %. **^{1}H-NMR (C_6D_6, 400 MHz, 25 °C) δ [ppm]:** 6.92-7.21 (m, 9 H, C$_6$*H*$_3$), 5.04 (s, 1 H, *γ*-C*H*), 4.10 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH$_3$)$_2$), 3.45 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH$_3$)$_2$), 2.77 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH$_3$)$_2$), 1.72 (s, 6 H, CC*H*$_3$), 1.70 (d, 6 H, $^3J_{HH}$ = 6.6 Hz, CH(C*H*$_3$)$_2$), 1.53 (s, 2 H, C*H*$_2$), 1.48 (d, 6 H, $^3J_{HH}$ = 6.6 Hz, CH(C*H*$_3$)$_2$), 1.42 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, CH(C*H*$_3$)$_2$), 1.29 (d, 6 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3$)$_2$), 1.14 (s, 6 H, C(C*H*$_3$)$_2$), 1.12 (d, 6 H,

$^{3}J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$), 1.10 (d, 6 H, $^{3}J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 0.81 (s, 6 H, C(CH_3)$_2$). **^{13}C{^{1}H}-NMR (C_6D_6, 100 MHz, 25 °C) δ [ppm]:** 251.6 ($C_{q,Carbene}$), 167.5 (N*C*CH$_3$), 147.4 (*C*$_6$H$_3$), 146.3 (*C*$_6$H$_3$), 143.3 (*C*$_6$H$_3$), 143.0 (*C*$_6$H$_3$), 136.4 (*C*$_6$H$_3$), 129.5 (*C*$_6$H$_3$), 126.9 (*C*$_6$H$_3$), 126.1 (*C*$_6$H$_3$), 125.1 (*C*$_6$H$_3$), 123.8 (*C*$_6$H$_3$), 97.7 (γ-*C*H), 80.7 (*C*(CH$_3$)$_2$), 63.1 (*C*(CH$_3$)$_2$), 50.8 (*C*H$_2$), 37.8 (C(*C*H$_3$)$_2$), 31.9 (C(*C*H$_3$)$_2$), 30.6 (*C*H(CH$_3$)$_2$), 29.4 (*C*H$_3$), 29.0 (*C*H(CH$_3$)$_2$), 28.2 (*C*H(CH$_3$)$_2$), 27.9 (*C*H$_3$), 26.0 (*C*H$_3$), 24.9 (*C*H$_3$), 24.8 (*C*H$_3$), 24.6 (C*C*H$_3$). **IR ν [cm^{-1}]:** 3058, 2960, 2924, 2864, 2756, 1527, 1464, 1435, 1382, 1353, 1314, 1252, 1234, 1202, 1175, 1130, 1109, 1080, 1040, 1021, 1001, 965, 934, 857, 794, 757, 778, 728, 694, 638, 569, 527, 438, 404.

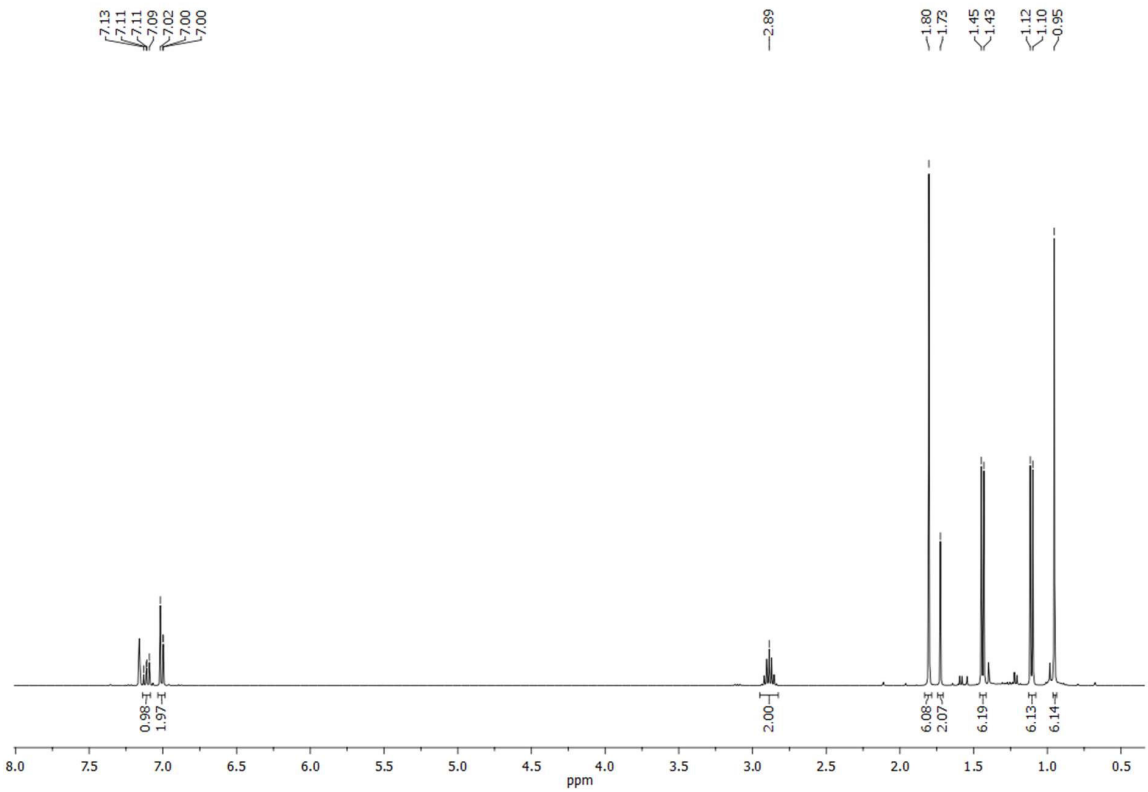


Fig. S1 ^{1}H NMR spectrum of (^{Me}cAAC)AsCl in C_6D_6.

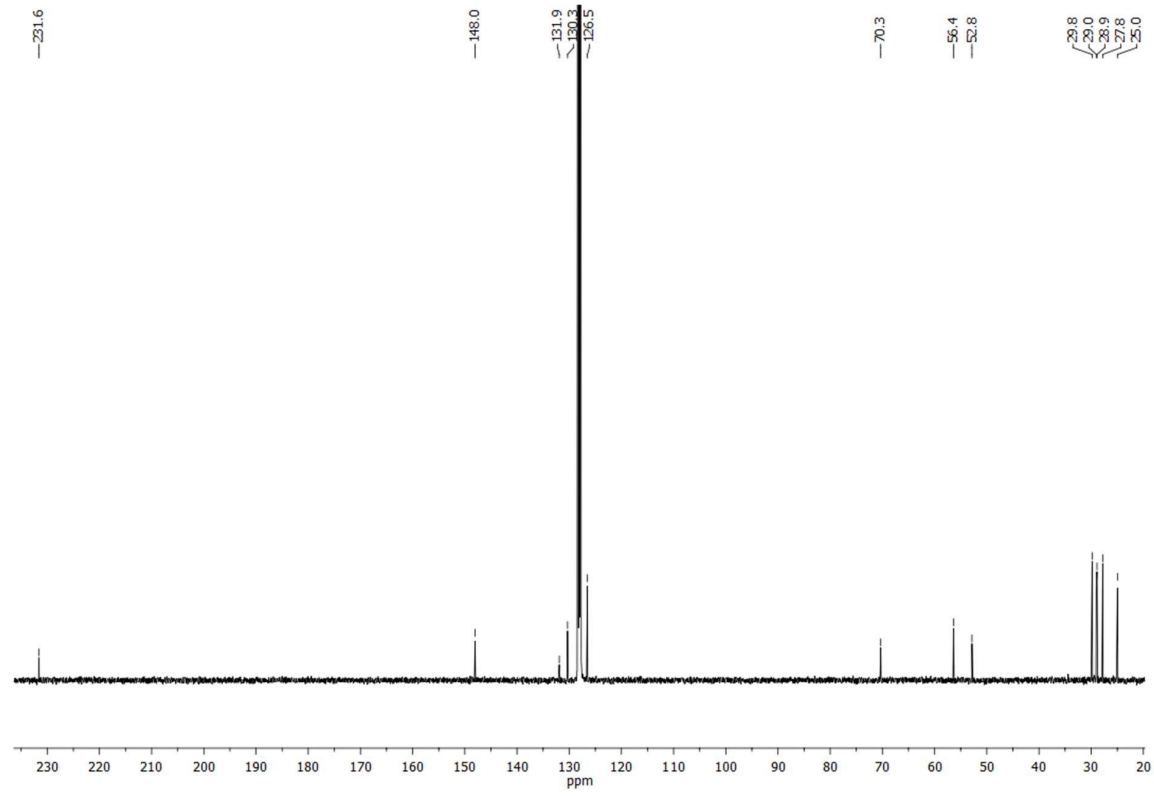


Fig. S2 ^{13}C NMR spectrum of (^{Me}cAAC)AsCl in C_6D_6.

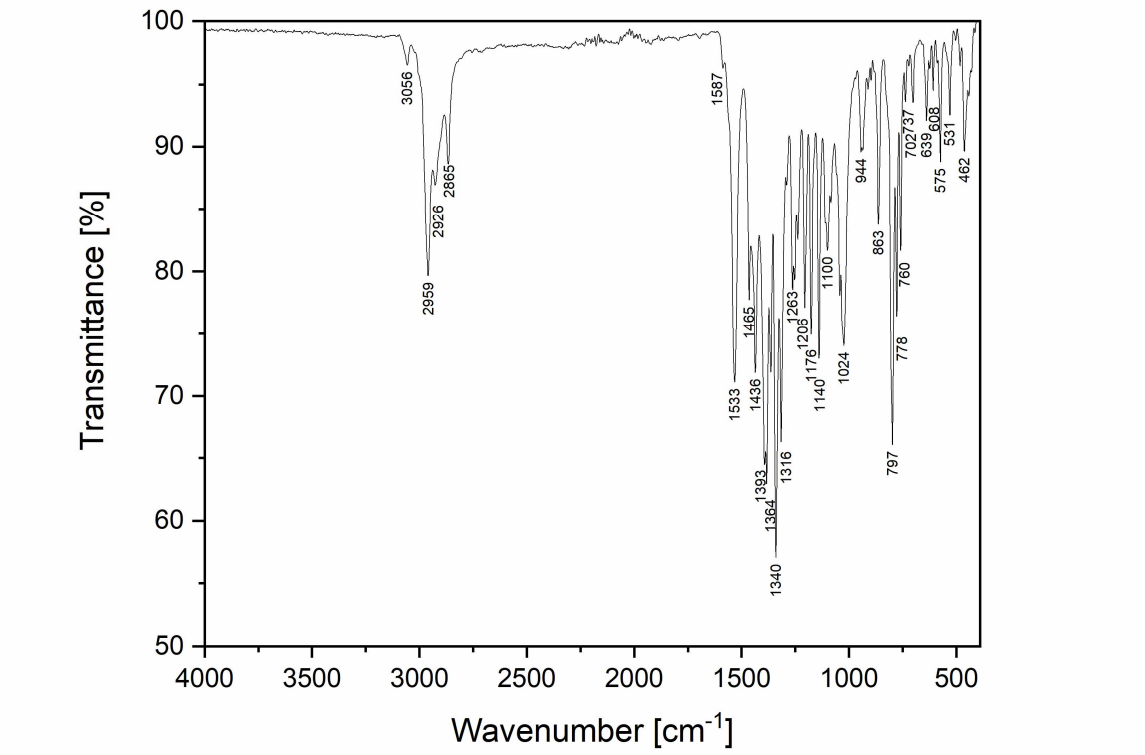


Fig. S3 IR spectrum of (^{Me}cAAC)AsCl.

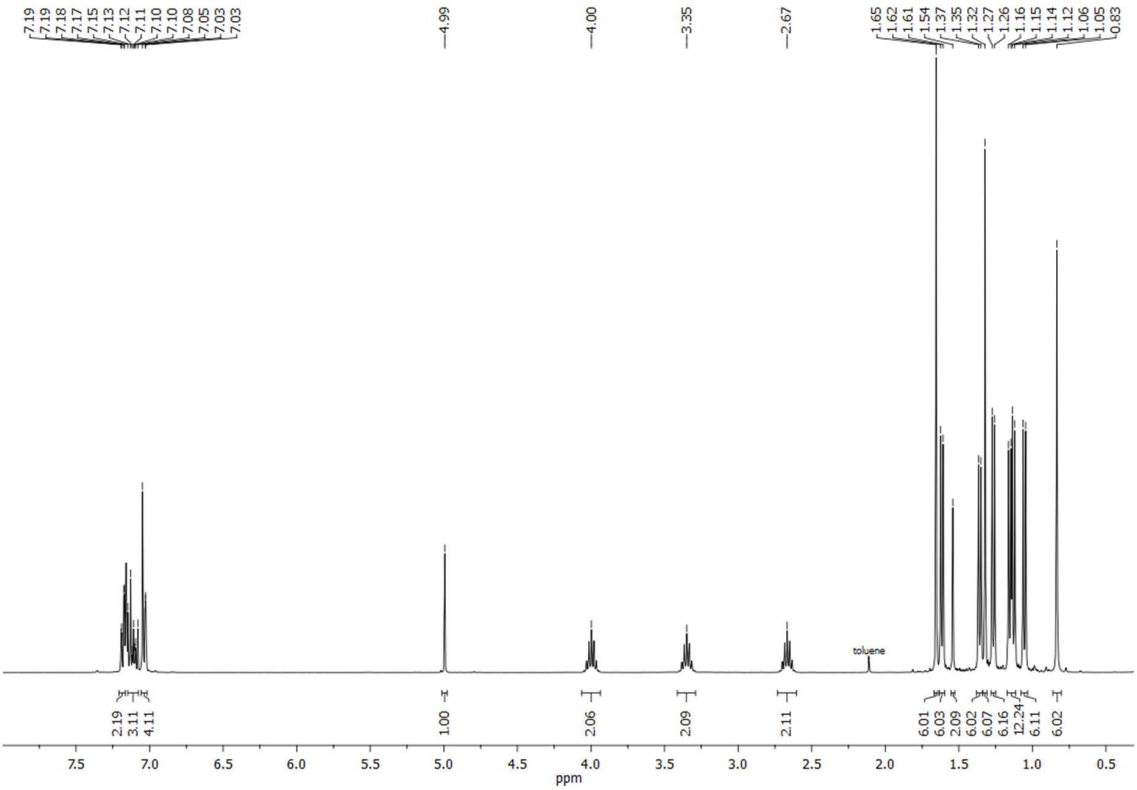


Fig. S4 ^{1}H NMR spectrum of (^{Me}cAAC)AsGa(Cl)L **1** in C_6D_6.

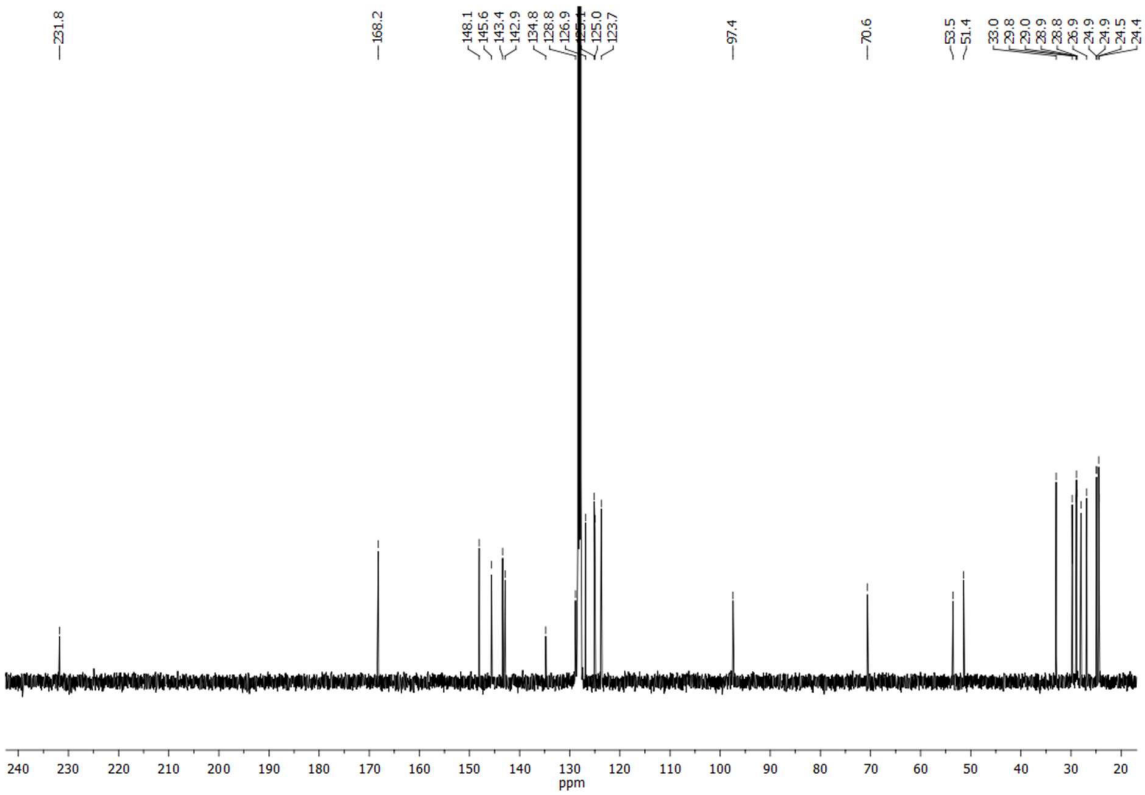


Fig. S5 ^{13}C NMR spectrum of (^{Me}cAAC)AsGa(Cl)L **1** in C_6D_6.

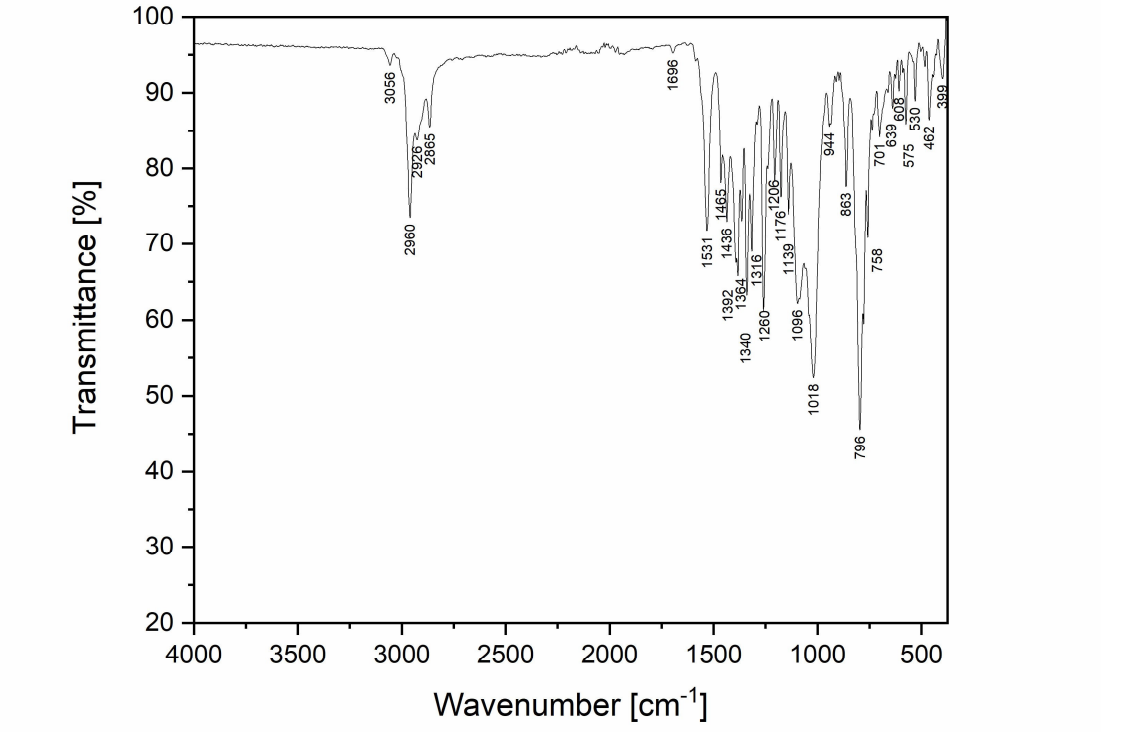


Fig. S6 IR spectrum of (^{Me}cAAC)AsGa(Cl)L **1**.

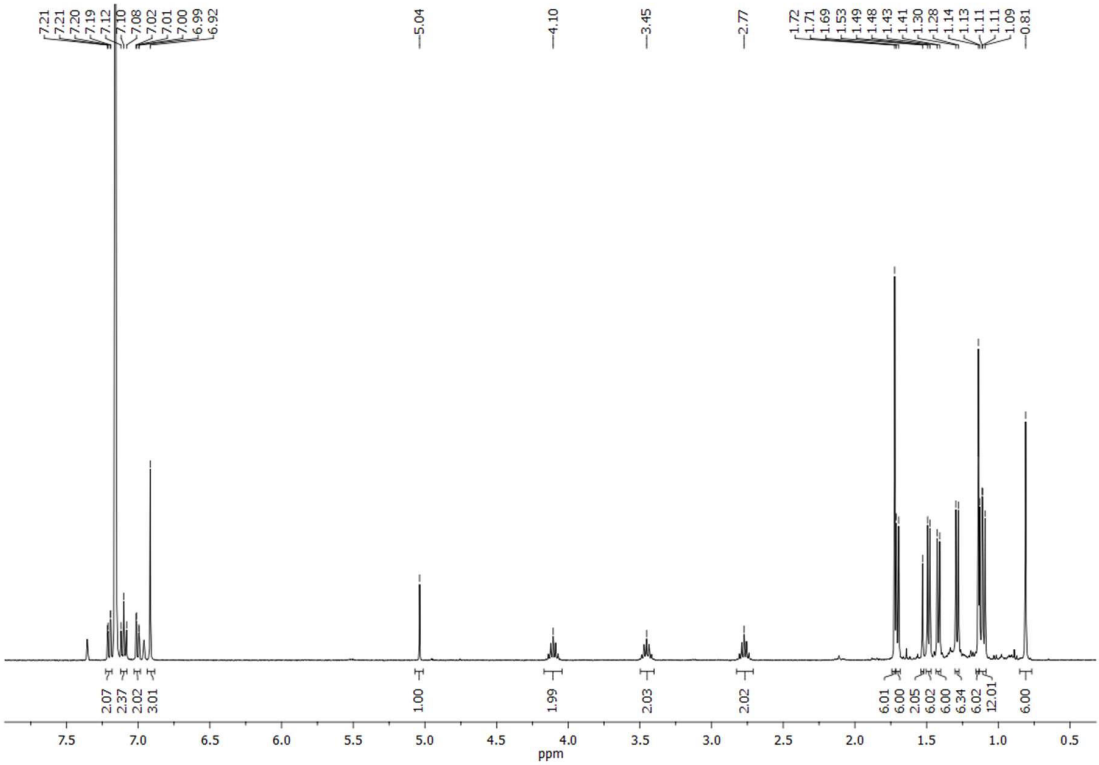


Fig. S7 ^{1}H NMR spectrum of (^{Me}cAAC)BiGa(Cl)L **3** in C_6D_6.

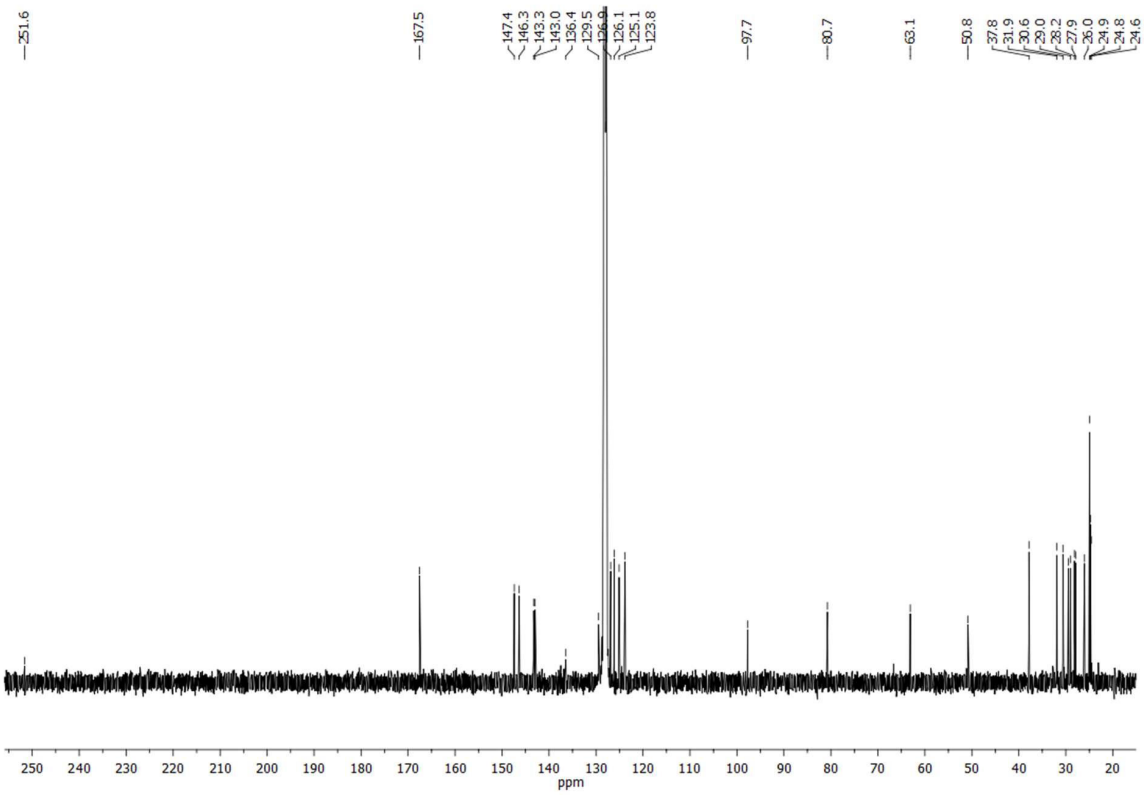


Fig. S8 ^{13}C NMR spectrum of (^{Me}cAAC)BiGa(Cl)L **3** in C_6D_6.

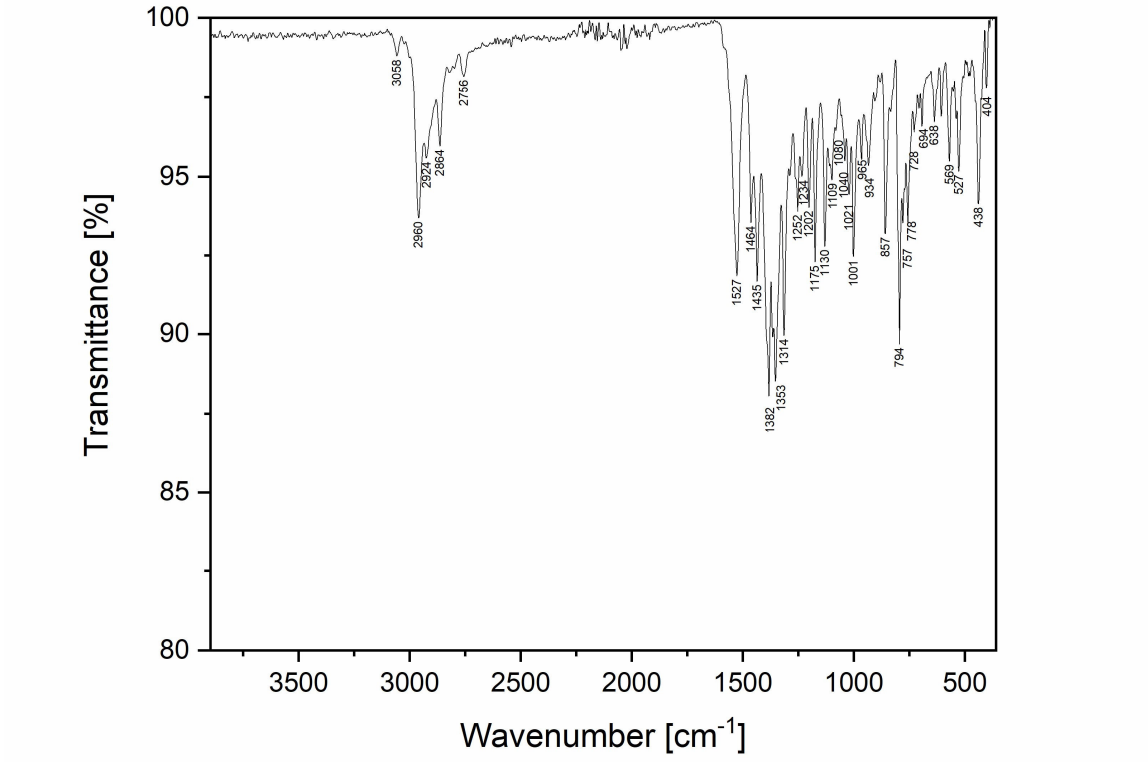


Fig. S9 IR spectrum of ([Me]cAAC)BiGa(Cl)L **3**.

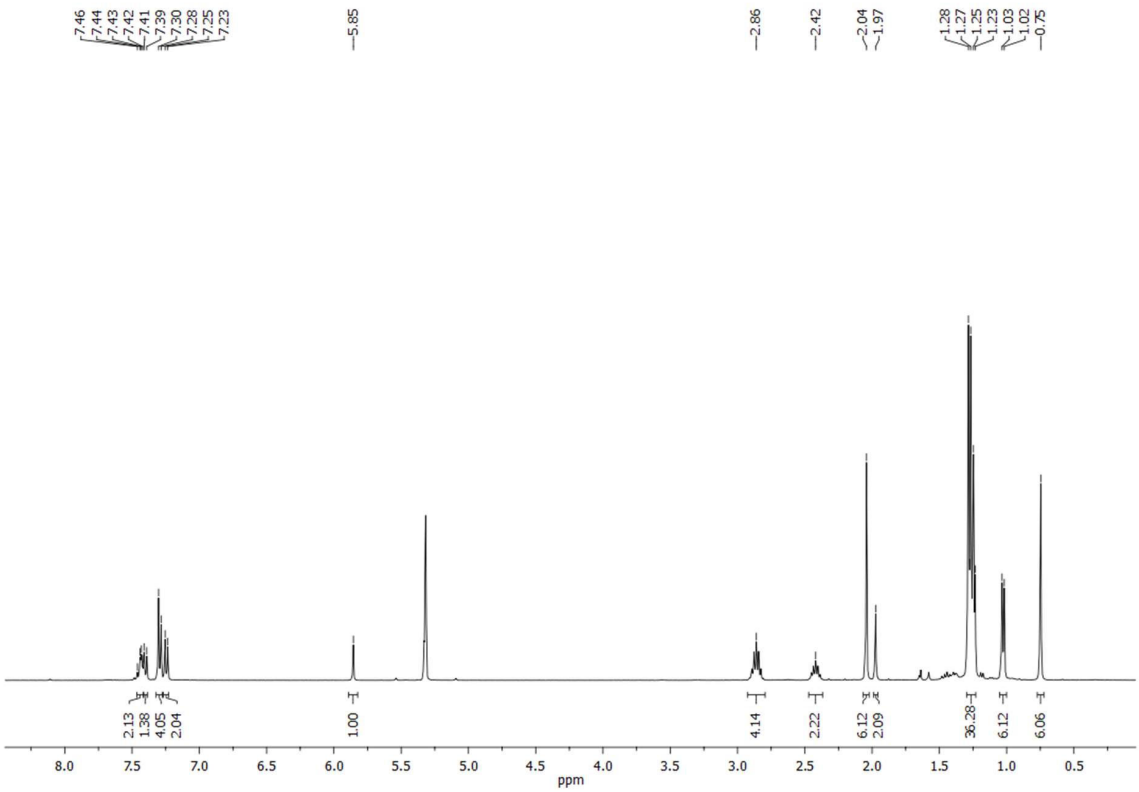


Fig. S10 ^{1}H NMR spectrum of [([Me]cAAC)AsGaL][Al(OC(CF$_3$)$_3$)$_4$] **4** in C*D*$_2$Cl$_2$.

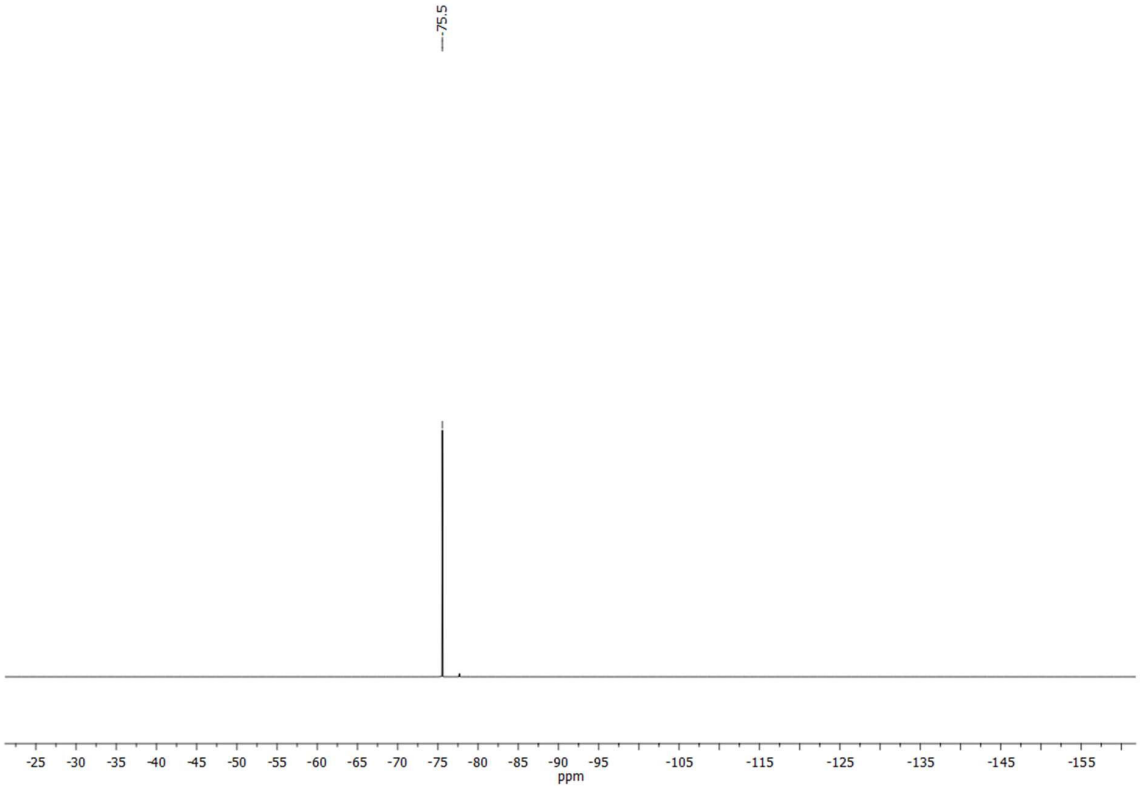


Fig. S11 ^{19}F NMR spectrum of [(^{Me}cAAC)AsGaL][Al(OC(CF$_3$)$_3$)$_4$] **4** in CD_2Cl_2.

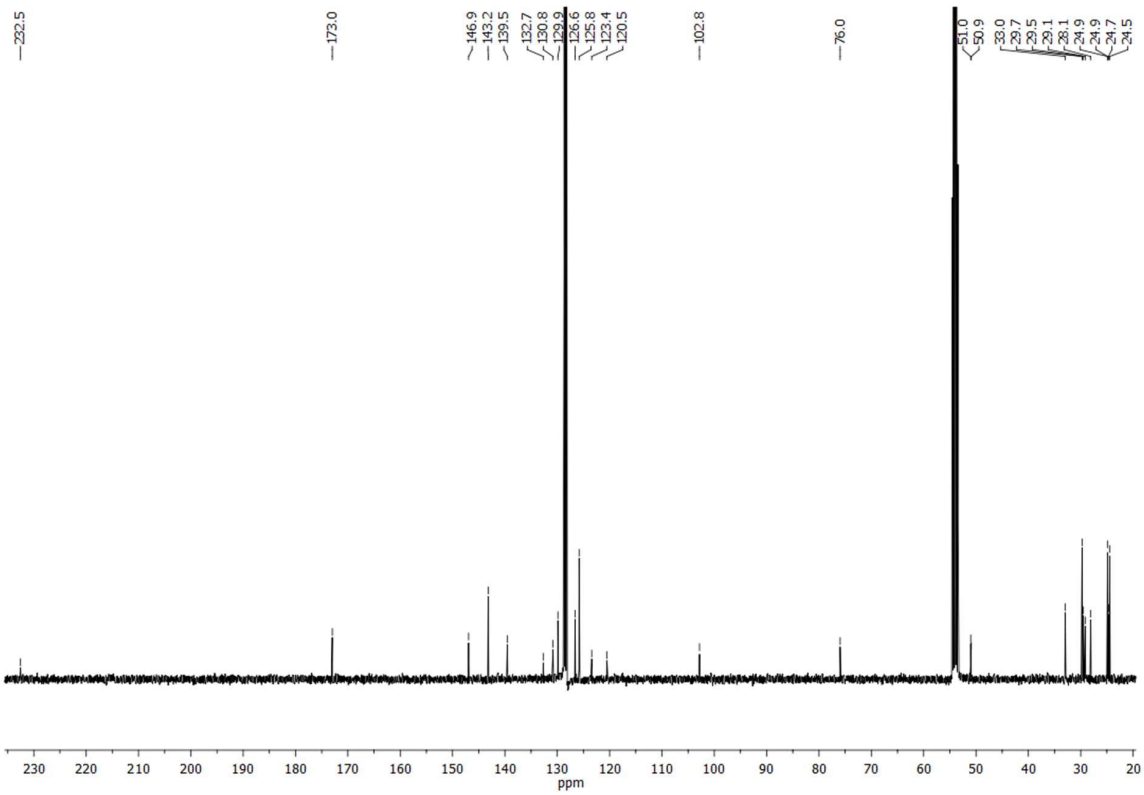


Fig. S12 ^{13}C NMR spectrum of [(^{Me}cAAC)AsGaL][Al(OC(CF$_3$)$_3$)$_4$] **4** in CD_2Cl_2.

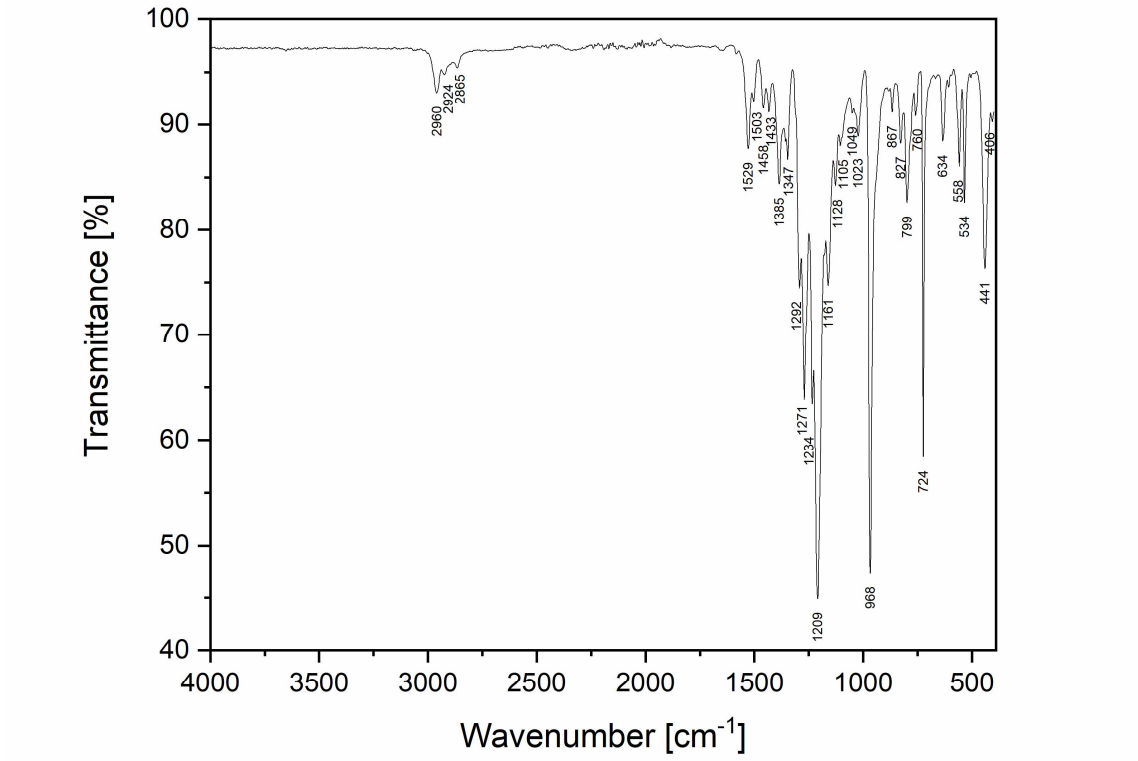


Fig. S13 IR spectrum of [(^{Me}cAAC)AsGaL][Al(OC(CF$_3$)$_3$)$_4$] **4**.

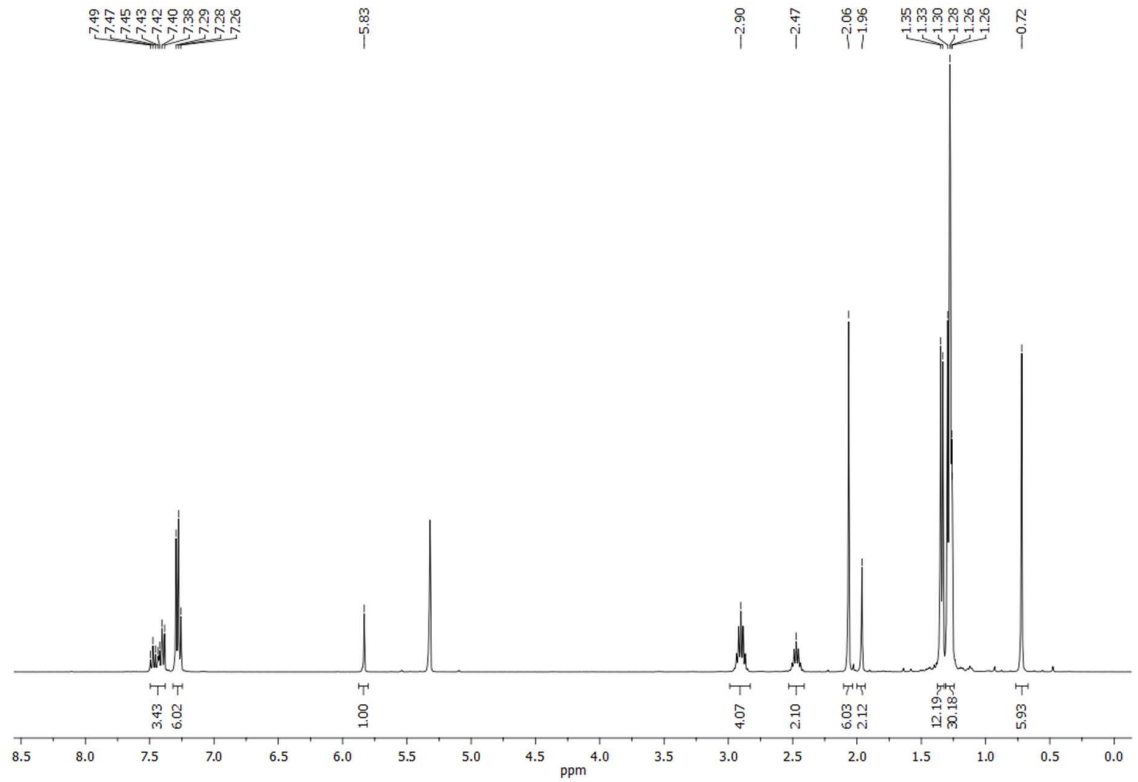


Fig. S14 ^{1}H NMR spectrum of [(^{Me}cAAC)SbGaL][Al(OC(CF$_3$)$_3$)$_4$] **5** in CD_2Cl$_2$.

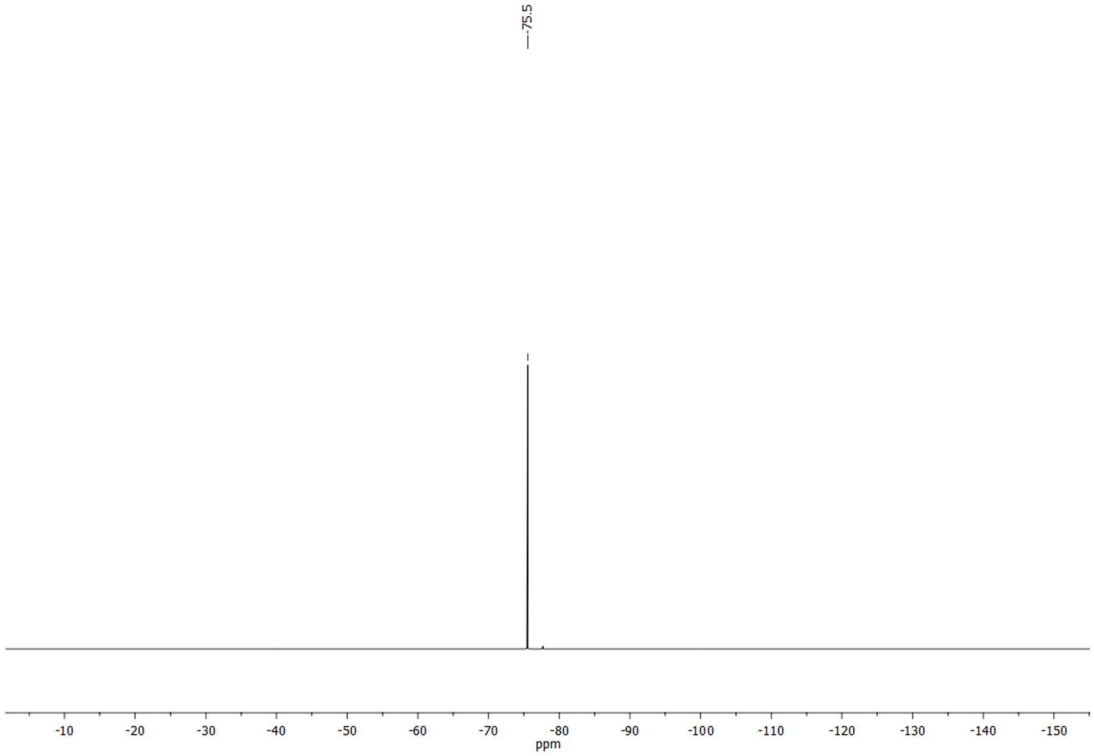


Fig. S15 ^{19}F NMR spectrum of [(^{Me}cAAC)SbGaL][Al(OC(CF$_3$)$_3$)$_4$] **5** in C*D*$_2$Cl$_2$.

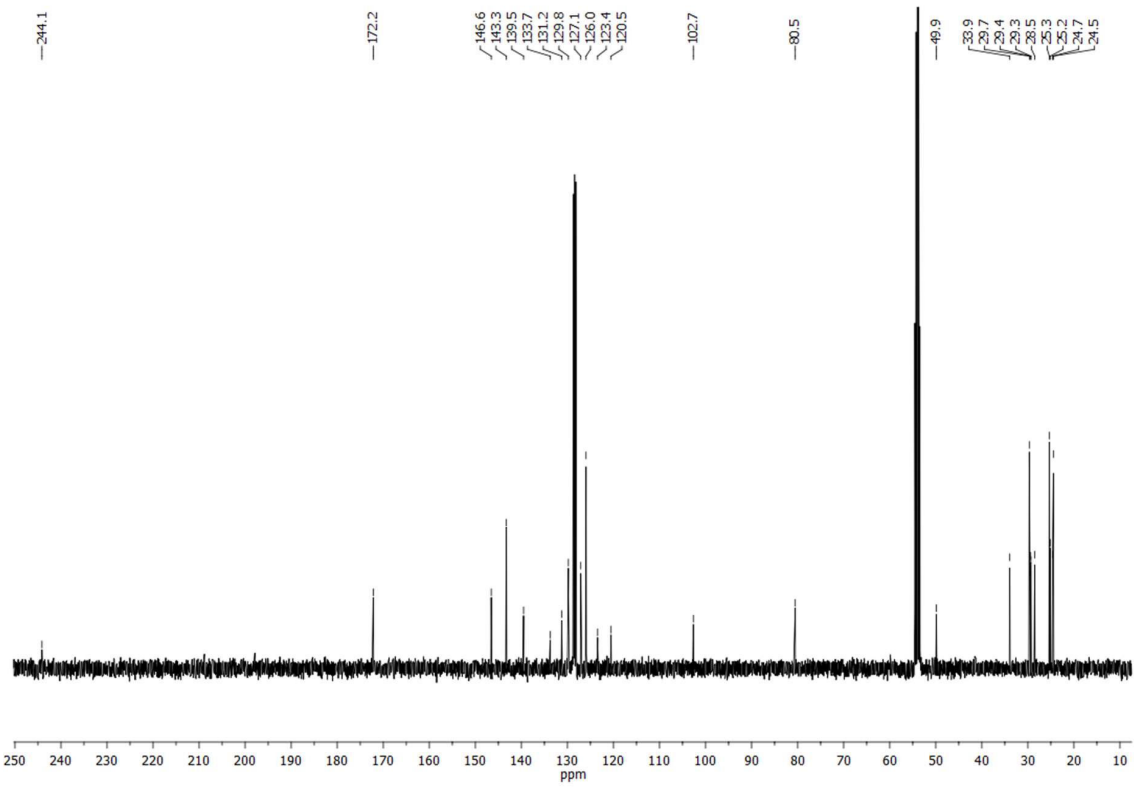


Fig. S16 ^{13}C NMR spectrum of [(^{Me}cAAC)SbGaL][Al(OC(CF$_3$)$_3$)$_4$] **5** in C*D*$_2$Cl$_2$.

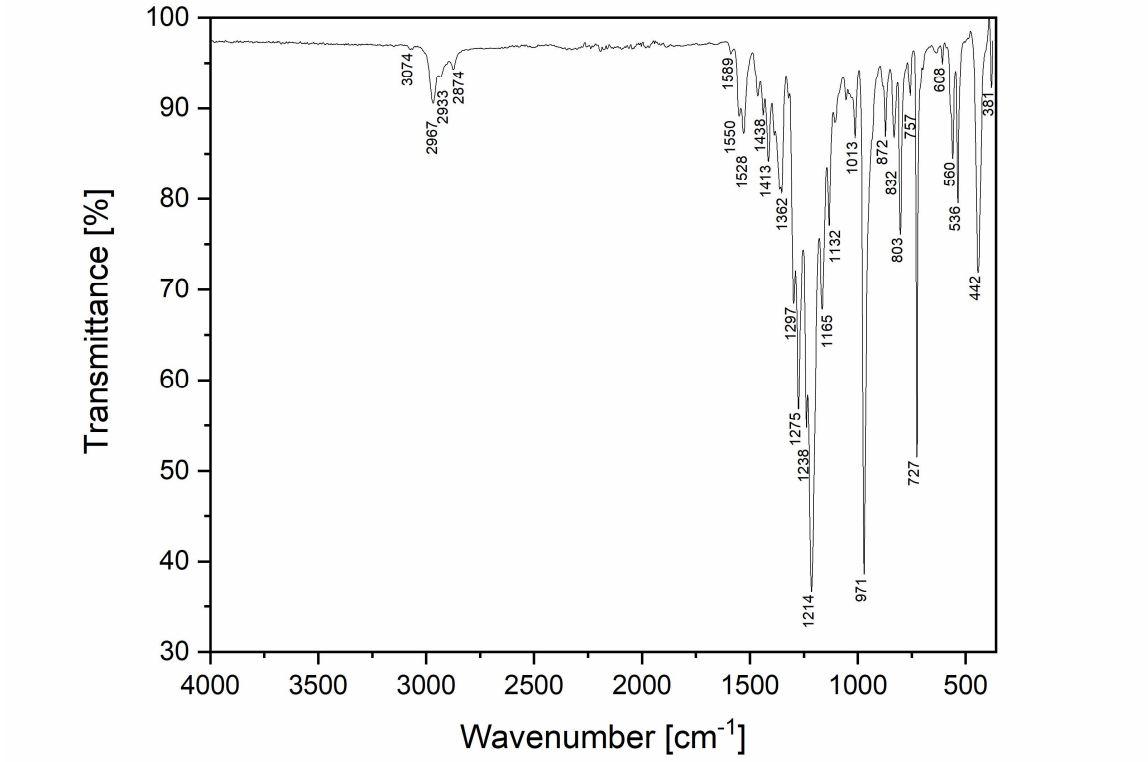


Fig. S17 IR spectrum of [(^{Me}cAAC)SbGaL][Al(OC(CF$_3$)$_3$)$_4$] **5**.

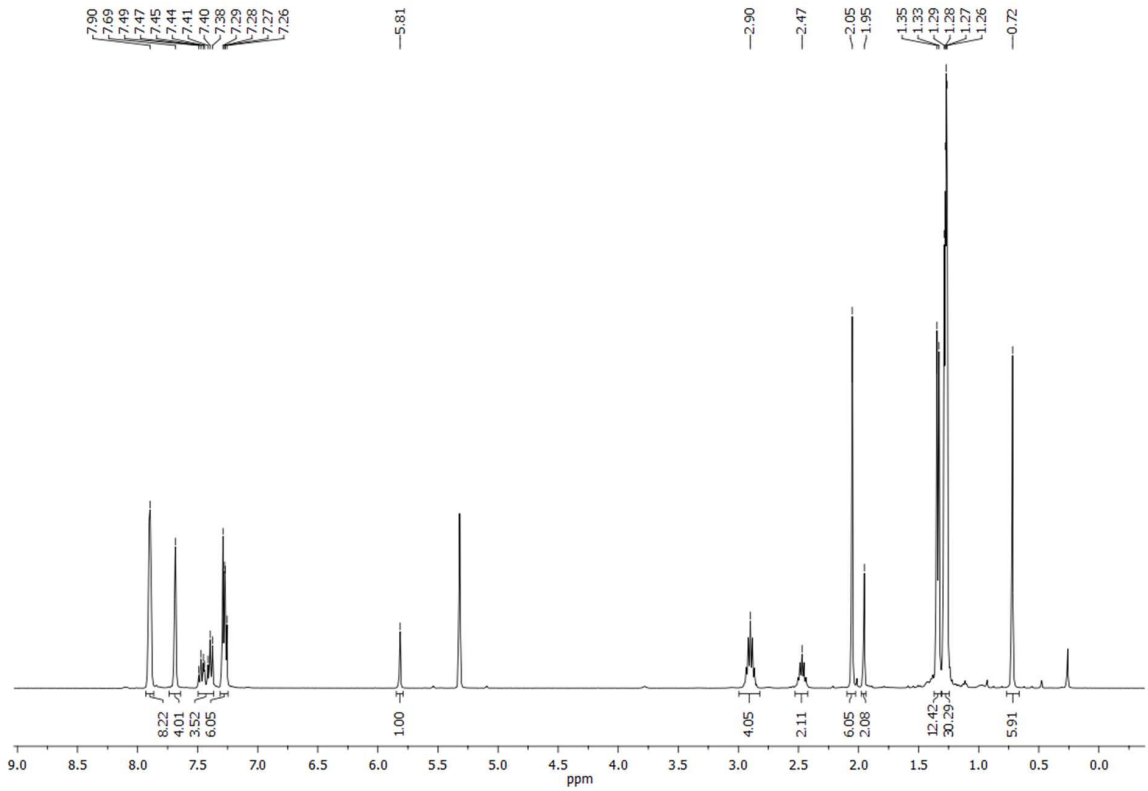


Fig. S18 ^{1}H NMR spectrum of [(^{Me}cAAC)SbGaL][B(C$_6$H$_3$(CF$_3$)$_2$)$_4$] **6** in CD_2Cl$_2$.

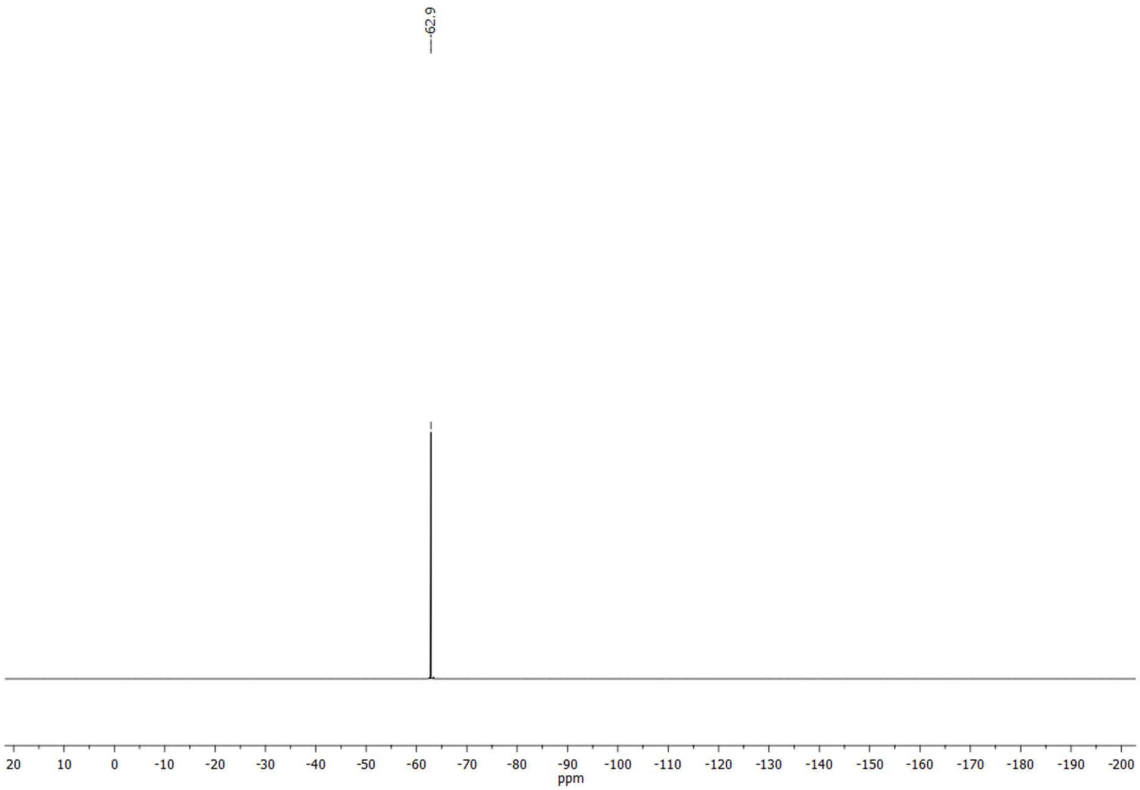


Fig. S19 ^{19}F NMR spectrum of [(^{Me}cAAC)SbGaL][B($C_6H_3(CF_3)_2)_4$] **6** in CD_2Cl_2.

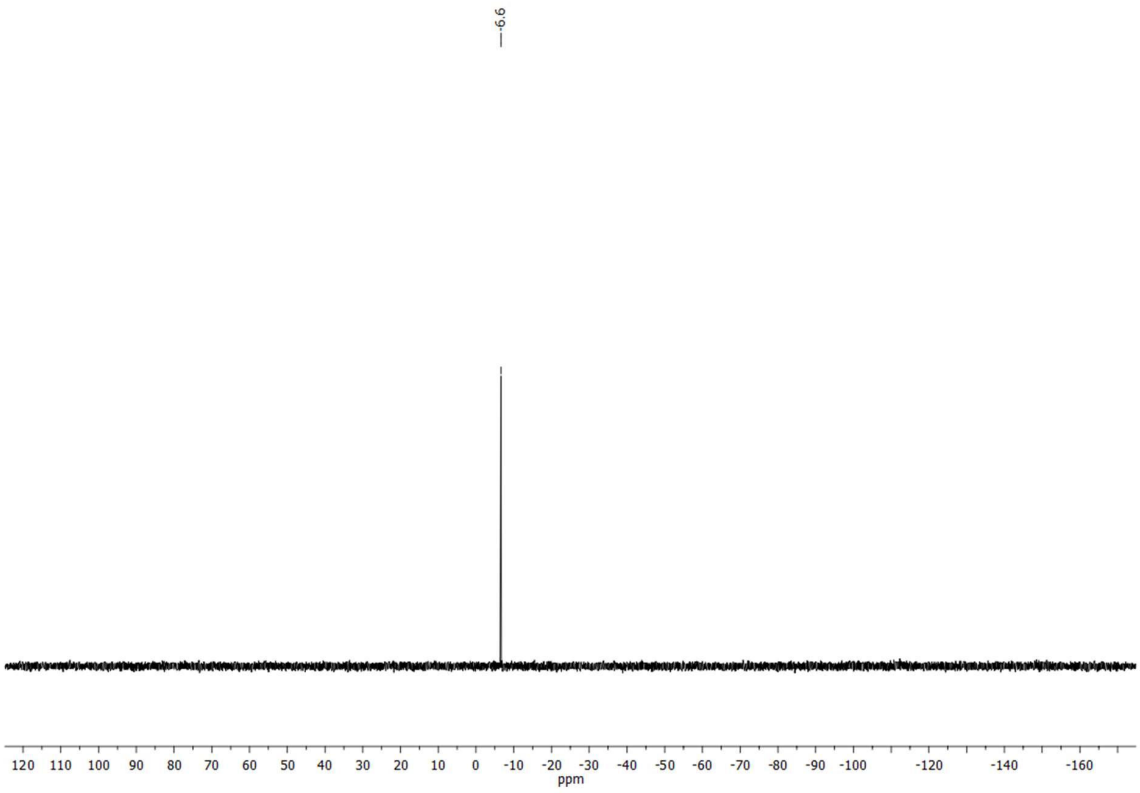


Fig. S20 ^{11}B NMR spectrum of [(^{Me}cAAC)SbGaL][B($C_6H_3(CF_3)_2)_4$] **6** in CD_2Cl_2.

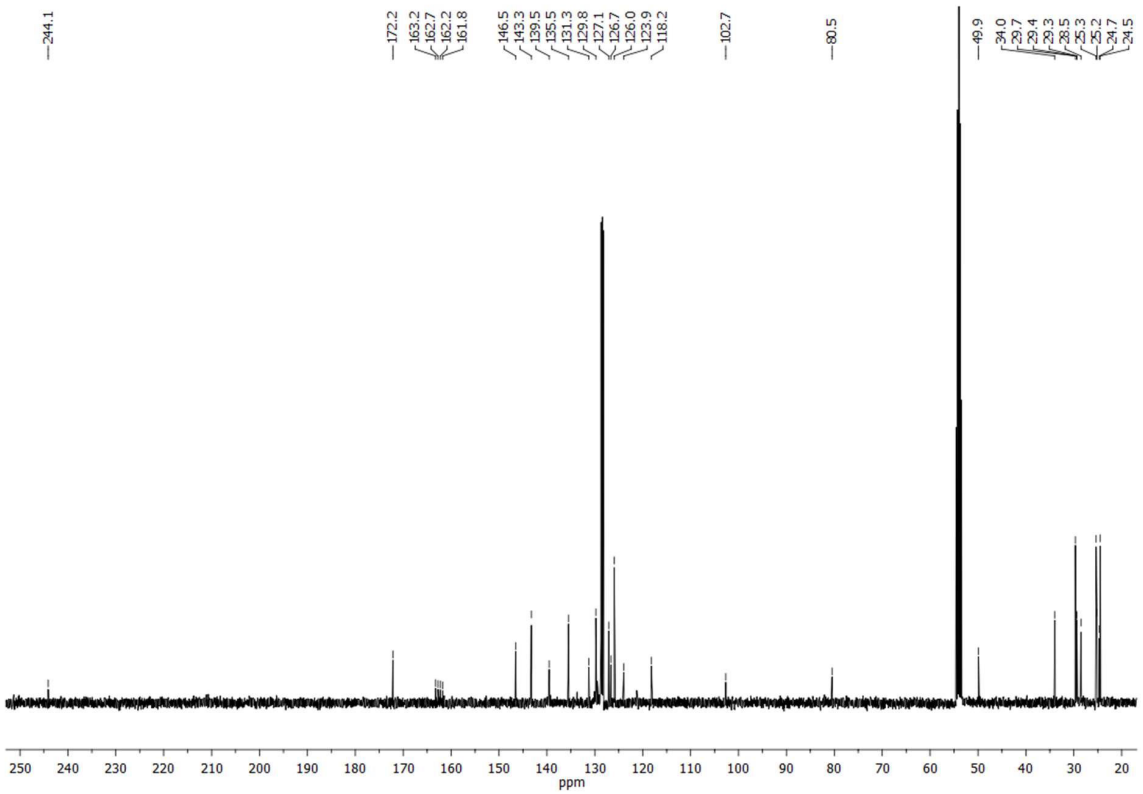


Fig. S21 ^{13}C NMR spectrum of [(^{Me}cAAC)SbGaL][B($C_6H_3(CF_3)_2)_4$] **6** in CD_2Cl_2.

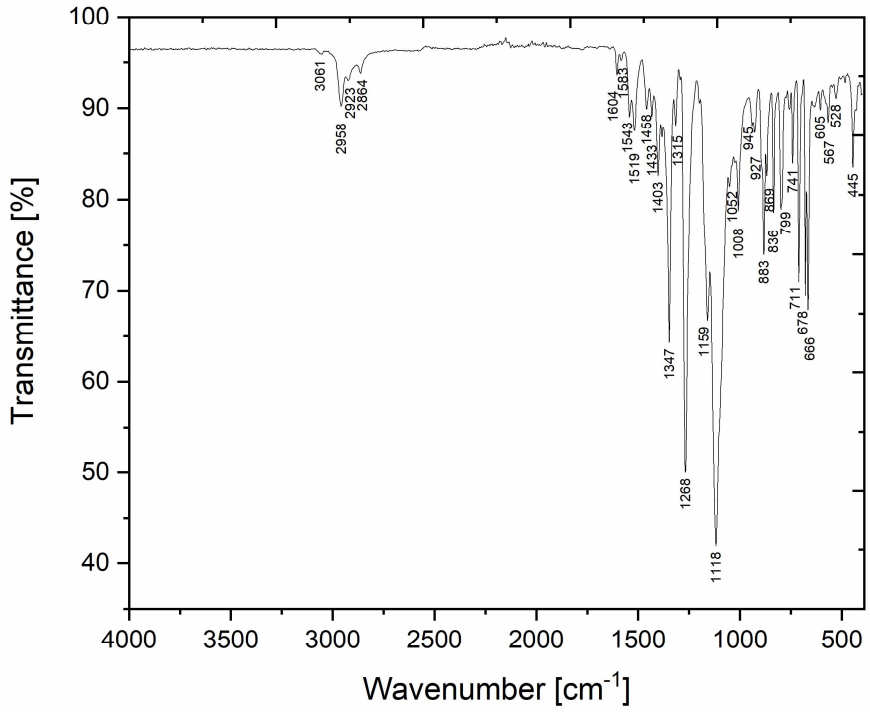


Fig. S22 IR spectrum of [(^{Me}cAAC)SbGaL][B($C_6H_3(CF_3)_2)_4$] **6**.

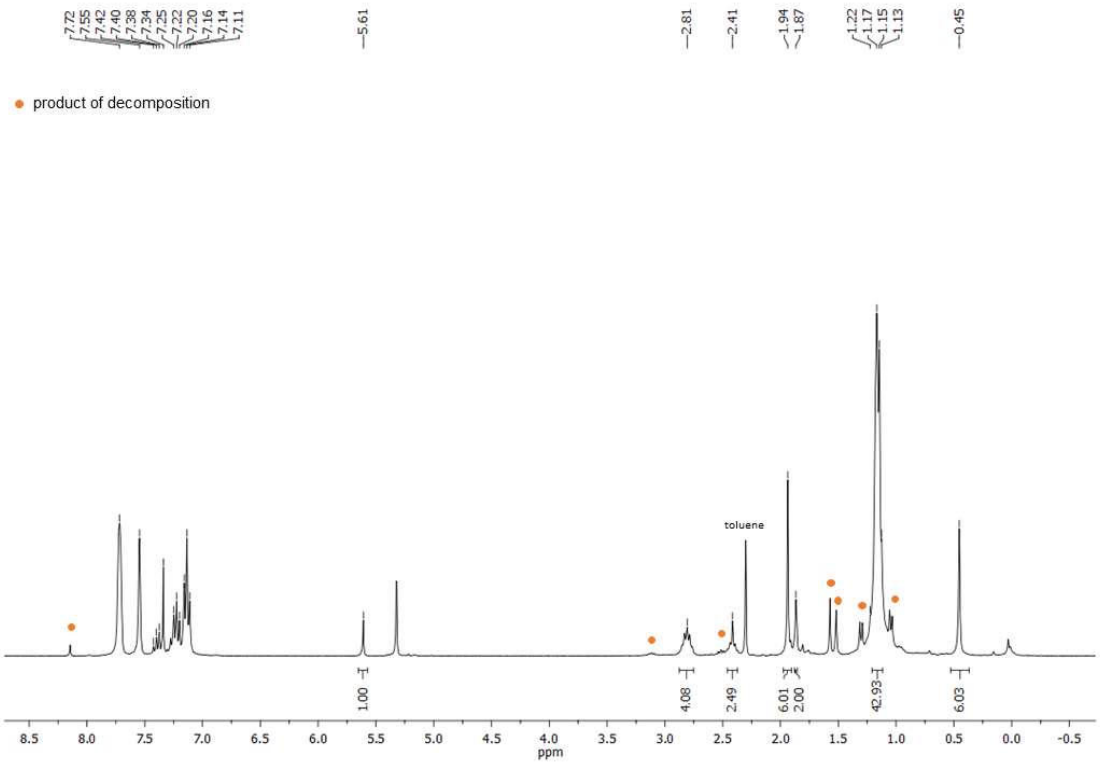


Fig. S23 ^{1}H NMR spectrum of [(^{Me}cAAC)BiGaL][B($C_6H_3(CF_3)_2)_4$] **7** in CD_2Cl_2 at -40 °C.

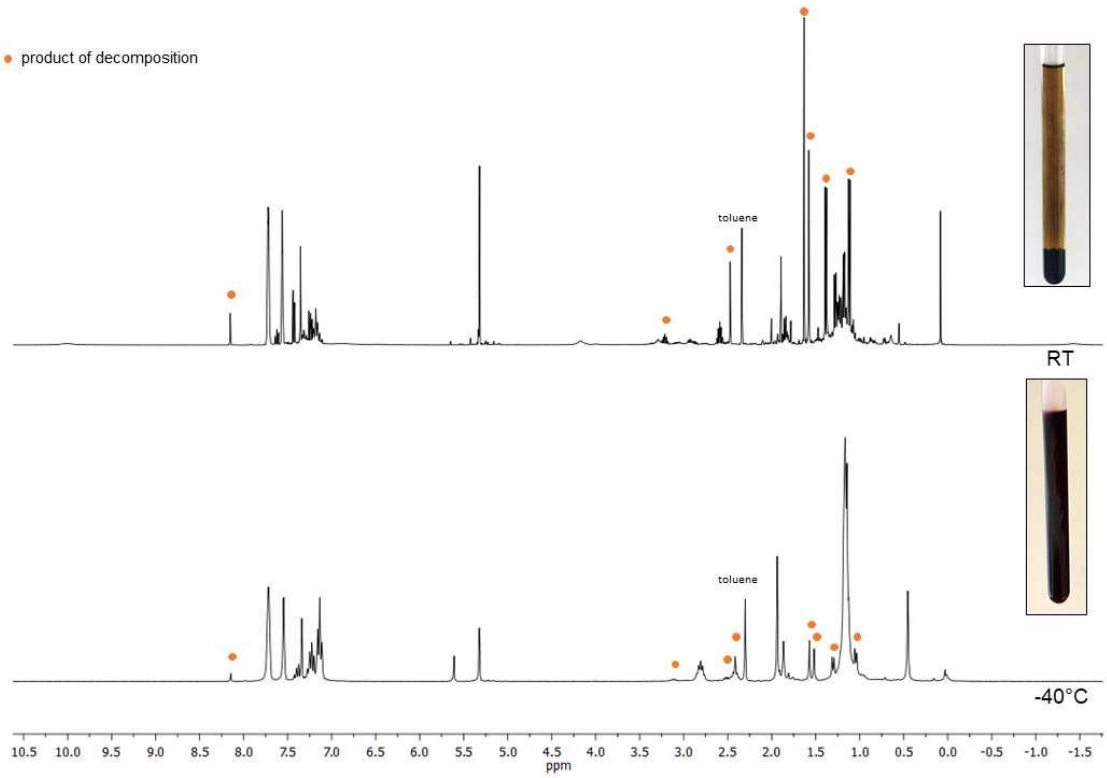


Fig. S24 ^{1}H NMR spectrum of [(^{Me}cAAC)BiGaL][B($C_6H_3(CF_3)_2)_4$] **7** in CD_2Cl_2 at -40 °C (below) and after 5 minutes at ambient temperature (above).

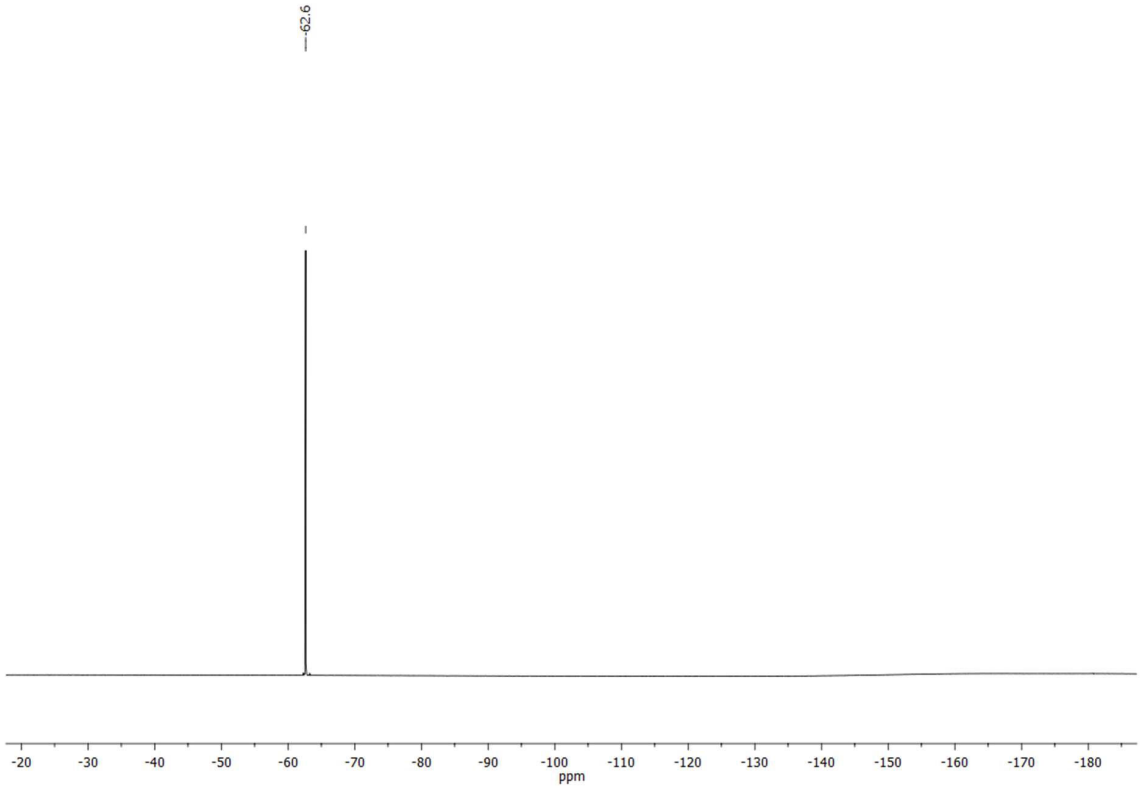


Fig. S25 ^{19}F NMR spectrum of [(^{Me}cAAC)BiGaL]B($C_6H_3(CF_3)_2)_4$] **7** in CD_2Cl_2 at -40 °C.

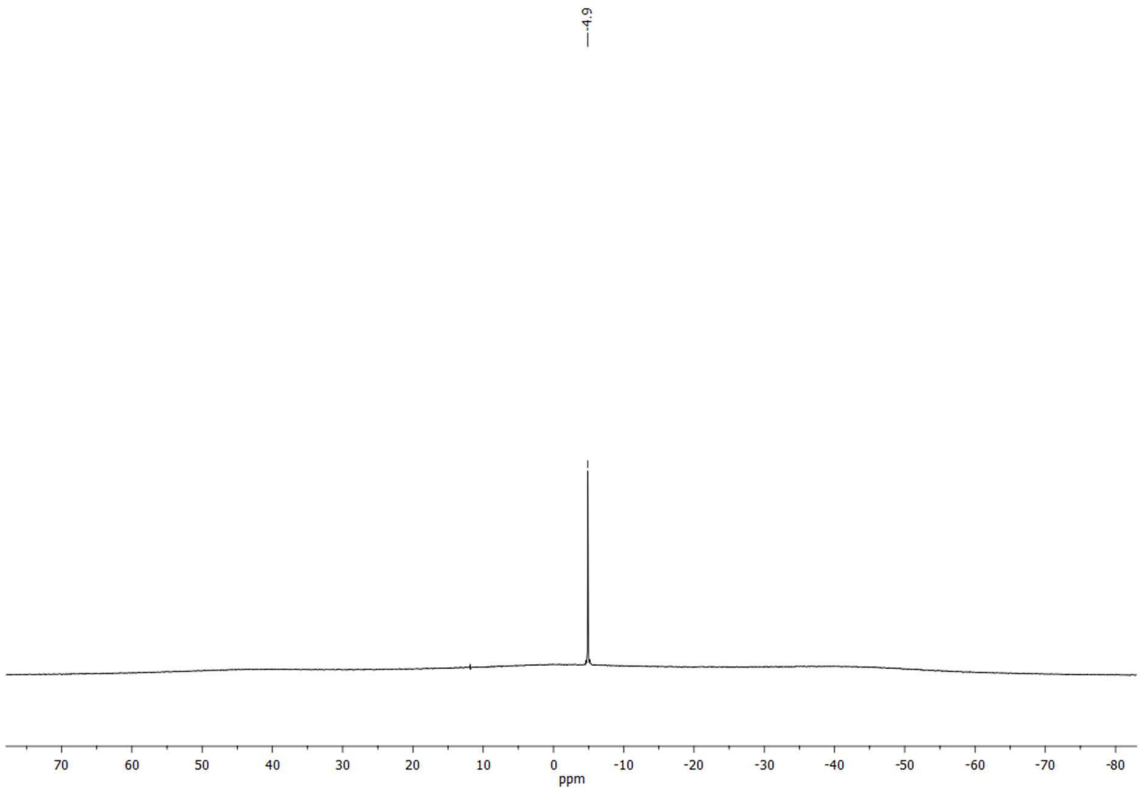


Fig. S26 ^{11}B NMR spectrum of [(^{Me}cAAC)BiGaL][B($C_6H_3(CF_3)_2)_4$] **7** in CD_2Cl_2 at -40 °C.

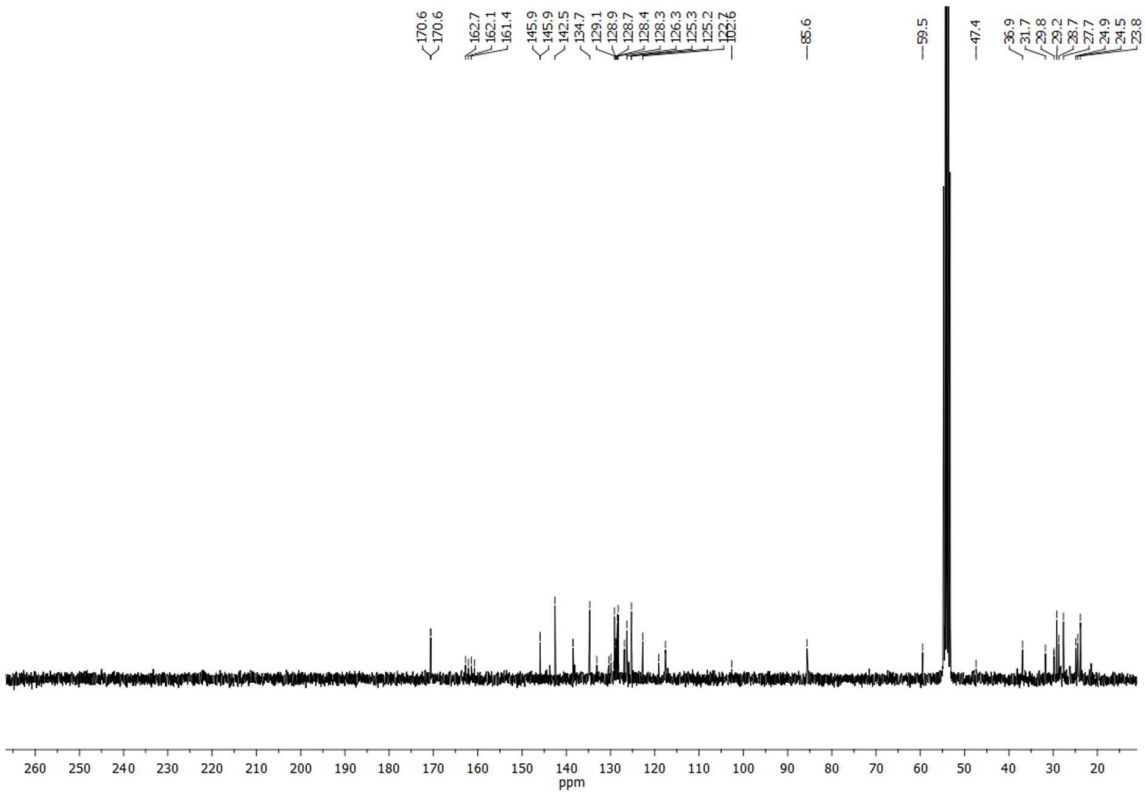


Fig. S27 ^{13}C NMR spectrum of [(^{Me}cAAC)BiGaL][B($C_6H_3(CF_3)_2)_4$] **7** in CD_2Cl_2 at -40 °C.

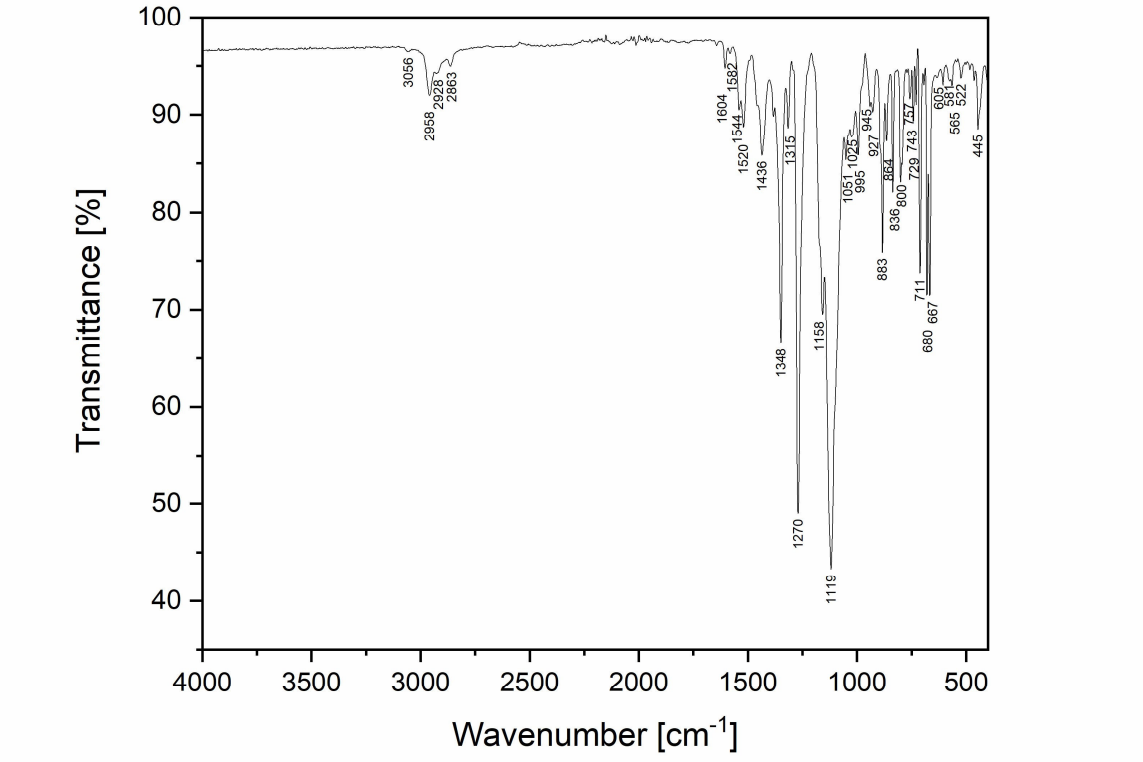


Fig. S28 IR spectrum of [(^{Me}cAAC)BiGaL][B($C_6H_3(CF_3)_2)_4$] **7**.

D) Crystallographic Part

Single-crystal X-ray analyses. The crystals were mounted on nylon loops in inert oil. Data of **1**, **3** and **4**, were collected on a Bruker AXS D8 Venture diffractometer with Photon II detector (mono-chromated Cu_{Ka} radiation, l = 1.54178 Å, micro-focus source) at 100(2) K. Data of **6**, **7** and CAACAsCl (jk_631) were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated Mo_{Ka} radiation, l = 0.71073 Å) at 100(2) K. The structures were solved by Direct Methods (SHELXS-97)[16] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2017)[17,18]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans and in case of **7** numerically form indexed faces (Bruker AXS APEX2). Hydrogen atoms were refined using a riding model or rigid methyl groups. In **1** the whole molecule is disordered over a mirror plane. A solution in the corresponding non-centrosymmetric space group did not resolve the disorder, thus this model was discarded. RIGU restraints were applied to all anisotropic displacement parameters. Considering the vast disorder quantitative results may be unreliable and should be carefully assessed. On the surface of the crystal of **3** grew several small satellite crystals that could not be removed. Independent lattices for two of them could be identified, however the corresponding reflections were too weak for a successful treatment as non-merohedral twin. The obtained intensity data for the main crystal is likely distorted by overlaps. The molecule shows a full-body disorder over a mirror-plane. This cannot be resolved by choosing the non-centrosymmetric subgroup without the mirror-plane ($Pna2_1$). The local symmetry was ignored in the refinement (negative PART) and RIGU restraints were applied to all anisotropic displacement parameter. The combination of disorder and unresolved twinning problems renders quantitative results unreliable and they should not be discussed. The determination of the connectivity can be considered successful. In **4** the entire anion is disordered. All corresponding bond lengths and angles were restrained to be equal (SADI). RIGU and SIMU restraints were applied to all the anion's anisotropic displacement parameters. Atoms in close proximity were refined with common displacement parameters (EADP). In addition, O1 and C1 of residues 4 and 6 were refined with common coordinates (EXYZ). One of the cation's isopropyl group is disordered over two positions. All its corresponding bond lengths and angles were restrained to be equal (SADI). As1 and Ga1 are disordered over two positions. SADI restraints were used in the refinement of their bond lengths and RIGU and SIMU restraints for their displacement parameters. In the course of the measurement ice formed on the crystal. The resulting diffraction reduced the quality of part of the data. In combination with the vast disorder and consequent use of re- and constraints quantitative results are biased and unreliable and should be critically assessed and conclusions backed up by other analytical means. In **6** the dichloromethane molecule is disordered over two positions. Its corresponding bond lengths and angles were restrained to be equal with SADI and its displacement parameters were restrained with RIGU. Two CF_3 groups show rotational disorder. One group was modelled with two the other with three alternate orientations. For the latter the occupancies were constrained to the values of the free variables in the last refinement runs to ensure convergence. All bond lengths and angles of these groups were restrained to be equal (SADI) and RIGU, SIMU and ISOR restraints were applied to the displacement parameters. Still, the displacement ellipsoids suggest that this is only a mediocre description, however the electron density is too diffuse to identify and refine further orientations. In **7** the dichloromethane molecule is disordered over two positions. The bond lengths were restrained to be equal with SADI and RIGU restraints were used for the displacement

parameters. The residual electron density near several CF_3 suggests rotational disorder. In the two most pronounced cases a refinement with two alternate positions was attempted, however this led to highly unrealistic displacement parameters even with strict restraints applied. Since the improvement in the R-values was neglectable this model was discarded. The electron density map shows high residual peaks near heavy atoms. A semi-empirical absorption correction from multi-scans yielded the same results. The same could be observed for data collected from another specimen with Cu_{Ka} radiation. Truncating the data at high angle reduces the height of these peaks (and the *R*-values) thus they likely result from a combination of lower quality high angle data and Fourier truncation effects. The crystal of CAACAsCl (jk_631) was pseudo-merohedrally twinned and the model refined as a 2-component twin with the twin law (-1 0 0 0 -1 0 1 0 1).

CCDC-2096524 (**1**), -2096525 (**3**), -2096526 (**4**), -2096527 (**6**), -2096528 (**7**), and -2096530 (^{Me}cAACAsCl) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic details of (^{Me}cAAC)AsCl, **1** and **3**.

	(^{Me}cAAC)AsCl	**1**	**3**
Empirical formula	$C_{20}H_{31}AsClN$	$C_{49}H_{72}AsClGaN_3$	$C_{49}H_{72}BiClGaN_3$
M [g mol^{-1}]	395,83	883.18	1017.24
Crystal size [mm]	0.297 × 0.100 × 0.090	0.226 × 0.191 × 0.070	0.108 × 0.052 × 0.039
T [K]	100(2)	100(2)	100(2)
Crystal system	monoclinic	orthorhombic	orthorhombic
Space group	$P2_1/c$	*Pnma*	*Pnma*
a [Å]	10.726(4)	10.0473(7)	10.0866(10)
b [Å]	9.032(3)	19.2234(13)	19.113(2)
c [Å]	21.484(9)	24.0765(16)	24.736(2)
α [°]	90	90	90
β [°]	104.334(7)	90	90
γ [°]	90	90	90
V [Å^3]	2016.6(13)	4650.2(5)	4768.8(8)
Z	4	4	4
D_{calcd} [g cm^{-3}]	1304	1.261	1.417
$\mu(K_\alpha$ [mm^{-1}])	1818	2.382	8.614
Transmissions	0.75/0.60	0.75/0.63	0.75/0.53
F(000)	832	1872	2072
Index ranges	-16 ≤ h ≤ 16	-12 ≤ h ≤ 12	-12 ≤ h ≤ 12
	-13 ≤ k ≤ 13	-24 ≤ k ≤ 21	-24 ≤ k ≤ 24
	-33 ≤ l ≤ 33	-30 ≤ l ≤ 30	-31 ≤ l ≤ 31
θ_{max} [°]	33442	80.283	80.734
Reflections collected	46739	99176	128478
Independent reflections	8007	5237	5367
R_{int}	0,0537	0.0370	0.1083
Refined parameters	217	508	514
R_1 [$I > 2\sigma(I)$]	0,028	0.0350	0.0512
wR_2 [all data]	0,0663	0.0779	0.1305
GooF	972	1.182	1.121
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	0.565/-0.328	0.534/-0.613	2.890/-1.604

Table S2. Crystallographic details of **4**, **6** and **7**.

	4	**6**	**7**
Empirical formula	$C_{65}H_{72}AlAsF_{36}GaN_3O_4$	$C_{81.50}H_{85}BClF_{24}GaN_3Sb$	$C_{81.50}H_{85}BBiClF_{24}GaN_3$
M [g mol^{-1}]	1814.87	1800.25	1887.48
Crystal size [mm]	0.138 × 0.111 × 0.083	0.315 × 0.132 × 0.071	0.275 × 0.206 × 0.181
T [K]	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a [Å]	12.6547(18)	17.3927(9)	17.4708(6)
b [Å]	16.649(2)	20.2713(10)	20.3196(8)
c [Å]	18.452(3)	23.9571(13)	23.9981(9)
α [°]	94.858(7)	75.938(2)	75.7399(18)
β [°]	93.130(7)	85.836(3)	85.4334(18)
γ [°]	98.688(7)	84.655(2)	84.4827(17)
V [Å^3]	3820.2(9)	8147.0(7)	8204.7(5)
Z	2	4	4
D_{calcd} [g cm^{-3}]	1.578	1.468	1.528
μ(K_α [mm^{-1}])	2.317	0.795	2.602
Transmissions	0.75/0.64	0.75/0.57	0.39/0.27
F(000)	1832	3660	3788
Index ranges	-16 ≤ h ≤ 16	-24 ≤ h ≤ 25	-26 ≤ h ≤ 26
	-21 ≤ k ≤ 21	-29 ≤ k ≤ 29	-31 ≤ k ≤ 31
	-23 ≤ l ≤ 23	-34 ≤ l ≤ 34	-36 ≤ l ≤ 36
θ_{max} [°]	81.278	30.774	33.228
Reflections collected	203578	429472	595788
Independent reflections	16547	50542	62816
R_{int}	0.1093	0.0800	0.055
Refined parameters	1521	2175	2090
R_1 [$I > 2\sigma(I)$]	0.0866	0.0414	0.0595
wR_2 [all data]	0.2701	0.1012	0.1563
GooF	1.014	1.080	1.057
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	2.126/-0.522	1.207/-0.879	10.002/-4.288

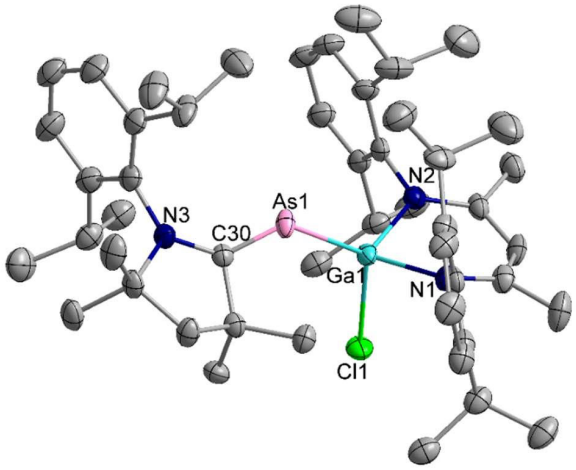


Fig. S29. Solid state structure of **1**. Hydrogen atoms and minor component of the disorder are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S3 Bond lengths [Å] for **1**.

Ga(1)-N(2)	1.940(10)	C(8)-C(9)	1.372(10)	C(30)-C(31)	1.522(5)
Ga(1)-N(1)	2.021(9)	C(9)-C(10)	1.417(12)	C(31)-C(35)	1.524(5)
Ga(1)-Cl(1)	2.2482(6)	C(10)-C(11)	1.396(6)	C(31)-C(32)	1.537(5)
Ga(1)-As(1)	2.4201(4)	C(11)-C(15)	1.536(5)	C(31)-C(34)	1.539(5)
As(1)-C(30)	1.869(3)	C(12)-C(14)	1.514(10)	C(32)-C(33)	1.521(8)
N(1)-C(3)	1.323(10)	C(12)-C(13)	1.525(13)	C(33)-C(37)	1.519(7)
N(1)-C(18)	1.451(8)	C(15)-C(17)	1.522(6)	C(33)-C(36)	1.534(7)
N(2)-C(1)	1.347(10)	C(15)-C(16)	1.541(5)	C(38)-C(43)	1.409(8)
N(2)-C(6)	1.456(9)	C(18)-C(23)	1.378(8)	C(38)-C(39)	1.411(5)
N(3)-C(30)	1.357(4)	C(18)-C(19)	1.427(14)	C(39)-C(40)	1.407(6)
N(3)-C(38)	1.449(4)	C(19)-C(20)	1.388(10)	C(39)-C(44)	1.504(6)
N(3)-C(33)	1.512(6)	C(19)-C(24)	1.509(10)	C(40)-C(41)	1.376(7)
C(1)-C(2)	1.394(7)	C(20)-C(21)	1.376(10)	C(41)-C(42)	1.372(8)
C(1)-C(4)	1.511(7)	C(21)-C(22)	1.359(12)	C(42)-C(43)	1.396(8)
C(2)-C(3)	1.384(6)	C(22)-C(23)	1.408(6)	C(43)-C(47)	1.528(6)
C(3)-C(5)	1.516(7)	C(23)-C(27)	1.522(6)	C(44)-C(46)	1.546(5)
C(6)-C(11)	1.397(8)	C(24)-C(26)	1.545(12)	C(44)-C(45)	1.550(16)
C(6)-C(7)	1.427(14)	C(24)-C(25)	1.545(13)	C(47)-C(49)	1.529(6)
C(7)-C(8)	1.390(9)	C(27)-C(29)	1.523(7)	C(47)-C(48)	1.543(6)
C(7)-C(12)	1.507(9)	C(27)-C(28)	1.538(6)		

Table S4 Bond angles [°] for **1**.

N(2)-Ga(1)-N(1)	94.3(2)	C(21)-C(20)-C(19)	122.1(10)
N(2)-Ga(1)-Cl(1)	103.5(3)	C(22)-C(21)-C(20)	118.7(9)
N(1)-Ga(1)-Cl(1)	97.5(2)	C(21)-C(22)-C(23)	122.4(6)
N(2)-Ga(1)-As(1)	127.3(3)	C(18)-C(23)-C(22)	118.3(5)
N(1)-Ga(1)-As(1)	104.6(2)	C(18)-C(23)-C(27)	123.3(5)

Cl(1)-Ga(1)-As(1)	121.48(2)	C(22)-C(23)-C(27)	118.4(5)
C(30)-As(1)-Ga(1)	109.47(10)	C(19)-C(24)-C(26)	111.7(8)
C(3)-N(1)-C(18)	119.6(7)	C(19)-C(24)-C(25)	112.4(9)
C(3)-N(1)-Ga(1)	118.4(5)	C(26)-C(24)-C(25)	109.9(8)
C(18)-N(1)-Ga(1)	121.9(6)	C(23)-C(27)-C(29)	110.9(4)
C(1)-N(2)-C(6)	118.3(8)	C(23)-C(27)-C(28)	112.0(4)
C(1)-N(2)-Ga(1)	121.4(6)	C(29)-C(27)-C(28)	109.4(5)
C(6)-N(2)-Ga(1)	119.8(6)	N(3)-C(30)-C(31)	108.0(3)
C(30)-N(3)-C(38)	124.6(3)	N(3)-C(30)-As(1)	120.0(2)
C(30)-N(3)-C(33)	114.9(4)	C(31)-C(30)-As(1)	132.0(2)
C(38)-N(3)-C(33)	120.2(3)	C(30)-C(31)-C(35)	114.2(3)
N(2)-C(1)-C(2)	122.8(6)	C(30)-C(31)-C(32)	102.6(3)
N(2)-C(1)-C(4)	120.2(6)	C(35)-C(31)-C(32)	110.3(3)
C(2)-C(1)-C(4)	117.0(4)	C(30)-C(31)-C(34)	109.6(3)
C(3)-C(2)-C(1)	128.8(3)	C(35)-C(31)-C(34)	108.8(3)
N(1)-C(3)-C(2)	124.4(5)	C(32)-C(31)-C(34)	111.3(3)
N(1)-C(3)-C(5)	119.0(5)	C(33)-C(32)-C(31)	107.7(4)
C(2)-C(3)-C(5)	116.6(5)	N(3)-C(33)-C(37)	111.7(5)
C(11)-C(6)-C(7)	121.9(6)	N(3)-C(33)-C(32)	100.5(4)
C(11)-C(6)-N(2)	122.5(6)	C(37)-C(33)-C(32)	111.9(5)
C(7)-C(6)-N(2)	115.5(7)	N(3)-C(33)-C(36)	111.7(4)
C(8)-C(7)-C(6)	116.9(8)	C(37)-C(33)-C(36)	108.1(5)
C(8)-C(7)-C(12)	119.7(9)	C(32)-C(33)-C(36)	112.9(4)
C(6)-C(7)-C(12)	123.2(8)	C(43)-C(38)-C(39)	120.9(4)
C(9)-C(8)-C(7)	122.2(10)	C(43)-C(38)-N(3)	119.2(4)
C(8)-C(9)-C(10)	120.3(8)	C(39)-C(38)-N(3)	119.8(3)
C(11)-C(10)-C(9)	119.4(5)	C(40)-C(39)-C(38)	117.2(4)
C(10)-C(11)-C(6)	119.1(5)	C(40)-C(39)-C(44)	118.2(4)
C(10)-C(11)-C(15)	117.1(4)	C(38)-C(39)-C(44)	124.4(3)
C(6)-C(11)-C(15)	123.8(4)	C(41)-C(40)-C(39)	121.9(4)
C(7)-C(12)-C(14)	111.4(7)	C(42)-C(41)-C(40)	120.1(4)
C(7)-C(12)-C(13)	114.5(9)	C(41)-C(42)-C(43)	120.9(6)
C(14)-C(12)-C(13)	110.6(7)	C(42)-C(43)-C(38)	118.8(5)
C(17)-C(15)-C(11)	112.6(3)	C(42)-C(43)-C(47)	118.1(6)
C(17)-C(15)-C(16)	109.6(3)	C(38)-C(43)-C(47)	122.9(5)
C(11)-C(15)-C(16)	110.2(3)	C(39)-C(44)-C(46)	113.0(3)
C(23)-C(18)-C(19)	120.4(6)	C(39)-C(44)-C(45)	109.4(12)
C(23)-C(18)-N(1)	120.9(6)	C(46)-C(44)-C(45)	109.4(6)
C(19)-C(18)-N(1)	118.6(7)	C(43)-C(47)-C(49)	110.1(4)
C(20)-C(19)-C(18)	117.9(8)	C(43)-C(47)-C(48)	113.1(4)
C(20)-C(19)-C(24)	121.9(9)	C(49)-C(47)-C(48)	109.2(3)
C(18)-C(19)-C(24)	120.1(8)		

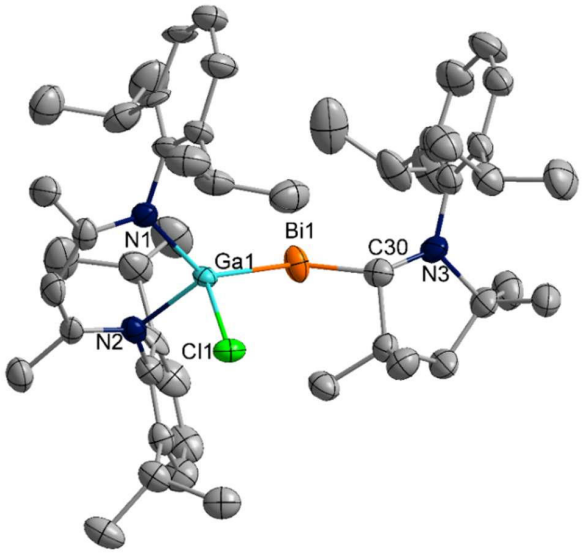


Fig. S30. Solid state structure of **3**. Hydrogen atoms and minor component of the disorder are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S5 Bond lengths [Å] for **3**.

Bi(1)-C(30)	2.199(8)	C(7)-C(8)	1.428(14)	C(27)-C(28)	1.530(12)
Bi(1)-Ga(1)	2.732(2)	C(7)-C(12)	1.513(15)	C(27)-C(29)	1.535(14)
Ga(1)-N(1)	1.93(2)	C(8)-C(9)	1.35(3)	C(30)-C(31)	1.528(12)
Ga(1)-N(2)	2.02(2)	C(9)-C(10)	1.43(2)	C(31)-C(47)	1.514(11)
Ga(1)-Cl(1)	2.276(2)	C(10)-C(11)	1.398(17)	C(31)-C(46)	1.534(13)
N(1)-C(1)	1.31(2)	C(11)-C(15)	1.51(2)	C(31)-C(32)	1.544(12)
N(1)-C(6)	1.460(16)	C(12)-C(13)	1.527(16)	C(32)-C(33)	1.501(18)
N(2)-C(3)	1.355(19)	C(12)-C(14)	1.544(17)	C(34)-C(39)	1.411(16)
N(2)-C(18)	1.423(18)	C(15)-C(17)	1.525(19)	C(34)-C(35)	1.425(14)
N(3)-C(30)	1.338(11)	C(15)-C(16)	1.552(18)	C(35)-C(36)	1.404(14)
N(3)-C(34)	1.459(10)	C(18)-C(19)	1.40(2)	C(35)-C(40)	1.483(13)
N(3)-C(33)	1.534(14)	C(18)-C(23)	1.414(16)	C(36)-C(37)	1.402(17)
C(1)-C(2)	1.390(15)	C(19)-C(20)	1.33(2)	C(37)-C(38)	1.34(2)
C(1)-C(4)	1.513(16)	C(19)-C(24)	1.531(18)	C(38)-C(39)	1.391(19)
C(2)-C(3)	1.414(17)	C(20)-C(21)	1.36(3)	C(39)-C(43)	1.526(15)
C(3)-C(5)	1.495(16)	C(21)-C(22)	1.42(3)	C(40)-C(42)	1.557(15)
C(49)-C(33)	1.53(2)	C(22)-C(23)	1.378(15)	C(40)-C(41)	1.59(4)
C(48)-C(33)	1.539(18)	C(23)-C(27)	1.531(12)	C(43)-C(44)	1.540(15)
C(6)-C(7)	1.364(18)	C(24)-C(25)	1.522(18)	C(43)-C(45)	1.546(15)
C(6)-C(11)	1.44(2)	C(24)-C(26)	1.536(17)		

Table S6 Bond angles [°] for **3**.

C(30)-Bi(1)-Ga(1)	103.0(2)	C(19)-C(20)-C(21)	127(2)
N(1)-Ga(1)-N(2)	95.0(4)	C(20)-C(21)-C(22)	116.4(17)
N(1)-Ga(1)-Cl(1)	104.7(7)	C(23)-C(22)-C(21)	120.3(13)

N(2)-Ga(1)-Cl(1)	98.3(7)	C(22)-C(23)-C(18)	119.3(11)
N(1)-Ga(1)-Bi(1)	132.6(7)	C(22)-C(23)-C(27)	117.3(10)
N(2)-Ga(1)-Bi(1)	101.2(6)	C(18)-C(23)-C(27)	123.3(10)
Cl(1)-Ga(1)-Bi(1)	116.35(15)	C(25)-C(24)-C(19)	112.3(12)
C(1)-N(1)-C(6)	120.5(16)	C(25)-C(24)-C(26)	111.4(11)
C(1)-N(1)-Ga(1)	120.3(12)	C(19)-C(24)-C(26)	112.6(14)
C(6)-N(1)-Ga(1)	119.2(14)	C(28)-C(27)-C(23)	111.0(7)
C(3)-N(2)-C(18)	119.7(17)	C(28)-C(27)-C(29)	110.6(8)
C(3)-N(2)-Ga(1)	119.7(12)	C(23)-C(27)-C(29)	111.6(8)
C(18)-N(2)-Ga(1)	120.5(13)	N(3)-C(30)-C(31)	108.6(7)
C(30)-N(3)-C(34)	123.3(7)	N(3)-C(30)-Bi(1)	120.4(6)
C(30)-N(3)-C(33)	114.7(8)	C(31)-C(30)-Bi(1)	131.0(5)
C(34)-N(3)-C(33)	121.7(8)	C(47)-C(31)-C(30)	113.6(7)
N(1)-C(1)-C(2)	124.4(12)	C(47)-C(31)-C(46)	109.4(7)
N(1)-C(1)-C(4)	119.2(12)	C(30)-C(31)-C(46)	109.0(7)
C(2)-C(1)-C(4)	116.2(10)	C(47)-C(31)-C(32)	111.0(8)
C(1)-C(2)-C(3)	129.2(7)	C(30)-C(31)-C(32)	102.3(7)
N(2)-C(3)-C(2)	121.6(13)	C(46)-C(31)-C(32)	111.4(8)
N(2)-C(3)-C(5)	121.4(13)	C(33)-C(32)-C(31)	108.4(9)
C(2)-C(3)-C(5)	117.0(10)	C(32)-C(33)-N(3)	100.6(9)
C(7)-C(6)-C(11)	121.9(12)	C(32)-C(33)-C(49)	113.7(11)
C(7)-C(6)-N(1)	120.7(13)	N(3)-C(33)-C(49)	110.4(12)
C(11)-C(6)-N(1)	117.4(14)	C(32)-C(33)-C(48)	113.9(12)
C(6)-C(7)-C(8)	118.2(11)	N(3)-C(33)-C(48)	111.1(10)
C(6)-C(7)-C(12)	124.2(10)	C(49)-C(33)-C(48)	107.2(11)
C(8)-C(7)-C(12)	117.6(11)	C(39)-C(34)-C(35)	121.8(9)
C(9)-C(8)-C(7)	121.6(14)	C(39)-C(34)-N(3)	119.6(9)
C(8)-C(9)-C(10)	120.6(17)	C(35)-C(34)-N(3)	118.6(8)
C(11)-C(10)-C(9)	119.0(17)	C(36)-C(35)-C(34)	116.5(9)
C(10)-C(11)-C(6)	118.4(15)	C(36)-C(35)-C(40)	117.6(9)
C(10)-C(11)-C(15)	121.3(16)	C(34)-C(35)-C(40)	125.7(8)
C(6)-C(11)-C(15)	120.2(13)	C(37)-C(36)-C(35)	121.3(10)
C(7)-C(12)-C(13)	111.6(9)	C(38)-C(37)-C(36)	120.0(11)
C(7)-C(12)-C(14)	111.7(9)	C(37)-C(38)-C(39)	122.9(16)
C(13)-C(12)-C(14)	110.4(11)	C(38)-C(39)-C(34)	117.4(13)
C(11)-C(15)-C(17)	114.5(14)	C(38)-C(39)-C(43)	118.9(14)
C(11)-C(15)-C(16)	110.1(13)	C(34)-C(39)-C(43)	123.4(11)
C(17)-C(15)-C(16)	108.8(11)	C(35)-C(40)-C(42)	112.5(9)
C(19)-C(18)-C(23)	120.0(14)	C(35)-C(40)-C(41)	107(2)
C(19)-C(18)-N(2)	118.0(14)	C(42)-C(40)-C(41)	111.2(12)
C(23)-C(18)-N(2)	122.1(14)	C(39)-C(43)-C(44)	112.8(10)
C(20)-C(19)-C(18)	117.4(16)	C(39)-C(43)-C(45)	110.3(10)
C(20)-C(19)-C(24)	119.6(17)	C(44)-C(43)-C(45)	109.7(9)
C(18)-C(19)-C(24)	122.7(14)		

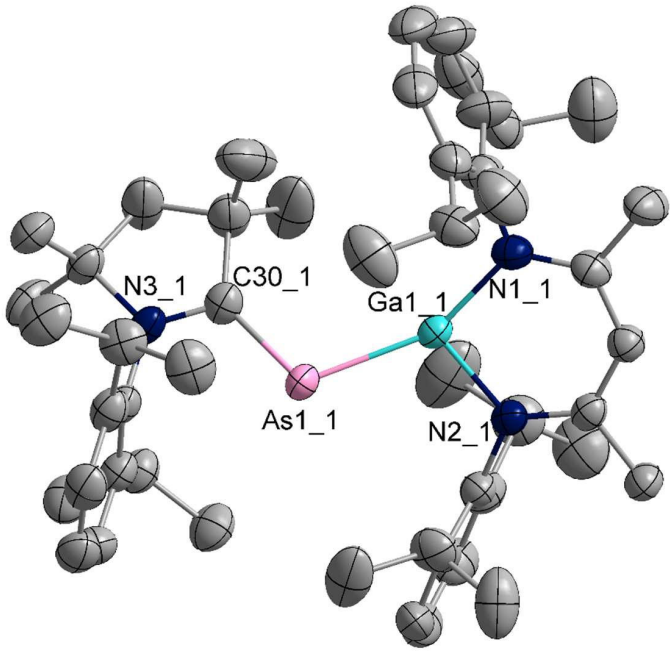


Fig. S31. Solid state structure of **4**. Hydrogen atoms, anionic part and minor component of the disorder are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S7 Bond lengths [Å] for **4**.

Al(1)-O17	1.548(14)	C331-C481	1.500(8)	F75-C45	1.372(9)
Al(1)-O18	1.64(2)	C331-C491	1.518(10)	F85-C45	1.285(9)
Al(1)-O19	1.665(18)	C341-C351	1.394(6)	F95-C45	1.355(9)
Al(1)-O14	1.721(3)	C341-C391	1.408(6)	O15-C15	1.368(7)
Al(1)-O16	1.721(3)	C351-C361	1.397(6)	C15-C45	1.542(9)
Al(1)-O12	1.728(4)	C351-C401	1.534(6)	C15-C25	1.545(9)
Al(1)-O13	1.731(6)	C361-C371	1.376(7)	C15-C35	1.547(9)
Al(1)-O15	1.787(6)	C371-C381	1.350(8)	F16-C26	1.331(12)
As11-C301	1.892(4)	C381-C391	1.410(6)	F26-C26	1.334(12)
As11-Ga11	2.3410(10)	C391-C431	1.519(7)	F36-C26	1.333(10)
Ga11-N11	1.904(4)	C401-C421	1.534(6)	F46-C36	1.312(12)
Ga11-N21	1.910(3)	C401-C411	1.541(7)	F56-C36	1.344(12)
As1'1-C301	1.813(7)	C431-C441	1.533(7)	F66-C36	1.325(12)
As1'1-Ga1'1	2.385(11)	C431-C451	1.551(7)	F76-C46	1.320(11)
Ga1'1-N11	1.992(9)	F12-C22	1.343(7)	F86-C46	1.318(12)
Ga1'1-N21	2.041(8)	F22-C22	1.334(7)	F96-C46	1.318(11)
N11-C11	1.339(6)	F32-C22	1.326(7)	O16-C16	1.345(5)
N11-C61	1.449(5)	F42-C32	1.340(7)	C16-C26	1.529(9)
N21-C31	1.330(5)	F52-C32	1.325(7)	C16-C36	1.552(9)
N21-C181	1.455(5)	F62-C32	1.309(7)	C16-C46	1.571(9)
N31-C301	1.309(5)	F72-C42	1.327(6)	F17-C27	1.331(13)
N31-C341	1.463(5)	F82-C42	1.320(8)	F27-C27	1.325(13)

N31-C311	1.525(5)	F92-C42	1.327(6)	F37-C27	1.338(13)
C11-C21	1.390(6)	O12-C12	1.341(6)	F47-C37	1.324(13)
C11-C41	1.508(6)	C12-C22	1.543(8)	F57-C37	1.347(13)
C21-C31	1.398(5)	C12-C32	1.553(7)	F67-C37	1.341(13)
C31-C51	1.505(5)	C12-C42	1.577(7)	F77-C47	1.315(13)
C61-C111	1.404(7)	F13-C23	1.321(7)	F87-C47	1.336(13)
C61-C71	1.415(7)	F23-C23	1.326(7)	F97-C47	1.333(13)
C71-C81	1.405(8)	F33-C23	1.332(7)	O17-C17	1.333(12)
C71-C12'1	1.480(13)	F43-C33	1.331(7)	C17-C37	1.541(12)
C71-C121	1.558(13)	F53-C33	1.336(8)	C17-C47	1.547(12)
C81-C91	1.362(10)	F63-C33	1.319(8)	C17-C27	1.559(12)
C91-C101	1.379(10)	F73-C43	1.341(8)	O18-C18	1.349(13)
C101-C111	1.395(7)	F83-C43	1.338(8)	C18-C38	1.539(13)
C111-C151	1.519(8)	F93-C43	1.327(8)	C18-C28	1.547(13)
C121-C141	1.520(14)	O13-C13	1.361(7)	C18-C48	1.550(13)
C121-C131	1.531(12)	C13-C33	1.541(8)	C28-F28	1.328(13)
C12'1-C13'1	1.517(14)	C13-C23	1.545(8)	C28-F18	1.333(13)
C12'1-C14'1	1.525(12)	C13-C43	1.563(8)	C28-F38	1.335(13)
C151-C171	1.513(8)	F14-C24	1.329(11)	C38-F68	1.325(13)
C151-C161	1.568(9)	F24-C24	1.321(12)	C38-F48	1.331(13)
C181-C231	1.400(6)	F34-C24	1.307(10)	C38-F58	1.332(13)
C181-C191	1.409(6)	F44-C34	1.309(12)	C48-F88	1.330(13)
C191-C201	1.396(7)	F54-C34	1.335(10)	C48-F98	1.333(13)
C191-C241	1.538(7)	F64-C34	1.315(11)	C48-F78	1.336(13)
C201-C211	1.373(9)	F74-C44	1.368(9)	F19-C29	1.331(14)
C211-C221	1.364(9)	F84-C44	1.290(11)	F29-C29	1.333(14)
C221-C231	1.412(7)	F94-C44	1.334(11)	F39-C29	1.325(14)
C231-C271	1.509(7)	O14-C14	1.345(5)	F49-C39	1.330(14)
C241-C261	1.530(8)	C14-C44	1.535(8)	F59-C39	1.327(14)
C241-C251	1.537(10)	C14-C34	1.560(9)	F69-C39	1.316(13)
C271-C281	1.518(9)	C14-C24	1.567(8)	F79-C49	1.329(14)
C271-C291	1.527(8)	F15-C25	1.305(9)	F89-C49	1.330(14)
C301-C331	1.537(6)	F25-C25	1.379(8)	F99-C49	1.333(14)
C311-C471	1.504(6)	F35-C25	1.341(8)	O19-C19	1.345(14)
C311-C461	1.519(7)	F45-C35	1.308(10)	C19-C49	1.545(13)
C311-C321	1.521(6)	F55-C35	1.352(8)	C19-C29	1.549(13)
C321-C331	1.542(7)	F65-C35	1.374(10)	C19-C39	1.557(13)

Table S8 Bond angles [°] for **4**.

C301-As11-Ga11	112.06(13)	F83-C43-C13	111.6(5)
N11-Ga11-N21	97.97(14)	F73-C43-C13	112.0(6)
N11-Ga11-As11	147.29(11)	C14-O14-Al(1)	147.7(3)
N21-Ga11-As11	110.52(10)	O14-C14-C44	111.7(4)
C301-As1'1-Ga1'1	111.8(4)	O14-C14-C34	112.4(4)
N11-Ga1'1-N21	91.0(4)	C44-C14-C34	108.4(6)
N11-Ga1'1-As1'1	108.4(6)	O14-C14-C24	107.5(4)
N21-Ga1'1-As1'1	114.1(4)	C44-C14-C24	108.1(5)
C11-N11-C61	119.3(3)	C34-C14-C24	108.5(7)
C11-N11-Ga11	123.1(3)	F34-C24-F24	105.6(11)
C61-N11-Ga11	117.4(3)	F34-C24-F14	110.6(10)
C11-N11-Ga1'1	125.5(3)	F24-C24-F14	109.4(12)
C61-N11-Ga1'1	114.0(4)	F34-C24-C14	112.2(8)
C31-N21-C181	119.3(3)	F24-C24-C14	111.1(9)
C31-N21-Ga11	122.7(3)	F14-C24-C14	107.9(7)
C181-N21-Ga11	117.7(2)	F44-C34-F64	112.5(12)
C31-N21-Ga1'1	122.9(3)	F44-C34-F54	103.9(12)
C181-N21-Ga1'1	113.6(3)	F64-C34-F54	107.7(12)
C301-N31-C341	121.7(3)	F44-C34-C14	110.2(10)
C301-N31-C311	115.9(3)	F64-C34-C14	110.9(9)
C341-N31-C311	122.4(3)	F54-C34-C14	111.5(8)
N11-C11-C21	123.1(4)	F84-C44-F94	104.9(11)
N11-C11-C41	119.7(4)	F84-C44-F74	116.9(11)
C21-C11-C41	117.1(4)	F94-C44-F74	105.2(8)
C11-C21-C31	128.6(4)	F84-C44-C14	109.3(8)
N21-C31-C21	123.8(3)	F94-C44-C14	109.0(8)
N21-C31-C51	119.4(3)	F74-C44-C14	111.1(7)
C21-C31-C51	116.8(3)	C15-O15-Al(1)	143.7(5)
C111-C61-C71	123.2(4)	O15-C15-C45	106.7(6)
C111-C61-N11	118.0(4)	O15-C15-C25	115.4(6)
C71-C61-N11	118.8(4)	C45-C15-C25	109.3(6)
C81-C71-C61	114.9(5)	O15-C15-C35	106.3(6)
C81-C71-C12'1	121.5(7)	C45-C15-C35	111.3(6)
C61-C71-C12'1	121.5(6)	C25-C15-C35	107.8(6)
C81-C71-C121	122.9(6)	F15-C25-F35	110.1(7)
C61-C71-C121	121.1(6)	F15-C25-F25	111.2(7)
C91-C81-C71	123.1(6)	F35-C25-F25	104.7(6)
C81-C91-C101	120.4(5)	F15-C25-C15	111.6(6)
C91-C101-C111	120.6(5)	F35-C25-C15	112.3(7)
C101-C111-C61	117.7(5)	F25-C25-C15	106.6(6)
C101-C111-C151	119.1(5)	F45-C35-F55	110.2(7)
C61-C111-C151	123.2(4)	F45-C35-F65	110.7(9)
C141-C121-C131	108.7(10)	F55-C35-F65	105.1(8)

C141-C121-C71	110.3(11)	F45-C35-C15	111.1(7)
C131-C121-C71	117.3(10)	F55-C35-C15	112.3(7)
C71-C12'1-C13'1	101.3(10)	F65-C35-C15	107.2(7)
C71-C12'1-C14'1	115.8(10)	F85-C45-F95	109.1(8)
C13'1-C12'1-C14'1	108.8(10)	F85-C45-F75	111.8(7)
C171-C151-C111	112.6(5)	F95-C45-F75	104.2(7)
C171-C151-C161	109.2(5)	F85-C45-C15	112.6(7)
C111-C151-C161	112.4(5)	F95-C45-C15	109.3(6)
C231-C181-C191	121.8(4)	F75-C45-C15	109.4(6)
C231-C181-N21	120.3(4)	C16-O16-Al(1)	147.7(3)
C191-C181-N21	117.9(3)	O16-C16-C26	113.2(5)
C201-C191-C181	118.1(5)	O16-C16-C36	108.0(5)
C201-C191-C241	120.6(4)	C26-C16-C36	111.2(6)
C181-C191-C241	121.3(4)	O16-C16-C46	106.7(5)
C211-C201-C191	120.8(5)	C26-C16-C46	109.0(7)
C221-C211-C201	120.8(5)	C36-C16-C46	108.6(6)
C211-C221-C231	121.4(5)	F16-C26-F36	104.9(13)
C181-C231-C221	117.1(4)	F16-C26-F26	107.1(12)
C181-C231-C271	122.6(4)	F36-C26-F26	110.6(10)
C221-C231-C271	120.3(4)	F16-C26-C16	110.7(11)
C261-C241-C251	110.9(5)	F36-C26-C16	111.5(8)
C261-C241-C191	112.4(5)	F26-C26-C16	111.7(9)
C251-C241-C191	109.2(5)	F46-C36-F66	108.8(15)
C231-C271-C281	110.5(4)	F46-C36-F56	107.5(15)
C231-C271-C291	112.6(5)	F66-C36-F56	110.0(15)
C281-C271-C291	109.0(4)	F46-C36-C16	112.9(12)
N31-C301-C331	109.7(4)	F66-C36-C16	110.6(10)
N31-C301-As1'1	131.0(4)	F56-C36-C16	107.1(10)
C331-C301-As1'1	112.6(4)	F96-C46-F86	106.5(10)
N31-C301-As11	116.8(3)	F96-C46-F76	109.4(11)
C331-C301-As11	133.5(3)	F86-C46-F76	110.0(11)
C471-C311-C461	107.3(4)	F96-C46-C16	109.0(8)
C471-C311-C321	116.4(5)	F86-C46-C16	112.9(9)
C461-C311-C321	111.4(4)	F76-C46-C16	109.0(9)
C471-C311-N31	110.7(3)	C17-O17-Al(1)	169.6(15)
C461-C311-N31	111.3(3)	O17-C17-C37	110.3(13)
C321-C311-N31	99.7(3)	O17-C17-C47	111.5(13)
C311-C321-C331	109.1(4)	C37-C17-C47	106.8(11)
C481-C331-C491	113.3(6)	O17-C17-C27	114.7(12)
C481-C331-C301	112.5(5)	C37-C17-C27	107.7(11)
C491-C331-C301	107.8(4)	C47-C17-C27	105.3(12)
C481-C331-C321	109.3(5)	F27-C27-F17	107.7(18)
C491-C331-C321	112.1(5)	F27-C27-F37	115.6(19)
C301-C331-C321	101.4(4)	F17-C27-F37	112.4(19)

C351-C341-C391	121.8(4)	F27-C27-C17	107.8(13)
C351-C341-N31	119.4(3)	F17-C27-C17	108.4(16)
C391-C341-N31	118.7(4)	F37-C27-C17	104.7(15)
C341-C351-C361	117.6(4)	F47-C37-F67	116.8(17)
C341-C351-C401	124.6(4)	F47-C37-F57	111.7(18)
C361-C351-C401	117.8(4)	F67-C37-F57	102.8(15)
C371-C361-C351	121.5(4)	F47-C37-C17	106.1(12)
C381-C371-C361	120.2(4)	F67-C37-C17	111.5(14)
C371-C381-C391	121.7(4)	F57-C37-C17	107.8(14)
C341-C391-C381	117.0(4)	F77-C47-F97	116.6(18)
C341-C391-C431	125.1(4)	F77-C47-F87	113.0(18)
C381-C391-C431	117.8(4)	F97-C47-F87	107.4(18)
C351-C401-C421	110.4(4)	F77-C47-C17	107.4(13)
C351-C401-C411	111.4(4)	F97-C47-C17	105.2(15)
C421-C401-C411	108.7(4)	F87-C47-C17	106.5(15)
C391-C431-C441	112.1(4)	C18-O18-Al(1)	161(2)
C391-C431-C451	109.8(4)	O18-C18-C38	109.7(15)
C441-C431-C451	109.8(4)	O18-C18-C28	109.2(14)
C12-O12-Al(1)	146.7(3)	C38-C18-C28	109.6(12)
O12-C12-C22	110.7(4)	O18-C18-C48	107.2(13)
O12-C12-C32	107.4(4)	C38-C18-C48	110.8(12)
C22-C12-C32	110.0(5)	C28-C18-C48	110.2(12)
O12-C12-C42	111.8(4)	F28-C28-F18	105.3(17)
C22-C12-C42	108.7(4)	F28-C28-F38	109.2(18)
C32-C12-C42	108.2(4)	F18-C28-F38	109.6(18)
F32-C22-F22	107.6(6)	F28-C28-C18	111.5(16)
F32-C22-F12	107.7(5)	F18-C28-C18	111.2(14)
F22-C22-F12	107.4(6)	F38-C28-C18	110.0(14)
F32-C22-C12	112.9(5)	F68-C38-F48	111.8(19)
F22-C22-C12	110.6(5)	F68-C38-F58	108.4(18)
F12-C22-C12	110.5(5)	F48-C38-F58	109.2(18)
F62-C32-F52	107.4(5)	F68-C38-C18	109.0(15)
F62-C32-F42	108.4(5)	F48-C38-C18	109.9(15)
F52-C32-F42	107.6(5)	F58-C38-C18	108.3(14)
F62-C32-C12	111.3(5)	F88-C48-F98	107.8(18)
F52-C32-C12	113.1(5)	F88-C48-F78	110.6(18)
F42-C32-C12	108.8(5)	F98-C48-F78	105.8(19)
F82-C42-F92	106.5(5)	F88-C48-C18	112.2(16)
F82-C42-F72	108.5(5)	F98-C48-C18	110.7(16)
F92-C42-F72	108.1(5)	F78-C48-C18	109.5(15)
F82-C42-C12	111.5(5)	C19-O19-Al(1)	159.4(17)
F92-C42-C12	109.7(4)	O19-C19-C49	110.9(14)
F72-C42-C12	112.3(5)	O19-C19-C29	112.4(15)
C13-O13-Al(1)	149.5(7)	C49-C19-C29	108.1(13)

O13-C13-C33	113.5(6)	O19-C19-C39	104.9(14)
O13-C13-C23	105.5(5)	C49-C19-C39	110.9(14)
C33-C13-C23	110.3(5)	C29-C19-C39	109.7(14)
O13-C13-C43	109.7(5)	F39-C29-F19	111(2)
C33-C13-C43	108.4(6)	F39-C29-F29	110(2)
C23-C13-C43	109.4(5)	F19-C29-F29	109(2)
F13-C23-F23	106.7(6)	F39-C29-C19	109.9(17)
F13-C23-F33	107.0(5)	F19-C29-C19	108.6(18)
F23-C23-F33	108.4(5)	F29-C29-C19	109.7(18)
F13-C23-C13	112.4(5)	F69-C39-F59	113(2)
F23-C23-C13	110.1(5)	F69-C39-F49	111(2)
F33-C23-C13	112.0(6)	F59-C39-F49	109(2)
F63-C33-F43	108.8(6)	F69-C39-C19	109.8(18)
F63-C33-F53	107.2(6)	F59-C39-C19	107.1(17)
F43-C33-F53	107.8(6)	F49-C39-C19	107.2(16)
F63-C33-C13	111.7(6)	F79-C49-F89	111(2)
F43-C33-C13	112.2(6)	F79-C49-F99	105.0(19)
F53-C33-C13	109.0(5)	F89-C49-F99	110(2)
F93-C43-F83	106.8(6)	F79-C49-C19	111.1(15)
F93-C43-F73	107.7(6)	F89-C49-C19	109.0(15)
F83-C43-F73	106.7(6)	F99-C49-C19	110.7(18)
F93-C43-C13	111.8(5)		

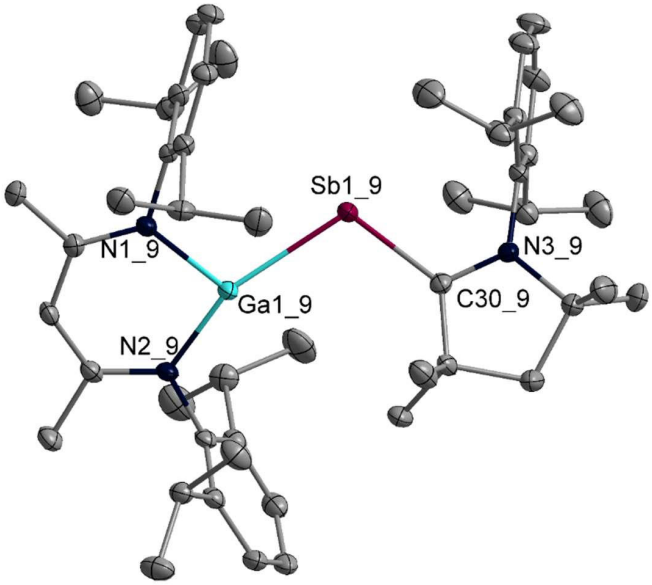


Fig. S32. Solid state structure of **6**. Hydrogen atoms, anionic part are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S9 Bond lengths [Å] for **6**.

B(1)-C17	1.633(3)	C55-C85	1.502(3)	C279-C289	1.526(4)
B(1)-C18	1.641(3)	F16-C76	1.332(9)	C279-C299	1.529(3)
B(1)-C16	1.643(3)	F26-C76	1.312(9)	C309-C339	1.510(3)
B(1)-C15	1.644(3)	F36-C76	1.304(10)	C319-C479	1.519(4)
B(2)-C12	1.634(3)	F1'6-C76	1.325(7)	C319-C469	1.528(3)
B(2)-C11	1.640(3)	F2'6-C76	1.342(6)	C319-C329	1.534(3)
B(2)-C14	1.641(3)	F3'6-C76	1.327(6)	C329-C339	1.548(3)
B(2)-C13	1.643(3)	F46-C86	1.335(3)	C339-C489	1.528(3)
F11-C71	1.339(3)	F56-C86	1.330(3)	C339-C499	1.534(3)
F21-C71	1.336(3)	F66-C86	1.317(3)	C349-C359	1.409(3)
F31-C71	1.345(3)	C16-C26	1.397(3)	C349-C399	1.411(3)
F41-C81	1.337(3)	C16-C66	1.399(3)	C359-C369	1.394(3)
F51-C81	1.338(3)	C26-C36	1.400(3)	C359-C409	1.520(3)
F61-C81	1.339(3)	C36-C46	1.383(4)	C369-C379	1.372(4)
C11-C21	1.398(3)	C36-C76	1.495(4)	C379-C389	1.382(4)
C11-C61	1.401(3)	C46-C56	1.387(4)	C389-C399	1.396(3)
C21-C31	1.388(3)	C56-C66	1.385(3)	C399-C439	1.522(3)
C31-C41	1.387(3)	C56-C86	1.494(4)	C409-C419	1.532(3)
C31-C71	1.501(3)	F17-C77	1.334(3)	C409-C429	1.534(4)
C41-C51	1.389(3)	F27-C77	1.336(3)	C439-C449	1.530(4)
C51-C61	1.385(3)	F37-C77	1.329(3)	C439-C459	1.540(3)
C51-C81	1.501(3)	F47-C87	1.321(3)	Sb110-C3010	2.113(2)
F12-C72	1.314(7)	F57-C87	1.341(3)	Sb110-Ga110	2.5561(3)
F22-C72	1.332(7)	F67-C87	1.330(3)	Ga110-N110	1.9069(17)
F32-C72	1.334(7)	C17-C27	1.402(3)	Ga110-N210	1.9299(17)

F3'2-C72	1.348(10)	C17-C67	1.403(3)	N110-C110	1.350(3)
F1'2-C72	1.336(10)	C27-C37	1.389(3)	N110-C610	1.448(2)
F2'2-C72	1.291(10)	C37-C47	1.384(3)	N210-C310	1.322(3)
F1"2-C72	1.324(13)	C37-C77	1.502(3)	N210-C1810	1.449(3)
F2"2-C72	1.325(12)	C47-C57	1.391(3)	N310-C3010	1.324(3)
F3"2-C72	1.325(13)	C57-C67	1.390(3)	N310-C3410	1.452(3)
F42-C82	1.330(3)	C57-C87	1.495(3)	N310-C3110	1.520(3)
F52-C82	1.334(3)	F18-C78	1.339(3)	C110-C210	1.390(3)
F62-C82	1.350(3)	F28-C78	1.337(3)	C110-C410	1.504(3)
C12-C62	1.399(3)	F38-C78	1.341(3)	C210-C310	1.403(3)
C12-C22	1.400(3)	F48-C88	1.333(3)	C310-C510	1.509(3)
C22-C32	1.391(3)	F58-C88	1.336(3)	C610-C1110	1.393(3)
C32-C42	1.386(3)	F68-C88	1.316(3)	C610-C710	1.407(3)
C32-C72	1.494(3)	C18-C68	1.400(3)	C710-C810	1.395(3)
C42-C52	1.382(3)	C18-C28	1.403(3)	C710-C1210	1.525(4)
C52-C62	1.389(3)	C28-C38	1.401(3)	C810-C910	1.379(4)
C52-C82	1.499(3)	C38-C48	1.383(3)	C910-C1010	1.377(4)
F13-C73	1.332(3)	C38-C78	1.500(3)	C1010-C1110	1.399(3)
F23-C73	1.335(3)	C48-C58	1.383(3)	C1110-C1510	1.516(4)
F33-C73	1.330(3)	C58-C68	1.394(3)	C1210-C1310	1.524(4)
F43-C83	1.328(3)	C58-C88	1.496(3)	C1210-C1410	1.534(4)
F53-C83	1.335(3)	Sb19-C309	2.114(2)	C1510-C1710	1.515(4)
F63-C83	1.344(3)	Sb19-Ga19	2.5485(3)	C1510-C1610	1.530(4)
C13-C23	1.398(3)	Ga19-N29	1.9007(17)	C1810-C2310	1.400(3)
C13-C63	1.401(3)	Ga19-N19	1.9224(17)	C1810-C1910	1.409(3)
C23-C33	1.390(3)	N19-C19	1.334(3)	C1910-C2010	1.397(3)
C33-C43	1.386(3)	N19-C69	1.446(3)	C1910-C2410	1.515(3)
C33-C73	1.489(3)	N29-C39	1.349(3)	C2010-C2110	1.374(4)
C43-C53	1.386(3)	N29-C189	1.450(3)	C2110-C2210	1.380(4)
C53-C63	1.394(3)	N39-C309	1.324(3)	C2210-C2310	1.398(3)
C53-C83	1.496(3)	N39-C349	1.459(3)	C2310-C2710	1.523(3)
F14-C74	1.339(3)	N39-C319	1.518(3)	C2410-C2610	1.522(3)
F24-C74	1.332(3)	C19-C29	1.398(3)	C2410-C2510	1.525(3)
F34-C74	1.342(3)	C19-C49	1.505(3)	C2710-C2910	1.526(4)
F44-C84	1.332(3)	C29-C39	1.384(3)	C2710-C2810	1.526(3)
F54-C84	1.340(3)	C39-C59	1.506(3)	C3010-C3310	1.518(3)
F64-C84	1.340(3)	C69-C79	1.398(3)	C3110-C4610	1.522(4)
C14-C24	1.404(3)	C69-C119	1.405(3)	C3110-C4710	1.525(4)
C14-C64	1.409(3)	C79-C89	1.394(3)	C3110-C3210	1.527(3)
C24-C34	1.387(3)	C79-C129	1.522(3)	C3210-C3310	1.548(3)
C34-C44	1.385(3)	C89-C99	1.379(3)	C3310-C4910	1.525(3)
C34-C74	1.504(3)	C99-C109	1.385(4)	C3310-C4810	1.532(4)
C44-C54	1.391(3)	C109-C119	1.396(3)	C3410-C3510	1.411(3)
C54-C64	1.384(3)	C119-C159	1.524(3)	C3410-C3910	1.411(3)

C54-C84	1.502(3)	C129-C139	1.525(3)	C3510-C3610	1.393(3)
F15-C75	1.316(3)	C129-C149	1.529(3)	C3510-C4010	1.518(3)
F25-C75	1.344(3)	C159-C169	1.521(3)	C3610-C3710	1.373(4)
F35-C75	1.318(3)	C159-C179	1.528(3)	C3710-C3810	1.381(4)
F45-C85	1.335(3)	C189-C239	1.400(3)	C3810-C3910	1.392(3)
F55-C85	1.333(3)	C189-C199	1.405(3)	C3910-C4310	1.523(3)
F65-C85	1.345(3)	C199-C209	1.389(3)	C4010-C4110	1.531(3)
C15-C65	1.404(3)	C199-C249	1.520(3)	C4010-C4210	1.543(3)
C15-C25	1.405(3)	C209-C219	1.385(3)	C4310-C4410	1.533(4)
C25-C35	1.389(3)	C219-C229	1.382(3)	C4310-C4510	1.536(4)
C35-C45	1.388(3)	C229-C239	1.396(3)	C111-Cl111	1.739(11)
C35-C75	1.499(3)	C239-C279	1.514(3)	C111-Cl211	1.747(11)
C45-C55	1.382(3)	C249-C259	1.519(3)	C112-Cl112	1.739(9)
C55-C65	1.388(3)	C249-C269	1.524(3)	C112-Cl212	1.753(9)

Table S10 Bond angles [°] for **6**.

C17-B(1)-C18	114.19(17)	C48-C38-C28	120.7(2)
C17-B(1)-C16	112.54(18)	C48-C38-C78	119.61(19)
C18-B(1)-C16	103.23(16)	C28-C38-C78	119.6(2)
C17-B(1)-C15	104.66(16)	C58-C48-C38	118.73(19)
C18-B(1)-C15	112.38(18)	C48-C58-C68	120.3(2)
C16-B(1)-C15	110.00(17)	C48-C58-C88	120.8(2)
C12-B(2)-C11	111.97(18)	C68-C58-C88	118.9(2)
C12-B(2)-C14	112.85(17)	C58-C68-C18	122.6(2)
C11-B(2)-C14	103.71(16)	F28-C78-F18	106.6(2)
C12-B(2)-C13	105.35(16)	F28-C78-F38	106.40(18)
C11-B(2)-C13	112.29(17)	F18-C78-F38	106.5(2)
C14-B(2)-C13	110.86(17)	F28-C78-C38	112.1(2)
C21-C11-C61	115.60(19)	F18-C78-C38	112.58(18)
C21-C11-B(2)	122.52(18)	F38-C78-C38	112.2(2)
C61-C11-B(2)	121.73(18)	F68-C88-F48	106.8(2)
C31-C21-C11	122.3(2)	F68-C88-F58	106.4(2)
C41-C31-C21	120.99(19)	F48-C88-F58	105.4(2)
C41-C31-C71	120.0(2)	F68-C88-C58	113.2(2)
C21-C31-C71	118.84(19)	F48-C88-C58	112.8(2)
C31-C41-C51	117.7(2)	F58-C88-C58	111.7(2)
C61-C51-C41	120.98(19)	C309-Sb19-Ga19	109.44(6)
C61-C51-C81	118.84(19)	N29-Ga19-N19	96.36(7)
C41-C51-C81	120.1(2)	N29-Ga19-Sb19	153.19(5)
C51-C61-C11	122.36(19)	N19-Ga19-Sb19	107.91(5)
F21-C71-F11	107.08(18)	C19-N19-C69	119.94(17)
F21-C71-F31	106.6(2)	C19-N19-Ga19	124.99(14)
F11-C71-F31	105.56(19)	C69-N19-Ga19	115.03(13)

F21-C71-C31	113.02(19)	C39-N29-C189	118.97(17)
F11-C71-C31	112.74(19)	C39-N29-Ga19	123.70(14)
F31-C71-C31	111.38(19)	C189-N29-Ga19	117.23(13)
F41-C81-F51	106.92(19)	C309-N39-C349	121.35(18)
F41-C81-F61	106.82(18)	C309-N39-C319	114.95(17)
F51-C81-F61	106.02(17)	C349-N39-C319	123.69(16)
F41-C81-C51	112.95(18)	N19-C19-C29	122.36(19)
F51-C81-C51	111.72(18)	N19-C19-C49	120.34(18)
F61-C81-C51	111.99(19)	C29-C19-C49	117.30(18)
C62-C12-C22	115.67(19)	C39-C29-C19	128.24(19)
C62-C12-B(2)	121.71(19)	N29-C39-C29	124.15(19)
C22-C12-B(2)	122.36(19)	N29-C39-C59	118.35(19)
C32-C22-C12	122.1(2)	C29-C39-C59	117.50(19)
C42-C32-C22	121.1(2)	C79-C69-C119	122.89(19)
C42-C32-C72	119.5(2)	C79-C69-N19	119.28(18)
C22-C32-C72	119.4(2)	C119-C69-N19	117.69(19)
C52-C42-C32	117.8(2)	C89-C79-C69	117.3(2)
C42-C52-C62	121.0(2)	C89-C79-C129	120.0(2)
C42-C52-C82	119.6(2)	C69-C79-C129	122.71(18)
C62-C52-C82	119.3(2)	C99-C89-C79	120.9(2)
C52-C62-C12	122.3(2)	C89-C99-C109	120.8(2)
F1"2-C72-F3"2	106.3(13)	C99-C109-C119	120.6(2)
F1"2-C72-F2"2	106.0(12)	C109-C119-C69	117.2(2)
F3"2-C72-F2"2	106.2(12)	C109-C119-C159	121.0(2)
F12-C72-F22	105.6(6)	C69-C119-C159	121.74(19)
F12-C72-F32	106.3(6)	C79-C129-C139	112.83(19)
F22-C72-F32	104.9(6)	C79-C129-C149	110.36(18)
F2'2-C72-F1'2	107.5(10)	C139-C129-C149	110.5(2)
F2'2-C72-F3'2	107.0(8)	C169-C159-C119	112.3(2)
F1'2-C72-F3'2	103.4(9)	C169-C159-C179	110.4(2)
F2'2-C72-C32	118.2(9)	C119-C159-C179	112.7(2)
F12-C72-C32	114.1(5)	C239-C189-C199	123.12(19)
F1"2-C72-C32	111.1(18)	C239-C189-N29	119.44(19)
F3"2-C72-C32	115.6(16)	C199-C189-N29	117.40(19)
F2"2-C72-C32	111.1(15)	C209-C199-C189	117.2(2)
F22-C72-C32	110.8(6)	C209-C199-C249	121.5(2)
F32-C72-C32	114.4(6)	C189-C199-C249	121.19(19)
F1'2-C72-C32	110.6(9)	C219-C209-C199	121.0(2)
F3'2-C72-C32	109.2(8)	C229-C219-C209	120.5(2)
F42-C82-F52	107.2(2)	C219-C229-C239	121.2(2)
F42-C82-F62	106.58(19)	C229-C239-C189	116.9(2)
F52-C82-F62	106.1(2)	C229-C239-C279	120.1(2)
F42-C82-C52	113.1(2)	C189-C239-C279	123.0(2)
F52-C82-C52	113.0(2)	C259-C249-C199	113.73(18)

F62-C82-C52	110.6(2)	C259-C249-C269	109.9(2)
C23-C13-C63	115.53(19)	C199-C249-C269	111.02(18)
C23-C13-B(2)	121.31(19)	C239-C279-C289	111.6(2)
C63-C13-B(2)	123.11(19)	C239-C279-C299	111.7(2)
C33-C23-C13	122.6(2)	C289-C279-C299	110.4(2)
C43-C33-C23	120.9(2)	N39-C309-C339	109.85(18)
C43-C33-C73	120.4(2)	N39-C309-Sb19	117.41(15)
C23-C33-C73	118.7(2)	C339-C309-Sb19	132.42(15)
C53-C43-C33	117.9(2)	N39-C319-C479	112.11(19)
C43-C53-C63	121.0(2)	N39-C319-C469	111.2(2)
C43-C53-C83	120.1(2)	C479-C319-C469	108.1(2)
C63-C53-C83	118.9(2)	N39-C319-C329	99.78(16)
C53-C63-C13	122.1(2)	C479-C319-C329	113.4(2)
F33-C73-F13	106.7(2)	C469-C319-C329	112.2(2)
F33-C73-F23	105.7(2)	C319-C329-C339	107.03(17)
F13-C73-F23	105.7(2)	C309-C339-C489	112.41(18)
F33-C73-C33	113.2(2)	C309-C339-C499	109.44(19)
F13-C73-C33	112.4(2)	C489-C339-C499	109.95(18)
F23-C73-C33	112.7(2)	C309-C339-C329	102.28(17)
F43-C83-F53	107.3(2)	C489-C339-C329	110.87(19)
F43-C83-F63	105.8(2)	C499-C339-C329	111.71(19)
F53-C83-F63	105.98(19)	C359-C349-C399	122.0(2)
F43-C83-C53	112.60(19)	C359-C349-N39	119.9(2)
F53-C83-C53	112.9(2)	C399-C349-N39	117.93(19)
F63-C83-C53	111.76(19)	C369-C359-C349	117.0(2)
C24-C14-C64	115.6(2)	C369-C359-C409	118.2(2)
C24-C14-B(2)	123.29(18)	C349-C359-C409	124.8(2)
C64-C14-B(2)	120.89(18)	C379-C369-C359	122.1(2)
C34-C24-C14	121.88(19)	C369-C379-C389	120.2(2)
C44-C34-C24	121.7(2)	C379-C389-C399	121.0(2)
C44-C34-C74	118.4(2)	C389-C399-C349	117.6(2)
C24-C34-C74	119.88(19)	C389-C399-C439	118.0(2)
C34-C44-C54	117.5(2)	C349-C399-C439	124.3(2)
C64-C54-C44	121.1(2)	C359-C409-C419	111.4(2)
C64-C54-C84	120.5(2)	C359-C409-C429	111.5(2)
C44-C54-C84	118.3(2)	C419-C409-C429	109.2(2)
C54-C64-C14	122.2(2)	C399-C439-C449	111.4(2)
F24-C74-F14	106.9(2)	C399-C439-C459	111.19(19)
F24-C74-F34	106.74(19)	C449-C439-C459	109.3(2)
F14-C74-F34	105.98(18)	C3010-Sb110-Ga110	109.03(6)
F24-C74-C34	112.70(19)	N110-Ga110-N210	95.89(7)
F14-C74-C34	112.15(19)	N110-Ga110-Sb110	152.81(5)
F34-C74-C34	111.9(2)	N210-Ga110-Sb110	108.19(5)
F44-C84-F64	106.4(2)	C110-N110-C610	118.93(17)

F44-C84-F54	106.6(2)	C110-N110-Ga110	123.96(14)
F64-C84-F54	106.1(2)	C610-N110-Ga110	116.84(13)
F44-C84-C54	112.3(2)	C310-N210-C1810	121.41(17)
F64-C84-C54	112.7(2)	C310-N210-Ga110	125.59(14)
F54-C84-C54	112.2(2)	C1810-N210-Ga110	112.99(12)
C65-C15-C25	115.32(19)	C3010-N310-C3410	121.54(18)
C65-C15-B(1)	120.19(19)	C3010-N310-C3110	114.32(18)
C25-C15-B(1)	124.43(18)	C3410-N310-C3110	124.11(17)
C35-C25-C15	122.25(19)	N110-C110-C210	123.84(19)
C45-C35-C25	121.1(2)	N110-C110-C410	118.25(18)
C45-C35-C75	117.4(2)	C210-C110-C410	117.90(18)
C25-C35-C75	121.5(2)	C110-C210-C310	128.11(19)
C55-C45-C35	117.8(2)	N210-C310-C210	122.43(18)
C45-C55-C65	121.2(2)	N210-C310-C510	120.60(18)
C45-C55-C85	120.3(2)	C210-C310-C510	116.94(18)
C65-C55-C85	118.4(2)	C1110-C610-C710	122.71(19)
C55-C65-C15	122.3(2)	C1110-C610-N110	118.67(19)
F15-C75-F35	107.9(2)	C710-C610-N110	118.57(19)
F15-C75-F25	105.3(2)	C810-C710-C610	117.0(2)
F35-C75-F25	104.6(2)	C810-C710-C1210	121.6(2)
F15-C75-C35	113.5(2)	C610-C710-C1210	121.4(2)
F35-C75-C35	113.0(2)	C910-C810-C710	121.2(2)
F25-C75-C35	111.9(2)	C1010-C910-C810	120.6(2)
F55-C85-F45	107.26(19)	C910-C1010-C1110	120.8(2)
F55-C85-F65	106.8(2)	C610-C1110-C1010	117.6(2)
F45-C85-F65	106.53(19)	C610-C1110-C1510	123.0(2)
F55-C85-C55	112.97(19)	C1010-C1110-C1510	119.4(2)
F45-C85-C55	112.0(2)	C1310-C1210-C710	113.6(2)
F65-C85-C55	110.89(18)	C1310-C1210-C1410	110.1(2)
C26-C16-C66	115.8(2)	C710-C1210-C1410	111.4(2)
C26-C16-B(1)	124.5(2)	C1710-C1510-C1110	112.1(2)
C66-C16-B(1)	119.5(2)	C1710-C1510-C1610	110.3(2)
C16-C26-C36	122.3(2)	C1110-C1510-C1610	111.7(2)
C46-C36-C26	120.3(2)	C2310-C1810-C1910	123.17(19)
C46-C36-C76	120.1(2)	C2310-C1810-N210	118.87(19)
C26-C36-C76	119.5(2)	C1910-C1810-N210	117.64(19)
C36-C46-C56	118.2(2)	C2010-C1910-C1810	116.8(2)
C66-C56-C46	121.1(2)	C2010-C1910-C2410	121.4(2)
C66-C56-C86	118.0(2)	C1810-C1910-C2410	121.80(19)
C46-C56-C86	120.7(2)	C2110-C2010-C1910	121.1(2)
C56-C66-C16	122.2(2)	C2010-C2110-C2210	120.9(2)
F36-C76-F26	108.8(8)	C2110-C2210-C2310	121.0(2)
F1'6-C76-F3'6	106.6(6)	C2210-C2310-C1810	117.0(2)
F36-C76-F16	106.5(9)	C2210-C2310-C2710	119.8(2)

F26-C76-F16	104.9(9)	C1810-C2310-C2710	123.22(19)
F1'6-C76-F2'6	105.0(6)	C1910-C2410-C2610	113.5(2)
F3'6-C76-F2'6	105.7(6)	C1910-C2410-C2510	113.06(19)
F36-C76-C36	117.1(10)	C2610-C2410-C2510	109.5(2)
F26-C76-C36	110.1(6)	C2310-C2710-C2910	111.9(2)
F1'6-C76-C36	114.8(5)	C2310-C2710-C2810	111.6(2)
F3'6-C76-C36	111.4(6)	C2910-C2710-C2810	109.6(2)
F16-C76-C36	108.7(8)	N310-C3010-C3310	110.22(18)
F2'6-C76-C36	112.6(4)	N310-C3010-Sb110	117.79(15)
F66-C86-F56	108.5(2)	C3310-C3010-Sb110	131.62(15)
F66-C86-F46	106.2(3)	N310-C3110-C4610	111.7(2)
F56-C86-F46	104.0(2)	N310-C3110-C4710	111.2(2)
F66-C86-C56	112.6(2)	C4610-C3110-C4710	108.7(2)
F56-C86-C56	112.9(2)	N310-C3110-C3210	100.40(17)
F46-C86-C56	112.0(2)	C4610-C3110-C3210	113.3(2)
C27-C17-C67	115.5(2)	C4710-C3110-C3210	111.5(2)
C27-C17-B(1)	121.08(18)	C3110-C3210-C3310	107.16(18)
C67-C17-B(1)	123.03(18)	C3010-C3310-C4910	112.15(19)
C37-C27-C17	122.4(2)	C3010-C3310-C4810	109.17(19)
C47-C37-C27	121.1(2)	C4910-C3310-C4810	110.8(2)
C47-C37-C77	120.6(2)	C3010-C3310-C3210	102.20(18)
C27-C37-C77	118.3(2)	C4910-C3310-C3210	109.90(19)
C37-C47-C57	117.8(2)	C4810-C3310-C3210	112.4(2)
C67-C57-C47	121.0(2)	C3510-C3410-C3910	121.7(2)
C67-C57-C87	120.9(2)	C3510-C3410-N310	120.3(2)
C47-C57-C87	118.1(2)	C3910-C3410-N310	117.94(19)
C57-C67-C17	122.3(2)	C3610-C3510-C3410	117.3(2)
F37-C77-F17	106.48(19)	C3610-C3510-C4010	118.2(2)
F37-C77-F27	107.3(2)	C3410-C3510-C4010	124.4(2)
F17-C77-F27	105.8(2)	C3710-C3610-C3510	122.0(2)
F37-C77-C37	113.3(2)	C3610-C3710-C3810	119.8(2)
F17-C77-C37	111.5(2)	C3710-C3810-C3910	121.5(2)
F27-C77-C37	112.05(18)	C3810-C3910-C3410	117.7(2)
F47-C87-F67	107.7(2)	C3810-C3910-C4310	118.0(2)
F47-C87-F57	105.5(2)	C3410-C3910-C4310	124.3(2)
F67-C87-F57	105.1(2)	C3510-C4010-C4110	111.3(2)
F47-C87-C57	112.8(2)	C3510-C4010-C4210	111.3(2)
F67-C87-C57	113.1(2)	C4110-C4010-C4210	108.9(2)
F57-C87-C57	112.1(2)	C3910-C4310-C4410	111.0(2)
C68-C18-C28	115.88(19)	C3910-C4310-C4510	111.5(2)
C68-C18-B(1)	120.91(19)	C4410-C4310-C4510	109.4(2)
C28-C18-B(1)	122.83(19)	Cl111-C111-Cl211	112.9(8)
C38-C28-C18	121.7(2)	Cl112-C112-Cl212	112.1(6)

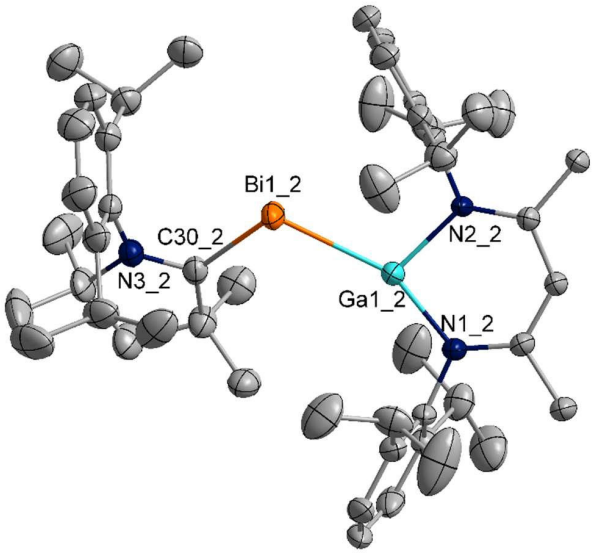


Fig. S33. Solid state structure of **7**. Hydrogen atoms, the anionic part and minor component of the disorder are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S11 Bond lengths [Å] for **7**.

Bi11-C301	2.244(3)	C112-C152	1.530(6)	C313-B13	1.650(5)
Bi11-Ga11	2.6465(4)	C122-C132	1.521(9)	C323-C333	1.387(5)
Ga11-N21	1.911(3)	C122-C142	1.523(8)	C333-C343	1.391(5)
Ga11-N11	1.923(3)	C152-C162	1.530(7)	C333-C373	1.498(6)
N11-C11	1.329(4)	C152-C172	1.537(7)	C343-C353	1.390(5)
N11-C61	1.441(4)	C182-C232	1.408(5)	C353-C363	1.388(5)
N21-C31	1.338(4)	C182-C192	1.409(6)	C353-C383	1.503(5)
N21-C181	1.440(4)	C192-C202	1.396(5)	C413-C423	1.403(5)
N31-C301	1.322(4)	C192-C242	1.533(6)	C413-C463	1.405(5)
N31-C341	1.447(5)	C202-C212	1.378(7)	C413-B13	1.637(5)
N31-C311	1.525(5)	C212-C222	1.371(7)	C423-C433	1.389(5)
C11-C21	1.400(5)	C222-C232	1.400(5)	C433-C443	1.394(5)
C11-C41	1.507(5)	C232-C272	1.507(6)	C433-C473	1.500(5)
C21-C31	1.400(5)	C242-C262	1.529(7)	C443-C453	1.388(5)
C31-C51	1.504(5)	C242-C252	1.530(7)	C453-C463	1.390(5)
C61-C71	1.394(5)	C272-C282	1.505(7)	C453-C483	1.503(5)
C61-C111	1.411(5)	C272-C292	1.533(6)	F114-C174	1.336(5)
C71-C81	1.395(5)	C302-C332	1.515(5)	F124-C174	1.336(5)
C71-C121	1.525(5)	C312-C462	1.524(8)	F134-C174	1.327(5)
C81-C91	1.393(6)	C312-C472	1.525(7)	F144-C184	1.330(6)
C91-C101	1.375(6)	C312-C322	1.534(6)	F154-C184	1.308(6)
C101-C111	1.403(5)	C322-C332	1.543(6)	F164-C184	1.336(6)
C111-C151	1.517(6)	C332-C492	1.529(6)	F214-C274	1.330(5)
C121-C131	1.524(6)	C332-C482	1.541(6)	F224-C274	1.347(5)
C121-C141	1.533(6)	C342-C392	1.404(5)	F234-C274	1.337(5)

C151-C161	1.514(6)	C342-C352	1.413(5)	F244-C284	1.313(6)
C151-C171	1.543(7)	C352-C362	1.400(6)	F254-C284	1.306(5)
C181-C231	1.386(5)	C352-C402	1.515(6)	F264-C284	1.348(6)
C181-C191	1.413(5)	C362-C372	1.380(7)	F314-C374	1.313(6)
C191-C201	1.396(5)	C372-C382	1.369(7)	F324-C374	1.331(5)
C191-C241	1.517(5)	C382-C392	1.400(6)	F334-C374	1.321(7)
C201-C211	1.397(6)	C392-C432	1.516(6)	F344-C384	1.339(5)
C211-C221	1.374(6)	C402-C422	1.535(7)	F354-C384	1.336(5)
C221-C231	1.403(5)	C402-C412	1.541(8)	F364-C384	1.344(5)
C231-C271	1.522(6)	C432-C442	1.531(6)	F374-C474	1.311(6)
C241-C261	1.521(6)	C432-C452	1.533(6)	F384-C474	1.318(6)
C241-C251	1.529(6)	F113-C173	1.311(6)	F394-C474	1.323(6)
C271-C281	1.520(7)	F123-C173	1.311(6)	F404-C484	1.316(6)
C271-C291	1.530(7)	F133-C173	1.294(5)	F414-C484	1.314(7)
C301-C331	1.518(5)	F143-C183	1.348(6)	F424-C484	1.338(7)
C311-C461	1.517(6)	F153-C183	1.336(5)	C114-C124	1.404(5)
C311-C471	1.528(6)	F163-C183	1.335(5)	C114-C164	1.410(5)
C311-C321	1.540(6)	F213-C273	1.328(5)	C114-B14	1.626(5)
C321-C331	1.542(6)	F223-C273	1.328(5)	C124-C134	1.397(5)
C331-C481	1.527(5)	F233-C273	1.339(5)	C134-C144	1.377(5)
C331-C491	1.540(6)	F243-C283	1.328(5)	C134-C174	1.500(6)
C341-C391	1.403(5)	F253-C283	1.325(5)	C144-C154	1.393(6)
C341-C351	1.412(6)	F263-C283	1.340(5)	C154-C164	1.391(5)
C351-C361	1.406(6)	F313-C373	1.345(5)	C154-C184	1.500(6)
C351-C401	1.519(6)	F323-C373	1.337(5)	C214-C224	1.403(5)
C361-C371	1.391(7)	F333-C373	1.327(6)	C214-C264	1.404(5)
C371-C381	1.375(7)	F343-C383	1.340(5)	C214-B14	1.648(5)
C381-C391	1.403(6)	F353-C383	1.333(5)	C224-C234	1.391(5)
C391-C431	1.528(6)	F363-C383	1.334(5)	C234-C244	1.382(5)
C401-C411	1.537(7)	F413-C473	1.349(5)	C234-C274	1.506(5)
C401-C421	1.539(6)	F423-C473	1.325(5)	C244-C254	1.390(5)
C431-C451	1.530(7)	F433-C473	1.340(5)	C254-C264	1.395(5)
C431-C441	1.531(6)	F443-C483	1.331(5)	C254-C284	1.498(6)
Bi12-C302	2.255(3)	F453-C483	1.336(4)	C314-C324	1.402(5)
Bi12-Ga12	2.6524(4)	F463-C483	1.344(4)	C314-C364	1.407(5)
Ga12-N12	1.920(3)	C113-C123	1.399(5)	C314-B14	1.639(5)
Ga12-N22	1.932(3)	C113-C163	1.405(5)	C324-C334	1.393(5)
N12-C12	1.342(4)	C113-B13	1.635(5)	C334-C344	1.393(5)
N12-C62	1.447(4)	C123-C133	1.394(5)	C334-C374	1.503(6)
N22-C32	1.330(4)	C133-C143	1.387(5)	C344-C354	1.385(5)
N22-C182	1.441(4)	C133-C173	1.495(5)	C354-C364	1.400(5)
N32-C302	1.308(4)	C143-C153	1.384(5)	C354-C384	1.497(5)
N32-C342	1.454(5)	C153-C163	1.390(5)	C414-C464	1.395(5)
N32-C312	1.523(5)	C153-C183	1.504(5)	C414-C424	1.407(5)

C12-C22	1.391(5)	C213-C223	1.402(5)	C414-B14	1.644(5)
C12-C42	1.504(5)	C213-C263	1.409(5)	C424-C434	1.386(5)
C22-C32	1.404(5)	C213-B13	1.639(5)	C434-C444	1.383(7)
C32-C52	1.501(5)	C223-C233	1.395(5)	C434-C474	1.506(6)
C62-C72	1.402(5)	C233-C243	1.389(5)	C444-C454	1.377(6)
C62-C112	1.406(5)	C233-C273	1.504(5)	C454-C464	1.398(5)
C72-C82	1.398(5)	C243-C253	1.386(5)	C454-C484	1.495(7)
C72-C122	1.516(6)	C253-C263	1.391(5)	Cl15-C15	1.746(11)
C82-C92	1.388(7)	C253-C283	1.497(5)	Cl25-C15	1.743(10)
C92-C102	1.366(8)	C313-C363	1.402(5)	Cl16-C16	1.744(13)
C102-C112	1.398(6)	C313-C323	1.404(5)	Cl26-C16	1.743(13)

Table S12 Bond angles [°] for **7**.

C301-Bi11-Ga11	107.78(9)	F133-C173-F123	106.8(5)
N21-Ga11-N11	95.95(12)	F113-C173-F123	104.2(5)
N21-Ga11-Bi11	154.78(9)	F133-C173-C133	113.3(4)
N11-Ga11-Bi11	106.95(9)	F113-C173-C133	112.5(4)
C11-N11-C61	120.4(3)	F123-C173-C133	113.4(4)
C11-N11-Ga11	125.4(2)	F163-C183-F153	107.2(4)
C61-N11-Ga11	114.2(2)	F163-C183-F143	106.9(4)
C31-N21-C181	119.2(3)	F153-C183-F143	106.1(4)
C31-N21-Ga11	124.2(2)	F163-C183-C153	113.0(4)
C181-N21-Ga11	116.5(2)	F153-C183-C153	112.5(3)
C301-N31-C341	121.1(3)	F143-C183-C153	110.7(4)
C301-N31-C311	114.7(3)	C223-C213-C263	115.7(3)
C341-N31-C311	124.2(3)	C223-C213-B13	123.4(3)
N11-C11-C21	122.6(3)	C263-C213-B13	120.9(3)
N11-C11-C41	120.7(3)	C233-C223-C213	122.1(3)
C21-C11-C41	116.7(3)	C243-C233-C223	121.2(3)
C11-C21-C31	127.8(3)	C243-C233-C273	119.7(3)
N21-C31-C21	124.0(3)	C223-C233-C273	119.0(3)
N21-C31-C51	118.8(3)	C253-C243-C233	117.7(3)
C21-C31-C51	117.2(3)	C243-C253-C263	121.3(3)
C71-C61-C111	122.4(3)	C243-C253-C283	120.4(3)
C71-C61-N11	119.6(3)	C263-C253-C283	118.3(3)
C111-C61-N11	117.8(3)	C253-C263-C213	122.0(3)
C61-C71-C81	118.0(3)	F223-C273-F213	107.4(4)
C61-C71-C121	122.3(3)	F223-C273-F233	106.2(4)
C81-C71-C121	119.7(3)	F213-C273-F233	105.8(3)
C91-C81-C71	120.5(4)	F223-C273-C233	112.9(3)
C101-C91-C81	120.6(4)	F213-C273-C233	112.3(3)
C91-C101-C111	121.0(4)	F233-C273-C233	111.8(3)
C101-C111-C61	117.2(4)	F253-C283-F243	107.1(4)

C101-C111-C151	121.1(3)	F253-C283-F263	106.0(4)
C61-C111-C151	121.7(3)	F243-C283-F263	106.0(3)
C131-C121-C71	112.7(3)	F253-C283-C253	112.1(3)
C131-C121-C141	110.4(4)	F243-C283-C253	112.7(3)
C71-C121-C141	110.5(3)	F263-C283-C253	112.4(3)
C161-C151-C111	112.1(4)	C363-C313-C323	115.9(3)
C161-C151-C171	110.3(4)	C363-C313-B13	123.2(3)
C111-C151-C171	112.1(4)	C323-C313-B13	120.6(3)
C231-C181-C191	123.2(3)	C333-C323-C313	122.1(3)
C231-C181-N21	119.9(3)	C323-C333-C343	121.1(3)
C191-C181-N21	116.8(3)	C323-C333-C373	120.7(3)
C201-C191-C181	116.7(3)	C343-C333-C373	118.2(3)
C201-C191-C241	121.7(3)	C353-C343-C333	117.6(3)
C181-C191-C241	121.6(3)	C363-C353-C343	121.3(3)
C191-C201-C211	121.2(4)	C363-C353-C383	119.7(3)
C221-C211-C201	120.0(4)	C343-C353-C383	119.0(3)
C211-C221-C231	121.3(4)	C353-C363-C313	122.0(3)
C181-C231-C221	117.5(4)	F333-C373-F323	106.8(4)
C181-C231-C271	122.6(3)	F333-C373-F313	106.4(4)
C221-C231-C271	119.9(3)	F323-C373-F313	105.8(4)
C191-C241-C261	110.7(3)	F333-C373-C333	112.4(4)
C191-C241-C251	113.9(3)	F323-C373-C333	112.5(4)
C261-C241-C251	109.8(4)	F313-C373-C333	112.6(3)
C281-C271-C231	110.9(4)	F353-C383-F363	107.1(4)
C281-C271-C291	110.5(4)	F353-C383-F343	106.9(3)
C231-C271-C291	112.0(4)	F363-C383-F343	106.2(3)
N31-C301-C331	110.1(3)	F353-C383-C353	112.2(3)
N31-C301-Bi11	117.1(2)	F363-C383-C353	112.5(3)
C331-C301-Bi11	132.5(2)	F343-C383-C353	111.6(3)
C461-C311-N31	111.7(3)	C423-C413-C463	115.6(3)
C461-C311-C471	108.3(4)	C423-C413-B13	122.5(3)
N31-C311-C471	111.1(3)	C463-C413-B13	121.8(3)
C461-C311-C321	113.2(4)	C433-C423-C413	122.2(3)
N31-C311-C321	100.1(3)	C423-C433-C443	121.3(3)
C471-C311-C321	112.5(4)	C423-C433-C473	118.9(3)
C311-C321-C331	107.3(3)	C443-C433-C473	119.6(3)
C301-C331-C481	111.8(3)	C453-C443-C433	117.4(3)
C301-C331-C491	108.6(3)	C443-C453-C463	121.2(3)
C481-C331-C491	110.0(3)	C443-C453-C483	120.1(3)
C301-C331-C321	102.7(3)	C463-C453-C483	118.5(3)
C481-C331-C321	111.8(3)	C453-C463-C413	122.3(3)
C491-C331-C321	111.7(3)	F423-C473-F433	107.3(3)
C391-C341-C351	121.8(3)	F423-C473-F413	106.7(3)
C391-C341-N31	120.4(3)	F433-C473-F413	105.0(3)

C351-C341-N31	117.6(3)	F423-C473-C433	113.4(3)
C361-C351-C341	117.8(4)	F433-C473-C433	112.8(3)
C361-C351-C401	117.4(4)	F413-C473-C433	111.0(3)
C341-C351-C401	124.8(4)	F443-C483-F453	107.0(3)
C371-C361-C351	121.2(4)	F443-C483-F463	106.0(3)
C381-C371-C361	119.4(4)	F453-C483-F463	106.5(3)
C371-C381-C391	122.4(4)	F443-C483-C453	112.1(3)
C381-C391-C341	117.4(4)	F453-C483-C453	112.9(3)
C381-C391-C431	118.0(4)	F463-C483-C453	112.0(3)
C341-C391-C431	124.6(3)	C113-B13-C413	111.8(3)
C351-C401-C411	111.5(4)	C113-B13-C213	105.5(3)
C351-C401-C421	111.4(4)	C413-B13-C213	112.0(3)
C411-C401-C421	109.1(4)	C113-B13-C313	112.8(3)
C391-C431-C451	111.3(4)	C413-B13-C313	103.8(3)
C391-C431-C441	111.7(4)	C213-B13-C313	111.1(3)
C451-C431-C441	108.9(4)	C124-C114-C164	115.6(3)
C302-Bi12-Ga12	107.56(9)	C124-C114-B14	121.1(3)
N12-Ga12-N22	95.57(13)	C164-C114-B14	123.0(3)
N12-Ga12-Bi12	154.33(9)	C134-C124-C114	122.2(3)
N22-Ga12-Bi12	107.33(9)	C144-C134-C124	121.1(4)
C12-N12-C62	119.6(3)	C144-C134-C174	120.9(3)
C12-N12-Ga12	124.1(2)	C124-C134-C174	118.1(3)
C62-N12-Ga12	116.0(2)	C134-C144-C154	118.2(3)
C32-N22-C182	122.0(3)	C164-C154-C144	120.8(3)
C32-N22-Ga12	125.7(2)	C164-C154-C184	120.7(4)
C182-N22-Ga12	112.3(2)	C144-C154-C184	118.4(4)
C302-N32-C342	121.5(3)	C154-C164-C114	122.1(3)
C302-N32-C312	114.0(3)	F134-C174-F124	106.2(4)
C342-N32-C312	124.5(3)	F134-C174-F114	107.4(4)
N12-C12-C22	124.0(3)	F124-C174-F114	105.5(4)
N12-C12-C42	118.3(3)	F134-C174-C134	113.4(4)
C22-C12-C42	117.6(3)	F124-C174-C134	111.6(3)
C12-C22-C32	128.2(3)	F114-C174-C134	112.2(3)
N22-C32-C22	122.2(3)	F154-C184-F144	108.6(5)
N22-C32-C52	120.2(3)	F154-C184-F164	105.9(4)
C22-C32-C52	117.6(3)	F144-C184-F164	104.5(4)
C72-C62-C112	122.4(3)	F154-C184-C154	112.5(4)
C72-C62-N12	118.8(3)	F144-C184-C154	113.2(4)
C112-C62-N12	118.7(3)	F164-C184-C154	111.6(4)
C82-C72-C62	117.9(4)	C224-C214-C264	115.5(3)
C82-C72-C122	119.5(4)	C224-C214-B14	120.3(3)
C62-C72-C122	122.6(3)	C264-C214-B14	124.1(3)
C92-C82-C72	120.3(4)	C234-C224-C214	122.1(3)
C102-C92-C82	120.7(4)	C244-C234-C224	121.4(3)

C92-C102-C112	121.7(4)	C244-C234-C274	120.4(3)
C102-C112-C62	116.9(4)	C224-C234-C274	118.1(3)
C102-C112-C152	122.8(4)	C234-C244-C254	117.8(3)
C62-C112-C152	120.3(4)	C244-C254-C264	120.8(3)
C72-C122-C132	112.1(5)	C244-C254-C284	117.2(3)
C72-C122-C142	111.5(4)	C264-C254-C284	122.0(3)
C132-C122-C142	110.0(5)	C254-C264-C214	122.3(3)
C112-C152-C162	113.0(4)	F214-C274-F234	107.3(3)
C112-C152-C172	111.4(4)	F214-C274-F224	106.7(3)
C162-C152-C172	110.4(5)	F234-C274-F224	106.4(3)
C232-C182-C192	122.4(3)	F214-C274-C234	112.3(3)
C232-C182-N22	118.7(3)	F234-C274-C234	112.8(3)
C192-C182-N22	118.5(3)	F224-C274-C234	110.9(3)
C202-C192-C182	117.4(4)	F254-C284-F244	109.5(4)
C202-C192-C242	119.3(4)	F254-C284-F264	104.2(4)
C182-C192-C242	123.3(3)	F244-C284-F264	104.2(4)
C212-C202-C192	120.8(4)	F254-C284-C254	113.3(4)
C222-C212-C202	121.1(4)	F244-C284-C254	113.1(4)
C212-C222-C232	121.1(4)	F264-C284-C254	111.9(4)
C222-C232-C182	117.1(4)	C324-C314-C364	115.8(3)
C222-C232-C272	122.0(4)	C324-C314-B14	121.3(3)
C182-C232-C272	120.8(3)	C364-C314-B14	122.5(3)
C262-C242-C252	109.8(5)	C334-C324-C314	122.4(3)
C262-C242-C192	111.6(4)	C324-C334-C344	120.8(3)
C252-C242-C192	111.8(4)	C324-C334-C374	118.8(3)
C282-C272-C232	113.3(3)	C344-C334-C374	120.4(3)
C282-C272-C292	109.3(4)	C354-C344-C334	118.0(3)
C232-C272-C292	112.8(4)	C344-C354-C364	121.1(3)
N32-C302-C332	111.0(3)	C344-C354-C384	118.8(3)
N32-C302-Bi12	117.3(2)	C364-C354-C384	120.1(3)
C332-C302-Bi12	131.2(2)	C354-C364-C314	121.9(3)
N32-C312-C462	111.1(4)	F314-C374-F334	105.9(5)
N32-C312-C472	111.2(4)	F314-C374-F324	106.8(4)
C462-C312-C472	109.1(5)	F334-C374-F324	105.8(4)
N32-C312-C322	100.6(3)	F314-C374-C334	112.9(4)
C462-C312-C322	112.4(4)	F334-C374-C334	112.1(4)
C472-C312-C322	112.2(4)	F324-C374-C334	112.8(4)
C312-C322-C332	106.9(3)	F354-C384-F344	106.5(3)
C302-C332-C492	111.8(3)	F354-C384-F364	106.4(4)
C302-C332-C482	108.8(3)	F344-C384-F364	106.3(3)
C492-C332-C482	110.0(4)	F354-C384-C354	112.7(3)
C302-C332-C322	102.3(3)	F344-C384-C354	112.0(4)
C492-C332-C322	111.1(4)	F364-C384-C354	112.5(3)
C482-C332-C322	112.5(4)	C464-C414-C424	115.7(3)

C392-C342-C352	122.2(3)	C464-C414-B14	124.4(3)
C392-C342-N32	120.3(3)	C424-C414-B14	119.6(3)
C352-C342-N32	117.3(3)	C434-C424-C414	121.9(4)
C362-C352-C342	117.2(4)	C444-C434-C424	121.2(4)
C362-C352-C402	118.6(4)	C444-C434-C474	121.0(4)
C342-C352-C402	124.2(4)	C424-C434-C474	117.7(4)
C372-C362-C352	121.6(4)	C454-C444-C434	118.2(4)
C382-C372-C362	119.8(4)	C444-C454-C464	120.8(4)
C372-C382-C392	122.2(4)	C444-C454-C484	119.9(4)
C382-C392-C342	117.1(4)	C464-C454-C484	119.3(4)
C382-C392-C432	118.0(4)	C414-C464-C454	122.2(4)
C342-C392-C432	124.9(3)	F374-C474-F384	106.7(5)
C352-C402-C422	111.2(4)	F374-C474-F394	109.0(5)
C352-C402-C412	111.0(4)	F384-C474-F394	104.4(4)
C422-C402-C412	109.0(5)	F374-C474-C434	112.6(4)
C392-C432-C442	111.9(4)	F384-C474-C434	111.7(4)
C392-C432-C452	111.6(4)	F394-C474-C434	112.0(5)
C442-C432-C452	108.7(4)	F414-C484-F404	108.8(5)
C123-C113-C163	115.7(3)	F414-C484-F424	102.6(6)
C123-C113-B13	122.5(3)	F404-C484-F424	105.3(4)
C163-C113-B13	121.6(3)	F414-C484-C454	112.8(4)
C133-C123-C113	122.3(3)	F404-C484-C454	113.6(5)
C143-C133-C123	121.0(3)	F424-C484-C454	112.9(4)
C143-C133-C173	119.5(3)	C114-B14-C314	114.6(3)
C123-C133-C173	119.5(3)	C114-B14-C414	112.7(3)
C153-C143-C133	117.7(3)	C314-B14-C414	103.2(3)
C143-C153-C163	121.5(3)	C114-B14-C214	104.8(3)
C143-C153-C183	119.4(3)	C314-B14-C214	112.0(3)
C163-C153-C183	119.1(3)	C414-B14-C214	109.7(3)
C153-C163-C113	121.9(3)	Cl25-C15-Cl15	112.5(6)
F133-C173-F113	105.7(5)	Cl26-C16-Cl16	112.9(10)

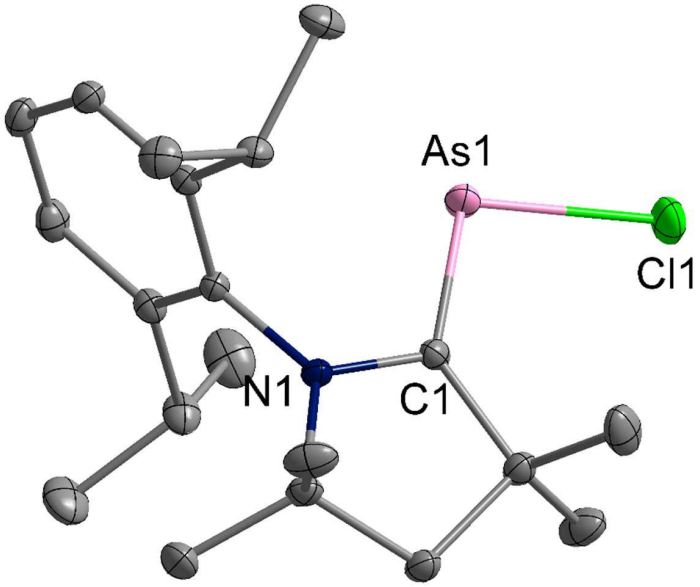


Fig. S34. Solid state structure of (^{Me}cAACAs)Cl. Hydrogen atoms are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S15 Bond lengths [Å] for (^{Me}cAAC)AsCl.

As(1)-C(1)	1.8675(14)	C(2)-C(3)	1.537(2)	C(7)-C(8)	1.382(2)
As(1)-Cl(1)	2.2467(8)	C(3)-C(4)	1.547(2)	C(8)-C(9)	1.388(2)
N(1)-C(1)	1.3514(18)	C(4)-C(19)	1.532(2)	C(9)-C(10)	1.396(2)
N(1)-C(5)	1.4427(18)	C(4)-C(20)	1.542(2)	C(10)-C(14)	1.527(2)
N(1)-C(2)	1.5145(17)	C(5)-C(10)	1.4145(19)	C(11)-C(13)	1.5291(19)
C(1)-C(4)	1.5244(19)	C(5)-C(6)	1.4180(19)	C(11)-C(12)	1.541(2)
C(2)-C(18)	1.520(2)	C(6)-C(7)	1.399(2)	C(14)-C(15)	1.537(2)
C(2)-C(17)	1.530(2)	C(6)-C(11)	1.5171(19)	C(14)-C(16)	1.539(2)

Table S16 Bond angles [°] for (^{Me}cAAC)AsCl.

C(1)-As(1)-Cl(1)	101.91(5)	C(20)-C(4)-C(3)	109.05(12)
C(1)-N(1)-C(5)	119.50(11)	C(10)-C(5)-C(6)	121.07(12)
C(1)-N(1)-C(2)	114.56(11)	C(10)-C(5)-N(1)	118.17(12)
C(5)-N(1)-C(2)	125.88(11)	C(6)-C(5)-N(1)	120.63(12)
N(1)-C(1)-C(4)	109.54(11)	C(7)-C(6)-C(5)	118.16(12)
N(1)-C(1)-As(1)	117.07(10)	C(7)-C(6)-C(11)	118.41(12)
C(4)-C(1)-As(1)	133.38(10)	C(5)-C(6)-C(11)	123.43(12)
N(1)-C(2)-C(18)	110.72(12)	C(8)-C(7)-C(6)	121.33(13)
N(1)-C(2)-C(17)	112.36(11)	C(7)-C(8)-C(9)	119.78(13)
C(18)-C(2)-C(17)	108.66(13)	C(8)-C(9)-C(10)	121.74(13)
N(1)-C(2)-C(3)	99.70(10)	C(9)-C(10)-C(5)	117.85(13)
C(18)-C(2)-C(3)	113.36(12)	C(9)-C(10)-C(14)	118.20(12)
C(17)-C(2)-C(3)	111.89(13)	C(5)-C(10)-C(14)	123.94(13)
C(2)-C(3)-C(4)	108.07(11)	C(6)-C(11)-C(13)	112.00(12)

C(1)-C(4)-C(19)	110.28(12)	C(6)-C(11)-C(12)	110.22(12)
C(1)-C(4)-C(20)	112.46(12)	C(13)-C(11)-C(12)	109.99(12)
C(19)-C(4)-C(20)	109.90(13)	C(10)-C(14)-C(15)	111.70(12)
C(1)-C(4)-C(3)	102.42(11)	C(10)-C(14)-C(16)	110.65(13)
C(19)-C(4)-C(3)	112.58(12)	C(15)-C(14)-C(16)	109.64(13)

E) Computational Details

All calculations were performed by using the program package Gaussian 16[19] and Amsterdam Density Functional[20] (ADF). The geometrical parameters of all stationary points were optimized by means of the density functional B3LYP[21] together with the dispersion correction with Becke-Johnson damping[22] (D3BJ) using Gaussian 16. The basis set def2-TZVP was applied. For all structures C1 symmetry was applied. Frequency calculations were carried out at each of the stationary points to verify the nature of the stationary point. It turned out that all products have no imaginary frequency. Natural bond orbital analysis was performed using the NBO[23] version 3.1 implemented in Gaussian 16. The bond energy analysis calculations[24] were carried out using Amsterdam Density Functional (ADF).

Table S17. NBO charges [e] of the Ga-E-C-N units calculated by means of B3LYP-D3BJ/def2-TZVP.

Compound	E	Ga	E	C	N
8	N	1.729	-1.054	0.518	-0.462
9	P	1.355	-0.226	0.007	-0.443
1	As	1.301	-0.187	0.045	-0.449
2	Sb	1.170	0.030	-0.003	-0.457
3	Bi	1.134	0.051	0.047	-0.466
10	N	1.858	-1.094	0.540	-0.411
11	P	1.425	-0.192	0.057	-0.400
4-An$^-$	As	1.335	-0.124	0.107	-0.407
6-An$^-$	Sb	1.173	0.133	0.063	-0.416
7-An$^-$	Bi	1.122	0.176	0.105	-0.421

Table S18. Wiberg Bond Index in the Ga-E-C-N units calculated by means of B3LYP-D3BJ/def2-TZVP.

Compound	E	Ga–E	E–C	C–N
8	N	0.5769	1.7519	1.1200
9	P	0.9355	1.5284	1.2012
1	As	0.9697	1.4548	1.2246
2	Sb	1.0283	1.2880	1.2488
3	Bi	1.0316	1.2220	1.2646
10	N	0.7324	1.6017	1.2368
11	P	1.1458	1.3756	1.3150
4-An$^-$	As	1.2069	1.2869	1.3467
6-An$^-$	Sb	1.2577	1.0802	1.3817
7-An$^-$	Bi	1.2529	0.9993	1.4033

Table S19. Mayer Bond Index in the Ga-E-C-N units calculated by means of B3LYP-D3BJ/def2-TZVP.

Compound	E	Ga–E	E–C	C–N
8	N	1.150	1.730	1.177
9	P	1.043	1.672	1.255
1	As	1.026	1.633	1.271
2	Sb	1.045	1.313	1.299
3	Bi	1.020	1.285	1.315
10	N	1.500	1.418	1.315
11	P	1.457	1.363	1.385
4-An$^-$	As	1.333	1.348	1.411
6-An$^-$	Sb	1.290	1.122	1.450
7-An$^-$	Bi	1.234	1.052	1.473

Table S20. Bond orbitals in the Ga-E-C-N units calculated by means of B3LYP-D3BJ/def2-TZVP.

Compound	E	Ga–E		E–C[b]	
		Ga	E	E	C
10	N	[a]	[a]	s 49%	s 37%
		[a]	[a]	p 51%	p 63%
		[a]	[a]	d <1%	d <1%
11	P	s 83%	s 11%	s 21%	s 38%
		p 16%	p 89%	p 78%	p 61%
		d <1%	d <1%	d <1%	d <1%
4-An$^-$	As	s 84%	s 9%	s 16%	s 37%
		p 16%	p 91%	p 84%	p 63%
		d <1%	d <1%	d <1%	d <1%
6-An$^-$	Sb	s 82%	s 8%	s 10%	s 36%
		p 18%	p 92%	p 90%	p 64%
		d <1%	d <1%	d <1%	d <1%
7-An$^-$	Bi	s 82%	s 5%	s 6%	s 35%
		p 18%	p 94%	p 93%	p 65%
		d <1%	d <1%	d <1%	d <1%

[a] no localized single bond was calculated. [b] only the data for the single bond are listed

Table S21. Analysis of the total bonding energy calculated by means of B3LYP-D3BJ/TZP. The bond energy is computed as an energy difference between molecule and fragments. The total bonding energy (ΔE) consists of the Pauli repulsion (ΔE_{Pauli}), the electrostatic interaction (ΔV_{elstat}), orbital interactions (ΔE_{oi}) and the dispersion energy (ΔE_{Disp}). The values are given in kcal/mol.

	E	bond break	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}	ΔE_{Disp}	ΔE
8	N	homolytic E–C	1091.92	-360.14	-920.63	-32.99	-221.85
		heterolytic E–C	898.26	-380.88	-680.25	-32.99	-195.87
9	P	homolytic E–C	576.68	-234.35	-469.94	-30.51	-158.12
		heterolytic E–C	415.38	-249.48	-261.76	-30.51	-126.37
1	As	homolytic E–C	506.04	-218.63	-400.27	-29.54	-142.41
		heterolytic E–C	368.81	-240.65	-209.13	-29.54	-110.51
2	Sb	homolytic E–C	416.91	-190.81	-323.04	-27.37	-124.31
		heterolytic E–C	309.86	-215.18	-158.60	-27.37	-91.29
3	Bi	homolytic E–C	376.72	-170.53	-295.07	-26.81	-115.68
		heterolytic E–C	248.93	-187.08	-117.34	-26.81	-82.30
10	N	homolytic Ga–E	284.17	-176.98	-177.77	-29.88	-100.45
		homolytic E–C	646.03	-307.98	-496.35	-31.68	-189.98
		heterolytic E–C	1030.10	-423.29	-782.32	-31.68	-207.20
11	P	homolytic Ga–E	164.29	-119.10	-110.07	-27.74	-92.62
		homolytic E–C	317.67	-184.68	-242.87	-30.46	-140.34
		heterolytic E–C	418.26	-252.08	-270.70	-30.46	-134.99
4-An$^-$	As	homolytic Ga–E	150.84	-114.22	-103.03	-26.72	-93.13
		homolytic E–C	260.21	-160.47	-199.13	-29.35	-128.74
		heterolytic E–C	342.36	-230.34	-201.08	-29.35	-118.41
6-An$^-$	Sb	homolytic Ga–E	133.30	-102.82	-95.44	-25.81	-90.77
		homolytic E–C	202.31	-129.72	-161.91	-27.99	-117.32
		heterolytic E–C	264.35	-193.78	-140.81	-27.99	-98.24
7-An$^-$	Bi	homolytic Ga–E	122.68	-97.16	-92.27	-25.21	-91.95
		homolytic E–C	170.47	-112.70	-143.87	-27.15	-113.24
		heterolytic E–C	219.33	-171.92	-110.20	-27.15	-89.95

F) Cartesian Coordinates and Absolute Energies for All Calculated Compounds

Table S22. Absolute energies [au] calculated by means B3LYP-D3BJ/def2-TZVP.

	E
8	-4515.989361
9	-4802.591021
1	-6697.135165
2	-4701.548809
3	-4675.923625
10	-4055.503746
11	-4342.106761
4-An$^-$	-6236.652200
6-An$^-$	-4241.071753
7-An$^-$	-4215.451160

Cartesian coordinates of the optimized geometry for **8** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	2.33302200	-1.96753100	-0.62422500
C	1.45763000	-1.07719000	-1.21989500
Ga	-0.81431700	0.70882300	-0.94029300
N	-0.70055800	2.47351500	-0.03425100
N	-2.61374900	0.27660900	-0.25005000
Cl	-1.36898000	1.34872800	-3.04345100
C	-3.47635900	1.30558600	-0.30393400
C	-3.09546000	2.64045400	-0.21951600
H	-3.89677900	3.36141400	-0.25111900
C	-1.82902200	3.15586000	0.10612000
C	-4.94818300	1.02581200	-0.47247200
H	-5.53125000	1.93669400	-0.36375800
H	-5.31741300	0.28024500	0.22668800
H	-5.10789000	0.62788000	-1.47709200
C	-1.81184700	4.53477100	0.71400800
H	-2.69746900	5.08895000	0.41048500
H	-0.92071600	5.09875300	0.45549500
H	-1.83315700	4.44255200	1.80275000
C	-3.15298500	-0.99238800	0.15720400
C	-3.43676500	-1.99741300	-0.77727400
C	-4.09971000	-3.14533800	-0.34137700
H	-4.33802100	-3.92037200	-1.05793900
C	-4.46865200	-3.30605900	0.98136200
H	-4.99654800	-4.19689100	1.29689300
C	-4.13102200	-2.33049900	1.90644700
H	-4.38588600	-2.47746000	2.94702700
C	-3.45844800	-1.17496600	1.52341000
C	-3.05228900	-1.89183000	-2.23806600
H	-2.53810000	-0.94680300	-2.39405300
C	-4.27510100	-1.88602300	-3.16252700
H	-4.96082400	-1.07712600	-2.90895400
H	-4.82850300	-2.82525600	-3.09815400
H	-3.96235900	-1.74869500	-4.19914800
C	-2.08969100	-3.02325100	-2.61639300
H	-1.76929000	-2.92011500	-3.65331100
H	-2.56491100	-3.99990500	-2.50673700
H	-1.20500700	-3.00599300	-1.97974900
C	-3.06141100	-0.15595900	2.57976200
H	-2.27585800	0.45825000	2.14439200
C	-4.21699900	0.77401000	2.97499900
H	-3.89281800	1.46276500	3.75821000
H	-5.05964500	0.19663700	3.36242500
H	-4.57043200	1.37045600	2.13737800
C	-2.48858600	-0.81823100	3.83781200
H	-2.10024300	-0.05463800	4.51323800
H	-1.67902600	-1.50405200	3.59575900
H	-3.25282600	-1.37276800	4.38496600
C	0.51433000	3.06795400	0.45530100
C	1.33946400	3.78350000	-0.43031900
C	2.44604200	4.44461800	0.09921800
H	3.09140000	5.00959200	-0.55817100
C	2.73719600	4.39170300	1.45285000
H	3.60073600	4.91582600	1.84215000
C	1.93701200	3.64575700	2.30078500
H	2.18848800	3.58126900	3.35060900
C	0.81912200	2.96774500	1.82158300
C	1.03484000	3.86703500	-1.91611200
H	0.54388500	2.94037600	-2.20313000
C	2.29203700	4.00497000	-2.77848800
H	2.03401000	3.84533800	-3.82629600
H	3.05353500	3.27609200	-2.50267900
H	2.73153600	5.00161600	-2.70001500
C	0.05051000	4.99590200	-2.25282200
H	0.42677400	5.95925800	-1.89995500
H	-0.92949200	4.82465200	-1.81368400
H	-0.08593500	5.05724500	-3.33381700
C	0.00107600	2.09788900	2.75534200

H	-0.97029600	1.93802700	2.29174100
C	0.67580000	0.72759600	2.90765400
H	1.68015000	0.84002800	3.31761400
H	0.76264000	0.21404300	1.95012900
H	0.10915900	0.09059100	3.58555600
C	-0.25403400	2.74463700	4.11905200
H	-0.68372300	3.74303600	4.01732300
H	0.66191900	2.83253100	4.70580800
H	-0.94946500	2.13283600	4.69608200
C	1.88507400	-0.95271900	-2.70643400
C	3.14858200	-1.83049600	-2.79456400
H	3.21138500	-2.36690400	-3.74165600
H	4.03888900	-1.20433500	-2.71289400
C	3.10643800	-2.78503800	-1.59456100
C	2.23278500	0.50830600	-3.00139100
H	1.34143500	1.12820900	-3.02502000
H	2.71484300	0.58309600	-3.97891500
H	2.91788500	0.90583500	-2.25160800
C	0.80645400	-1.43214600	-3.68007100
H	-0.12328600	-0.88803200	-3.54263500
H	0.60876000	-2.49590200	-3.57195700
H	1.14263100	-1.25745800	-4.70476600
C	4.50124000	-3.15173400	-1.09721200
H	5.12068300	-2.27650500	-0.92466300
H	4.99285100	-3.76601700	-1.85315600
H	4.45311900	-3.72915900	-0.17360900
C	2.37082400	-4.09096500	-1.93331400
H	1.34020800	-3.90997400	-2.23144700
H	2.36303200	-4.76450800	-1.07841100
H	2.87941300	-4.59796900	-2.75538400
C	2.49477000	-2.06663000	0.79109000
C	3.47833000	-1.26717100	1.40495700
C	3.65763700	-1.37337600	2.78087400
H	4.40555700	-0.76313700	3.26942300
C	2.88482200	-2.23894200	3.53889100
H	3.03701000	-2.30708400	4.60878600
C	1.90989000	-3.00532000	2.92531200
H	1.29524200	-3.66540600	3.52348200
C	1.69461100	-2.93122000	1.54943200
C	4.30393900	-0.26228500	0.62231100
H	4.19021900	-0.49316400	-0.43359300
C	3.76676600	1.15550000	0.82406400
H	4.33332400	1.87106000	0.22555300
H	3.84652100	1.45800400	1.86848000
H	2.72021200	1.22410300	0.53663400
C	5.79747400	-0.32771200	0.95682300
H	6.36081100	0.32055900	0.28243600
H	6.18918200	-1.34157800	0.86435300
H	5.99605300	0.01275100	1.97450900
C	0.56912600	-3.73455500	0.93551700
H	0.57732200	-3.54629000	-0.13465100
C	-0.77740000	-3.24455700	1.46564900
H	-0.86935300	-2.17351500	1.30866300
H	-0.87970500	-3.44947800	2.53310700
H	-1.60226200	-3.73658000	0.95103800
C	0.73252700	-5.24078500	1.16253100
H	0.65251200	-5.49047700	2.22241700
H	1.70058000	-5.60216500	0.81265800
H	-0.04876300	-5.79056000	0.63352400
N	0.53779000	-0.48188300	-0.57141800

Cartesian coordinates of the optimized geometry for **9** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	-3.23786400	-0.48139600	-0.90948000
C	-1.91256100	-0.43108300	-1.21675800
P	-0.77628700	0.04310300	0.00598100
Ga	1.40341700	0.15817100	-0.73810200

N	2.66349300	-1.15828800	0.08807300
N	2.20165400	1.73818700	0.16647600
Cl	2.24512300	0.35275100	-2.82405700
C	3.50905600	1.73477000	0.41902900
C	4.29903200	0.58209000	0.42063300
H	5.34827500	0.73661000	0.62029400
C	3.88327200	-0.75696200	0.42197200
C	4.20075900	3.03297600	0.74798900
H	5.22376100	2.85509400	1.06895900
H	3.67139500	3.57984100	1.52645200
H	4.21707900	3.67619400	-0.13265700
C	4.91694600	-1.74852200	0.89995200
H	5.86495200	-1.55033600	0.39944700
H	4.62741400	-2.77855500	0.72167600
H	5.08319200	-1.61679500	1.96946100
C	1.44591500	2.93169000	0.43683700
C	1.34374300	3.94481600	-0.53029400
C	0.67479800	5.12072800	-0.19352000
H	0.59100900	5.90993700	-0.92901100
C	0.12293400	5.29779000	1.06231200
H	-0.38206700	6.22247200	1.31120100
C	0.19465300	4.27294300	1.99156300
H	-0.27040000	4.40485200	2.95782000
C	0.83221400	3.07089700	1.69639600
C	1.89385300	3.78521900	-1.93329000
H	2.49689300	2.88108400	-1.96328300
C	2.78443300	4.95391600	-2.36805200
H	3.59884900	5.12686800	-1.66269300
H	2.21927300	5.88398800	-2.45349000
H	3.22304800	4.74429700	-3.34543600
C	0.73719500	3.59098500	-2.92222400
H	1.11712500	3.34542400	-3.91501700
H	0.13426400	4.49935800	-2.99567400
H	0.08457400	2.78123700	-2.60063500
C	0.85498500	1.95328600	2.72543400
H	0.97149800	1.01822500	2.17962900
C	2.05117200	2.07822200	3.67797600
H	2.03833200	1.27023900	4.41256200
H	2.01828800	3.02673600	4.21900500
H	2.99924100	2.02574200	3.14370700
C	-0.45714100	1.85758800	3.50846400
H	-0.43543500	0.99310800	4.16991600
H	-1.30665200	1.74142300	2.83701600
H	-0.62417700	2.73642900	4.13342800
C	2.23489800	-2.49742900	0.38091200
C	2.18117600	-3.45947400	-0.64845500
C	1.73188200	-4.73835800	-0.32835600
H	1.68372500	-5.49224900	-1.10059400
C	1.34833200	-5.06922700	0.96247800
H	0.99972200	-6.06956800	1.18580600
C	1.41364400	-4.11589900	1.96065100
H	1.11149000	-4.37567800	2.96661500
C	1.85526900	-2.82057400	1.69499400
C	2.64335400	-3.14598600	-2.06171600
H	2.34619200	-2.12594700	-2.29120700
C	2.02498100	-4.05420400	-3.12681700
H	2.23360600	-3.64444700	-4.11606500
H	0.94471700	-4.13773400	-3.01718500
H	2.44793100	-5.06097200	-3.09613700
C	4.17328600	-3.18541100	-2.18968000
H	4.56573600	-4.15514800	-1.87402200
H	4.64998900	-2.41025500	-1.59631900
H	4.46137500	-3.02255400	-3.22978000
C	1.92483500	-1.82906500	2.84383900
H	2.29118900	-0.87996800	2.45640800
C	0.54502900	-1.57595500	3.45775200
H	0.10237000	-2.50305100	3.82478600
H	-0.14056100	-1.13810600	2.73430400
H	0.63380100	-0.89519100	4.30496700

C	2.90255400	-2.29883400	3.93063700
H	3.88214100	-2.54006400	3.51957000
H	2.52809000	-3.19228600	4.43401200
H	3.03005600	-1.52070300	4.68586100
C	-1.74721300	-0.84300200	-2.68114000
C	-3.14304800	-1.39950100	-3.04160700
H	-3.40741100	-1.19431000	-4.07847100
H	-3.13995300	-2.48292600	-2.91017300
C	-4.14314700	-0.78351800	-2.06065900
C	-0.70213800	-1.94507900	-2.84855600
H	0.30260800	-1.56612500	-2.69759300
H	-0.75167200	-2.34386400	-3.86443100
H	-0.87731700	-2.75993400	-2.14567600
C	-1.36708700	0.36268400	-3.55212300
H	-0.36880200	0.71297800	-3.30772300
H	-2.06143500	1.19203900	-3.42714000
H	-1.36971000	0.06962500	-4.60432500
C	-5.25830600	-1.75405100	-1.68207500
H	-4.86976900	-2.72262500	-1.38139200
H	-5.90425900	-1.90529700	-2.54786800
H	-5.87008400	-1.35591000	-0.87199600
C	-4.79666600	0.48351700	-2.62666300
H	-4.06384800	1.23749500	-2.90243500
H	-5.48875500	0.91974000	-1.90973600
H	-5.36386100	0.22094900	-3.52100600
C	-3.69306200	-0.27467300	0.43625900
C	-3.74111400	-1.38478500	1.30172700
C	-4.12872400	-1.17421200	2.62212900
H	-4.16818200	-2.01399000	3.30318600
C	-4.44795100	0.09247200	3.08303300
H	-4.74342500	0.23612600	4.11466500
C	-4.37323700	1.17597900	2.22528000
H	-4.59973800	2.16644300	2.59715500
C	-3.98508700	1.02108200	0.89561200
C	-3.34756700	-2.78751200	0.86997400
H	-3.16313600	-2.76745700	-0.20148400
C	-2.03947100	-3.23701900	1.52960900
H	-1.76407600	-4.23500200	1.18370200
H	-2.13704400	-3.27137200	2.61651900
H	-1.22790600	-2.55887900	1.27961300
C	-4.46230000	-3.80480800	1.14397000
H	-4.19851400	-4.77585300	0.71972100
H	-5.41456400	-3.49064800	0.71642400
H	-4.61176600	-3.94628000	2.21575500
C	-3.84979600	2.25883000	0.02851900
H	-3.53682000	1.93789700	-0.96046400
C	-2.75995000	3.20072100	0.55088600
H	-1.80041900	2.69287000	0.59869900
H	-2.99975100	3.57776500	1.54692000
H	-2.65251800	4.06044100	-0.11298300
C	-5.18288800	3.00633400	-0.10259600
H	-5.47975400	3.44497900	0.85198300
H	-5.99127600	2.34975500	-0.42593300
H	-5.09231000	3.81936300	-0.82571500

Cartesian coordinates of the optimized geometry for **1** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	-3.30805500	-0.35956900	-0.91070700
C	-1.99028500	-0.36365300	-1.21247300
Ga	1.48232200	0.10390500	-0.72524000
N	2.69846300	-1.27310600	0.07156400
N	2.38076400	1.64303900	0.16010600
Cl	2.26619200	0.26162100	-2.83848600
C	3.68896700	1.57509500	0.39558700
C	4.42041100	0.38415300	0.38909900
H	5.47832100	0.48638900	0.57707600
C	3.93990500	-0.93366300	0.39121100

C	4.44873600	2.83837700	0.70991600
H	5.45392600	2.61014600	1.05468300
H	3.93745100	3.43412400	1.46392500
H	4.51956900	3.45653000	-0.18611600
C	4.93180300	-1.97739100	0.84677700
H	5.86797300	-1.84551600	0.30350300
H	4.57394500	-2.99072300	0.69894200
H	5.15152200	-1.83766600	1.90545000
C	1.67723900	2.86731800	0.43029000
C	1.60619500	3.87890800	-0.54094400
C	0.96207700	5.07161600	-0.21387500
H	0.90232500	5.85920400	-0.95349900
C	0.40061400	5.26512500	1.03482700
H	-0.08889100	6.20052300	1.27448300
C	0.44452800	4.24392800	1.97024700
H	-0.02589900	4.39070300	2.93157000
C	1.06223800	3.02875600	1.68744900
C	2.15927400	3.70315800	-1.94097800
H	2.72210000	2.77345400	-1.97252700
C	3.10250000	4.83617800	-2.35954700
H	3.91813000	4.96863100	-1.64696200
H	2.57748400	5.78995600	-2.43993200
H	3.53867600	4.61686200	-3.33593600
C	1.00372200	3.56682700	-2.94093700
H	1.38116700	3.30998700	-3.93176900
H	0.44274000	4.50168200	-3.01447000
H	0.31330800	2.78480700	-2.63007300
C	1.06408300	1.92003000	2.72664700
H	1.12314000	0.97545500	2.18739600
C	2.29297000	1.99533700	3.64236100
H	2.26167900	1.19590000	4.38580500
H	2.32159000	2.94956900	4.17338400
H	3.22121800	1.89079100	3.08230100
C	-0.22375700	1.88985900	3.55349400
H	-0.22758100	1.01772600	4.20521400
H	-1.10224600	1.83078100	2.91199900
H	-0.31716600	2.76950900	4.19267500
C	2.19992100	-2.58873900	0.36032800
C	2.08175900	-3.53866800	-0.67494800
C	1.56025200	-4.79124400	-0.36050600
H	1.46273700	-5.53525600	-1.13767200
C	1.16368500	-5.10749400	0.92993600
H	0.75826900	-6.08718400	1.14894700
C	1.28722600	-4.16511400	1.93301800
H	0.97322000	-4.41275500	2.93836800
C	1.80314500	-2.89623900	1.67333200
C	2.54288800	-3.23958200	-2.09140400
H	2.30002400	-2.20244700	-2.30834300
C	1.85882400	-4.10021800	-3.15579600
H	2.07902400	-3.69436200	-4.14417000
H	0.77693300	-4.11989400	-3.03265400
H	2.22109100	-5.13073600	-3.13919800
C	4.06607000	-3.36535400	-2.24013900
H	4.40532600	-4.36089100	-1.94357700
H	4.59393100	-2.62876900	-1.64098500
H	4.35092600	-3.20351100	-3.28132200
C	1.93138800	-1.91708800	2.82769100
H	2.31770200	-0.97675200	2.43798200
C	0.57651700	-1.62722300	3.48019900
H	0.11892300	-2.54139600	3.86128000
H	-0.11694700	-1.17161900	2.77528300
H	0.70689100	-0.94845500	4.32381600
C	2.92135600	-2.42718300	3.88495200
H	3.88464400	-2.68687800	3.44800800
H	2.53468800	-3.31871700	4.38265200
H	3.08606800	-1.66425000	4.64852000
C	-1.82345000	-0.75142500	-2.67731900
C	-3.23741300	-1.24491200	-3.06271600
H	-3.48770400	-0.99804200	-4.09385500

H	-3.27504600	-2.33110900	-2.96501400
C	-4.22185900	-0.62050200	-2.06967200
C	-0.81637200	-1.88737000	-2.85739700
H	0.19787200	-1.55094000	-2.67105600
H	-0.85796600	-2.25301600	-3.88604300
H	-1.03764200	-2.71546200	-2.18367700
C	-1.38573200	0.45921100	-3.51510700
H	-0.37909900	0.76526900	-3.24590900
H	-2.05066300	1.31108500	-3.38014500
H	-1.38222900	0.19039600	-4.57373100
C	-5.35876000	-1.56962100	-1.70474800
H	-4.99051600	-2.54956900	-1.41529100
H	-6.00609900	-1.69656800	-2.57342400
H	-5.96325500	-1.16825800	-0.89084300
C	-4.83899500	0.67429300	-2.60928400
H	-4.08417600	1.40870300	-2.87891400
H	-5.51112800	1.11986900	-1.87950800
H	-5.42110800	0.44418000	-3.50289400
C	-3.76323800	-0.13486000	0.43383900
C	-3.86397600	-1.24280800	1.29819800
C	-4.26544100	-1.01774300	2.61217200
H	-4.34856300	-1.85598500	3.29105400
C	-4.54118900	0.25982400	3.07007800
H	-4.84898200	0.41397200	4.09656200
C	-4.40336300	1.34068500	2.21710700
H	-4.59143900	2.33927700	2.58835400
C	-4.00106100	1.17292500	0.89312900
C	-3.51027100	-2.66036700	0.87924100
H	-3.28559100	-2.64943800	-0.18506500
C	-2.24690800	-3.16091400	1.59069000
H	-1.99829700	-4.16910100	1.25380700
H	-2.38988800	-3.19222500	2.67284600
H	-1.39919200	-2.51582600	1.37449700
C	-4.67299700	-3.63324900	1.11479200
H	-4.43261700	-4.61456500	0.70047400
H	-5.59764400	-3.28393800	0.65559000
H	-4.86347700	-3.76648200	2.18109400
C	-3.79302400	2.41078800	0.03909100
H	-3.46805700	2.08603100	-0.94527800
C	-2.68110100	3.30654500	0.59896200
H	-1.74274500	2.76282600	0.67131900
H	-2.93655300	3.68865500	1.58932400
H	-2.52155500	4.16405100	-0.05737100
C	-5.09005000	3.21583600	-0.11598600
H	-5.38672700	3.66232100	0.83494700
H	-5.91997200	2.59797100	-0.45945400
H	-4.94877500	4.02781500	-0.83205600
As	-0.76239000	0.07512400	0.12122000

Cartesian coordinates of the optimized geometry for **2** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	-3.47072500	-0.25458500	-0.90460400
C	-2.15566700	-0.29366900	-1.18076500
Ga	1.59261700	0.06042200	-0.71250900
N	2.79964800	-1.37272300	0.00846300
N	2.62702800	1.55677400	0.10540500
Cl	2.23883900	0.18501200	-2.87910000
C	3.94099500	1.42848800	0.26367200
C	4.61214400	0.20293100	0.22475800
H	5.68277600	0.25475900	0.35297000
C	4.07147200	-1.09170700	0.25478600
C	4.77853500	2.65600000	0.51553800
H	5.76733200	2.38464600	0.87670800
H	4.30444500	3.32448600	1.23136500
H	4.89181600	3.21429400	-0.41517600
C	5.04240400	-2.18194500	0.64321600
H	5.92615400	-2.11901700	0.00724800

H	4.61466900	-3.17525600	0.55821800
H	5.37474400	-2.03063400	1.67025600
C	1.97636000	2.80356800	0.39673200
C	1.87657700	3.80526300	-0.58160500
C	1.23288100	4.99768600	-0.25063400
H	1.15044000	5.77691400	-0.99698500
C	0.69369200	5.19810700	1.00609000
H	0.19696200	6.12979700	1.24533600
C	0.77460700	4.19033400	1.95445500
H	0.32761400	4.34595100	2.92524900
C	1.40250500	2.98045600	1.67279400
C	2.39707300	3.62501100	-1.99381500
H	2.92305300	2.67480300	-2.04651800
C	3.37493500	4.73069100	-2.40823100
H	4.20471100	4.82242200	-1.70594300
H	2.88167300	5.70319500	-2.46238600
H	3.78807000	4.51447600	-3.39536000
C	1.22512200	3.54799500	-2.98087100
H	1.58187800	3.28972300	-3.97895200
H	0.70109000	4.50508300	-3.03758200
H	0.50819100	2.78897500	-2.67354300
C	1.45841500	1.88928300	2.72972500
H	1.42574800	0.93307100	2.20629300
C	2.77310500	1.91861300	3.52122100
H	2.77294100	1.13560600	4.28267700
H	2.89732100	2.87994100	4.02480200
H	3.63736600	1.75588100	2.88012800
C	0.26502500	1.92725600	3.68667100
H	0.27589700	1.04758300	4.32842700
H	-0.67976200	1.93427900	3.14327800
H	0.29752500	2.80237600	4.33825700
C	2.25275600	-2.66597700	0.31162800
C	2.04162000	-3.60038800	-0.72317100
C	1.47244400	-4.82836200	-0.39452900
H	1.30522300	-5.55978900	-1.17181300
C	1.11170200	-5.13417300	0.90861500
H	0.66787900	-6.09449400	1.13872600
C	1.31763500	-4.20433100	1.91007200
H	1.02985700	-4.44299700	2.92529900
C	1.88527000	-2.96059700	1.63654900
C	2.44264700	-3.30916700	-2.15910100
H	2.24682800	-2.25735200	-2.35135800
C	1.65164900	-4.11370700	-3.19299100
H	1.83824200	-3.70521500	-4.18721000
H	0.57924400	-4.07348900	-3.00760200
H	1.95416400	-5.16337100	-3.21034000
C	3.94523800	-3.52014000	-2.39339300
H	4.24108700	-4.53859800	-2.12977600
H	4.54699600	-2.82620500	-1.81336000
H	4.18266700	-3.35712300	-3.44627000
C	2.10057100	-1.99376100	2.78816700
H	2.45849300	-1.05071400	2.37784900
C	0.80092200	-1.70888400	3.54738300
H	0.38586900	-2.62058700	3.97973800
H	0.04595400	-1.27153500	2.89541000
H	0.99191600	-1.01561800	4.36747600
C	3.16701300	-2.51597900	3.76193400
H	4.09871800	-2.75735600	3.25295600
H	2.82161700	-3.42188000	4.26432900
H	3.37973900	-1.76834500	4.52888400
C	-1.96397700	-0.65738000	-2.64535100
C	-3.38147800	-1.09998300	-3.07747700
H	-3.60210400	-0.81495000	-4.10546100
H	-3.45099700	-2.18705800	-3.01438100
C	-4.37108900	-0.47635900	-2.08847800
C	-0.98159700	-1.81660800	-2.82097900
H	0.03141500	-1.51555300	-2.57426600
H	-0.98493800	-2.14603800	-3.86258900
H	-1.25700900	-2.65988500	-2.18705200

C	-1.46476000	0.55753600	-3.44330500
H	-0.45862400	0.82674100	-3.13420900
H	-2.10822300	1.42614900	-3.30946900
H	-1.43439400	0.31124500	-4.50702400
C	-5.52901200	-1.41114100	-1.75979600
H	-5.17882400	-2.40058500	-1.48018500
H	-6.16188600	-1.51465400	-2.64220500
H	-6.14259500	-1.01409700	-0.95062300
C	-4.94807100	0.84258900	-2.60939700
H	-4.17134500	1.56771800	-2.83957200
H	-5.63061900	1.28227500	-1.88650600
H	-5.51062400	0.64691500	-3.52346200
C	-3.95291000	-0.03750200	0.43393900
C	-4.10105000	-1.15543400	1.28090300
C	-4.55525600	-0.94116000	2.57958400
H	-4.67909300	-1.78742800	3.24189300
C	-4.83345800	0.33316700	3.04353500
H	-5.18549500	0.47756500	4.05710200
C	-4.63676800	1.42315800	2.21490300
H	-4.82233300	2.41934500	2.59335900
C	-4.18047200	1.26920200	0.90650500
C	-3.74870300	-2.57600000	0.86830500
H	-3.44776800	-2.55910300	-0.17739400
C	-2.55447700	-3.11643000	1.66883000
H	-2.29053600	-4.11701300	1.32046100
H	-2.79218000	-3.18194400	2.73271300
H	-1.68239500	-2.47752900	1.54892000
C	-4.94530700	-3.52652200	1.01370300
H	-4.69921300	-4.50727000	0.60151200
H	-5.83210900	-3.15237100	0.50345900
H	-5.20493500	-3.66917300	2.06403700
C	-3.91280600	2.52301300	0.09128200
H	-3.52459500	2.21691700	-0.87685500
C	-2.84204200	3.41021700	0.74371400
H	-1.91328300	2.86352300	0.89079500
H	-3.17826300	3.79153600	1.71004900
H	-2.62710500	4.26794100	0.10340700
C	-5.19385100	3.34116600	-0.12535000
H	-5.53608900	3.77878600	0.81428800
H	-6.01052500	2.73707600	-0.51930200
H	-5.00715200	4.16041900	-0.82238200
Sb	-0.78140700	0.14609300	0.32405900

Cartesian coordinates of the optimized geometry for **3** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	-3.51209400	-0.02548700	-0.92887700
C	-2.20341400	-0.08910100	-1.20723800
Ga	1.66288900	-0.04870900	-0.71991300
N	2.68678300	-1.62765300	0.00581800
N	2.92210400	1.29893800	0.04440700
Cl	2.28945700	-0.07612200	-2.90283500
C	4.21016200	0.99636500	0.17270400
C	4.70442000	-0.31007800	0.14960900
H	5.77459600	-0.40505100	0.25352000
C	3.98996700	-1.51620100	0.22275200
C	5.21152300	2.10409500	0.37701700
H	6.17787300	1.70478600	0.67437900
H	4.87060800	2.81594300	1.12677900
H	5.33652100	2.65934000	-0.55380200
C	4.81141700	-2.71805400	0.62885600
H	5.71671900	-2.75727700	0.02268500
H	4.27226000	-3.65325200	0.52313400
H	5.12465600	-2.61328000	1.66791800
C	2.45690100	2.62663600	0.32601500
C	2.46884000	3.61691100	-0.66870500
C	2.01057700	4.89291900	-0.34213400
H	2.01555100	5.66519600	-1.10007400

C	1.54132000	5.18538800	0.92506300
H	1.19087500	6.18220200	1.16090800
C	1.50171900	4.18897400	1.88826500
H	1.10753900	4.41980600	2.86713500
C	1.94415600	2.89862500	1.61078000
C	2.90497100	3.33597200	-2.09285400
H	3.30967600	2.32750700	-2.13444500
C	3.99118500	4.30063200	-2.58185700
H	4.85485400	4.31005300	-1.91504700
H	3.61869900	5.32453000	-2.65177800
H	4.33329500	4.00558800	-3.57565300
C	1.68968500	3.37319900	-3.02915400
H	1.97157300	3.05338400	-4.03332100
H	1.27722900	4.38324500	-3.08933700
H	0.90425100	2.70851000	-2.67288200
C	1.86193300	1.81753300	2.67671200
H	1.66988700	0.87449400	2.16219800
C	3.18522400	1.64707200	3.43492200
H	3.08332700	0.87970700	4.20539700
H	3.47010900	2.58150500	3.92363100
H	3.99590400	1.34629200	2.77434100
C	0.71527600	2.04227300	3.66490700
H	0.60132700	1.16984100	4.30654200
H	-0.23115200	2.20599900	3.14893700
H	0.90431200	2.89903900	4.31422800
C	1.99614500	-2.84376100	0.33468400
C	1.68547000	-3.77311900	-0.67996700
C	1.01472600	-4.93951600	-0.31925400
H	0.77269300	-5.66796400	-1.07933300
C	0.65037100	-5.19000600	0.99467000
H	0.12960500	-6.10436500	1.24945600
C	0.94799400	-4.26195200	1.97407400
H	0.65325700	-4.45422900	2.99719800
C	1.61833400	-3.07830100	1.66834200
C	2.08718100	-3.54511500	-2.12768000
H	1.96376500	-2.48660600	-2.34208300
C	1.22537300	-4.31523000	-3.13083300
H	1.42476100	-3.94321800	-4.13677400
H	0.16125600	-4.19622200	-2.93181300
H	1.45380400	-5.38366800	-3.12771200
C	3.56690300	-3.86641700	-2.38229500
H	3.80101300	-4.89150600	-2.08451100
H	4.22683000	-3.19083300	-1.84587700
H	3.78927700	-3.76062800	-3.44562100
C	1.92619900	-2.10931900	2.79665500
H	2.38563100	-1.22175300	2.36494000
C	0.65319700	-1.66977000	3.52687700
H	0.13810500	-2.52230100	3.97245200
H	-0.04111400	-1.17353900	2.84948100
H	0.90243300	-0.97920200	4.33347300
C	2.92121200	-2.71105500	3.79895600
H	3.82894600	-3.06079700	3.30972300
H	2.47960300	-3.56196300	4.32161100
H	3.20157900	-1.96776800	4.54814400
C	-2.01688300	-0.52428600	-2.65133400
C	-3.45282000	-0.90668600	-3.08773300
H	-3.65111100	-0.63511700	-4.12376600
H	-3.57944900	-1.98690600	-2.99984500
C	-4.41468600	-0.20767700	-2.12171200
C	-1.10557900	-1.75131700	-2.73970400
H	-0.08105300	-1.49828500	-2.48737800
H	-1.10977200	-2.13757200	-3.76136600
H	-1.44390400	-2.54010400	-2.06720500
C	-1.42283600	0.60876200	-3.50202100
H	-0.40890900	0.83352100	-3.18091500
H	-2.01261900	1.52190700	-3.43257800
H	-1.38404600	0.30026400	-4.54915300
C	-5.63754700	-1.05215300	-1.78911200
H	-5.36123500	-2.05763200	-1.48485300

H	-6.26719100	-1.12953300	-2.67643800
H	-6.23005700	-0.59738900	-0.99461300
C	-4.88226800	1.14143400	-2.67639000
H	-4.04699900	1.80955200	-2.87447700
H	-5.56746100	1.63545100	-1.99289000
H	-5.41156600	0.97315300	-3.61554700
C	-3.98590500	0.11499600	0.42365400
C	-4.08556800	-1.05363600	1.20885700
C	-4.50636600	-0.92399100	2.52887700
H	-4.58885100	-1.80856800	3.14601300
C	-4.80575300	0.31524800	3.07065200
H	-5.12944500	0.39384600	4.10073300
C	-4.67461400	1.45283200	2.29570400
H	-4.88775100	2.42012800	2.73041200
C	-4.25322600	1.38314500	0.96741400
C	-3.72960100	-2.44109900	0.69854800
H	-3.49243200	-2.36211200	-0.36025400
C	-2.48222700	-3.00167100	1.39542700
H	-2.22825600	-3.98061500	0.98548400
H	-2.65123800	-3.11963000	2.46792200
H	-1.62516000	-2.34680800	1.25444100
C	-4.90116700	-3.42108500	0.85222300
H	-4.66326000	-4.36944600	0.36627800
H	-5.82106300	-3.03219100	0.41570600
H	-5.10001500	-3.63359100	1.90391600
C	-4.08371800	2.68142200	0.19922900
H	-3.68232300	2.44011000	-0.78180000
C	-3.08085100	3.62716600	0.87488600
H	-2.10825300	3.15195500	0.99094800
H	-3.43273100	3.94400600	1.85851000
H	-2.94633400	4.52281000	0.26513500
C	-5.42973300	3.39879700	0.02026200
H	-5.79810200	3.77156000	0.97789100
H	-6.19631700	2.73973400	-0.38733200
H	-5.32065000	4.25407500	-0.64941600
Bi	-0.74178300	0.49526000	0.32468200

Cartesian coordinates of the optimized geometry for **10** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	2.26391800	-1.79558000	-0.89919500
C	0.99344700	-1.34165100	-0.96915300
Ga	-0.96973900	0.39988200	0.22891800
N	-0.93668400	2.20240400	0.84270100
N	-2.74123300	-0.07521300	0.73513100
C	-3.47100500	0.71917500	1.53909600
C	-3.07454600	1.99010500	1.93960700
H	-3.77103800	2.51704600	2.57125200
C	-1.94630300	2.71967700	1.54994900
C	-4.79815100	0.21763200	2.03335700
H	-5.35204200	1.01545000	2.51953200
H	-4.64119700	-0.58519000	2.75565000
H	-5.39788400	-0.19705100	1.22587200
C	-1.91851300	4.17645900	1.91584000
H	-2.22964500	4.76773700	1.05102000
H	-0.92345200	4.51471200	2.18979500
H	-2.61152800	4.37742600	2.72849700
C	-3.35132500	-1.25470600	0.17088800
C	-3.33436800	-2.45808500	0.88601900
C	-3.93404400	-3.57150600	0.29920400
H	-3.93475800	-4.51519500	0.82695600
C	-4.52562500	-3.48958700	-0.94896700
H	-4.99033000	-4.36357300	-1.38580100
C	-4.51478500	-2.29125700	-1.64785200
H	-4.96690900	-2.24959100	-2.62770900
C	-3.92473500	-1.15032800	-1.11129900
C	-2.64717800	-2.59530700	2.23226300
H	-2.42869800	-1.59521000	2.60816300

C	-3.52736500	-3.29531200	3.27353700
H	-4.50613500	-2.82141800	3.35989200
H	-3.04640800	-3.26415800	4.25202700
H	-3.68962600	-4.34429200	3.02313700
C	-1.30685200	-3.32611400	2.07418100
H	-1.45535700	-4.31542700	1.63812900
H	-0.82807800	-3.45374100	3.04504800
H	-0.62407400	-2.77272600	1.42985100
C	0.15468000	3.06958200	0.46032000
C	1.30216900	3.10163500	1.26440500
C	2.29631900	4.01709600	0.92534200
H	3.19151100	4.07801400	1.52641200
C	2.16461000	4.84196400	-0.18011600
H	2.94933000	5.54602200	-0.42373400
C	1.04234400	4.75289300	-0.98812100
H	0.96498000	5.38507000	-1.86129000
C	0.01236500	3.86683300	-0.68405600
C	1.46268100	2.18142700	2.46272000
H	0.92747600	1.25739200	2.23258400
C	0.84684000	2.76882700	3.74005600
H	-0.22998500	2.90807000	3.65805300
H	1.29613100	3.73585500	3.97463400
H	1.02893300	2.10082900	4.58349700
C	2.91928600	1.79350400	2.70719200
H	2.97151500	1.01597900	3.46796900
H	3.50858800	2.63787800	3.06845100
H	3.38419400	1.41008600	1.80233900
C	-1.19255500	3.73269500	-1.59924800
H	-2.02057400	3.32696900	-1.01595600
C	-1.67142600	5.06241400	-2.18494600
H	-2.60171700	4.91440900	-2.73527000
H	-0.94687200	5.48401800	-2.88234500
H	-1.85295600	5.80145200	-1.40340200
C	-0.88164300	2.72432300	-2.71374700
H	-1.76029900	2.54150500	-3.33475700
H	-0.54247400	1.76955600	-2.30884500
H	-0.08129200	3.09713500	-3.35509200
C	0.27408700	-2.06082700	-2.12500000
C	1.41792700	-2.81688700	-2.82404600
H	1.09520700	-3.78224800	-3.21123200
H	1.78324300	-2.23022500	-3.66806400
C	2.54843500	-2.96276700	-1.79577500
C	3.29296900	-1.20402900	-0.09167000
C	4.08470900	-0.19567500	-0.67249900
C	5.19019500	0.26102900	0.03969500
H	5.82065900	1.02736500	-0.38933500
C	5.49980300	-0.25397600	1.28906600
H	6.37485300	0.09916300	1.81885200
C	4.66695400	-1.19157400	1.87317400
H	4.88623600	-1.54891800	2.87020600
C	3.53901600	-1.67005600	1.20701800
C	3.73323300	0.44275600	-2.00500000
H	3.03594400	-0.21634200	-2.51869500
C	3.00437100	1.77233000	-1.77495100
H	2.68820500	2.20462800	-2.72643500
H	3.65871100	2.49134200	-1.28199800
H	2.12677900	1.63474100	-1.14681900
C	4.94424000	0.64380700	-2.92056500
H	5.51367600	-0.27682600	-3.05031200
H	5.62328500	1.40130700	-2.52716900
H	4.61654000	0.98462500	-3.90416000
C	2.58415600	-2.59109500	1.94188900
H	1.83697300	-2.93808200	1.23130900
C	1.84561700	-1.80052700	3.03134600
H	1.29140300	-0.97135000	2.59288000
H	2.54809800	-1.39436400	3.76037900
H	1.14698300	-2.44476600	3.56565200
C	3.27324700	-3.81806600	2.54670200
H	2.53113400	-4.49684900	2.97056500

H	3.95514700	-3.53662200	3.35031200
H	3.85003800	-4.36792400	1.80330700
C	-0.36325400	-1.03934000	-3.06408800
H	-0.78017000	-1.54700700	-3.93503800
H	0.36529300	-0.30617100	-3.41137100
H	-1.17861700	-0.50635300	-2.57682200
C	-0.80156900	-3.01498600	-1.59985000
H	-1.56727000	-2.48009800	-1.04779000
H	-0.38962100	-3.78115700	-0.94714500
H	-1.28863100	-3.51356200	-2.43858200
C	3.92310500	-2.88536600	-2.45130800
H	4.05326500	-3.76330400	-3.08493800
H	4.72089500	-2.88628900	-1.70954300
H	4.02956700	-2.00454100	-3.07771900
C	2.46868400	-4.27603100	-1.01077600
H	1.52541600	-4.38455300	-0.48003600
H	3.27709100	-4.33726700	-0.28492100
H	2.57263900	-5.11695800	-1.69719200
C	-3.90615700	0.15385400	-1.89716500
H	-2.96067000	0.66062400	-1.67523000
C	-5.03147000	1.10855700	-1.47131300
H	-5.00956500	2.01072200	-2.08487900
H	-6.00427500	0.63282800	-1.60719900
H	-4.94626700	1.41601500	-0.43173400
C	-3.95588200	-0.04990900	-3.41303500
H	-3.75250500	0.89524200	-3.91748200
H	-3.22334400	-0.78062800	-3.75218900
H	-4.94253100	-0.38149300	-3.73922900
N	0.54947400	-0.42700400	-0.17737000

Cartesian coordinates of the optimized geometry for **11** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	2.82551600	-1.51366800	-0.80812300
C	1.51538100	-1.25147500	-0.80212500
P	0.96662600	0.08865000	0.18610500
Ga	-1.26155400	0.33725700	0.19102700
N	-1.66137000	2.16709800	0.67312300
N	-2.99421300	-0.39691800	0.50646300
C	-3.97213000	0.30254400	1.11029100
C	-3.88811900	1.65715100	1.41298900
H	-4.76564100	2.08747900	1.86836900
C	-2.84198800	2.55218600	1.15096000
C	-5.23183600	-0.41709000	1.50614100
H	-6.02531900	0.29232100	1.72431200
H	-5.04380100	-1.00618800	2.40612400
H	-5.56666700	-1.10898500	0.73759700
C	-3.10809700	4.01178500	1.38447000
H	-3.39077800	4.47950600	0.43789100
H	-2.22770000	4.53519400	1.74685600
H	-3.92998800	4.14541100	2.08337700
C	-3.22234800	-1.76405800	0.11231300
C	-3.01570000	-2.79215600	1.04253700
C	-3.21267600	-4.10447700	0.61515100
H	-3.05987200	-4.91909500	1.30960200
C	-3.59985700	-4.38122500	-0.68447000
H	-3.75224400	-5.40602600	-0.99660100
C	-3.78970200	-3.34820200	-1.59117400
H	-4.08543600	-3.58403400	-2.60277800
C	-3.60351900	-2.01927200	-1.21900600
C	-2.55754400	-2.51969600	2.46534100
H	-2.68312900	-1.45538600	2.66454900
C	-3.39260000	-3.27811700	3.50287900
H	-4.46032800	-3.09803200	3.37032300
H	-3.11572600	-2.96225800	4.50957300
H	-3.22892900	-4.35470700	3.44254300
C	-1.06476700	-2.83619400	2.63267300
H	-0.86573700	-3.88865200	2.42159700

H	-0.74668200	-2.63049000	3.65579600
H	-0.44650700	-2.23744000	1.96345400
C	-0.64700600	3.14801100	0.36700200
C	0.38074700	3.38305700	1.29400000
C	1.34283200	4.33478600	0.96240400
H	2.14430100	4.54356200	1.65629200
C	1.29875600	5.00978200	-0.24663300
H	2.05730200	5.74428400	-0.48290600
C	0.29678400	4.73159900	-1.16220700
H	0.28693200	5.24781900	-2.11197500
C	-0.69341500	3.79493400	-0.87728000
C	0.45645800	2.64611800	2.62101400
H	-0.07542300	1.69951000	2.50474500
C	-0.24910100	3.42555200	3.73980300
H	-1.30932400	3.56771100	3.53279700
H	0.20382900	4.41066500	3.86649600
H	-0.16339800	2.89030100	4.68700800
C	1.89304700	2.30502900	3.02816900
H	1.88223700	1.63832200	3.89136800
H	2.45312300	3.19592300	3.31591900
H	2.42973900	1.80662000	2.22191300
C	-1.74249400	3.44550500	-1.91961800
H	-2.57989800	2.96407600	-1.41377500
C	-2.30568600	4.66863000	-2.64732300
H	-3.12660100	4.37050100	-3.30123800
H	-1.55334400	5.15236100	-3.27119200
H	-2.68362300	5.41195200	-1.94396500
C	-1.16969700	2.42893700	-2.91834700
H	-1.93540600	2.10275500	-3.62492700
H	-0.77004400	1.54912300	-2.41014200
H	-0.34727600	2.86949500	-3.48486000
C	0.79984000	-2.20491200	-1.75258300
C	1.97293900	-2.83025400	-2.54119800
H	1.78445900	-3.87492900	-2.78262700
H	2.10006500	-2.29301500	-3.48163000
C	3.23776100	-2.66140500	-1.69225800
C	3.76291800	-0.73537000	-0.03162100
C	4.31607100	0.42452100	-0.60975400
C	5.23476300	1.15166600	0.14264500
H	5.67777200	2.04191300	-0.28218200
C	5.58083700	0.76576300	1.42643700
H	6.30266900	1.34219800	1.99012900
C	4.98042300	-0.34242600	1.99723000
H	5.22433400	-0.61344200	3.01524900
C	4.04988400	-1.10571900	1.29472800
C	3.91239000	0.96370500	-1.97231600
H	3.22692700	0.25280300	-2.43153900
C	3.15651900	2.29389600	-1.83090900
H	2.81224000	2.63561200	-2.80903300
H	3.80320400	3.06908700	-1.41701000
H	2.29163500	2.19399300	-1.17921600
C	5.11653100	1.14181400	-2.90629100
H	5.70820900	0.23163900	-2.99312900
H	5.77740800	1.93129300	-2.54627000
H	4.77971400	1.42851100	-3.90409000
C	3.34373500	-2.23277200	2.02768600
H	2.66574400	-2.72059100	1.33123000
C	2.48813700	-1.67902100	3.17711700
H	1.77229400	-0.94432500	2.81241000
H	3.11134000	-1.20238000	3.93523700
H	1.93830800	-2.48977600	3.65799900
C	4.32260700	-3.28425100	2.56457700
H	3.77567200	-4.12678000	2.99113100
H	4.95050600	-2.86779800	3.35340600
H	4.98357600	-3.66655500	1.78776600
C	-0.14135400	-1.47966500	-2.71121600
H	-0.49676700	-2.18123800	-3.46673700
H	0.35986100	-0.65334100	-3.21477900
H	-1.01368100	-1.08631600	-2.19365300

C	0.01453900	-3.25598200	-0.95709200
H	-0.79557600	-2.79657700	-0.39891200
H	0.64650300	-3.79099300	-0.25060800
H	-0.42470000	-3.98139100	-1.64235000
C	4.45536700	-2.31271800	-2.53906500
H	4.71674100	-3.17785000	-3.14892200
H	5.31601600	-2.06932300	-1.91670100
H	4.25683200	-1.47946800	-3.20696900
C	3.56271900	-3.90423400	-0.86245200
H	2.73287500	-4.21231300	-0.23099100
H	4.43282000	-3.73228200	-0.23321900
H	3.79775900	-4.72711800	-1.53780600
C	-3.82129500	-0.89149000	-2.22017500
H	-3.06328600	-0.12563200	-2.02522600
C	-5.19051400	-0.21571900	-2.04763100
H	-5.33433300	0.53834600	-2.82306600
H	-5.99238800	-0.95038100	-2.14045000
H	-5.29291600	0.28028500	-1.08585200
C	-3.65746700	-1.32772800	-3.67781100
H	-3.64292900	-0.44891900	-4.32324300
H	-2.73570500	-1.88300600	-3.84073000
H	-4.49100500	-1.95191000	-4.00343700

Cartesian coordinates of the optimized geometry for **4**-An$^-$ at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

As	0.96947300	0.28063900	0.12439300
Ga	-1.37240800	0.32126900	0.13779700
C	1.61483100	-1.25554400	-0.76975900
N	-3.07443400	-0.50263300	0.41671000
N	-1.90491700	2.13746200	0.56026000
N	2.92386100	-1.47061100	-0.72734100
C	0.94120200	-2.30568400	-1.63637100
C	-4.12238700	0.15862700	0.94113100
C	-3.19655600	-1.89834900	0.08199400
C	-3.13078400	2.47296800	0.94756200
C	-0.90654900	3.14650900	0.30353700
C	3.39303100	-2.67245600	-1.51478800
C	3.81667600	-0.61694700	0.02514000
C	2.14280500	-2.96477300	-2.35278400
C	-0.01161900	-1.69675100	-2.66295100
C	0.17752300	-3.30209900	-0.75292100
C	-4.13895900	1.52771000	1.18374300
C	-5.35389200	-0.62272000	1.30883800
C	-3.49437100	-2.24209000	-1.25077600
C	-2.97166600	-2.86488400	1.07232100
C	-3.49207300	3.92269600	1.10031900
C	-0.85689500	3.74003400	-0.96619500
C	0.04049700	3.43393100	1.30085500
C	4.60080100	-2.34064400	-2.38079200
C	3.76358900	-3.82551700	-0.58266200
C	4.36929400	0.51355700	-0.60931500
C	4.05450100	-0.88973500	1.38583800
H	1.99220100	-4.03388500	-2.49194300
H	2.26087900	-2.51776200	-3.34028600
H	-0.34386800	-2.47533500	-3.35053200
H	0.47309400	-0.90885800	-3.23933500
H	-0.89321700	-1.27581100	-2.18540200
H	-0.64948800	-2.81555900	-0.24455900
H	0.81781700	-3.75245800	0.00366000
H	-0.23582700	-4.09856600	-1.37202300
H	-5.06622300	1.92183400	1.56794500
H	-6.19788000	0.04386200	1.46335100
H	-5.17375400	-1.16639000	2.23852700
H	-5.61043900	-1.36114800	0.55349100
C	-3.58143900	-3.59694500	-1.56118900
C	-3.72680200	-1.17996400	-2.31878300
C	-3.06759800	-4.20641200	0.70553100

C	-2.59936000	-2.49180400	2.49755400
H	-3.77740600	4.32127700	0.12325000
H	-2.65644800	4.51829500	1.45678100
H	-4.34072200	4.04000200	1.76983200
C	0.15071800	4.66965400	-1.21231400
C	-1.81856700	3.34989500	-2.07557700
C	1.02223900	4.37691600	1.00601000
C	0.01229000	2.74906000	2.65810700
H	4.90213700	-3.23963800	-2.91906600
H	5.44591200	-2.01383300	-1.77569400
H	4.37252300	-1.57197000	-3.11359100
H	2.93937000	-4.12325200	0.06086500
H	4.61484600	-3.56134900	0.04032400
H	4.04844700	-4.68670500	-1.18724900
C	5.23891500	1.31228200	0.12955600
C	4.02532100	0.94836100	-2.02528300
C	4.93518400	-0.05580600	2.07137900
C	3.35256800	-1.98738700	2.16744600
H	-3.81241500	-3.90055400	-2.57154300
C	-3.37455600	-4.57023300	-0.59409800
C	-5.13081900	-0.56134500	-2.23233300
H	-3.01086000	-0.37026600	-2.13946400
C	-3.49065500	-1.68329200	-3.74450700
H	-2.89976700	-4.97480400	1.44753500
H	-2.81667000	-1.43305200	2.63839500
C	-3.41626600	-3.26546200	3.53793500
C	-1.09474000	-2.67775800	2.73945400
H	0.21558300	5.14141300	-2.18318300
C	1.07638200	4.99344700	-0.23425000
H	-2.64537900	2.79511800	-1.63131600
C	-1.12594900	2.41171000	-3.07522800
C	-2.42472700	4.56165200	-2.78965100
H	1.76398200	4.62344200	1.75185200
H	-0.46724600	1.77633000	2.52651600
C	-0.83241700	3.53568500	3.67043700
C	1.41119000	2.48514900	3.22258100
H	5.68198100	2.18083300	-0.33777400
C	5.53551400	1.02536200	1.45052700
H	3.35248900	0.20844600	-2.45699300
C	5.27137100	1.04736000	-2.91609800
C	3.28050700	2.29309900	-2.02645400
H	5.14108300	-0.25078100	3.11482800
H	2.71187000	-2.53863700	1.48339100
C	4.34175200	-2.97274200	2.80304100
C	2.44365100	-1.39050800	3.25260500
H	-3.45017100	-5.61665700	-0.85907300
H	-5.29147500	-0.01704100	-1.30549100
H	-5.89440500	-1.33739000	-2.31045700
H	-3.49643500	-0.83967200	-4.43533600
H	-5.27973800	0.14003400	-3.05479500
H	-4.28120400	-2.36486300	-4.06245000
H	-2.53791200	-2.19885500	-3.84784000
H	-4.48799700	-3.17821400	3.35385400
H	-3.20947800	-2.88084400	4.53753000
H	-3.16604000	-4.32703100	3.53929300
H	-0.80362600	-3.71921600	2.58922000
H	-0.83798500	-2.39892500	3.76261500
H	-0.49693800	-2.06310400	2.06568300
H	1.85109400	5.71950800	-0.44258700
H	-1.83139700	2.06691000	-3.83385300
H	-0.69899000	1.54076900	-2.57466200
H	-0.30679100	2.92534100	-3.58169700
H	-3.17884100	4.23701400	-3.50830400
H	-1.67034500	5.12485400	-3.34018600
H	-2.89865500	5.24466700	-2.08323900
H	-1.87151300	3.62308800	3.35585200
H	-0.43435200	4.54381000	3.80056100
H	-0.81918300	3.03930900	4.64229000
H	1.33750900	1.84625600	4.10360400

H	1.90146700	3.40861300	3.53418700
H	2.05004100	1.98654400	2.49418500
H	6.21920800	1.65689300	2.00260000
H	5.86054900	0.13198800	-2.90550200
H	5.92023300	1.86056200	-2.58845900
H	4.98110800	1.25665000	-3.94714600
H	2.99000000	2.55615400	-3.04549400
H	3.91736200	3.09325100	-1.64592100
H	2.38210700	2.25609400	-1.41426000
H	3.80369200	-3.80309000	3.26336100
H	4.92772100	-2.48817700	3.58513400
H	5.04151000	-3.38262000	2.07615100
H	1.71737900	-0.70397300	2.82133600
H	3.02661900	-0.84801500	3.99827500
H	1.90349600	-2.18767000	3.76620000

Cartesian coordinates of the optimized geometry for **6**-An$^-$ at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Sb	-0.95359800	0.49512600	0.03629500
Ga	1.59410600	0.26005100	-0.00852600
C	-1.83673600	-1.34288800	-0.57574300
N	3.27959000	-0.63004200	0.24933700
N	2.29460800	2.07730000	0.14345800
N	-3.14547500	-1.46678700	-0.44413800
C	-1.27150800	-2.54536000	-1.30721900
C	4.43132100	0.01808300	0.49679400
C	3.27571400	-2.06845200	0.17181500
C	3.57010300	2.37772200	0.34883800
C	1.28718100	3.09642700	0.00762600
C	-3.72496700	-2.74423200	-1.02737300
C	-3.95424200	-0.46653800	0.22157500
C	-2.44218200	-3.55189900	-1.25598800
C	-0.92098700	-2.13724400	-2.74936900
C	-0.03936400	-3.12603400	-0.62297300
C	4.56112600	1.40146200	0.52622600
C	5.66266300	-0.80315500	0.76112500
C	3.59256800	-2.67501800	-1.05616100
C	2.90949900	-2.81495700	1.29931900
C	3.99584300	3.81549700	0.43843200
C	0.81029800	3.39716300	-1.28143100
C	0.72204000	3.66528100	1.16034700
C	-4.48521300	-2.46696700	-2.32253600
C	-4.67033700	-3.42522000	-0.04735700
C	-4.50514500	0.60020600	-0.51632500
C	-4.11630800	-0.55943600	1.61952900
H	-2.50121300	-4.15264400	-2.16198500
H	-2.29117800	-4.23349000	-0.41832300
H	-1.78270000	-1.73835200	-3.28165300
H	-0.55548500	-3.00888100	-3.29486500
H	-0.14687300	-1.37395300	-2.75379300
H	-0.23661100	-3.35297200	0.42342500
H	0.80410500	-2.44327500	-0.66874000
H	0.26129000	-4.04786400	-1.12128900
H	5.55490700	1.77560100	0.71477200
H	5.49469000	-1.48259200	1.59721200
H	6.50956600	-0.16266200	0.98963200
H	5.91232700	-1.42377200	-0.09983400
C	3.50681100	-4.06141400	-1.13688800
C	3.99156300	-1.84360100	-2.26540600
C	2.83406900	-4.20099300	1.16524000
C	2.60313900	-2.16618800	2.63794600
H	3.92210600	4.15366900	1.47429000
H	3.36076600	4.46309500	-0.16027400
H	5.03178200	3.92636800	0.12599400
C	-0.24082100	4.30287500	-1.39262900
C	1.42614600	2.78554300	-2.52800900
C	-0.33808200	4.55437700	0.99300600
C	1.20697100	3.33431100	2.56194500

H	-5.36985300	-1.86547100	-2.13210500
H	-4.81493000	-3.41799600	-2.74112300
H	-3.87508600	-1.96485900	-3.06884700
H	-4.16154300	-3.72114900	0.86539400
H	-5.06827400	-4.32527200	-0.51665300
H	-5.51173100	-2.78151500	0.20753800
C	-5.28527000	1.52874800	0.17137100
C	-4.26825500	0.83459300	-1.99990200
C	-4.90438900	0.40088200	2.24807400
C	-3.44319700	-1.61030400	2.48821100
H	3.74588000	-4.55954100	-2.06571400
C	3.12388000	-4.81928500	-0.03882700
H	4.44684400	-0.92177200	-1.90195900
C	5.02736700	-2.53147400	-3.15781600
C	2.75965100	-1.44085400	-3.08506000
H	2.55039900	-4.80289500	2.01822800
H	2.83563100	-1.10376900	2.55786100
C	3.48067500	-2.73652400	3.75882500
C	1.11564100	-2.28400100	2.99355900
H	-0.62428700	4.55661100	-2.37088400
C	-0.81588600	4.87271300	-0.26744000
H	1.98865300	1.90015200	-2.22459500
C	2.43036600	3.75207600	-3.17120900
C	0.37910300	2.32231100	-3.54404400
H	-0.79705900	5.00199700	1.86414100
H	2.09212300	2.70417500	2.47717900
C	1.61191400	4.59743200	3.33287900
C	0.15814800	2.53593100	3.34759600
H	-5.72563200	2.35146400	-0.37462900
C	-5.49668300	1.42811400	1.53423600
H	-3.62099900	0.04335900	-2.37190300
C	-3.54734600	2.16814100	-2.25298800
C	-5.57938400	0.81201200	-2.79910100
H	-5.04858000	0.34591200	3.31820600
H	-2.88802400	-2.28785800	1.84139400
C	-2.42859900	-0.96920500	3.44689600
C	-4.46187700	-2.43227100	3.29025200
H	3.06250000	-5.89646000	-0.12226400
H	5.89157700	-2.86626400	-2.58259900
H	5.37693000	-1.83739700	-3.92312600
H	4.61071300	-3.39783300	-3.67337000
H	2.24196300	-2.32296300	-3.46465300
H	3.04627600	-0.81901000	-3.93476700
H	2.04225500	-0.87312700	-2.48736500
H	3.30482000	-2.19356400	4.68868500
H	4.54126300	-2.65827200	3.51559400
H	3.25995800	-3.78867600	3.94382400
H	0.81614900	-3.33037300	3.08095500
H	0.48491800	-1.81362600	2.23882800
H	0.91334100	-1.79638700	3.94849400
H	-1.63950400	5.56626600	-0.37415600
H	3.22762200	4.02267400	-2.47835200
H	1.93298300	4.67223900	-3.48304800
H	2.88770800	3.29901500	-4.05256900
H	-0.34913900	1.65803500	-3.07788300
H	0.86532700	1.78498200	-4.36002700
H	-0.15887400	3.16272400	-3.98426900
H	0.74765200	5.23002500	3.53947800
H	2.33188100	5.19733700	2.77500700
H	2.05937800	4.32839100	4.29094500
H	0.53158300	2.29902100	4.34552800
H	-0.09171300	1.60233500	2.84355400
H	-0.76498300	3.10685600	3.46083800
H	-6.10987800	2.15976100	2.04381800
H	-4.17101400	3.01367100	-1.95918900
H	-3.32598200	2.27309400	-3.31669800
H	-2.61044500	2.23169300	-1.70341000
H	-6.17419700	-0.07790600	-2.60159700
H	-5.36989100	0.85184700	-3.86923400

H	-6.19611200	1.67736300	-2.55271500
H	-2.92506500	-0.30420700	4.15514300
H	-1.68234000	-0.39209500	2.90390900
H	-1.91574800	-1.74375800	4.01962400
H	-3.95818600	-3.24562000	3.81549600
H	-5.23646100	-2.86141500	2.65714900
H	-4.95525500	-1.81482300	4.04180500

Cartesian coordinates of the optimized geometry for **7**-An$^-$ at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Bi	-0.90686500	0.56467000	-0.03000800
Ga	1.70620800	0.19627000	-0.03354800
C	-1.89301000	-1.38267800	-0.55115400
N	3.36052800	-0.75951700	0.21378100
N	2.49018500	1.98682800	0.11320200
N	-3.19784700	-1.46631000	-0.39933700
C	-1.36059000	-2.63625600	-1.21228900
C	4.54225500	-0.16154300	0.43948100
C	3.28430100	-2.19659500	0.16092800
C	3.77754100	2.23342300	0.31231700
C	1.51790300	3.04035700	-0.00367000
C	-3.81735100	-2.75686300	-0.91848900
C	-3.96403200	-0.41648900	0.24192400
C	-2.55650300	-3.60982500	-1.10542400
C	-0.99267900	-2.32117900	-2.67328500
C	-0.14080100	-3.19771500	-0.48845400
C	4.73025300	1.21579000	0.46809200
C	5.74228300	-1.03444900	0.68142600
C	2.91057200	-2.90511500	1.31090300
C	3.53633100	-2.83950700	-1.06326900
C	4.26318500	3.65128700	0.42105000
C	0.97266700	3.60975800	1.15925300
C	1.04512500	3.37486600	-1.28713000
C	-4.56457100	-2.52115800	-2.22945900
C	-4.78433200	-3.35784700	0.09140900
C	-4.08908500	-0.44712800	1.64697600
C	-4.49561900	0.63999300	-0.52383700
H	-2.63481400	-4.25626500	-1.97788000
H	-2.42071800	-4.24938200	-0.23268600
H	-1.84013000	-1.93037700	-3.23392500
H	-0.64816900	-3.23255800	-3.16496900
H	-0.19723600	-1.58105500	-2.71575300
H	-0.34686300	-3.36176100	0.56817200
H	0.71199600	-2.52884700	-0.56796300
H	0.14818100	-4.15059000	-0.93205000
H	5.74141200	1.54786800	0.64307100
H	5.56644400	-1.69685400	1.52962100
H	6.62331300	-0.43112500	0.88020800
H	5.93960800	-1.67481500	-0.17871700
C	2.76584100	-4.28792100	1.20523500
C	2.66582800	-2.21775100	2.64318100
C	3.38097300	-4.22143800	-1.11598800
C	3.94227800	-2.05092800	-2.29815500
H	4.25846800	3.95686400	1.46969300
H	3.62577100	4.34232400	-0.12372000
H	5.28567100	3.73225500	0.05823300
C	-0.06045300	4.53349700	1.00887900
C	1.45603300	3.24914900	2.55395900
C	0.02094000	4.31337900	-1.38079300
C	1.64323000	2.76541200	-2.54349700
H	-4.91625900	-3.48241400	-2.60464600
H	-3.93702600	-2.07151700	-2.99471100
H	-5.43461000	-1.88901900	-2.07490100
H	-4.28547200	-3.63093400	1.01656500
H	-5.21614900	-4.26298000	-0.33630500
H	-5.60134000	-2.67293600	0.31722300
C	-4.81670500	0.57091600	2.25737300

C	-3.44318600	-1.49601000	2.53880600
C	-5.21278100	1.63011300	0.14749300
C	-4.31439700	0.79181600	-2.02580900
H	2.47598100	-4.86026100	2.07629600
C	2.99365200	-4.94077500	0.00588300
H	2.95526500	-1.17154500	2.53984300
C	3.52967500	-2.81658600	3.75961000
C	1.18026500	-2.24593900	3.02516200
H	3.56949800	-4.74623200	-2.04187000
H	4.42846200	-1.13393000	-1.96388200
C	4.94601800	-2.79191300	-3.18491800
C	2.71015400	-1.63443500	-3.11099200
H	-0.50146000	4.98305200	1.88829700
C	-0.53294900	4.88414700	-0.24511800
H	2.30967800	2.57880500	2.45633100
C	1.92817000	4.48974100	3.32359100
C	0.37997300	2.49780400	3.34891300
H	-0.35788800	4.59318700	-2.35359500
H	2.14543300	1.83865600	-2.25868900
C	2.71420000	3.68950200	-3.14025100
C	0.59026100	2.39695900	-3.59115300
H	-4.93161400	0.56441000	3.33242900
C	-5.38427900	1.59508900	1.51910000
H	-2.93326300	-2.21990500	1.90542000
C	-2.38019400	-0.87197200	3.45521800
C	-4.48196800	-2.24279400	3.38758100
H	-5.63706800	2.44684300	-0.41979800
H	-3.70337400	-0.03460000	-2.38141800
C	-3.57571400	2.09025600	-2.38611100
C	-5.66181400	0.75901300	-2.76269200
H	2.87889800	-6.01509600	-0.05546200
H	3.40190300	-2.24741600	4.68164600
H	4.58834400	-2.80336300	3.49658000
H	3.25320600	-3.85082100	3.96918300
H	0.82486100	-3.27245500	3.13569300
H	0.56366000	-1.75453200	2.27200400
H	1.02152700	-1.73170300	3.97448500
H	5.80857000	-3.13500500	-2.61201900
H	5.30402700	-2.12947100	-3.97405600
H	4.49841500	-3.66031000	-3.67020800
H	2.16471800	-2.51165400	-3.46238300
H	3.00181700	-1.04166900	-3.97965600
H	2.01670900	-1.03381500	-2.51715700
H	-1.33473900	5.60468100	-0.33879100
H	1.09674400	5.16225600	3.53922900
H	2.67059500	5.05553200	2.75975200
H	2.37135500	4.19742400	4.27682900
H	0.75309600	2.23961000	4.34162900
H	0.08254600	1.57834600	2.84440900
H	-0.51434100	3.11041000	3.47550200
H	2.27790500	4.64772700	-3.42814900
H	3.15648300	3.23781600	-4.02990300
H	3.51594200	3.88840100	-2.42887400
H	-0.18381100	1.76134300	-3.15961500
H	1.06027300	1.85628200	-4.41426200
H	0.11168900	3.28025300	-4.01584100
H	-5.94875800	2.37349900	2.01549500
H	-2.82939400	-0.15936500	4.14864200
H	-1.61757700	-0.35129600	2.87876500
H	-1.89369000	-1.65031400	4.04560300
H	-4.00565900	-3.06153300	3.92968700
H	-5.28869500	-2.65515000	2.78405500
H	-4.93041000	-1.57872500	4.12748400
H	-4.15680700	2.96770800	-2.09918100
H	-3.41553800	2.13710700	-3.46472000
H	-2.60414800	2.15274900	-1.89856100
H	-6.26961600	-0.09931300	-2.48159500
H	-5.50254100	0.72656800	-3.84161900
H	-6.24336400	1.65523300	-2.54227500

G) References

[1] A. Schumann, J. Bresien, M. Fischer, C. Hering-Junghans, *Chem. Commun.* **2021**, *57*, 1014–1017.

[2] K. M. Melancon, M. B Gildner, T. W. Hudnall, *Chem. Eur. J.* **2018**, *24*, 9264–9268.

[3] A. Doddi, M. Weinhart, A. Hinz, D. Bockfeld, J. M. Goicoechea, M. Scheer, M. Tamm, *Chem. Commun.* **2017**, *53*, 6069–6072.

[4] A. Hinz, M. M. Hansmann, G. Bertrand, J. M. Goicoechea, *Chem. Eur. J.* **2018**, *24*, 9514–9519.

[5] S. Yao, Y. Grossheim, A. Kostenko, E. Ballestero-Martínez, S. Schutte, M. Bispinghoff, H. Grützmacher, M. Driess, *Angew. Chem. Int. Ed.* **2017**, *56*, 7465–7469.

[6] A. J Arduengo III, J. C. Calabrese, A. H. Cowley, H. V. R. Dias, J. R. Goerlich, W. J. Marshall, B. Riegel, *Inorg. Chem.* **1997**, *36*, 2151–2158.

[7] R. Kretschmer, D. A. Ruiz, C. E. Moore, A. L. Rheingold, G. Bertrand, *Angew. Chem., Int. Ed*. **2014**, *53*, 8176–8179; *Angew. Chem*. **2014**, *126*, 8315–8318.

[8] C. L. Dorsey, R. M. Mushinski, T. W. Hudnall, *Chem. Eur. J.* **2014**, *20*, 8914–8917.

[10] J. Krüger, C. Wölper, L. John, L. Song, P. R. Schreiner, S. Schulz, *Eur. J. Inorg. Chem.* **2019**, 1669–1678.

[11] G. Wang, L. A. Freeman, D. A. Dickie, R. Mokrai, Z. Benkő, R. J. Gilliard, *Chem. Eur. J.* 2019, *25*, 4335–4339.

[12] K. M. Melancon, M. B. Gildner, T. W. Hudnall, *Chem. Eur. J.* **2018**, *24*, 9264–9268.

[13] N. J. Hardman, B. E. Eichler, P. P. Power, *Chem. Commun*. **2000**, 1991-1992.

[14] I. Krossing, *Chem. Eur. J*. **2001**, *7*, 490–502.

[15] N. A. Yakelis, R. G. Bergman, *Organometallics* **2005**, *24*, 3579–3581.

[16] G. M. Sheldrick, *Acta Crystallogr.* **1990**, *A46*, 467–473.

[17] G. M. Sheldrick, SHELXL-2017, Program for the Refinement of Crystal Structures University of Göttingen, Göttingen (Germany) **2017**. See also: G.M. Sheldrick, Crystal structure refinement with SHELXL, *Acta Cryst.* **2015**, *C71*, 3–8.

[18] shelXle, *A Qt GUI for SHELXL*, C. B. Hübschle, G. M. Sheldrick, B. Dittrich, *J. Appl. Cryst.* **2011**, *44*, 1281–1284.

[19] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr.; , J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

[20] a) G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders, T. Ziegler, *J. Comput. Chem.* **2001**, *22*, 931−967. b) ADF 2020.1, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com. E.J. Baerends, T. Ziegler, A. J. Atkins, J. Autschbach, O. Baseggio, D. Bashford, A. Bérces, F. M. Bickelhaupt, C. Bo, P. M. Boerrigter, C. Cappelli, L. Cavallo, C. Daul, D. P. Chong, D. V. Chulhai, L. Deng, R. M. Dickson, J.M. Dieterich, F. Egidi, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, A. Förster, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S. J. A. van Gisbergen, A. Goez, A. W. Götz, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, S. Gusarov, F. E. Harris, P. van den Hoek, Z. Hu, C. R. Jacob, H. Jacobsen, L. Jensen, L. Joubert, J. W. Kaminski, G. van Kessel, C. König, F. Kootstra, A. Kovalenko, M. V. Krykunov, P. Lafiosca, E. van Lenthe, D. A. McCormack, M. Medves, A. Michalak, M. Mitoraj, S. M. Morton, J. Neugebauer, V. P. Nicu, L. Noodleman, V. P. Osinga, S. Patchkovskii, M. Pavanello, C. A. Peeples, P. H. T. Philipsen, D. Post, C. C. Pye, H. Ramanantoanina, P. Ramos, W. Ravenek, M. Reimann, J. I. Rodríguez, P. Ros, R. Rüger, P. R. T. Schipper, D. Schlüns, H. van Schoot, G. Schreckenbach, J. S. Seldenthuis, M. Seth, J. G. Snijders, M. Solà, M. Stener, M. Swart, D. Swerhone, V. Tognetti, G. te Velde, P.

Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T. A. Wesolowski, E. M. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo, A. L. Yakovlev.

[21] a) A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098−3100. b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785−789. c) B. Miehlich, A. Savin, H. Stoll, H. Preuss, *Chem. Phys. Lett.* **1989**, *157*, 200−206.

[22] S. Grimme, S. Ehrlich, L. Goerigk, *J. Comp. Chem.* **2011**, *32*, 1456−1465.

[23] A. E. Reed, L. A. Curtiss, F. Weinhold, *Chem. Rev.* **1988**, *88*, 899−926.

[24] F. M. Bickelhaupt, E. J. Baerends, *Rev. Comput. Chem.* **2000**, *15*, 1−86.

Supporting Information

Single Electron Oxidation of Carbene-Coordinated Pnictinidenes – Entry into Heteroleptic Radical Cations and Metalloid Clusters

Julia Krüger,[a] Julia Haak,[b] Christoph Wölper,[a] George E. Cutsail III,[a,b] Gebhard Haberhauer*[c] and Stephan Schulz*[a,d]*

Corresponding authors: George E. Cutsail III (george.cutsail@cec.mpg.de); Gebhard Haberhauer (gebhard.haberhauer@uni-due.de); Stephan Schulz (stephan.schulz@uni-due.de);

[a] MSc. J. Krüger, Dr. C. Wölper, Prof. Dr. S. Schulz, Institute of Inorganic Chemistry, University of Duisburg-Essen, Universitätsstraße 5-7, 45141 Essen (Germany).

[b] MSc. J. Haak, Dr. G. E. Cutsail III, Max Planck Institute for Chemical Energy Conversion (CEC) Stiftstraße 34–36, 45470 Mülheim an der Ruhr (Germany)

[c] Prof. Dr. G. Haberhauer, Institute of Organic Chemistry, University Duisburg-Essen, Universitätsstraße 5-7, 45141 Essen (Germany).

[d] Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Carl-Benz-Straße 199, 47057 Duisburg (Germany).

Contents

A) Experimental Procedure

General Synthetic methods

All manipulations were done in an atmosphere of purified Ar using Schlenk and glove-box techniques. Toluene and *n*-hexane were dried by an MBraun Solvent Purification System, benzene was dried over K and fluorobenzene over CaH_2. Deuterated solvents were dried over activated molecular sieves (4 Å) and degassed. The anhydrous nature of the solvents was verified by Karl Fischer titration. (^{Me}cAAC)EGa(Cl)L (E = As **I**, Sb **II**, Bi **III**)[1] and $[FeCp_2][B(C_6F_5)_4]$[2] were prepared according to literature methods. Microanalyses were performed at the laboratory for microanalysis of the University of Duisburg-Essen. Melting points were measured using a Thermo Scientific 9300 apparatus. Cyclic voltammetry measurements were performed in a glovebox using a Metrohm Autolab PGSTAT 204 potentiostat with a three electrodes setup consisting of a Pt disc (*d* = 1 mm) working electrode, Pt wire counter electrode, and Ag wire pseudo-reference electrode using ferrocene as the internal standard.

IR Spectroscopy. IR spectra were recorded with an ALPHA-T FT-IR spectrometer equipped with a single reflection ATR sampling module that is placed in a glovebox to guarantee inert gas conditions.

EPR Spectroscopy. For the EPR measurements, 10 mM fluorobenzene solutions of **1**, **2** and **3** were prepared in a glovebox in either 50 µL capillaries (Hirschmann), sealed with critoseal, or frozen in custom quartz EPR tubes. X-band samples of **1** and **2** were filled in 4 mm (OD) and X-band samples of **3** in 2.8 mm (OD) tubes. Q-band samples were measured in 2.8 mm (OD) tubes. CW X-band EPR spectra of **1** and **2** at room temperature (~9.43 GHz) and at 77 K (~9.45 GHz) were collected with a Bruker MS 5000 spectrometer. Spectra were collected with ~60 k points, to which an effective time constant of 0.05 s was applied. The spectra at room temperature were obtained with the following parameters: For **1**: 100 kHz field modulation frequency, 8 G modulation amplitude, 360 s scan time, single scan; For **2**: 100 kHz field modulation frequency, 8 G modulation amplitude, 240 s scan time, single scan, effective number of points = 1000, effective shots per point = 60. For the spectra at 77 K the following parameters were employed: For **1**: 100 kHz field modulation frequency, 8 G modulation amplitude, 360 s scan time, single scan; For **2**: 100 kHz field modulation frequency, 8 G modulation amplitude, 360 s scan time, five scans. CW X-band EPR spectra of **3** were collected at ~6 K on a Bruker Elexsys E500 equipped with an Oxford helium flow cryostat and temperature controller. Spectra were collected with the following parameters: modulation amplitude: 6 G; modulation frequency: 100 kHz; time constant: 81.92 ms; scan time: 336 s; eight scans. Q-band pulsed EPR measurements of **1** (~34.00 GHz) and **2** (~34.01 GHz) were collected on a Bruker Elexsys E580 spectrometer equipped with an Oxford helium flow cryostat and temperature controller. Spectra were measured at 15 K (**1**) and 12 K (**2**) and were obtained as free induction decays with the following parameters: For **1**: π_{inv} = 200 ns, repetition rate = 250 us, shots per point: 20, number of points: 8192, number of scans: 20; for **2**: π_{inv} = 400 ns, repetition rate = 250 us, shots per point: 25, number of points: 2048, number of scans: 36; The depicted approximate first derivatives of the spectra were created with the EasySpin function for field modulation ("fieldmod") with peak-to-peak modulation amplitudes of 7 G (**1**) and 17 G (**2**) and subsequently smoothed over 10 points (**1**) and 20 points (**2**). The EPR data was processed and analyzed in Matlab R2019b and simulated using the EasySpin package (v. 6.0.0-dev.30).[3] For the simulation of the room temperature spectra, the EasySpin function for

isotropic EPR spectra in the fast motion regime was used (“garlic”), while the solid-state function (“pepper”) was used for the simulation of the frozen solutions spectra.

Synthesis of [(^{Me}cAAC)EGa(Cl)L][B(C_6F_5)$_4$] (E = As 1, Sb 2, Bi 3)

(^{Me}cAAC)EGa(Cl)L (E = As **I**, Sb **II**) (0.032 mmol) and [FeCp$_2$][B(C_6F_5)$_4$] (29 mg; 0.032mmol) were weighed in a Schlenk flask, cooled to -78 °C and 3 mL of toluene were added. The cooling bath was removed, and the reaction mixture was stirred for 1 h at ambient temperature. The solvent was evaporated under vacuum and the residue was washed four times with 6 mL of a benzene/hexane solution (1:10). The brown powder was dried under vacuum to yield analytically pure [(^{Me}cAAC)EGa(Cl)L][B(C_6F_5)$_4$] (E = As **1**, Sb **2**).

1: Yield 29 mg (0.019 mmol; 58%). M.p.: 164 °C (dec.). Anal. Calcd. for $C_{73}H_{72}N_3ClF_{20}BGaAs$: C, 56.12; H, 4.65; N, 2.69. Found: C, 55.77; H, 4.62; N, 2.72 %. IR ν [cm^{-1}]: 2969, 2930, 2873, 1642, 1593, 1530, 1512, 1459, 1386, 1375, 1314, 1274, 1261, 1202, 1179, 1127, 1084, 1026, 977, 870, 800, 774, 755, 727, 684, 661, 609, 573, 536, 501, 441.

2: Yield 32 mg (0.020 mmol; 62%). M.p.: 121 °C (dec.). Anal. Calcd. for $C_{73}H_{72}N_3ClF_{20}BGaSb$: C, 54.49; H, 4.51; N, 2.61. Found: C, 53.89; H, 4.37; N, 2.69 %. IR ν [cm^{-1}]: 3020, 2954, 2920, 2861, 1637, 1524, 1507, 1454, 1380, 1308, 1271, 1258, 1198, 1175, 1081, 1023, 975, 867, 797, 771, 754, 724, 680, 658, 607, 571, 528, 507, 448.

Since the isolated yield of (^{Me}cAAC)BiGa(Cl)L (***III)*** *is low (24%), in situ synthesis of* ***III*** *is preferred. However, the reaction of* ***III*** *with [FeCp$_2$][B(C_6F_5)$_4$] was also carried out using an isolated sample of* ***III****.*

(^{Me}cAAC)BiCl$_3$ (40 mg; 0.067 mmol) and LGa (65 mg; 0.133 mmol) were combined in a Schlenk flask, cooled to –100 °C and 3 mL of toluene were added. The reaction mixture was warmed to –30 °C within 3 h, yielding a pink solution which was separated from metallic bismuth particles formed during the reaction, concentrated and overlayed with 5 mL of *n*-hexane. Storage at –30 °C for 12 h gave colorless crystals of LGaCl$_2$. The mother liquor containing **III** was transferred to a Schlenk flask, the solvent was removed and [FeCp$_2$][B(C_6F_5)$_4$] (30 mg; 0.034 mmol) were added. The mixture was cooled to –80 °C, 2 mL of toluene added and then suspension warmed to ambient temperature within 30 minutes. After stirring for 15 minutes at room temperature, the solvent was evaporated and the residue quickly washed four times with 6 mL of a benzene/hexane solution (1:10), yielding a red powder which was dried under vacuum to yield analytically pure [(^{Me}cAAC)BiGa(Cl)L][B(C_6F_5)$_4$] (**3**).

3: Yield 32 mg (0.018 mmol; 51%). M.p.: 110 °C (dec.). Anal. Calcd. for $C_{73}H_{72}N_3ClF_{20}BGaBi$: C, 51.69; H, 4.28; N, 2.48. Found: C, 51.51; H, 4.20; N, 2.49 %. IR ν [cm^{-1}]: 3031, 2953, 2918, 2861, 1637, 1506, 1454, 1373, 1311, 1271, 1258, 1199, 1174, 1078, 1052, 973, 932, 863, 812, 796, 771, 753, 723, 680, 657, 607, 571, 527, 477, 439.

B) Spectroscopic Characterization

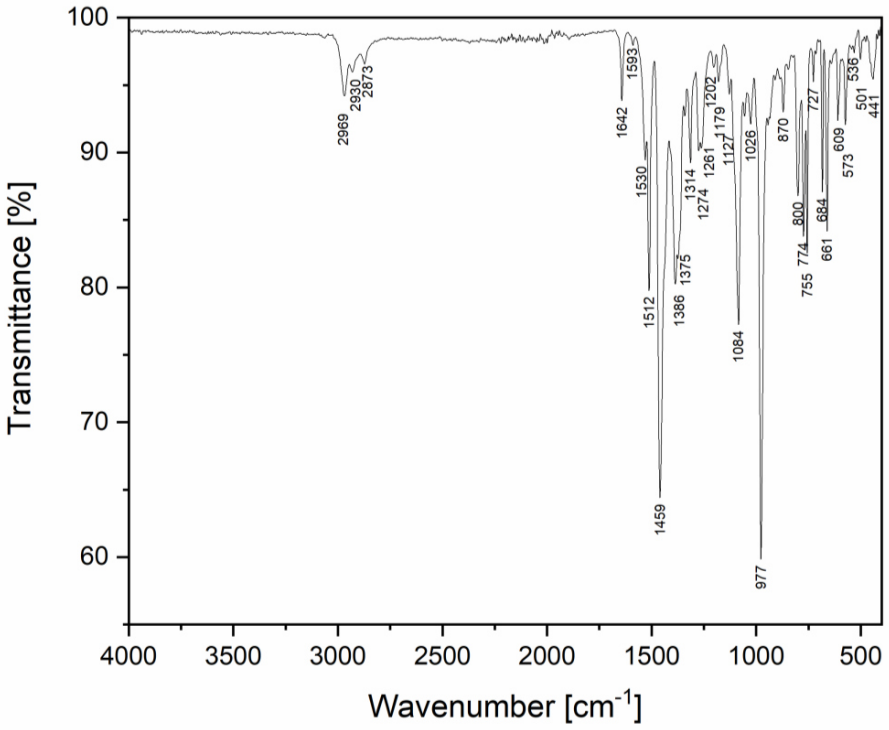


Fig. S1 IR spectrum of [(^{Me}cAAC)AsGa(Cl)L][B(C_6F_5)$_4$] **1**.

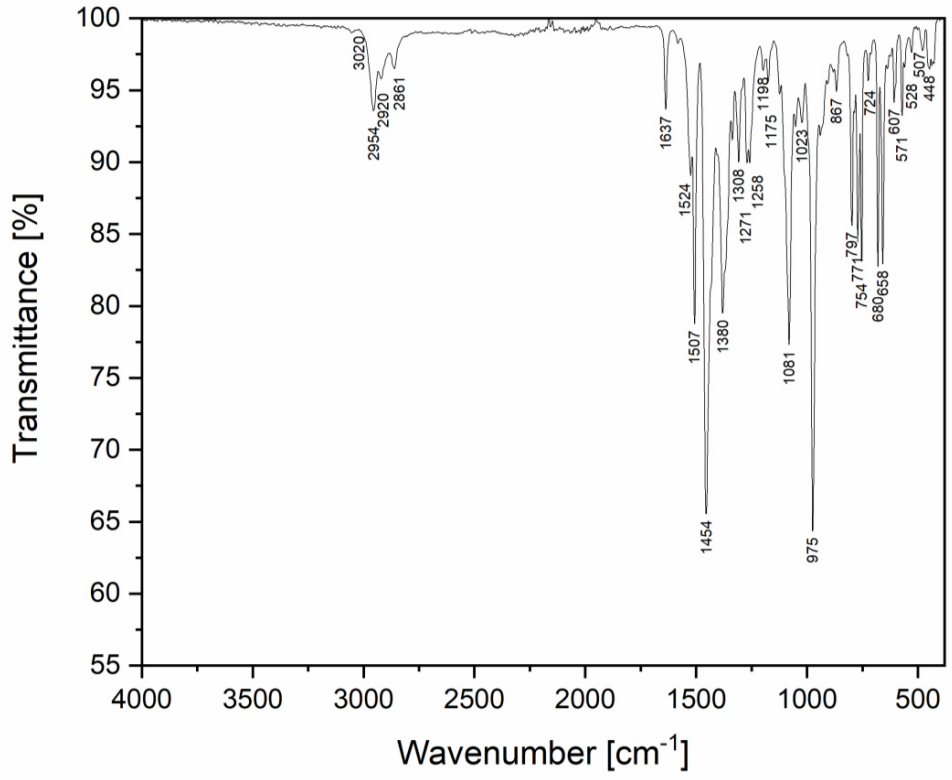


Fig. S2 IR spectrum of [(^{Me}cAAC)SbGa(Cl)L][B(C_6F_5)$_4$] **2**.

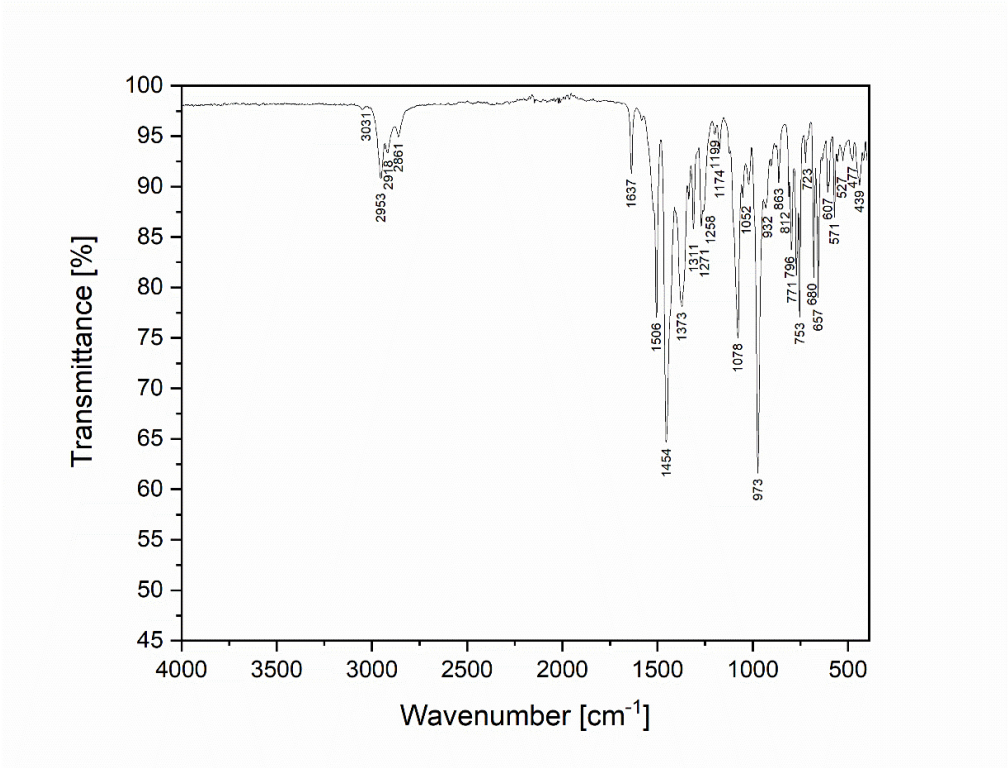


Fig. S3 IR spectrum of [(^{Me}cAAC)BiGa(Cl)L]B(C_6F_5)$_4$] **3**.

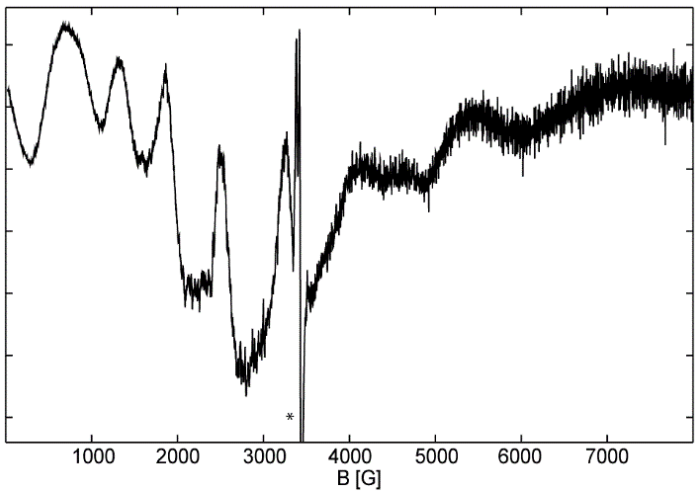


Fig. S4. As collected CW EPR spectrum of **3** at X-band frequency (~9.64 GHz). The asterisk indicates a small organic radical impurity. Spectrometer conditions are described in the Experimental Section.

C) Cyclic voltammetry

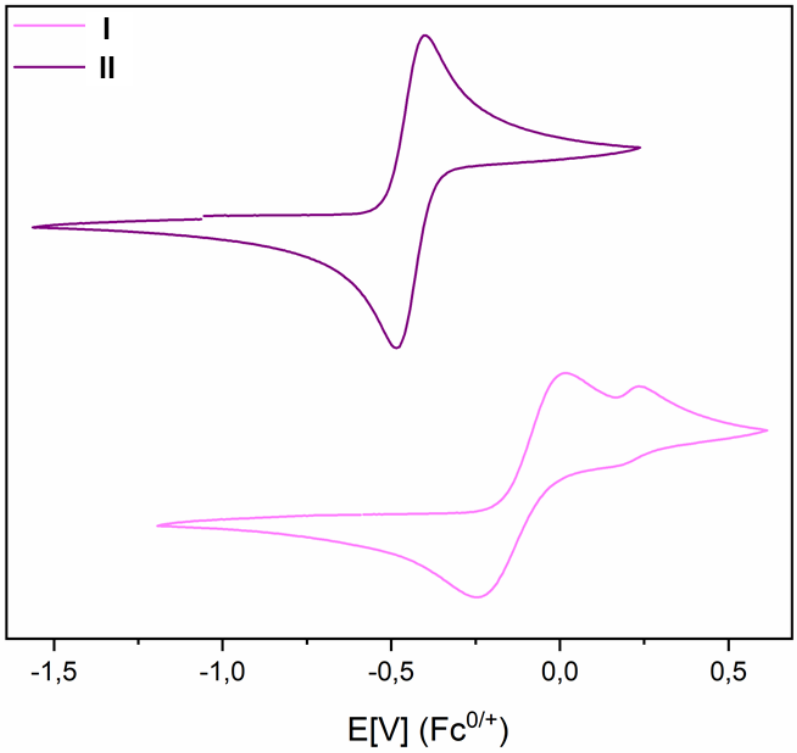


Fig. S5. Cyclic voltammograms of **I** and **II** in 1,2-difluorobenzene solution (1 mM) containing [*n*-Bu_4N][B(3,5-$(CF_3)_2$-$C_6H_3)_4$] (50 mM) as electrolyte at 100 mV s^{-1} scan rate. It is noted that on increasing the scan rate the intensity of the adsorption peak (which linearly increases with v) tends to become larger than that of the diffusive peak. At high scan rates the diffusive peak may completely disappear. Cyclic voltammetry measurement of **III** was not performed due to its fast decomposition at ambient temperature.

D) Crystallographic Part

Single-crystal X-ray analyses. Crystals were mounted on nylon loops in inert oil. Data were collected on a Bruker AXS D8 Venture diffractometer with Photon II detector (monochromated $Cu_{K\alpha}$ radiation, λ = 1.54178 Å, microfocus source) at 100(2) K (**1**·C_6H_5F, **2**·$C_6H_4F_2$, **4**·$C_6H_4F_2$) and on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) at 100(2) K (**1**). The structures were solved by Direct Methods (SHELXS-97)[4] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2017)[5,6]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX3). Hydrogen atoms were refined using a riding model or rigid methyl groups. In **1**·C_6H_5F the fluorobenzene molecule is disordered over a center of inversion. The crystals of **1** degraded when cooled to 100 K and barely diffracted. Likely this is caused by a phase transition and consequent loss of crystalinity. Thus, the measurement was done at 200 K. In **2**·$C_6H_4F_2$ the difluorobenzene molecule is disordered over two sites. Its corresponding bond lengths and angles were restrained to be equal (SADI) and RIGU restraints were applied to the anisotropic displacement parameters. The structure of **4**·$C_6H_4F_2$ contains highly disordered difluorobenzene of unknown occupancy. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run.[7] Since the amount of the solvent is not clear it was not included in the sum formula. Another solvent molecule was refined with partial occupancy. The displacement ellipsoids suggest disorder however due to the low quality of the data no second orientation could be resolved. The phenyl rings of the solvent molecules were constrained to a regular hexagon with edges of 1.39 Å of length (AFIX 66). Despite several attempts only crystals of substandard quality could be obtained. Depending on the θ-range up to two third of the reflections are un-observed with a mean $I/\sigma(I) < 2$ for resolutions larger than 0.8 Å. Due to the high R_{int} and the fact that all disagreeing reflections show higher observed than calculated intensities twinning cannot be excluded. However, no second orientation could be identified in the off-lattice background intensity. No twin-law for pseudo-merohedral twinning could be identified. RIGU restraints were applied to all displacement parameters of the model. Therefore, any information beyond the connectivity should be taken with care. [^{Me}cAACH][$BAr^F{}_4$] contains two disordered fluorobenzene molecules with an occupancy of 0.5. One is placed on a special position and the disorder of the other is correlated with this. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE[7] run. The molecules were included in the sum formula for completeness. The crystal diffracted weakly leading to limited data quality, hence bond lengths and angles should be handled with care.

CCDC-2096529 (**1**·C_6H_5F), -2142700 (**1**), -2128553 (**2**·$C_6H_4F_2$), -2128554 (**4**·$C_6H_4F_2$), and -2128555 ([^{Me}cAACH][$BAr^F{}_4$]) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic details of **1**·C_6H_5F and **1**.

	1·C_6H_5F	**1**
Empirical formula	$C_{76}H_{74.50}ABClF_{20.50}GaN_3$	$C_{73}H_{72}AsBClF_{20}GaN_3$
M [g mol^{-1}]	1610.28	1562.23
Crystal size [mm]	0.193 × 0.152 × 0.113	0.613 × 0.272 × 0.215
T [K]	100(2)	200(2)
Crystal system	triclinic	monoclinic
Space group	$P\bar{1}$	P 21/n
a [Å]	11.9276(10)	11.4567(8)
b [Å]	16.7053(15)	31.817(2)
c [Å]	18.715(2)	20.3269(16)
α [°]	79.617(9)	90
β [°]	82.916(8)	104.187(2)
γ [°]	88.472(8)	90
V [Å^3]	3640.0(7)	7183.6(9)
Z	2	4
D_{calcd} [g cm^{-3}]	1.469	1.444
μ(K_α [mm^{-1}])	2.218	0.973
Transmissions	0.75/0.61	0.75/0.66
F(000)	1644	3188
Index ranges	-15 ≤ h ≤ 15	-17 ≤ h ≤ 17
	-19 ≤ k ≤ 21	-49 ≤ k ≤ 49
	-23 ≤ l ≤ 23	-31 ≤ l ≤ 31
θ_{max} [°]	78.726	33.355
Reflections collected	130678	329491
Independent reflections	15509	27816
R_{int}	0.0703	0.0484
Refined parameters	955	919
R_1 [$I > 2\sigma(I)$]	0.0420	0.0622
wR_2 [all data]	0.1191	0.1637
GooF	1.029	1.059
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	1.185/-1.003	3.434/-2.280

Table S2. Crystallographic details of **2**·$C_6H_4F_2$, **4**·$C_6H_4F_2$ and [^{Me}cAACH][BAr$^F_4$].

	2·$C_6H_4F_2$	**4**·$C_6H_4F_2$	[^{Me}cAACH][BAr$^F_4$]
Empirical formula	$C_{79}H_{76}BClF_{22}GaN_3Sb$	$C_{122.04}H_{128.36}BBi_6Cl_3F_{23.68}Ga_3N_6$	$C_{50}H_{37}BF_{21}N$
M [g mol^{-1}]	1723.15	3709.35	1061.61
Crystal size [mm]	0.344 × 0.298 × 0.162	0.208 × 0.095 × 0.059	0.235 × 0.090 × 0.063
T [K]	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	orthorhombic
Space group	$P\bar{1}$	$P\bar{1}$	P*bcn*
a [Å]	15.1510(3)	17.4856(12)	20.3308(15)
b [Å]	15.1959(4)	20.1623(13)	17.7426(14)
c [Å]	19.0099(4)	23.0777(14)	25.7189(18)
α [°]	108.1949(10)	105.949(3)	90
β [°]	99.1442(11)	105.746(4)	90
γ [°]	108.2117(11)	106.656(4)	90
V [Å^3]	3786.68(15)	6932.1(8)	9277.4(12)
Z	2	2	8
D_{calcd} [g cm^{-3}]	1.511	1.777	1.520
μ(K_α [mm^{-1}])	4.468	16.446	1.310
Transmissions	0.75/0.53	0.32/0.13	0.75/0.64
F(000)	1746	3526	4304
Index ranges	-18 ≤ h ≤ 19	-20 ≤ h ≤ 21	-25 ≤ h ≤ 26
	-19 ≤ k ≤ 19	-25 ≤ k ≤ 25	-15 ≤ k ≤ 21
	-24 ≤ l ≤ 24	-28 ≤ l ≤ 28	-32 ≤ l ≤ 32
θ_{max} [°]	80.734	74.494	82.569
Reflections collected	203971	276065	194294
Independent reflections	16495	28215	10146
R_{int}	0.0437	0.1785	0.1240
Refined parameters	1064	1503	603
R_1 [$I > 2\sigma(I)$]	0.0294	0.0909	0.0568
wR_2 [all data]	0.0749	0.2388	0.1389
GooF	1.038	1.068	1.093
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	1.831/-1.219	4.182/-3.249	0.284/-0.226

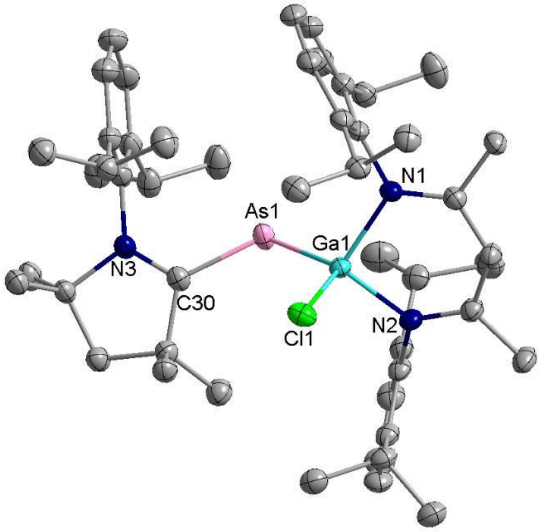


Fig. S6. Solid state structure of **1**·C_6H_5F. Hydrogen atoms, counter anion and solvent molecules are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S3 Bond lengths [Å] for **1**·C_6H_5F.

As(1)-C(30)	1.9406(19)	C(24)-C(25)	1.537(3)	F421-C421	1.352(2)
As(1)-Ga(1)	2.4670(4)	C(27)-C(29)	1.526(4)	F431-C431	1.338(2)
Ga(1)-N(2)	1.9240(16)	C(27)-C(28)	1.531(3)	F441-C441	1.339(2)
Ga(1)-N(1)	1.9436(16)	C(30)-C(33)	1.510(3)	F451-C451	1.347(2)
Ga(1)-Cl(1)	2.1824(5)	C(31)-C(46)	1.521(3)	F461-C461	1.348(2)
N(1)-C(1)	1.326(3)	C(31)-C(47)	1.527(3)	C111-C121	1.392(3)
N(1)-C(6)	1.451(2)	C(31)-C(32)	1.535(3)	C111-C161	1.393(3)
N(2)-C(3)	1.335(3)	C(32)-C(33)	1.542(3)	C111-B11	1.652(3)
N(2)-C(18)	1.450(2)	C(33)-C(48)	1.531(3)	C121-C131	1.376(3)
N(3)-C(30)	1.304(3)	C(33)-C(49)	1.537(3)	C131-C141	1.373(4)
N(3)-C(34)	1.455(3)	C(34)-C(35)	1.408(3)	C141-C151	1.373(3)
N(3)-C(31)	1.536(2)	C(34)-C(39)	1.409(3)	C151-C161	1.387(3)
C(1)-C(2)	1.407(3)	C(35)-C(36)	1.397(3)	C211-C261	1.391(3)
C(1)-C(4)	1.510(3)	C(35)-C(40)	1.526(3)	C211-C221	1.397(3)
C(2)-C(3)	1.392(3)	C(36)-C(37)	1.388(4)	C211-B11	1.648(3)
C(3)-C(5)	1.510(3)	C(37)-C(38)	1.374(4)	C221-C231	1.377(3)
C(6)-C(7)	1.406(3)	C(38)-C(39)	1.396(3)	C231-C241	1.373(3)
C(6)-C(11)	1.409(3)	C(39)-C(43)	1.521(3)	C241-C251	1.379(3)
C(7)-C(8)	1.400(3)	C(40)-C(42)	1.535(3)	C251-C261	1.387(3)
C(7)-C(12)	1.525(3)	C(40)-C(41)	1.536(3)	C311-C321	1.390(3)
C(8)-C(9)	1.380(3)	C(43)-C(45)	1.534(3)	C311-C361	1.393(3)
C(9)-C(10)	1.392(3)	C(43)-C(44)	1.537(3)	C311-B11	1.651(3)
C(10)-C(11)	1.396(3)	F121-C121	1.352(3)	C321-C331	1.379(3)
C(11)-C(15)	1.526(3)	F131-C131	1.349(3)	C331-C341	1.376(3)
C(12)-C(14)	1.534(3)	F141-C141	1.345(3)	C341-C351	1.367(3)
C(12)-C(13)	1.536(3)	F151-C151	1.346(3)	C351-C361	1.381(3)

C(15)-C(17)	1.523(3)	F161-C161	1.350(2)	C411-C461	1.388(3)
C(15)-C(16)	1.531(3)	F221-C221	1.354(2)	C411-C421	1.393(3)
C(18)-C(19)	1.406(3)	F231-C231	1.345(2)	C411-B11	1.650(3)
C(18)-C(23)	1.409(3)	F241-C241	1.336(2)	C421-C431	1.378(3)
C(19)-C(20)	1.403(3)	F251-C251	1.338(2)	C431-C441	1.382(3)
C(19)-C(24)	1.521(3)	F261-C261	1.345(2)	C441-C451	1.374(3)
C(20)-C(21)	1.383(3)	F321-C321	1.351(2)	C451-C461	1.388(3)
C(21)-C(22)	1.386(3)	F331-C331	1.340(2)	F12-C12	1.324(7)
C(22)-C(23)	1.393(3)	F341-C341	1.342(2)	C12-C22	1.358(6)
C(23)-C(27)	1.527(3)	F351-C351	1.347(3)	C12-C32	1.391(6)
C(24)-C(26)	1.531(3)	F361-C361	1.345(2)	C22-C32#1	1.381(6)

Table S4 Bond angles [°] for **1**·C_6H_5F.

C(30)-As(1)-Ga(1)	115.46(6)	C(35)-C(40)-C(41)	110.70(18)
N(2)-Ga(1)-N(1)	98.41(7)	C(42)-C(40)-C(41)	109.18(19)
N(2)-Ga(1)-Cl(1)	109.02(5)	C(39)-C(43)-C(45)	111.5(2)
N(1)-Ga(1)-Cl(1)	107.50(5)	C(39)-C(43)-C(44)	111.2(2)
N(2)-Ga(1)-As(1)	110.06(5)	C(45)-C(43)-C(44)	109.00(19)
N(1)-Ga(1)-As(1)	110.22(5)	C121-C111-C161	112.99(19)
Cl(1)-Ga(1)-As(1)	119.531(18)	C121-C111-B11	119.61(18)
C(1)-N(1)-C(6)	120.12(16)	C161-C111-B11	127.12(17)
C(1)-N(1)-Ga(1)	119.15(13)	F121-C121-C131	116.4(2)
C(6)-N(1)-Ga(1)	120.04(12)	F121-C121-C111	118.87(19)
C(3)-N(2)-C(18)	119.26(16)	C131-C121-C111	124.7(2)
C(3)-N(2)-Ga(1)	119.37(13)	F131-C131-C141	119.4(2)
C(18)-N(2)-Ga(1)	121.37(13)	F131-C131-C121	120.9(2)
C(30)-N(3)-C(34)	123.85(16)	C141-C131-C121	119.8(2)
C(30)-N(3)-C(31)	113.75(16)	F141-C141-C151	120.6(2)
C(34)-N(3)-C(31)	122.38(16)	F141-C141-C131	120.8(2)
N(1)-C(1)-C(2)	124.35(18)	C151-C141-C131	118.5(2)
N(1)-C(1)-C(4)	121.41(18)	F151-C151-C141	119.6(2)
C(2)-C(1)-C(4)	114.22(17)	F151-C151-C161	120.3(2)
C(3)-C(2)-C(1)	128.61(19)	C141-C151-C161	120.1(2)
N(2)-C(3)-C(2)	123.99(18)	F161-C161-C151	114.84(19)
N(2)-C(3)-C(5)	119.22(18)	F161-C161-C111	121.36(18)
C(2)-C(3)-C(5)	116.78(18)	C151-C161-C111	123.8(2)
C(7)-C(6)-C(11)	121.87(18)	C261-C211-C221	113.19(18)
C(7)-C(6)-N(1)	119.31(18)	C261-C211-B11	127.99(18)
C(11)-C(6)-N(1)	118.82(17)	C221-C211-B11	118.78(17)
C(8)-C(7)-C(6)	117.64(19)	F221-C221-C231	115.71(18)
C(8)-C(7)-C(12)	118.96(18)	F221-C221-C211	119.33(18)
C(6)-C(7)-C(12)	123.39(18)	C231-C221-C211	124.94(19)
C(9)-C(8)-C(7)	121.6(2)	F231-C231-C241	119.81(19)

C(8)-C(9)-C(10)	119.9(2)	F231-C231-C221	120.89(19)
C(9)-C(10)-C(11)	121.1(2)	C241-C231-C221	119.28(19)
C(10)-C(11)-C(6)	117.97(19)	F241-C241-C231	120.8(2)
C(10)-C(11)-C(15)	119.91(19)	F241-C241-C251	120.4(2)
C(6)-C(11)-C(15)	122.06(18)	C231-C241-C251	118.80(19)
C(7)-C(12)-C(14)	110.97(18)	F251-C251-C241	119.43(19)
C(7)-C(12)-C(13)	111.73(17)	F251-C251-C261	120.4(2)
C(14)-C(12)-C(13)	109.77(17)	C241-C251-C261	120.21(19)
C(17)-C(15)-C(11)	113.80(19)	F261-C261-C251	115.45(18)
C(17)-C(15)-C(16)	109.72(19)	F261-C261-C211	121.01(18)
C(11)-C(15)-C(16)	110.69(18)	C251-C261-C211	123.54(19)
C(19)-C(18)-C(23)	122.37(18)	C321-C311-C361	113.47(18)
C(19)-C(18)-N(2)	120.31(18)	C321-C311-B11	120.95(17)
C(23)-C(18)-N(2)	117.32(17)	C361-C311-B11	125.51(17)
C(20)-C(19)-C(18)	117.32(19)	F321-C321-C331	116.27(18)
C(20)-C(19)-C(24)	119.16(19)	F321-C321-C311	119.25(18)
C(18)-C(19)-C(24)	123.52(17)	C331-C321-C311	124.45(19)
C(21)-C(20)-C(19)	121.2(2)	F331-C331-C341	119.53(19)
C(20)-C(21)-C(22)	120.34(19)	F331-C331-C321	121.3(2)
C(21)-C(22)-C(23)	121.1(2)	C341-C331-C321	119.2(2)
C(22)-C(23)-C(18)	117.68(19)	F341-C341-C351	120.0(2)
C(22)-C(23)-C(27)	119.98(19)	F341-C341-C331	121.0(2)
C(18)-C(23)-C(27)	122.33(18)	C351-C341-C331	119.0(2)
C(19)-C(24)-C(26)	111.26(18)	F351-C351-C341	119.7(2)
C(19)-C(24)-C(25)	112.29(17)	F351-C351-C361	119.9(2)
C(26)-C(24)-C(25)	108.67(18)	C341-C351-C361	120.4(2)
C(29)-C(27)-C(23)	112.9(2)	F361-C361-C351	115.19(19)
C(29)-C(27)-C(28)	110.1(2)	F361-C361-C311	121.48(18)
C(23)-C(27)-C(28)	112.28(19)	C351-C361-C311	123.3(2)
N(3)-C(30)-C(33)	111.65(17)	C461-C411-C421	113.58(17)
N(3)-C(30)-As(1)	121.40(14)	C461-C411-B11	128.43(17)
C(33)-C(30)-As(1)	125.75(14)	C421-C411-B11	117.67(16)
C(46)-C(31)-C(47)	108.78(17)	F421-C421-C431	115.65(17)
C(46)-C(31)-C(32)	111.53(18)	F421-C421-C411	119.23(17)
C(47)-C(31)-C(32)	114.47(17)	C431-C421-C411	125.12(18)
C(46)-C(31)-N(3)	111.83(16)	F431-C431-C421	121.22(17)
C(47)-C(31)-N(3)	109.59(16)	F431-C431-C441	120.22(18)
C(32)-C(31)-N(3)	100.49(15)	C421-C431-C441	118.56(18)
C(31)-C(32)-C(33)	107.47(16)	F441-C441-C451	120.33(18)
C(30)-C(33)-C(48)	112.20(16)	F441-C441-C431	120.43(18)
C(30)-C(33)-C(49)	107.87(16)	C451-C441-C431	119.22(18)
C(48)-C(33)-C(49)	110.10(18)	F451-C451-C441	119.51(17)
C(30)-C(33)-C(32)	102.28(16)	F451-C451-C461	120.40(18)
C(48)-C(33)-C(32)	112.15(17)	C441-C451-C461	120.08(18)

C(49)-C(33)-C(32)	111.98(16)	F461-C461-C451	114.80(17)
C(35)-C(34)-C(39)	122.78(19)	F461-C461-C411	121.82(17)
C(35)-C(34)-N(3)	118.52(18)	C451-C461-C411	123.37(18)
C(39)-C(34)-N(3)	118.67(19)	C211-B11-C411	101.42(15)
C(36)-C(35)-C(34)	117.2(2)	C211-B11-C311	111.20(16)
C(36)-C(35)-C(40)	117.8(2)	C411-B11-C311	113.51(15)
C(34)-C(35)-C(40)	124.84(19)	C211-B11-C111	115.70(16)
C(37)-C(36)-C(35)	121.0(2)	C411-B11-C111	112.88(16)
C(38)-C(37)-C(36)	120.4(2)	C311-B11-C111	102.60(15)
C(37)-C(38)-C(39)	121.7(2)	F12-C12-C22	119.0(5)
C(38)-C(39)-C(34)	116.9(2)	F12-C12-C32	119.3(5)
C(38)-C(39)-C(43)	118.3(2)	C22-C12-C32	121.6(5)
C(34)-C(39)-C(43)	124.7(2)	C12-C22-C32#1	120.0(4)
C(35)-C(40)-C(42)	112.13(19)	C22#1-C32-C12	118.3(4)

Table S5 Bond lengths [Å] for **1**.

As(1)-C(30)	1.937(2)	C(24)-C(26)	1.530(6)	F351-C351	1.342(4)
As(1)-Ga(1)	2.4616(4)	C(24)-C(25)	1.538(5)	F361-C361	1.354(3)
Ga(1)-N(2)	1.925(2)	C(27)-C(28)	1.515(6)	F421-C421	1.339(4)
Ga(1)-N(1)	1.9310(18)	C(27)-C(29)	1.533(5)	F431-C431	1.349(4)
Ga(1)-Cl(1)	2.1725(7)	C(30)-C(33)	1.515(4)	F441-C441	1.339(4)
N(1)-C(1)	1.338(3)	C(31)-C(46)	1.499(5)	F451-C451	1.339(4)
N(1)-C(6)	1.445(3)	C(31)-C(47)	1.505(4)	F461-C461	1.357(4)
N(2)-C(3)	1.336(3)	C(31)-C(32)	1.519(5)	C111-C121	1.387(3)
N(2)-C(18)	1.450(3)	C(32)-C(33)	1.505(5)	C111-C161	1.390(3)
N(3)-C(30)	1.298(3)	C(33)-C(48)	1.498(6)	C111-B11	1.650(3)
N(3)-C(34)	1.462(3)	C(33)-C(49)	1.530(7)	C121-C131	1.385(4)
N(3)-C(31)	1.531(3)	C(34)-C(35)	1.398(4)	C131-C141	1.366(5)
C(1)-C(2)	1.392(3)	C(34)-C(39)	1.409(4)	C141-C151	1.375(4)
C(1)-C(4)	1.506(3)	C(35)-C(36)	1.388(4)	C151-C161	1.374(4)
C(2)-C(3)	1.397(3)	C(35)-C(40)	1.516(4)	C211-C221	1.384(3)
C(3)-C(5)	1.512(4)	C(36)-C(37)	1.365(6)	C211-C261	1.392(3)
C(6)-C(11)	1.402(3)	C(37)-C(38)	1.372(7)	C211-B11	1.654(3)
C(6)-C(7)	1.409(3)	C(38)-C(39)	1.384(5)	C221-C231	1.383(4)
C(7)-C(8)	1.393(3)	C(39)-C(43)	1.520(5)	C231-C241	1.372(4)
C(7)-C(12)	1.517(4)	C(40)-C(41)	1.525(4)	C241-C251	1.367(4)
C(8)-C(9)	1.378(4)	C(40)-C(42)	1.528(5)	C251-C261	1.384(4)
C(9)-C(10)	1.382(4)	C(43)-C(44)	1.537(5)	C311-C361	1.383(4)
C(10)-C(11)	1.396(3)	C(43)-C(45)	1.538(4)	C311-C321	1.396(3)
C(11)-C(15)	1.520(3)	F121-C121	1.346(3)	C311-B11	1.653(3)
C(12)-C(14)	1.521(5)	F131-C131	1.342(3)	C321-C331	1.376(4)
C(12)-C(13)	1.543(4)	F141-C141	1.342(3)	C331-C341	1.372(5)
C(15)-C(17)	1.521(4)	F151-C151	1.343(3)	C341-C351	1.366(5)

C(15)-C(16)	1.528(4)	F161-C161	1.356(3)	C351-C361	1.384(4)
C(18)-C(19)	1.403(5)	F221-C221	1.350(3)	C411-C461	1.382(4)
C(18)-C(23)	1.412(5)	F231-C231	1.339(3)	C411-C421	1.394(4)
C(19)-C(20)	1.406(4)	F241-C241	1.338(3)	C411-B11	1.648(3)
C(19)-C(24)	1.516(6)	F251-C251	1.344(3)	C421-C431	1.377(4)
C(20)-C(21)	1.372(8)	F261-C261	1.347(3)	C431-C441	1.358(6)
C(21)-C(22)	1.363(8)	F321-C321	1.343(3)	C441-C451	1.363(6)
C(22)-C(23)	1.394(5)	F331-C331	1.351(3)	C451-C461	1.388(4)
C(23)-C(27)	1.517(6)	F341-C341	1.335(4)		

Table S6 Bond angles [°] for **1**.

C(30)-As(1)-Ga(1)	114.86(7)	C(34)-C(39)-C(43)	125.7(3)
N(2)-Ga(1)-N(1)	98.31(8)	C(35)-C(40)-C(41)	111.0(3)
N(2)-Ga(1)-Cl(1)	109.05(7)	C(35)-C(40)-C(42)	111.6(3)
N(1)-Ga(1)-Cl(1)	107.08(6)	C(41)-C(40)-C(42)	109.5(3)
N(2)-Ga(1)-As(1)	111.59(6)	C(39)-C(43)-C(44)	110.3(3)
N(1)-Ga(1)-As(1)	109.97(6)	C(39)-C(43)-C(45)	111.2(3)
Cl(1)-Ga(1)-As(1)	118.80(3)	C(44)-C(43)-C(45)	109.0(2)
C(1)-N(1)-C(6)	118.62(18)	C121-C111-C161	112.7(2)
C(1)-N(1)-Ga(1)	119.68(15)	C121-C111-B11	126.8(2)
C(6)-N(1)-Ga(1)	121.61(14)	C161-C111-B11	120.3(2)
C(3)-N(2)-C(18)	119.0(2)	F121-C121-C131	114.7(2)
C(3)-N(2)-Ga(1)	120.12(15)	F121-C121-C111	121.2(2)
C(18)-N(2)-Ga(1)	120.86(16)	C131-C121-C111	124.1(3)
C(30)-N(3)-C(34)	123.7(2)	F131-C131-C141	120.1(3)
C(30)-N(3)-C(31)	113.7(2)	F131-C131-C121	120.2(3)
C(34)-N(3)-C(31)	122.6(2)	C141-C131-C121	119.7(3)
N(1)-C(1)-C(2)	123.9(2)	F141-C141-C131	120.7(3)
N(1)-C(1)-C(4)	119.9(2)	F141-C141-C151	120.1(3)
C(2)-C(1)-C(4)	116.1(2)	C131-C141-C151	119.2(2)
C(1)-C(2)-C(3)	128.9(2)	F151-C151-C161	121.1(3)
N(2)-C(3)-C(2)	123.9(2)	F151-C151-C141	120.0(3)
N(2)-C(3)-C(5)	120.1(2)	C161-C151-C141	118.9(3)
C(2)-C(3)-C(5)	116.0(2)	F161-C161-C151	116.0(2)
C(11)-C(6)-C(7)	121.8(2)	F161-C161-C111	118.8(2)
C(11)-C(6)-N(1)	117.81(18)	C151-C161-C111	125.2(2)
C(7)-C(6)-N(1)	120.4(2)	C221-C211-C261	112.9(2)
C(8)-C(7)-C(6)	117.6(2)	C221-C211-B11	119.34(19)
C(8)-C(7)-C(12)	118.8(2)	C261-C211-B11	127.6(2)
C(6)-C(7)-C(12)	123.6(2)	F221-C221-C231	115.6(2)
C(9)-C(8)-C(7)	121.4(2)	F221-C221-C211	119.3(2)
C(8)-C(9)-C(10)	120.2(2)	C231-C221-C211	125.0(2)
C(9)-C(10)-C(11)	121.0(2)	F231-C231-C241	119.5(2)

C(10)-C(11)-C(6)	117.9(2)	F231-C231-C221	121.3(2)
C(10)-C(11)-C(15)	119.7(2)	C241-C231-C221	119.2(2)
C(6)-C(11)-C(15)	122.3(2)	F241-C241-C251	121.1(2)
C(7)-C(12)-C(14)	110.3(3)	F241-C241-C231	120.1(3)
C(7)-C(12)-C(13)	112.9(3)	C251-C241-C231	118.8(2)
C(14)-C(12)-C(13)	109.4(3)	F251-C251-C241	119.8(2)
C(11)-C(15)-C(17)	113.4(2)	F251-C251-C261	120.0(3)
C(11)-C(15)-C(16)	111.5(2)	C241-C251-C261	120.2(2)
C(17)-C(15)-C(16)	110.2(2)	F261-C261-C251	115.3(2)
C(19)-C(18)-C(23)	123.2(3)	F261-C261-C211	120.9(2)
C(19)-C(18)-N(2)	119.4(3)	C251-C261-C211	123.8(2)
C(23)-C(18)-N(2)	117.4(3)	C361-C311-C321	113.2(2)
C(18)-C(19)-C(20)	115.8(4)	C361-C311-B11	127.6(2)
C(18)-C(19)-C(24)	124.5(2)	C321-C311-B11	118.8(2)
C(20)-C(19)-C(24)	119.7(4)	F321-C321-C331	116.2(2)
C(21)-C(20)-C(19)	121.8(4)	F321-C321-C311	119.5(2)
C(22)-C(21)-C(20)	121.1(3)	C331-C321-C311	124.3(3)
C(21)-C(22)-C(23)	121.0(4)	F331-C331-C341	119.7(3)
C(22)-C(23)-C(18)	117.1(4)	F331-C331-C321	120.8(3)
C(22)-C(23)-C(27)	119.5(4)	C341-C331-C321	119.4(3)
C(18)-C(23)-C(27)	123.3(3)	F341-C341-C351	121.2(3)
C(19)-C(24)-C(26)	112.8(3)	F341-C341-C331	119.7(3)
C(19)-C(24)-C(25)	111.1(4)	C351-C341-C331	119.2(3)
C(26)-C(24)-C(25)	109.5(3)	F351-C351-C341	120.8(3)
C(28)-C(27)-C(23)	113.1(4)	F351-C351-C361	119.5(3)
C(28)-C(27)-C(29)	108.4(4)	C341-C351-C361	119.7(3)
C(23)-C(27)-C(29)	112.7(4)	F361-C361-C311	120.7(2)
N(3)-C(30)-C(33)	111.0(2)	F361-C361-C351	115.2(3)
N(3)-C(30)-As(1)	121.16(18)	C311-C361-C351	124.1(3)
C(33)-C(30)-As(1)	126.7(2)	C461-C411-C421	113.3(3)
C(46)-C(31)-C(47)	106.9(3)	C461-C411-B11	119.5(2)
C(46)-C(31)-C(32)	118.2(4)	C421-C411-B11	126.9(2)
C(47)-C(31)-C(32)	110.1(3)	F421-C421-C431	114.7(3)
C(46)-C(31)-N(3)	110.0(2)	F421-C421-C411	121.7(2)
C(47)-C(31)-N(3)	111.6(2)	C431-C421-C411	123.6(3)
C(32)-C(31)-N(3)	99.8(2)	F431-C431-C441	119.7(3)
C(33)-C(32)-C(31)	108.6(3)	F431-C431-C421	120.3(4)
C(48)-C(33)-C(32)	114.8(4)	C441-C431-C421	120.0(3)
C(48)-C(33)-C(30)	111.4(3)	F441-C441-C431	120.4(4)
C(32)-C(33)-C(30)	102.5(3)	F441-C441-C451	119.8(4)
C(48)-C(33)-C(49)	108.8(5)	C431-C441-C451	119.7(3)
C(32)-C(33)-C(49)	110.1(4)	F451-C451-C441	121.5(3)
C(30)-C(33)-C(49)	109.1(4)	F451-C451-C461	119.8(4)
C(35)-C(34)-C(39)	122.6(3)	C441-C451-C461	118.8(3)

C(35)-C(34)-N(3)	119.7(2)	F461-C461-C411	119.0(3)
C(39)-C(34)-N(3)	117.7(2)	F461-C461-C451	116.5(3)
C(36)-C(35)-C(34)	117.3(3)	C411-C461-C451	124.5(3)
C(36)-C(35)-C(40)	117.6(3)	C411-B11-C111	113.69(19)
C(34)-C(35)-C(40)	125.0(3)	C411-B11-C311	101.20(19)
C(37)-C(36)-C(35)	121.4(4)	C111-B11-C311	112.59(18)
C(36)-C(37)-C(38)	120.1(4)	C411-B11-C211	113.54(18)
C(37)-C(38)-C(39)	122.3(3)	C111-B11-C211	102.40(18)
C(38)-C(39)-C(34)	116.3(3)	C311-B11-C211	113.93(19)
C(38)-C(39)-C(43)	117.9(3)		

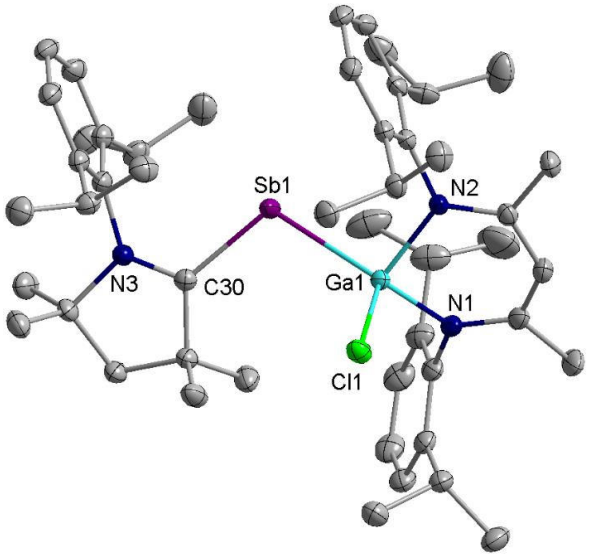


Fig. S7. Solid state structure of **2**·$C_6H_4F_2$. Hydrogen atoms, counter anion and solvent molecules are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S7 Bond lengths [Å] for **2**·$C_6H_4F_2$.

Sb11-C301	2.1807(17)	C311-C461	1.522(3)	C122-C132	1.380(3)
Sb11-Ga11	2.6621(2)	C311-C471	1.522(3)	C132-C142	1.369(3)
Ga11-N11	1.9419(14)	C311-C321	1.531(2)	C142-C152	1.377(3)
Ga11-N21	1.9449(14)	C321-C331	1.540(2)	C152-C162	1.378(3)
Ga11-Cl11	2.1979(4)	C331-C491	1.520(3)	C212-C222	1.387(3)
N11-C11	1.337(2)	C331-C481	1.536(3)	C212-C262	1.392(3)
N11-C61	1.449(2)	C341-C351	1.408(2)	C212-B12	1.648(3)
N21-C31	1.337(2)	C341-C391	1.409(2)	C222-C232	1.387(3)
N21-C181	1.450(2)	C351-C361	1.397(3)	C232-C242	1.374(3)
N31-C301	1.301(2)	C351-C401	1.526(3)	C242-C252	1.374(3)
N31-C341	1.466(2)	C361-C371	1.381(3)	C252-C262	1.380(3)
N31-C311	1.542(2)	C371-C381	1.382(3)	C312-C362	1.385(3)
C11-C21	1.398(3)	C381-C391	1.398(2)	C312-C322	1.392(3)
C11-C41	1.509(2)	C391-C431	1.523(3)	C312-B12	1.653(3)
C21-C31	1.397(2)	C401-C411	1.537(3)	C322-C332	1.378(3)
C31-C51	1.509(2)	C401-C421	1.538(3)	C332-C342	1.374(3)
C61-C111	1.406(3)	C431-C451	1.534(3)	C342-C352	1.373(3)
C61-C71	1.406(3)	C431-C441	1.538(3)	C352-C362	1.391(3)
C71-C81	1.400(3)	F122-C122	1.354(2)	C412-C422	1.391(3)
C71-C121	1.520(3)	F132-C132	1.352(2)	C412-C462	1.392(3)
C81-C91	1.378(3)	F142-C142	1.343(2)	C412-B12	1.655(3)
C91-C101	1.385(3)	F152-C152	1.347(2)	C422-C432	1.389(3)
C101-C111	1.394(3)	F162-C162	1.353(2)	C432-C442	1.368(4)
C111-C151	1.519(3)	F222-C222	1.349(2)	C442-C452	1.371(4)
C121-C141	1.535(3)	F232-C232	1.342(2)	C452-C462	1.387(3)

C121-C131	1.542(2)	F242-C242	1.341(2)	F13-C13	1.325(6)
C151-C161	1.527(4)	F252-C252	1.345(2)	F23-C23	1.335(6)
C151-C171	1.533(4)	F262-C262	1.351(2)	C13-C23	1.368(8)
C181-C191	1.403(2)	F322-C322	1.353(2)	C13-C63	1.368(8)
C181-C231	1.411(2)	F332-C332	1.345(2)	C23-C33	1.370(7)
C191-C201	1.400(2)	F342-C342	1.346(2)	C33-C43	1.368(7)
C191-C241	1.514(2)	F352-C352	1.343(2)	C43-C53	1.368(8)
C201-C211	1.374(3)	F362-C362	1.349(2)	C53-C63	1.371(8)
C211-C221	1.385(3)	F412-C422	1.348(3)	F14-C14	1.334(7)
C221-C231	1.392(3)	F422-C432	1.345(3)	F24-C24	1.314(7)
C231-C271	1.517(3)	F432-C442	1.346(2)	C14-C64	1.366(8)
C241-C261	1.531(2)	F442-C452	1.351(3)	C14-C24	1.374(8)
C241-C251	1.536(3)	F452-C462	1.349(3)	C24-C34	1.366(7)
C271-C281	1.527(3)	C112-C122	1.391(3)	C34-C44	1.363(9)
C271-C291	1.531(3)	C112-C162	1.396(3)	C44-C54	1.370(8)
C301-C331	1.518(2)	C112-B12	1.654(3)	C54-C64	1.371(7)

Table S8 Bond angles [°] for **2**·$C_6H_4F_2$.

C301-Sb11-Ga11	110.28(4)	F122-C122-C132	114.70(16)
N11-Ga11-N21	97.11(6)	F122-C122-C112	121.25(16)
N11-Ga11-Cl11	105.34(4)	C132-C122-C112	124.04(17)
N21-Ga11-Cl11	107.63(4)	F132-C132-C142	120.05(17)
N11-Ga11-Sb11	127.34(4)	F132-C132-C122	119.65(17)
N21-Ga11-Sb11	101.08(4)	C142-C132-C122	120.29(17)
Cl11-Ga11-Sb11	115.091(14)	F142-C142-C132	121.06(17)
C11-N11-C61	119.97(14)	F142-C142-C152	120.18(18)
C11-N11-Ga11	119.15(12)	C132-C142-C152	118.76(17)
C61-N11-Ga11	120.87(11)	F152-C152-C142	119.88(16)
C31-N21-C181	120.48(14)	F152-C152-C162	120.95(17)
C31-N21-Ga11	119.64(11)	C142-C152-C162	119.17(17)
C181-N21-Ga11	119.80(10)	F162-C162-C152	115.75(16)
C301-N31-C341	125.74(14)	F162-C162-C112	119.29(15)
C301-N31-C311	114.36(14)	C152-C162-C112	124.96(17)
C341-N31-C311	119.86(13)	C222-C212-C262	113.34(17)
N11-C11-C21	124.33(16)	C222-C212-B12	125.89(16)
N11-C11-C41	119.23(17)	C262-C212-B12	120.38(16)
C21-C11-C41	116.43(16)	F222-C222-C232	114.66(16)
C31-C21-C11	128.51(16)	F222-C222-C212	121.18(16)
N21-C31-C21	123.30(16)	C232-C222-C212	124.15(17)
N21-C31-C51	119.88(15)	F232-C232-C242	119.94(17)
C21-C31-C51	116.82(15)	F232-C232-C222	120.53(17)
C111-C61-C71	121.61(17)	C242-C232-C222	119.52(18)
C111-C61-N11	117.72(16)	F242-C242-C232	119.90(19)

C71-C61-N11	120.65(16)	F242-C242-C252	121.03(18)
C81-C71-C61	117.50(18)	C232-C242-C252	119.06(18)
C81-C71-C121	118.72(17)	F252-C252-C242	120.26(18)
C61-C71-C121	123.77(16)	F252-C252-C262	120.27(19)
C91-C81-C71	121.65(19)	C242-C252-C262	119.46(18)
C81-C91-C101	119.93(19)	F262-C262-C252	116.44(17)
C91-C101-C111	120.94(19)	F262-C262-C212	119.18(17)
C101-C111-C61	118.33(18)	C252-C262-C212	124.37(18)
C101-C111-C151	119.37(18)	C362-C312-C322	113.49(17)
C61-C111-C151	122.29(17)	C362-C312-B12	127.87(16)
C71-C121-C141	111.55(15)	C322-C312-B12	118.34(16)
C71-C121-C131	110.76(16)	F322-C322-C332	115.48(17)
C141-C121-C131	109.30(16)	F322-C322-C312	119.78(16)
C111-C151-C161	110.91(19)	C332-C322-C312	124.74(19)
C111-C151-C171	112.2(2)	F332-C332-C342	120.39(18)
C161-C151-C171	110.3(2)	F332-C332-C322	120.46(19)
C191-C181-C231	121.31(15)	C342-C332-C322	119.15(19)
C191-C181-N21	120.33(15)	F342-C342-C352	120.7(2)
C231-C181-N21	118.33(15)	F342-C342-C332	120.1(2)
C201-C191-C181	118.03(16)	C352-C342-C332	119.16(18)
C201-C191-C241	119.04(16)	F352-C352-C342	119.86(18)
C181-C191-C241	122.91(15)	F352-C352-C362	120.37(19)
C211-C201-C191	121.38(17)	C342-C352-C362	119.77(18)
C201-C211-C221	119.90(17)	F362-C362-C312	121.06(16)
C211-C221-C231	121.36(17)	F362-C362-C352	115.29(17)
C221-C231-C181	118.00(17)	C312-C362-C352	123.65(18)
C221-C231-C271	120.14(16)	C422-C412-C462	113.50(18)
C181-C231-C271	121.84(16)	C422-C412-B12	120.22(17)
C191-C241-C261	111.28(15)	C462-C412-B12	126.12(17)
C191-C241-C251	110.94(15)	F412-C422-C432	116.5(2)
C261-C241-C251	109.50(15)	F412-C422-C412	119.50(17)
C231-C271-C281	111.58(17)	C432-C422-C412	124.0(2)
C231-C271-C291	112.88(17)	F422-C432-C442	120.3(2)
C281-C271-C291	109.06(17)	F422-C432-C422	120.2(2)
N31-C301-C331	111.00(14)	C442-C432-C422	119.5(2)
N31-C301-Sb11	119.08(12)	F432-C442-C432	120.8(2)
C331-C301-Sb11	129.87(12)	F432-C442-C452	119.8(3)
C461-C311-C471	108.99(16)	C432-C442-C452	119.3(2)
C461-C311-C321	113.53(16)	F442-C452-C442	120.1(2)
C471-C311-C321	112.67(15)	F442-C452-C462	120.3(2)
C461-C311-N31	110.61(14)	C442-C452-C462	119.6(2)
C471-C311-N31	110.69(14)	F452-C462-C452	114.6(2)
C321-C311-N31	100.12(13)	F452-C462-C412	121.42(17)
C311-C321-C331	107.80(14)	C452-C462-C412	124.0(2)

C301-C331-C491	111.54(15)	C212-B12-C312	115.21(15)
C301-C331-C481	108.33(14)	C212-B12-C112	113.54(14)
C491-C331-C481	110.37(16)	C312-B12-C112	100.14(13)
C301-C331-C321	102.69(13)	C212-B12-C412	102.06(14)
C491-C331-C321	111.32(15)	C312-B12-C412	111.88(15)
C481-C331-C321	112.34(15)	C112-B12-C412	114.61(15)
C351-C341-C391	122.89(16)	F13-C13-C23	119.6(7)
C351-C341-N31	118.89(15)	F13-C13-C63	120.2(7)
C391-C341-N31	118.14(15)	C23-C13-C63	120.1(5)
C361-C351-C341	116.86(17)	F23-C23-C13	119.2(6)
C361-C351-C401	118.09(16)	F23-C23-C33	120.4(7)
C341-C351-C401	124.91(16)	C13-C23-C33	120.4(6)
C371-C361-C351	121.51(18)	C43-C33-C23	119.4(6)
C361-C371-C381	120.24(17)	C33-C43-C53	120.2(6)
C371-C381-C391	121.39(18)	C43-C53-C63	120.3(5)
C381-C391-C341	116.87(16)	C13-C63-C53	119.5(5)
C381-C391-C431	118.20(16)	F14-C14-C64	119.7(7)
C341-C391-C431	124.76(15)	F14-C14-C24	119.4(6)
C351-C401-C411	109.99(17)	C64-C14-C24	120.9(6)
C351-C401-C421	112.85(16)	F24-C24-C34	121.1(7)
C411-C401-C421	108.39(16)	F24-C24-C14	119.0(7)
C391-C431-C451	113.07(16)	C34-C24-C14	119.8(6)
C391-C431-C441	109.45(15)	C44-C34-C24	119.1(5)
C451-C431-C441	109.24(16)	C34-C44-C54	121.4(6)
C122-C112-C162	112.74(16)	C44-C54-C64	119.5(7)
C122-C112-B12	127.26(16)	C14-C64-C54	119.3(7)
C162-C112-B12	119.25(15)		

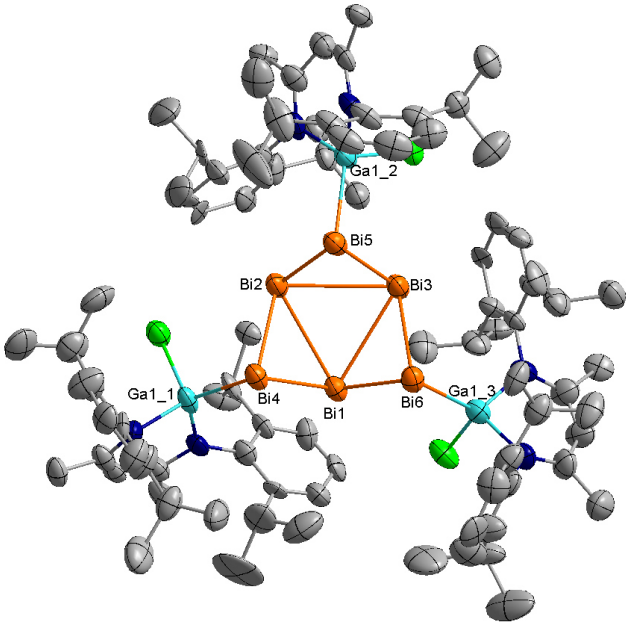


Fig. S8. Solid state structure of **4**·$C_6H_4F_2$. Hydrogen atoms, counter anion and solvent molecules are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S9 Bond lengths [Å] for **4**·$C_6H_4F_2$.

Bi(1)-Ga11	2.709(3)	C32-C52	1.49(3)	F25-C25	1.36(2)
Bi(1)-Bi(5)	2.9954(10)	C62-C112	1.40(3)	F35-C35	1.34(2)
Bi(1)-Bi(4)	2.9954(11)	C62-C72	1.41(3)	F45-C45	1.35(2)
Bi(2)-Ga13	2.700(2)	C72-C82	1.43(3)	F55-C55	1.37(2)
Bi(2)-Bi(6)	2.9924(11)	C72-C122	1.50(3)	F65-C65	1.35(2)
Bi(2)-Bi(5)	3.0041(11)	C82-C92	1.37(3)	C15-C25	1.38(3)
Bi(3)-Ga12	2.692(2)	C92-C102	1.37(3)	C15-C65	1.40(3)
Bi(3)-Bi(4)	2.9900(12)	C102-C112	1.40(3)	C25-C35	1.38(3)
Bi(3)-Bi(6)	3.0005(11)	C112-C152	1.49(3)	C35-C45	1.38(3)
Bi(4)-Bi(5)	3.3201(11)	C122-C132	1.54(4)	C45-C55	1.36(3)
Bi(4)-Bi(6)	3.3389(10)	C122-C142	1.54(4)	C55-C65	1.36(3)
Bi(5)-Bi(6)	3.3159(12)	C152-C172	1.51(3)	F26-C26	1.36(3)
B(1)-C15	1.63(3)	C152-C162	1.54(4)	F36-C36	1.34(3)
B(1)-C16	1.67(3)	C182-C192	1.39(3)	F46-C46	1.36(2)
B(1)-C17	1.67(3)	C182-C232	1.40(2)	F56-C56	1.36(3)
B(1)-C18	1.69(3)	C192-C202	1.40(2)	F66-C66	1.32(2)
Ga11-N21	1.899(17)	C192-C242	1.54(2)	C16-C26	1.38(3)
Ga11-N11	1.916(14)	C202-C212	1.38(2)	C16-C66	1.42(3)
Ga11-Cl11	2.211(5)	C212-C222	1.37(3)	C26-C36	1.39(3)
N11-C11	1.31(3)	C222-C232	1.41(3)	C36-C46	1.37(3)
N11-C61	1.49(3)	C232-C272	1.47(3)	C46-C56	1.35(3)
N21-C31	1.34(2)	C242-C252	1.54(3)	C56-C66	1.41(3)
N21-C181	1.47(2)	C242-C262	1.54(3)	F27-C27	1.33(2)
C11-C21	1.43(3)	C272-C292	1.54(3)	F37-C37	1.34(2)

C11-C41	1.52(2)	C272-C282	1.55(3)	F47-C47	1.37(2)
C21-C31	1.42(2)	Ga13-N13	1.912(15)	F57-C57	1.35(2)
C31-C51	1.52(3)	Ga13-N23	1.930(14)	F67-C67	1.36(2)
C61-C111	1.40(3)	Ga13-Cl13	2.228(6)	C17-C27	1.37(3)
C61-C71	1.41(3)	N13-C13	1.32(2)	C17-C67	1.39(2)
C71-C81	1.45(4)	N13-C63	1.47(2)	C27-C37	1.41(3)
C71-C121	1.51(4)	N23-C33	1.35(2)	C37-C47	1.37(3)
C81-C91	1.34(4)	N23-C183	1.43(2)	C47-C57	1.34(3)
C91-C101	1.38(4)	C13-C23	1.42(3)	C57-C67	1.39(3)
C101-C111	1.40(3)	C13-C43	1.47(3)	F28-C28	1.36(2)
C111-C151	1.52(3)	C23-C33	1.40(3)	F38-C38	1.37(3)
C151-C161	1.53(3)	C33-C53	1.50(3)	F48-C48	1.37(2)
C151-C171	1.54(3)	C63-C113	1.38(3)	F58-C58	1.35(2)
C141-C121	1.51(4)	C63-C73	1.42(3)	F68-C68	1.34(2)
C131-C121	1.51(4)	C73-C83	1.40(3)	C18-C28	1.37(3)
C181-C231	1.39(3)	C73-C123	1.52(3)	C18-C68	1.41(3)
C181-C191	1.41(3)	C83-C93	1.35(4)	C28-C38	1.37(3)
C191-C201	1.38(3)	C93-C103	1.36(4)	C38-C48	1.36(3)
C191-C241	1.45(3)	C103-C113	1.38(3)	C48-C58	1.37(3)
C201-C211	1.37(3)	C113-C153	1.53(4)	C58-C68	1.37(3)
C211-C221	1.40(3)	C123-C133	1.53(3)	F19-C19	1.28(3)
C221-C231	1.41(2)	C123-C143	1.56(3)	F29-C29	1.27(3)
C231-C271	1.51(3)	C153-C173	1.52(4)	C19-C29	1,39
C241-C251	1.44(3)	C153-C163	1.52(4)	C19-C69	1,39
C241-C261	1.61(3)	C183-C233	1.41(3)	C29-C39	1,39
C271-C291	1.52(3)	C183-C193	1.41(3)	C39-C49	1,39
C271-C281	1.54(3)	C193-C203	1.40(3)	C49-C59	1,39
Ga12-N12	1.915(19)	C193-C243	1.52(3)	C59-C69	1,39
Ga12-N22	1.925(14)	C203-C213	1.36(3)	F110-C110	1.35(2)
Ga12-Cl12	2.202(5)	C213-C223	1.41(3)	F210-C210	1.38(2)
N12-C12	1.35(3)	C223-C233	1.41(3)	C110-C210	1,39
N12-C62	1.47(3)	C233-C273	1.43(3)	C110-C610	1,39
N22-C32	1.33(3)	C243-C253	1.53(2)	C210-C310	1,39
N22-C182	1.46(2)	C243-C263	1.57(3)	C310-C410	1,39
C12-C22	1.38(3)	C273-C293	1.46(4)	C410-C510	1,39
C12-C42	1.51(3)	C273-C283	1.50(4)	C510-C610	1,39
C22-C32	1.44(3)				

Table S10 Bond angles [°] for **4**·$C_6H_4F_2$.

Ga11-Bi(1)-Bi(5)	92.62(5)	N23-Ga13-Cl13	103.5(5)
Ga11-Bi(1)-Bi(4)	87.65(6)	N13-Ga13-Bi(2)	111.7(5)
Bi(5)-Bi(1)-Bi(4)	67.31(3)	N23-Ga13-Bi(2)	124.4(5)
Ga13-Bi(2)-Bi(6)	92.25(5)	Cl13-Ga13-Bi(2)	111.65(14)

Ga13-Bi(2)-Bi(5)	88.73(6)	C13-N13-C63	116.1(15)
Bi(6)-Bi(2)-Bi(5)	67.14(3)	C13-N13-Ga13	121.8(14)
Ga12-Bi(3)-Bi(4)	92.36(6)	C63-N13-Ga13	122.0(11)
Ga12-Bi(3)-Bi(6)	87.92(6)	C33-N23-C183	121.1(15)
Bi(4)-Bi(3)-Bi(6)	67.75(3)	C33-N23-Ga13	117.6(13)
Bi(3)-Bi(4)-Bi(1)	93.08(3)	C183-N23-Ga13	121.4(11)
Bi(3)-Bi(4)-Bi(5)	99.45(3)	N13-C13-C23	120.6(18)
Bi(1)-Bi(4)-Bi(5)	56.34(2)	N13-C13-C43	123.5(18)
Bi(3)-Bi(4)-Bi(6)	56.28(2)	C23-C13-C43	115.8(16)
Bi(1)-Bi(4)-Bi(6)	99.91(3)	C33-C23-C13	128.4(18)
Bi(5)-Bi(4)-Bi(6)	59.73(2)	N23-C33-C23	123.9(17)
Bi(1)-Bi(5)-Bi(2)	92.14(3)	N23-C33-C53	118.2(18)
Bi(1)-Bi(5)-Bi(6)	100.43(3)	C23-C33-C53	117.8(17)
Bi(2)-Bi(5)-Bi(6)	56.26(2)	C113-C63-C73	120.4(19)
Bi(1)-Bi(5)-Bi(4)	56.34(2)	C113-C63-N13	119.2(19)
Bi(2)-Bi(5)-Bi(4)	99.13(3)	C73-C63-N13	120.3(19)
Bi(6)-Bi(5)-Bi(4)	60.42(2)	C83-C73-C63	118(2)
Bi(2)-Bi(6)-Bi(3)	91.37(3)	C83-C73-C123	120(2)
Bi(2)-Bi(6)-Bi(5)	56.60(3)	C63-C73-C123	122.5(19)
Bi(3)-Bi(6)-Bi(5)	99.33(3)	C93-C83-C73	122(3)
Bi(2)-Bi(6)-Bi(4)	98.95(3)	C83-C93-C103	119(2)
Bi(3)-Bi(6)-Bi(4)	55.98(2)	C93-C103-C113	123(3)
Bi(5)-Bi(6)-Bi(4)	59.85(2)	C63-C113-C103	118(2)
C15-B(1)-C16	115.4(18)	C63-C113-C153	124(2)
C15-B(1)-C17	103.3(14)	C103-C113-C153	118(2)
C16-B(1)-C17	112.4(15)	C73-C123-C133	113(2)
C15-B(1)-C18	114.2(15)	C73-C123-C143	110(2)
C16-B(1)-C18	100.9(14)	C133-C123-C143	111(2)
C17-B(1)-C18	111.0(17)	C173-C153-C163	110(3)
N21-Ga11-N11	97.1(7)	C173-C153-C113	113(2)
N21-Ga11-Cl11	104.4(5)	C163-C153-C113	111(3)
N11-Ga11-Cl11	104.7(5)	C233-C183-C193	120.1(18)
N21-Ga11-Bi(1)	124.0(4)	C233-C183-N23	119.9(18)
N11-Ga11-Bi(1)	110.9(5)	C193-C183-N23	120(2)
Cl11-Ga11-Bi(1)	113.19(17)	C203-C193-C183	119(2)
C11-N11-C61	119.6(15)	C203-C193-C243	118.4(18)
C11-N11-Ga11	121.4(14)	C183-C193-C243	122.5(18)
C61-N11-Ga11	118.9(12)	C213-C203-C193	122(2)
C31-N21-C181	120.2(17)	C203-C213-C223	120(2)
C31-N21-Ga11	118.9(13)	C213-C223-C233	121(2)
C181-N21-Ga11	120.6(12)	C183-C233-C223	119(2)
N11-C11-C21	121.3(16)	C183-C233-C273	123(2)
N11-C11-C41	123(2)	C223-C233-C273	118(2)
C21-C11-C41	116.0(19)	C193-C243-C253	111.7(17)

C31-C21-C11	127.3(19)	C193-C243-C263	111.7(17)
N21-C31-C21	124(2)	C253-C243-C263	107.8(16)
N21-C31-C51	120.9(17)	C233-C273-C293	117(3)
C21-C31-C51	115.1(18)	C233-C273-C283	116(2)
C111-C61-C71	127(2)	C293-C273-C283	107(2)
C111-C61-N11	117.9(18)	C25-C15-C65	113.1(19)
C71-C61-N11	115(2)	C25-C15-B(1)	127.3(17)
C61-C71-C81	111(2)	C65-C15-B(1)	119.4(17)
C61-C71-C121	124(2)	F25-C25-C35	114.5(17)
C81-C71-C121	125(2)	F25-C25-C15	120.9(17)
C91-C81-C71	126(3)	C35-C25-C15	124.6(19)
C81-C91-C101	119(3)	F35-C35-C25	121.0(18)
C91-C101-C111	122(3)	F35-C35-C45	119.1(19)
C101-C111-C61	115(2)	C25-C35-C45	119.9(19)
C101-C111-C151	120(2)	F45-C45-C55	122(2)
C61-C111-C151	125(2)	F45-C45-C35	121(2)
C111-C151-C161	110.3(18)	C55-C45-C35	117(2)
C111-C151-C171	112(2)	C45-C55-C65	122(2)
C161-C151-C171	110(2)	C45-C55-F55	118(2)
C71-C121-C131	110(2)	C65-C55-F55	119.7(19)
C71-C121-C141	109(3)	F65-C65-C55	117.6(18)
C131-C121-C141	110(2)	F65-C65-C15	119.3(19)
C231-C181-C191	121.9(17)	C55-C65-C15	123(2)
C231-C181-N21	120.4(16)	C26-C16-C66	114.4(18)
C191-C181-N21	117.5(17)	C26-C16-B(1)	121(2)
C201-C191-C181	118(2)	C66-C16-B(1)	124.4(19)
C201-C191-C241	118(2)	F26-C26-C16	120.4(18)
C181-C191-C241	123.0(17)	F26-C26-C36	115.2(19)
C211-C201-C191	121(2)	C16-C26-C36	124(2)
C201-C211-C221	121.9(19)	F36-C36-C46	120(2)
C211-C221-C231	119(2)	F36-C36-C26	120(2)
C181-C231-C221	118.5(19)	C46-C36-C26	120(2)
C181-C231-C271	123.8(16)	C56-C46-F46	120(2)
C221-C231-C271	117.5(18)	C56-C46-C36	119(2)
C251-C241-C191	123(3)	F46-C46-C36	121(2)
C251-C241-C261	110(2)	C46-C56-F56	123(2)
C191-C241-C261	109.6(19)	C46-C56-C66	122(2)
C231-C271-C291	112.7(17)	F56-C56-C66	115(2)
C231-C271-C281	111.8(18)	F66-C66-C56	118(2)
C291-C271-C281	109.2(18)	F66-C66-C16	120.9(17)
N12-Ga12-N22	97.1(7)	C56-C66-C16	121(2)
N12-Ga12-Cl12	105.8(5)	C27-C17-C67	115.1(17)
N22-Ga12-Cl12	103.2(4)	C27-C17-B(1)	126.5(17)
N12-Ga12-Bi(3)	111.2(5)	C67-C17-B(1)	117.6(16)

N22-Ga12-Bi(3)	125.0(5)	F27-C27-C17	122.6(18)
Cl12-Ga12-Bi(3)	112.25(18)	F27-C27-C37	115.2(18)
C12-N12-C62	118.6(19)	C17-C27-C37	122.2(19)
C12-N12-Ga12	119.6(15)	F37-C37-C47	122(2)
C62-N12-Ga12	121.1(14)	F37-C37-C27	119(2)
C32-N22-C182	120.5(15)	C47-C37-C27	119.3(19)
C32-N22-Ga12	119.1(13)	C57-C47-F47	120(2)
C182-N22-Ga12	120.2(12)	C57-C47-C37	121(2)
N12-C12-C22	122(2)	F47-C47-C37	119.4(19)
N12-C12-C42	121(2)	C47-C57-F57	120.3(18)
C22-C12-C42	117(2)	C47-C57-C67	118.5(19)
C12-C22-C32	131(2)	F57-C57-C67	121.2(18)
N22-C32-C22	120.9(18)	F67-C67-C17	121.9(16)
N22-C32-C52	121.6(19)	F67-C67-C57	114.0(16)
C22-C32-C52	117.4(19)	C17-C67-C57	123.9(18)
C112-C62-C72	123(2)	C28-C18-C68	114.9(18)
C112-C62-N12	116.6(19)	C28-C18-B(1)	128.2(18)
C72-C62-N12	119.6(19)	C68-C18-B(1)	116.8(18)
C62-C72-C82	115(2)	F28-C28-C18	121.5(17)
C62-C72-C122	124(2)	F28-C28-C38	115.5(19)
C82-C72-C122	121(2)	C18-C28-C38	123(2)
C92-C82-C72	124(2)	C48-C38-F38	120.1(19)
C102-C92-C82	117(2)	C48-C38-C28	120(2)
C92-C102-C112	124(2)	F38-C38-C28	119.5(19)
C62-C112-C102	116(2)	C38-C48-F48	120(2)
C62-C112-C152	124(2)	C38-C48-C58	119.8(18)
C102-C112-C152	119(2)	F48-C48-C58	120.0(19)
C72-C122-C132	111(2)	F58-C58-C68	121(2)
C72-C122-C142	111(2)	F58-C58-C48	119.8(17)
C132-C122-C142	108(2)	C68-C58-C48	119.1(19)
C112-C152-C172	116(2)	F68-C68-C58	116.4(18)
C112-C152-C162	113(2)	F68-C68-C18	120.7(17)
C172-C152-C162	109(2)	C58-C68-C18	123(2)
C192-C182-C232	121.4(18)	F19-C19-C29	119(3)
C192-C182-N22	121.4(14)	F19-C19-C69	121(3)
C232-C182-N22	117.1(17)	C29-C19-C69	120
C182-C192-C202	119.3(16)	F29-C29-C19	118(3)
C182-C192-C242	123.4(17)	F29-C29-C39	122(3)
C202-C192-C242	117.2(17)	C19-C29-C39	120
C212-C202-C192	120(2)	C49-C39-C29	120
C222-C212-C202	121.1(19)	C39-C49-C59	120
C212-C222-C232	120.5(16)	C69-C59-C49	120
C182-C232-C222	117.8(19)	C59-C69-C19	120
C182-C232-C272	122.8(19)	F110-C110-C210	117.9(15)

C222-C232-C272	119.1(17)	F110-C110-C610	122.1(15)
C252-C242-C262	110.8(17)	C210-C110-C610	120
C252-C242-C192	112.9(15)	F210-C210-C310	121.6(16)
C262-C242-C192	109.4(16)	F210-C210-C110	118.4(17)
C232-C272-C292	115(2)	C310-C210-C110	120
C232-C272-C282	113(2)	C210-C310-C410	120
C292-C272-C282	109.4(18)	C310-C410-C510	120
N13-Ga13-N23	97.2(6)	C410-C510-C610	120
N13-Ga13-Cl13	106.4(5)	C510-C610-C110	120

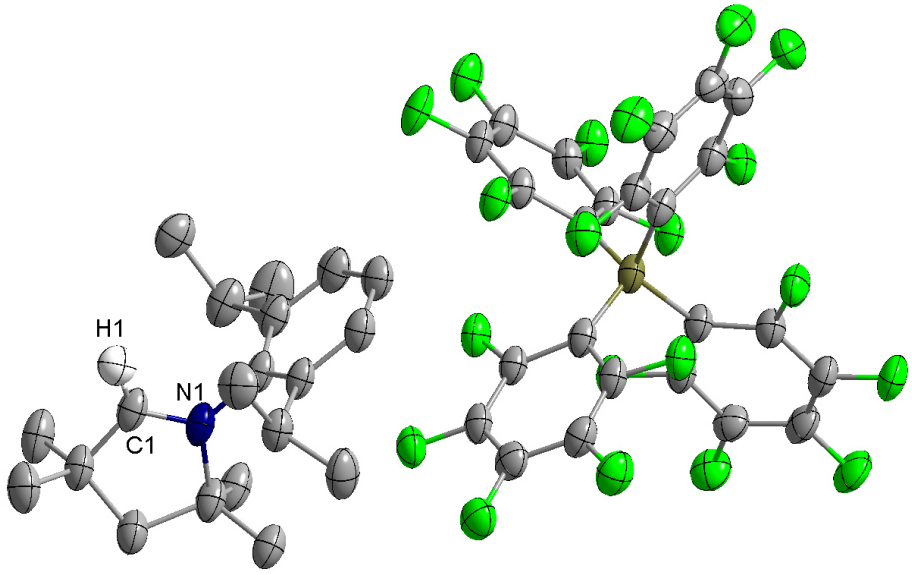


Fig. S9. Solid state structure of [^{Me}cAACH][BAr$^{F}_{4}$]. Hydrogen atoms except H1, counter anion and solvent molecules are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S11 Bond lengths [Å] for [^{Me}cAACH][BAr$^{F}_{4}$].

N11-C11	1.280(3)	F142-C142	1.353(3)	C142-C152	1.378(4)
N11-C51	1.455(4)	F152-C152	1.347(3)	C152-C162	1.371(4)
N11-C21	1.549(4)	F162-C162	1.360(3)	C212-C262	1.394(4)
C11-C41	1.485(4)	F222-C222	1.352(3)	C212-C222	1.396(4)
C21-C171	1.522(4)	F232-C232	1.355(3)	C212-B12	1.641(4)
C21-C181	1.532(4)	F242-C242	1.337(3)	C222-C232	1.366(4)
C21-C31	1.537(4)	F252-C252	1.348(3)	C232-C242	1.374(4)
C31-C41	1.548(4)	F262-C262	1.359(3)	C242-C252	1.386(4)
C41-C191	1.532(4)	F322-C322	1.356(3)	C252-C262	1.368(4)
C41-C201	1.546(4)	F332-C332	1.341(3)	C312-C362	1.390(4)
C51-C101	1.404(4)	F342-C342	1.340(3)	C312-C322	1.394(3)
C51-C61	1.405(4)	F352-C352	1.351(3)	C312-B12	1.648(4)
C61-C71	1.384(4)	F362-C362	1.356(3)	C322-C332	1.365(4)
C61-C111	1.528(4)	F412-C422	1.348(3)	C332-C342	1.381(4)
C71-C81	1.384(4)	F422-C432	1.342(3)	C342-C352	1.372(4)
C81-C91	1.370(4)	F432-C442	1.347(3)	C352-C362	1.379(4)
C91-C101	1.396(4)	F442-C452	1.346(3)	C412-C462	1.383(4)
C101-C141	1.518(4)	F452-C462	1.352(3)	C412-C422	1.390(4)
C111-C121	1.530(4)	C112-C162	1.386(4)	C412-B12	1.651(4)
C111-C131	1.531(4)	C112-C122	1.395(4)	C422-C432	1.382(4)
C141-C151	1.530(4)	C112-B12	1.654(4)	C432-C442	1.374(4)
C141-C161	1.530(4)	C122-C132	1.385(4)	C442-C452	1.370(4)
F122-C122	1.345(3)	C132-C142	1.365(4)	C452-C462	1.386(4)
F132-C132	1.357(3)				

Table S12 Bond angles [°] for [^{Me}cAACH][BAr$^{F}_{4}$].

C11-N11-C51	123.4(3)	F222-C222-C212	120.6(2)
C11-N11-C21	112.3(2)	C232-C222-C212	124.3(2)
C51-N11-C21	124.1(2)	F232-C232-C222	120.6(2)
N11-C11-C41	114.9(3)	F232-C232-C242	118.6(3)
C171-C21-C181	109.0(2)	C222-C232-C242	120.9(2)
C171-C21-C31	112.9(3)	F242-C242-C232	121.1(3)
C181-C21-C31	113.9(2)	F242-C242-C252	121.1(3)
C171-C21-N11	111.3(2)	C232-C242-C252	117.8(3)
C181-C21-N11	109.0(3)	F252-C252-C262	121.4(3)
C31-C21-N11	100.4(2)	F252-C252-C242	119.3(3)
C21-C31-C41	108.0(3)	C262-C252-C242	119.3(3)
C11-C41-C191	111.6(3)	F262-C262-C252	115.9(2)
C11-C41-C201	107.0(3)	F262-C262-C212	118.6(2)
C191-C41-C201	110.2(2)	C252-C262-C212	125.5(3)
C11-C41-C31	101.4(2)	C362-C312-C322	112.8(2)
C191-C41-C31	113.1(3)	C362-C312-B12	127.8(2)
C201-C41-C31	113.2(3)	C322-C312-B12	119.0(2)
C101-C51-C61	122.8(3)	F322-C322-C332	116.0(2)
C101-C51-N11	118.7(2)	F322-C322-C312	118.7(2)
C61-C51-N11	118.5(2)	C332-C322-C312	125.3(2)
C71-C61-C51	117.3(3)	F332-C332-C322	120.9(2)
C71-C61-C111	119.4(3)	F332-C332-C342	119.9(2)
C51-C61-C111	123.3(3)	C322-C332-C342	119.2(2)
C81-C71-C61	121.1(3)	F342-C342-C352	120.5(2)
C91-C81-C71	120.5(3)	F342-C342-C332	121.0(2)
C81-C91-C101	121.4(3)	C352-C342-C332	118.5(2)
C91-C101-C51	116.7(3)	F352-C352-C342	118.9(2)
C91-C101-C141	120.0(2)	F352-C352-C362	120.8(2)
C51-C101-C141	123.1(3)	C342-C352-C362	120.3(2)
C61-C111-C121	110.7(2)	F362-C362-C352	114.9(2)
C61-C111-C131	111.8(3)	F362-C362-C312	121.2(2)
C121-C111-C131	110.6(3)	C352-C362-C312	123.9(2)
C101-C141-C151	109.6(3)	C462-C412-C422	113.8(2)
C101-C141-C161	112.8(2)	C462-C412-B12	126.6(2)
C151-C141-C161	110.4(3)	C422-C412-B12	119.1(2)
C162-C112-C122	113.0(3)	F412-C422-C432	116.2(2)
C162-C112-B12	119.9(2)	F412-C422-C412	119.6(2)
C122-C112-B12	126.7(2)	C432-C422-C412	124.2(3)
F122-C122-C132	115.6(2)	F422-C432-C442	119.9(2)
F122-C122-C112	121.2(2)	F422-C432-C422	120.9(3)
C132-C122-C112	123.1(3)	C442-C432-C422	119.1(3)

F132-C132-C142	119.6(3)	F432-C442-C452	120.2(3)
F132-C132-C122	119.7(3)	F432-C442-C432	120.3(3)
C142-C132-C122	120.6(3)	C452-C442-C432	119.5(2)
F142-C142-C132	121.0(3)	F442-C452-C442	120.1(2)
F142-C142-C152	120.3(3)	F442-C452-C462	120.5(3)
C132-C142-C152	118.7(3)	C442-C452-C462	119.4(3)
F152-C152-C162	121.2(3)	F452-C462-C412	121.1(2)
F152-C152-C142	119.7(3)	F452-C462-C452	115.0(2)
C162-C152-C142	119.0(3)	C412-C462-C452	123.9(3)
F162-C162-C152	115.7(3)	C212-B12-C312	114.4(2)
F162-C162-C112	118.9(2)	C212-B12-C412	101.7(2)
C152-C162-C112	125.4(3)	C312-B12-C412	113.0(2)
C262-C212-C222	112.2(3)	C212-B12-C112	113.8(2)
C262-C212-B12	119.8(2)	C312-B12-C112	101.0(2)
C222-C212-B12	127.4(2)	C412-B12-C112	113.5(2)
F222-C222-C232	115.1(2)		

E) Computational Details

All calculations were performed by using the program package Gaussian 16[8] and Amsterdam Density Functional[9] (ADF). The geometrical parameters of all stationary points were optimized by means of the density functional B3LYP[10] together with the dispersion correction with Becke-Johnson damping[11] (D3BJ) using Gaussian 16. The basis set def2-TZVP was applied. For all structures C1 symmetry was applied. Frequency calculations were carried out at each of the stationary points to verify the nature of the stationary point. It turned out that all products have no imaginary frequency. Natural bond orbital analysis was performed using the NBO[12] version 3.1 implemented in Gaussian 16. The bond energy analysis calculations[13] were carried out using Amsterdam Density Functional (ADF).

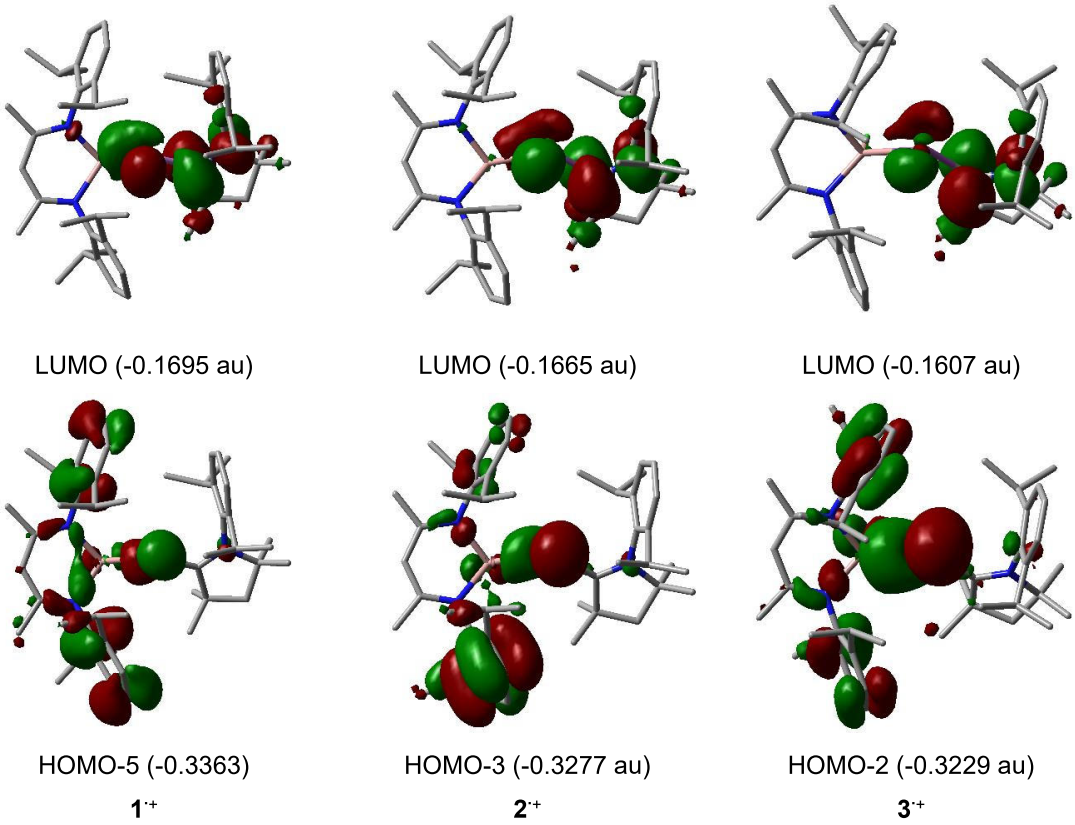


Figure S10. Selected orbitals (α electron) of **1**·+ (left), **2**·+ (middle), and **3**·+ (right) calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.03). Hydrogen atoms are omitted for clarity. HOMO-5 of **1**·+, HOMO-3 of **2**·+, and HOMO-2 of **3**·+ represent the electron lone pair at the pnictogen center E.

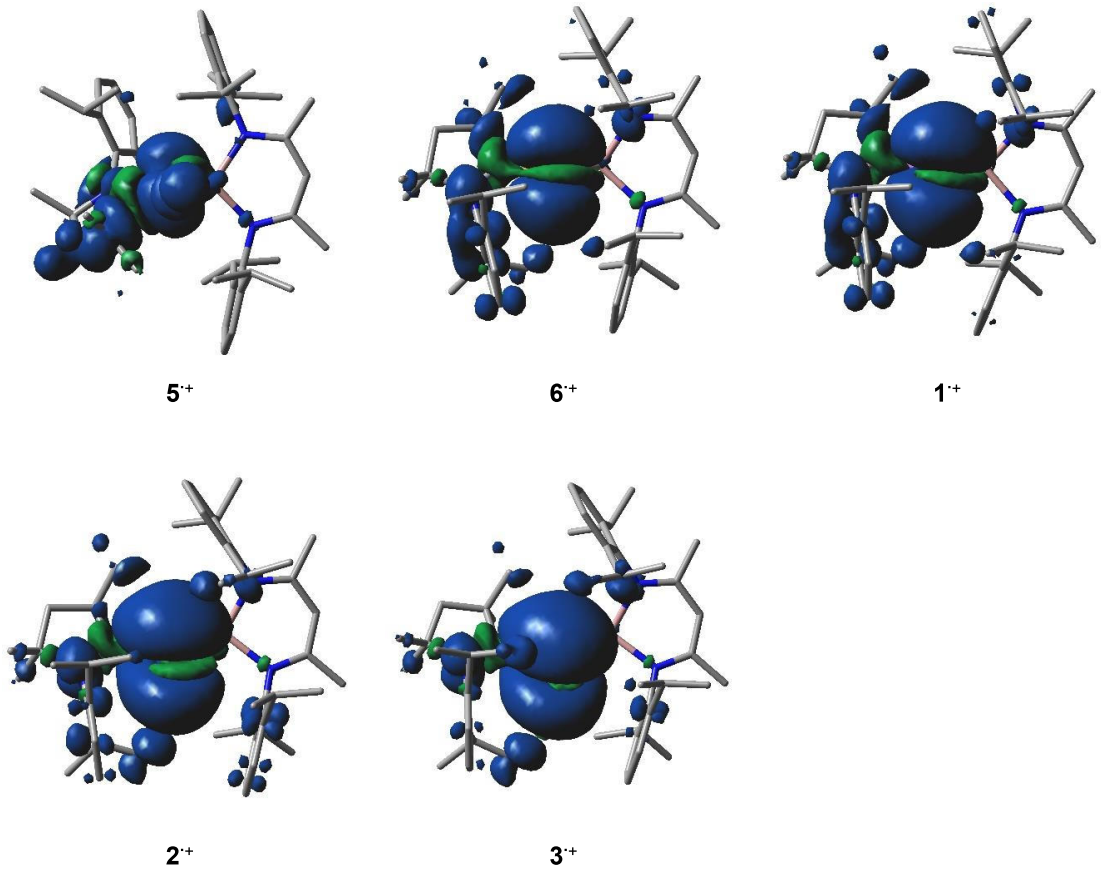


Figure S11. Spin density plots for **1**$^{\cdot+}$, **2**$^{\cdot+}$, **3**$^{\cdot+}$, **5**$^{\cdot+}$ and **6**$^{\cdot+}$ calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.0004). Hydrogen atoms are omitted for clarity.

Table S13. NBO charges [e] of the Ga-E-C-N units calculated by means of B3LYP-D3BJ/def2-TZVP.

Compound	E	Ga	E	C	N
IV	N	1.729	-1.054	0.518	-0.462
V	P	1.355	-0.226	0.007	-0.443
I	As	1.301	-0.187	0.045	-0.449
II	Sb	1.170	0.030	-0.003	-0.457
III	Bi	1.134	0.051	0.047	-0.466
5$^{\bullet+}$	N	1.716	-0.507	0.446	-0.384
6$^{\bullet+}$	P	1.428	0.156	0.091	-0.342
1$^{\bullet+}$	As	1.380	0.186	0.157	-0.357
2$^{\bullet+}$	Sb	1.227	0.477	0.090	-0.371
3$^{\bullet+}$	Bi	1.169	0.544	0.129	-0.379

Table S14. Wiberg Bond Index in the Ga-E-C-N units calculated by means of B3LYP-D3BJ/def2-TZVP.

Compound	E	Ga–E	E–C	C–N
IV	N	0.5769	1.7519	1.1200
V	P	0.9355	1.5284	1.2012
I	As	0.9697	1.4548	1.2246
II	Sb	1.0283	1.2880	1.2488
III	Bi	1.0316	1.2220	1.2646
5$^{\bullet+}$	N	0.4155	1.6170	1.2841
6$^{\bullet+}$	P	0.7230	1.1319	1.4669
1$^{\bullet+}$	As	0.7689	1.0350	1.4948
2$^{\bullet+}$	Sb	0.8865	0.8004	1.5171
3$^{\bullet+}$	Bi	0.9155	0.7198	1.5350

Table S15. Mayer Bond Index in the Ga-E-C-N units calculated by means of B3LYP-D3BJ/def2-TZVP.

Compound	E	Ga–E	E–C	C–N
IV	N	1.150	1.730	1.177
V	P	1.043	1.672	1.255
I	As	1.026	1.633	1.271
II	Sb	1.045	1.313	1.299
III	Bi	1.020	1.285	1.315
5$^{\bullet+}$	N	0.833	1.299	1.375
6$^{\bullet+}$	P	0.791	1.210	1.523
1$^{\bullet+}$	As	0.803	1.127	1.551
2$^{\bullet+}$	Sb	0.888	0.927	1.600
3$^{\bullet+}$	Bi	0.887	0.839	1.629

Table S16. Analysis of the total bonding energy calculated by means of B3LYP-D3BJ/TZP. The bond energy is computed as an energy difference between molecule and fragments. The total bonding energy (ΔE) consists of the Pauli repulsion (ΔE_{Pauli}), the electrostatic interaction (ΔV_{elstat}), orbital interactions (ΔE_{oi}) and the dispersion energy (ΔE_{Disp}). The values are given in kcal/mol.

Compound	E	bond break	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}	ΔE_{Disp}	ΔE
IV	N	homolytic	1091.92	-360.14	-920.63	-32.99	-221.85
		heterolytic	898.26	-380.88	-680.25	-32.99	-195.87
V	P	homolytic	576.68	-234.35	-469.94	-30.51	-158.12
		heterolytic	415.38	-249.48	-261.76	-30.51	-126.37
I	As	homolytic	506.04	-218.63	-400.27	-29.54	-142.41
		heterolytic	368.81	-240.65	-209.13	-29.54	-110.51
II	Sb	homolytic	416.91	-190.81	-323.04	-27.37	-124.31
		heterolytic	309.86	-215.18	-158.60	-27.37	-91.29
III	Bi	homolytic	376.72	-170.53	-295.07	-26.81	-115.68
		heterolytic	248.93	-187.08	-117.34	-26.81	-82.30
5$^{\bullet+}$	N	homolytic	128.56	-78.23	-123.04	-27.70	-100.41
		heterolytic	238.13	-108.70	-220.08	-27.70	-118.34
6$^{\bullet+}$	P	homolytic	266.72	-151.81	-196.85	-33.43	-115.37
		heterolytic	445.24	-245.10	-295.68	-33.43	-128.96
1$^{\bullet+}$	As	homolytic	218.12	-130.88	-161.63	-32.51	-106.91
		heterolytic	351.96	-218.60	-220.08	-32.51	-119.24
2$^{\bullet+}$	Sb	homolytic	171.66	-107.26	-134.31	-29.37	-99.27
		heterolytic	262.80	-184.78	-154.62	-29.37	-105.97
3$^{\bullet+}$	Bi	homolytic	140.47	-90.33	-118.78	-28.13	-96.77
		heterolytic	197.69	-157.19	-108.79	-28.13	-96.42

F) Cartesian Coordinates and Absolute Energies for All Calculated Compounds

Table S17. Absolute energies [au] calculated by means B3LYP-D3BJ/def2-TZVP.

	E
IV	-4515.989361
V	-4802.591021
I	-6697.135165
II	-4701.548809
III	-4675.923625
$\mathbf{5}^{\bullet+}$	-4515.750552
$\mathbf{6}^{\bullet+}$	-4802.376374
$\mathbf{1}^{\bullet+}$	-6696.928659
$\mathbf{2}^{\bullet+}$	-4701.356089
$\mathbf{3}^{\bullet+}$	-4675.739184

Cartesian coordinates of the optimized geometry for **IV** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	2.33302200	-1.96753100	-0.62422500
C	1.45763000	-1.07719000	-1.21989500
Ga	-0.81431700	0.70882300	-0.94029300
N	-0.70055800	2.47351500	-0.03425100
N	-2.61374900	0.27660900	-0.25005000
Cl	-1.36898000	1.34872800	-3.04345100
C	-3.47635900	1.30558600	-0.30393400
C	-3.09546000	2.64045400	-0.21951600
H	-3.89677900	3.36141400	-0.25111900
C	-1.82902200	3.15586000	0.10612000
C	-4.94818300	1.02581200	-0.47247200
H	-5.53125000	1.93669400	-0.36375800
H	-5.31741300	0.28024500	0.22668800
H	-5.10789000	0.62788000	-1.47709200
C	-1.81184700	4.53477100	0.71400800
H	-2.69746900	5.08895000	0.41048500
H	-0.92071600	5.09875300	0.45549500
H	-1.83315700	4.44255200	1.80275000
C	-3.15298500	-0.99238800	0.15720400
C	-3.43676500	-1.99741300	-0.77727400
C	-4.09971000	-3.14533800	-0.34137700
H	-4.33802100	-3.92037200	-1.05793900
C	-4.46865200	-3.30605900	0.98136200
H	-4.99654800	-4.19689100	1.29689300
C	-4.13102200	-2.33049900	1.90644700
H	-4.38588600	-2.47746000	2.94702700
C	-3.45844800	-1.17496600	1.52341000
C	-3.05228900	-1.89183000	-2.23806600
H	-2.53810000	-0.94680300	-2.39405300
C	-4.27510100	-1.88602300	-3.16252700
H	-4.96082400	-1.07712600	-2.90895400
H	-4.82850300	-2.82525600	-3.09815400
H	-3.96235900	-1.74869500	-4.19914800
C	-2.08969100	-3.02325100	-2.61639300
H	-1.76929000	-2.92011500	-3.65331100
H	-2.56491100	-3.99990500	-2.50673700
H	-1.20500700	-3.00599300	-1.97974900
C	-3.06141100	-0.15595900	2.57976200
H	-2.27585800	0.45825000	2.14439200
C	-4.21699900	0.77401000	2.97499900
H	-3.89281800	1.46276500	3.75821000
H	-5.05964500	0.19663700	3.36242500
H	-4.57043200	1.37045600	2.13737800
C	-2.48858600	-0.81823100	3.83781200
H	-2.10024300	-0.05463800	4.51323800
H	-1.67902600	-1.50405200	3.59575900
H	-3.25282600	-1.37276800	4.38496600

C	0.51433000	3.06795400	0.45530100
C	1.33946400	3.78350000	-0.43031900
C	2.44604200	4.44461800	0.09921800
H	3.09140000	5.00959200	-0.55817100
C	2.73719600	4.39170300	1.45285000
H	3.60073600	4.91582600	1.84215000
C	1.93701200	3.64575700	2.30078500
H	2.18848800	3.58126900	3.35060900
C	0.81912200	2.96774500	1.82158300
C	1.03484000	3.86703500	-1.91611200
H	0.54388500	2.94037600	-2.20313000
C	2.29203700	4.00497000	-2.77848800
H	2.03401000	3.84533800	-3.82629600
H	3.05353500	3.27609200	-2.50267900
H	2.73153600	5.00161600	-2.70001500
C	0.05051000	4.99590200	-2.25282200
H	0.42677400	5.95925800	-1.89995500
H	-0.92949200	4.82465200	-1.81368400
H	-0.08593500	5.05724500	-3.33381700
C	0.00107600	2.09788900	2.75534200
H	-0.97029600	1.93802700	2.29174100
C	0.67580000	0.72759600	2.90765400
H	1.68015000	0.84002800	3.31761400
H	0.76264000	0.21404300	1.95012900
H	0.10915900	0.09059100	3.58555600
C	-0.25403400	2.74463700	4.11905200
H	-0.68372300	3.74303600	4.01732300
H	0.66191900	2.83253100	4.70580800
H	-0.94946500	2.13283600	4.69608200
C	1.88507400	-0.95271900	-2.70643400
C	3.14858200	-1.83049600	-2.79456400
H	3.21138500	-2.36690400	-3.74165600
H	4.03888900	-1.20433500	-2.71289400
C	3.10643800	-2.78503800	-1.59456100
C	2.23278500	0.50830600	-3.00139100
H	1.34143500	1.12820900	-3.02502000
H	2.71484300	0.58309600	-3.97891500
H	2.91788500	0.90583500	-2.25160800
C	0.80645400	-1.43214600	-3.68007100
H	-0.12328600	-0.88803200	-3.54263500
H	0.60876000	-2.49590200	-3.57195700
H	1.14263100	-1.25745800	-4.70476600
C	4.50124000	-3.15173400	-1.09721200
H	5.12068300	-2.27650500	-0.92466300
H	4.99285100	-3.76601700	-1.85315600
H	4.45311900	-3.72915900	-0.17360900
C	2.37082400	-4.09096500	-1.93331400
H	1.34020800	-3.90997400	-2.23144700
H	2.36303200	-4.76450800	-1.07841100
H	2.87941300	-4.59796900	-2.75538400
C	2.49477000	-2.06663000	0.79109000
C	3.47833000	-1.26717100	1.40495700
C	3.65763700	-1.37337600	2.78087400
H	4.40555700	-0.76313700	3.26942300
C	2.88482200	-2.23894200	3.53889100
H	3.03701000	-2.30708400	4.60878600
C	1.90989000	-3.00532000	2.92531200
H	1.29524200	-3.66540600	3.52348200
C	1.69461100	-2.93122000	1.54943200
C	4.30393900	-0.26228500	0.62231100
H	4.19021900	-0.49316400	-0.43359300
C	3.76676600	1.15550000	0.82406400
H	4.33332400	1.87106000	0.22555300
H	3.84652100	1.45800400	1.86848000
H	2.72021200	1.22410300	0.53663400
C	5.79747400	-0.32771200	0.95682300
H	6.36081100	0.32055900	0.28243600
H	6.18918200	-1.34157800	0.86435300
H	5.99605300	0.01275100	1.97450900

C	0.56912600	-3.73455500	0.93551700
H	0.57732200	-3.54629000	-0.13465100
C	-0.77740000	-3.24455700	1.46564900
H	-0.86935300	-2.17351500	1.30866300
H	-0.87970500	-3.44947800	2.53310700
H	-1.60226200	-3.73658000	0.95103800
C	0.73252700	-5.24078500	1.16253100
H	0.65251200	-5.49047700	2.22241700
H	1.70058000	-5.60216500	0.81265800
H	-0.04876300	-5.79056000	0.63352400
N	0.53779000	-0.48188300	-0.57141800

Cartesian coordinates of the optimized geometry for **V** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	-3.23786400	-0.48139600	-0.90948000
C	-1.91256100	-0.43108300	-1.21675800
P	-0.77628700	0.04310300	0.00598100
Ga	1.40341700	0.15817100	-0.73810200
N	2.66349300	-1.15828800	0.08807300
N	2.20165400	1.73818700	0.16647600
Cl	2.24512300	0.35275100	-2.82405700
C	3.50905600	1.73477000	0.41902900
C	4.29903200	0.58209000	0.42063300
H	5.34827500	0.73661000	0.62029400
C	3.88327200	-0.75696200	0.42197200
C	4.20075900	3.03297600	0.74798900
H	5.22376100	2.85509400	1.06895900
H	3.67139500	3.57984100	1.52645200
H	4.21707900	3.67619400	-0.13265700
C	4.91694600	-1.74852200	0.89995200
H	5.86495200	-1.55033600	0.39944700
H	4.62741400	-2.77855500	0.72167600
H	5.08319200	-1.61679500	1.96946100
C	1.44591500	2.93169000	0.43683700
C	1.34374300	3.94481600	-0.53029400
C	0.67479800	5.12072800	-0.19352000
H	0.59100900	5.90993700	-0.92901100
C	0.12293400	5.29779000	1.06231200
H	-0.38206700	6.22247200	1.31120100
C	0.19465300	4.27294300	1.99156300
H	-0.27040000	4.40485200	2.95782000
C	0.83221400	3.07089700	1.69639600
C	1.89385300	3.78521900	-1.93329000
H	2.49689300	2.88108400	-1.96328300
C	2.78443300	4.95391600	-2.36805200
H	3.59884900	5.12686800	-1.66269300
H	2.21927300	5.88398800	-2.45349000
H	3.22304800	4.74429700	-3.34543600
C	0.73719500	3.59098500	-2.92222400
H	1.11712500	3.34542400	-3.91501700
H	0.13426400	4.49935800	-2.99567400
H	0.08457400	2.78123700	-2.60063500
C	0.85498500	1.95328600	2.72543400
H	0.97149800	1.01822500	2.17962900
C	2.05117200	2.07822200	3.67797600
H	2.03833200	1.27023900	4.41256200
H	2.01828800	3.02673600	4.21900500
H	2.99924100	2.02574200	3.14370700
C	-0.45714100	1.85758800	3.50846400
H	-0.43543500	0.99310800	4.16991600
H	-1.30665200	1.74142300	2.83701600
H	-0.62417700	2.73642900	4.13342800
C	2.23489800	-2.49742900	0.38091200
C	2.18117600	-3.45947400	-0.64845500
C	1.73188200	-4.73835800	-0.32835600
H	1.68372500	-5.49224900	-1.10059400
C	1.34833200	-5.06922700	0.96247800

H	0.99972200	-6.06956800	1.18580600
C	1.41364400	-4.11589900	1.96065100
H	1.11149000	-4.37567800	2.96661500
C	1.85526900	-2.82057400	1.69499400
C	2.64335400	-3.14598600	-2.06171600
H	2.34619200	-2.12594700	-2.29120700
C	2.02498100	-4.05420400	-3.12681700
H	2.23360600	-3.64444700	-4.11606500
H	0.94471700	-4.13773400	-3.01718500
H	2.44793100	-5.06097200	-3.09613700
C	4.17328600	-3.18541100	-2.18968000
H	4.56573600	-4.15514800	-1.87402200
H	4.64998900	-2.41025500	-1.59631900
H	4.46137500	-3.02255400	-3.22978000
C	1.92483500	-1.82906500	2.84383900
H	2.29118900	-0.87996800	2.45640800
C	0.54502900	-1.57595500	3.45775200
H	0.10237000	-2.50305100	3.82478600
H	-0.14056100	-1.13810600	2.73430400
H	0.63380100	-0.89519100	4.30496700
C	2.90255400	-2.29883400	3.93063700
H	3.88214100	-2.54006400	3.51957000
H	2.52809000	-3.19228600	4.43401200
H	3.03005600	-1.52070300	4.68586100
C	-1.74721300	-0.84300200	-2.68114000
C	-3.14304800	-1.39950100	-3.04160700
H	-3.40741100	-1.19431000	-4.07847100
H	-3.13995300	-2.48292600	-2.91017300
C	-4.14314700	-0.78351800	-2.06065900
C	-0.70213800	-1.94507900	-2.84855600
H	0.30260800	-1.56612500	-2.69759300
H	-0.75167200	-2.34386400	-3.86443100
H	-0.87731700	-2.75993400	-2.14567600
C	-1.36708700	0.36268400	-3.55212300
H	-0.36880200	0.71297800	-3.30772300
H	-2.06143500	1.19203900	-3.42714000
H	-1.36971000	0.06962500	-4.60432500
C	-5.25830600	-1.75405100	-1.68207500
H	-4.86976900	-2.72262500	-1.38139200
H	-5.90425900	-1.90529700	-2.54786800
H	-5.87008400	-1.35591000	-0.87199600
C	-4.79666600	0.48351700	-2.62666300
H	-4.06384800	1.23749500	-2.90243500
H	-5.48875500	0.91974000	-1.90973600
H	-5.36386100	0.22094900	-3.52100600
C	-3.69306200	-0.27467300	0.43625900
C	-3.74111400	-1.38478500	1.30172700
C	-4.12872400	-1.17421200	2.62212900
H	-4.16818200	-2.01399000	3.30318600
C	-4.44795100	0.09247200	3.08303300
H	-4.74342500	0.23612600	4.11466500
C	-4.37323700	1.17597900	2.22528000
H	-4.59973800	2.16644300	2.59715500
C	-3.98508700	1.02108200	0.89561200
C	-3.34756700	-2.78751200	0.86997400
H	-3.16313600	-2.76745700	-0.20148400
C	-2.03947100	-3.23701900	1.52960900
H	-1.76407600	-4.23500200	1.18370200
H	-2.13704400	-3.27137200	2.61651900
H	-1.22790600	-2.55887900	1.27961300
C	-4.46230000	-3.80480800	1.14397000
H	-4.19851400	-4.77585300	0.71972100
H	-5.41456400	-3.49064800	0.71642400
H	-4.61176600	-3.94628000	2.21575500
C	-3.84979600	2.25883000	0.02851900
H	-3.53682000	1.93789700	-0.96046400
C	-2.75995000	3.20072100	0.55088600
H	-1.80041900	2.69287000	0.59869900
H	-2.99975100	3.57776500	1.54692000

H	-2.65251800	4.06044100	-0.11298300
C	-5.18288800	3.00633400	-0.10259600
H	-5.47975400	3.44497900	0.85198300
H	-5.99127600	2.34975500	-0.42593300
H	-5.09231000	3.81936300	-0.82571500

Cartesian coordinates of the optimized geometry for **I** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	-3.30805500	-0.35956900	-0.91070700
C	-1.99028500	-0.36365300	-1.21247300
Ga	1.48232200	0.10390500	-0.72524000
N	2.69846300	-1.27310600	0.07156400
N	2.38076400	1.64303900	0.16010600
Cl	2.26619200	0.26162100	-2.83848600
C	3.68896700	1.57509500	0.39558700
C	4.42041100	0.38415300	0.38909900
H	5.47832100	0.48638900	0.57707600
C	3.93990500	-0.93366300	0.39121100
C	4.44873600	2.83837700	0.70991600
H	5.45392600	2.61014600	1.05468300
H	3.93745100	3.43412400	1.46392500
H	4.51956900	3.45653000	-0.18611600
C	4.93180300	-1.97739100	0.84677700
H	5.86797300	-1.84551600	0.30350300
H	4.57394500	-2.99072300	0.69894200
H	5.15152200	-1.83766600	1.90545000
C	1.67723900	2.86731800	0.43029000
C	1.60619500	3.87890800	-0.54094400
C	0.96207700	5.07161600	-0.21387500
H	0.90232500	5.85920400	-0.95349900
C	0.40061400	5.26512500	1.03482700
H	-0.08889100	6.20052300	1.27448300
C	0.44452800	4.24392800	1.97024700
H	-0.02589900	4.39070300	2.93157000
C	1.06223800	3.02875600	1.68744900
C	2.15927400	3.70315800	-1.94097800
H	2.72210000	2.77345400	-1.97252700
C	3.10250000	4.83617800	-2.35954700
H	3.91813000	4.96863100	-1.64696200
H	2.57748400	5.78995600	-2.43993200
H	3.53867600	4.61686200	-3.33593600
C	1.00372200	3.56682700	-2.94093700
H	1.38116700	3.30998700	-3.93176900
H	0.44274000	4.50168200	-3.01447000
H	0.31330800	2.78480700	-2.63007300
C	1.06408300	1.92003000	2.72664700
H	1.12314000	0.97545500	2.18739600
C	2.29297000	1.99533700	3.64236100
H	2.26167900	1.19590000	4.38580500
H	2.32159000	2.94956900	4.17338400
H	3.22121800	1.89079100	3.08230100
C	-0.22375700	1.88985900	3.55349400
H	-0.22758100	1.01772600	4.20521400
H	-1.10224600	1.83078100	2.91199900
H	-0.31716600	2.76950900	4.19267500
C	2.19992100	-2.58873900	0.36032800
C	2.08175900	-3.53866800	-0.67494800
C	1.56025200	-4.79124400	-0.36050600
H	1.46273700	-5.53525600	-1.13767200
C	1.16368500	-5.10749400	0.92993600
H	0.75826900	-6.08718400	1.14894700
C	1.28722600	-4.16511400	1.93301800
H	0.97322000	-4.41275500	2.93836800
C	1.80314500	-2.89623900	1.67333200
C	2.54288800	-3.23958200	-2.09140400
H	2.30002400	-2.20244700	-2.30834300
C	1.85882400	-4.10021800	-3.15579600

H	2.07902400	-3.69436200	-4.14417000
H	0.77693300	-4.11989400	-3.03265400
H	2.22109100	-5.13073600	-3.13919800
C	4.06607000	-3.36535400	-2.24013900
H	4.40532600	-4.36089100	-1.94357700
H	4.59393100	-2.62876900	-1.64098500
H	4.35092600	-3.20351100	-3.28132200
C	1.93138800	-1.91708800	2.82769100
H	2.31770200	-0.97675200	2.43798200
C	0.57651700	-1.62722300	3.48019900
H	0.11892300	-2.54139600	3.86128000
H	-0.11694700	-1.17161900	2.77528300
H	0.70689100	-0.94845500	4.32381600
C	2.92135600	-2.42718300	3.88495200
H	3.88464400	-2.68687800	3.44800800
H	2.53468800	-3.31871700	4.38265200
H	3.08606800	-1.66425000	4.64852000
C	-1.82345000	-0.75142500	-2.67731900
C	-3.23741300	-1.24491200	-3.06271600
H	-3.48770400	-0.99804200	-4.09385500
H	-3.27504600	-2.33110900	-2.96501400
C	-4.22185900	-0.62050200	-2.06967200
C	-0.81637200	-1.88737000	-2.85739700
H	0.19787200	-1.55094000	-2.67105600
H	-0.85796600	-2.25301600	-3.88604300
H	-1.03764200	-2.71546200	-2.18367700
C	-1.38573200	0.45921100	-3.51510700
H	-0.37909900	0.76526900	-3.24590900
H	-2.05066300	1.31108500	-3.38014500
H	-1.38222900	0.19039600	-4.57373100
C	-5.35876000	-1.56962100	-1.70474800
H	-4.99051600	-2.54956900	-1.41529100
H	-6.00609900	-1.69656800	-2.57342400
H	-5.96325500	-1.16825800	-0.89084300
C	-4.83899500	0.67429300	-2.60928400
H	-4.08417600	1.40870300	-2.87891400
H	-5.51112800	1.11986900	-1.87950800
H	-5.42110800	0.44418000	-3.50289400
C	-3.76323800	-0.13486000	0.43383900
C	-3.86397600	-1.24280800	1.29819800
C	-4.26544100	-1.01774300	2.61217200
H	-4.34856300	-1.85598500	3.29105400
C	-4.54118900	0.25982400	3.07007800
H	-4.84898200	0.41397200	4.09656200
C	-4.40336300	1.34068500	2.21710700
H	-4.59143900	2.33927700	2.58835400
C	-4.00106100	1.17292500	0.89312900
C	-3.51027100	-2.66036700	0.87924100
H	-3.28559100	-2.64943800	-0.18506500
C	-2.24690800	-3.16091400	1.59069000
H	-1.99829700	-4.16910100	1.25380700
H	-2.38988800	-3.19222500	2.67284600
H	-1.39919200	-2.51582600	1.37449700
C	-4.67299700	-3.63324900	1.11479200
H	-4.43261700	-4.61456500	0.70047400
H	-5.59764400	-3.28393800	0.65559000
H	-4.86347700	-3.76648200	2.18109400
C	-3.79302400	2.41078800	0.03909100
H	-3.46805700	2.08603100	-0.94527800
C	-2.68110100	3.30654500	0.59896200
H	-1.74274500	2.76282600	0.67131900
H	-2.93655300	3.68865500	1.58932400
H	-2.52155500	4.16405100	-0.05737100
C	-5.09005000	3.21583600	-0.11598600
H	-5.38672700	3.66232100	0.83494700
H	-5.91997200	2.59797100	-0.45945400
H	-4.94877500	4.02781500	-0.83205600
As	-0.76239000	0.07512400	0.12122000

Cartesian coordinates of the optimized geometry for **II** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	-3.47072500	-0.25458500	-0.90460400
C	-2.15566700	-0.29366900	-1.18076500
Ga	1.59261700	0.06042200	-0.71250900
N	2.79964800	-1.37272300	0.00846300
N	2.62702800	1.55677400	0.10540500
Cl	2.23883900	0.18501200	-2.87910000
C	3.94099500	1.42848800	0.26367200
C	4.61214400	0.20293100	0.22475800
H	5.68277600	0.25475900	0.35297000
C	4.07147200	-1.09170700	0.25478600
C	4.77853500	2.65600000	0.51553800
H	5.76733200	2.38464600	0.87670800
H	4.30444500	3.32448600	1.23136500
H	4.89181600	3.21429400	-0.41517600
C	5.04240400	-2.18194500	0.64321600
H	5.92615400	-2.11901700	0.00724800
H	4.61466900	-3.17525600	0.55821800
H	5.37474400	-2.03063400	1.67025600
C	1.97636000	2.80356800	0.39673200
C	1.87657700	3.80526300	-0.58160500
C	1.23288100	4.99768600	-0.25063400
H	1.15044000	5.77691400	-0.99698500
C	0.69369200	5.19810700	1.00609000
H	0.19696200	6.12979700	1.24533600
C	0.77460700	4.19033400	1.95445500
H	0.32761400	4.34595100	2.92524900
C	1.40250500	2.98045600	1.67279400
C	2.39707300	3.62501100	-1.99381500
H	2.92305300	2.67480300	-2.04651800
C	3.37493500	4.73069100	-2.40823100
H	4.20471100	4.82242200	-1.70594300
H	2.88167300	5.70319500	-2.46238600
H	3.78807000	4.51447600	-3.39536000
C	1.22512200	3.54799500	-2.98087100
H	1.58187800	3.28972300	-3.97895200
H	0.70109000	4.50508300	-3.03758200
H	0.50819100	2.78897500	-2.67354300
C	1.45841500	1.88928300	2.72972500
H	1.42574800	0.93307100	2.20629300
C	2.77310500	1.91861300	3.52122100
H	2.77294100	1.13560600	4.28267700
H	2.89732100	2.87994100	4.02480200
H	3.63736600	1.75588100	2.88012800
C	0.26502500	1.92725600	3.68667100
H	0.27589700	1.04758300	4.32842700
H	-0.67976200	1.93427900	3.14327800
H	0.29752500	2.80237600	4.33825700
C	2.25275600	-2.66597700	0.31162800
C	2.04162000	-3.60038800	-0.72317100
C	1.47244400	-4.82836200	-0.39452900
H	1.30522300	-5.55978900	-1.17181300
C	1.11170200	-5.13417300	0.90861500
H	0.66787900	-6.09449400	1.13872600
C	1.31763500	-4.20433100	1.91007200
H	1.02985700	-4.44299700	2.92529900
C	1.88527000	-2.96059700	1.63654900
C	2.44264700	-3.30916700	-2.15910100
H	2.24682800	-2.25735200	-2.35135800
C	1.65164900	-4.11370700	-3.19299100
H	1.83824200	-3.70521500	-4.18721000
H	0.57924400	-4.07348900	-3.00760200
H	1.95416400	-5.16337100	-3.21034000
C	3.94523800	-3.52014000	-2.39339300
H	4.24108700	-4.53859800	-2.12977600
H	4.54699600	-2.82620500	-1.81336000

H	4.18266700	-3.35712300	-3.44627000
C	2.10057100	-1.99376100	2.78816700
H	2.45849300	-1.05071400	2.37784900
C	0.80092200	-1.70888400	3.54738300
H	0.38586900	-2.62058700	3.97973800
H	0.04595400	-1.27153500	2.89541000
H	0.99191600	-1.01561800	4.36747600
C	3.16701300	-2.51597900	3.76193400
H	4.09871800	-2.75735600	3.25295600
H	2.82161700	-3.42188000	4.26432900
H	3.37973900	-1.76834500	4.52888400
C	-1.96397700	-0.65738000	-2.64535100
C	-3.38147800	-1.09998300	-3.07747700
H	-3.60210400	-0.81495000	-4.10546100
H	-3.45099700	-2.18705800	-3.01438100
C	-4.37108900	-0.47635900	-2.08847800
C	-0.98159700	-1.81660800	-2.82097900
H	0.03141500	-1.51555300	-2.57426600
H	-0.98493800	-2.14603800	-3.86258900
H	-1.25700900	-2.65988500	-2.18705200
C	-1.46476000	0.55753600	-3.44330500
H	-0.45862400	0.82674100	-3.13420900
H	-2.10822300	1.42614900	-3.30946900
H	-1.43439400	0.31124500	-4.50702400
C	-5.52901200	-1.41114100	-1.75979600
H	-5.17882400	-2.40058500	-1.48018500
H	-6.16188600	-1.51465400	-2.64220500
H	-6.14259500	-1.01409700	-0.95062300
C	-4.94807100	0.84258900	-2.60939700
H	-4.17134500	1.56771800	-2.83957200
H	-5.63061900	1.28227500	-1.88650600
H	-5.51062400	0.64691500	-3.52346200
C	-3.95291000	-0.03750200	0.43393900
C	-4.10105000	-1.15543400	1.28090300
C	-4.55525600	-0.94116000	2.57958400
H	-4.67909300	-1.78742800	3.24189300
C	-4.83345800	0.33316700	3.04353500
H	-5.18549500	0.47756500	4.05710200
C	-4.63676800	1.42315800	2.21490300
H	-4.82233300	2.41934500	2.59335900
C	-4.18047200	1.26920200	0.90650500
C	-3.74870300	-2.57600000	0.86830500
H	-3.44776800	-2.55910300	-0.17739400
C	-2.55447700	-3.11643000	1.66883000
H	-2.29053600	-4.11701300	1.32046100
H	-2.79218000	-3.18194400	2.73271300
H	-1.68239500	-2.47752900	1.54892000
C	-4.94530700	-3.52652200	1.01370300
H	-4.69921300	-4.50727000	0.60151200
H	-5.83210900	-3.15237100	0.50345900
H	-5.20493500	-3.66917300	2.06403700
C	-3.91280600	2.52301300	0.09128200
H	-3.52459500	2.21691700	-0.87685500
C	-2.84204200	3.41021700	0.74371400
H	-1.91328300	2.86352300	0.89079500
H	-3.17826300	3.79153600	1.71004900
H	-2.62710500	4.26794100	0.10340700
C	-5.19385100	3.34116600	-0.12535000
H	-5.53608900	3.77878600	0.81428800
H	-6.01052500	2.73707600	-0.51930200
H	-5.00715200	4.16041900	-0.82238200
Sb	-0.78140700	0.14609300	0.32405900

Cartesian coordinates of the optimized geometry for **III** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

N	-3.51209400	-0.02548700	-0.92887700
C	-2.20341400	-0.08910100	-1.20723800

Ga	1.66288900	-0.04870900	-0.71991300
N	2.68678300	-1.62765300	0.00581800
N	2.92210400	1.29893800	0.04440700
Cl	2.28945700	-0.07612200	-2.90283500
C	4.21016200	0.99636500	0.17270400
C	4.70442000	-0.31007800	0.14960900
H	5.77459600	-0.40505100	0.25352000
C	3.98996700	-1.51620100	0.22275200
C	5.21152300	2.10409500	0.37701700
H	6.17787300	1.70478600	0.67437900
H	4.87060800	2.81594300	1.12677900
H	5.33652100	2.65934000	-0.55380200
C	4.81141700	-2.71805400	0.62885600
H	5.71671900	-2.75727700	0.02268500
H	4.27226000	-3.65325200	0.52313400
H	5.12465600	-2.61328000	1.66791800
C	2.45690100	2.62663600	0.32601500
C	2.46884000	3.61691100	-0.66870500
C	2.01057700	4.89291900	-0.34213400
H	2.01555100	5.66519600	-1.10007400
C	1.54132000	5.18538800	0.92506300
H	1.19087500	6.18220200	1.16090800
C	1.50171900	4.18897400	1.88826500
H	1.10753900	4.41980600	2.86713500
C	1.94415600	2.89862500	1.61078000
C	2.90497100	3.33597200	-2.09285400
H	3.30967600	2.32750700	-2.13444500
C	3.99118500	4.30063200	-2.58185700
H	4.85485400	4.31005300	-1.91504700
H	3.61869900	5.32453000	-2.65177800
H	4.33329500	4.00558800	-3.57565300
C	1.68968500	3.37319900	-3.02915400
H	1.97157300	3.05338400	-4.03332100
H	1.27722900	4.38324500	-3.08933700
H	0.90425100	2.70851000	-2.67288200
C	1.86193300	1.81753300	2.67671200
H	1.66988700	0.87449400	2.16219800
C	3.18522400	1.64707200	3.43492200
H	3.08332700	0.87970700	4.20539700
H	3.47010900	2.58150500	3.92363100
H	3.99590400	1.34629200	2.77434100
C	0.71527600	2.04227300	3.66490700
H	0.60132700	1.16984100	4.30654200
H	-0.23115200	2.20599900	3.14893700
H	0.90431200	2.89903900	4.31422800
C	1.99614500	-2.84376100	0.33468400
C	1.68547000	-3.77311900	-0.67996700
C	1.01472600	-4.93951600	-0.31925400
H	0.77269300	-5.66796400	-1.07933300
C	0.65037100	-5.19000600	0.99467000
H	0.12960500	-6.10436500	1.24945600
C	0.94799400	-4.26195200	1.97407400
H	0.65325700	-4.45422900	2.99719800
C	1.61833400	-3.07830100	1.66834200
C	2.08718100	-3.54511500	-2.12768000
H	1.96376500	-2.48660600	-2.34208300
C	1.22537300	-4.31523000	-3.13083300
H	1.42476100	-3.94321800	-4.13677400
H	0.16125600	-4.19622200	-2.93181300
H	1.45380400	-5.38366800	-3.12771200
C	3.56690300	-3.86641700	-2.38229500
H	3.80101300	-4.89150600	-2.08451100
H	4.22683000	-3.19083300	-1.84587700
H	3.78927700	-3.76062800	-3.44562100
C	1.92619900	-2.10931900	2.79665500
H	2.38563100	-1.22175300	2.36494000
C	0.65319700	-1.66977000	3.52687700
H	0.13810500	-2.52230100	3.97245200
H	-0.04111400	-1.17353900	2.84948100

H	0.90243300	-0.97920200	4.33347300
C	2.92121200	-2.71105500	3.79895600
H	3.82894600	-3.06079700	3.30972300
H	2.47960300	-3.56196300	4.32161100
H	3.20157900	-1.96776800	4.54814400
C	-2.01688300	-0.52428600	-2.65133400
C	-3.45282000	-0.90668600	-3.08773300
H	-3.65111100	-0.63511700	-4.12376600
H	-3.57944900	-1.98690600	-2.99984500
C	-4.41468600	-0.20767700	-2.12171200
C	-1.10557900	-1.75131700	-2.73970400
H	-0.08105300	-1.49828500	-2.48737800
H	-1.10977200	-2.13757200	-3.76136600
H	-1.44390400	-2.54010400	-2.06720500
C	-1.42283600	0.60876200	-3.50202100
H	-0.40890900	0.83352100	-3.18091500
H	-2.01261900	1.52190700	-3.43257800
H	-1.38404600	0.30026400	-4.54915300
C	-5.63754700	-1.05215300	-1.78911200
H	-5.36123500	-2.05763200	-1.48485300
H	-6.26719100	-1.12953300	-2.67643800
H	-6.23005700	-0.59738900	-0.99461300
C	-4.88226800	1.14143400	-2.67639000
H	-4.04699900	1.80955200	-2.87447700
H	-5.56746100	1.63545100	-1.99289000
H	-5.41156600	0.97315300	-3.61554700
C	-3.98590500	0.11499600	0.42365400
C	-4.08556800	-1.05363600	1.20885700
C	-4.50636600	-0.92399100	2.52887700
H	-4.58885100	-1.80856800	3.14601300
C	-4.80575300	0.31524800	3.07065200
H	-5.12944500	0.39384600	4.10073300
C	-4.67461400	1.45283200	2.29570400
H	-4.88775100	2.42012800	2.73041200
C	-4.25322600	1.38314500	0.96741400
C	-3.72960100	-2.44109900	0.69854800
H	-3.49243200	-2.36211200	-0.36025400
C	-2.48222700	-3.00167100	1.39542700
H	-2.22825600	-3.98061500	0.98548400
H	-2.65123800	-3.11963000	2.46792200
H	-1.62516000	-2.34680800	1.25444100
C	-4.90116700	-3.42108500	0.85222300
H	-4.66326000	-4.36944600	0.36627800
H	-5.82106300	-3.03219100	0.41570600
H	-5.10001500	-3.63359100	1.90391600
C	-4.08371800	2.68142200	0.19922900
H	-3.68232300	2.44011000	-0.78180000
C	-3.08085100	3.62716600	0.87488600
H	-2.10825300	3.15195500	0.99094800
H	-3.43273100	3.94400600	1.85851000
H	-2.94633400	4.52281000	0.26513500
C	-5.42973300	3.39879700	0.02026200
H	-5.79810200	3.77156000	0.97789100
H	-6.19631700	2.73973400	-0.38733200
H	-5.32065000	4.25407500	-0.64941600
Bi	-0.74178300	0.49526000	0.32468200

Cartesian coordinates of the optimized geometry for **5**$^{\bullet+}$ at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	-1.20063500	0.51601600	-0.18854800
C	1.12104800	-1.40143400	-1.08826200
Cl	-1.82335000	0.83713400	-2.25728900
N	-1.03899900	2.16295100	0.78880200
N	-2.57002900	-0.41344100	0.81859800
N	2.40191100	-1.72161100	-0.87653000
C	0.55107900	-2.23327800	-2.28553700
C	-1.98145800	2.45938200	1.69697000

C	-0.02336300	3.15796200	0.50983000
C	-3.22859000	0.25277300	1.77153800
C	-3.03594300	-1.72573300	0.42365900
C	2.87801300	-2.89680000	-1.70934800
C	3.35614900	-0.94552900	-0.11757200
C	1.55691500	-3.39622900	-2.30299700
C	-0.87031400	-2.73626100	-2.08702700
C	0.62830000	-1.37753100	-3.55826800
C	-2.95877100	1.57227500	2.14409500
C	-2.03259900	3.84567600	2.27997900
C	-0.23410700	4.13754100	-0.47246700
C	1.14097800	3.14488300	1.30322700
C	-4.35973400	-0.39973000	2.52453000
C	-4.10916400	-1.83371000	-0.47835200
C	-2.41843700	-2.86455800	0.97222900
C	3.51846200	-3.96567000	-0.83127300
C	3.90157000	-2.47033000	-2.76189900
C	3.98827600	0.14266400	-0.75063200
C	3.73310400	-1.36768900	1.16838500
H	1.16900000	-4.21045600	-1.69046400
H	1.68798000	-3.77545500	-3.31551900
H	-1.59693400	-1.92923700	-2.10775200
H	-0.98168400	-3.28352400	-1.15534700
H	-1.11313400	-3.41562000	-2.90534800
H	1.63875200	-1.05004500	-3.78487500
H	-0.01191500	-0.50355000	-3.48307700
H	0.27859900	-1.98504100	-4.39455000
H	-3.61371700	1.96481800	2.90618700
H	-2.56387400	4.49932400	1.58676800
H	-1.04685500	4.27280100	2.43297000
H	-2.57546300	3.84086900	3.22119400
C	0.74212200	5.12227000	-0.63281400
C	-1.46233400	4.19800300	-1.36205600
C	2.07088800	4.16245700	1.11219500
C	1.40225500	2.05879400	2.33819600
H	-5.28692800	0.13228100	2.31207000
H	-4.17858700	-0.30638500	3.59519400
H	-4.49415500	-1.44572500	2.27666500
C	-4.56488600	-3.11185300	-0.80209100
C	-4.81914900	-0.64200800	-1.09885300
C	-2.92876800	-4.11418000	0.62886000
C	-1.23864900	-2.76706000	1.92738500
H	4.42955300	-3.59962000	-0.36152200
H	3.78633500	-4.81530100	-1.45996000
H	2.83648600	-4.31883800	-0.06145400
H	4.77582400	-2.02405200	-2.29067100
H	3.50208700	-1.76771300	-3.48615300
H	4.23268500	-3.35612000	-3.30351200
C	5.08705600	0.71561700	-0.11464600
C	3.48815100	0.74159900	-2.05215700
C	4.84864500	-0.76945900	1.75045000
C	2.92944300	-2.37068900	1.97404800
H	0.59922100	5.88795800	-1.38287100
C	1.87403100	5.14833200	0.15757700
H	-2.10707300	3.35556300	-1.11940500
C	-2.27030300	5.48524300	-1.14527300
C	-1.06918600	4.07737400	-2.84110000
H	2.96895000	4.18622900	1.70971800
H	1.05828400	1.11488300	1.90226500
C	0.64320900	2.26063900	3.65861600
C	2.88919100	1.90606600	2.64906000
H	-5.39132100	-3.21747900	-1.49112400
C	-3.99364000	-4.24176400	-0.24845200
H	-4.27238000	0.26189500	-0.83681000
C	-6.25243700	-0.50016600	-0.56517000
C	-4.85049000	-0.73785700	-2.63025400
H	-2.48714700	-5.00642200	1.04611900
H	-0.65167700	-1.89227400	1.64042000
C	-1.69378000	-2.56094900	3.37874600

C	-0.31666800	-3.98689000	1.84310500
H	5.59881600	1.54283500	-0.58593200
C	5.54080500	0.23930000	1.10426600
H	2.81669100	0.02523300	-2.51442100
C	2.66530500	2.00592900	-1.77324800
C	4.60499300	1.03823700	-3.05704500
H	5.17075600	-1.09121600	2.73110400
H	2.20764300	-2.83353100	1.30519400
C	2.13595800	-1.64127400	3.06793400
C	3.78108200	-3.47721000	2.60420500
H	2.61040400	5.93064300	0.02784600
H	-1.69276100	6.36610000	-1.42930900
H	-2.57272500	5.61394900	-0.10650600
H	-3.17221300	5.46853000	-1.75917100
H	-0.51681700	4.95896300	-3.17028100
H	-1.96106300	3.99099200	-3.46318400
H	-0.44842400	3.20123300	-3.01788400
H	0.86455900	3.24294700	4.08017400
H	0.96176600	1.50841200	4.38231100
H	-0.43377700	2.16918800	3.55102200
H	3.26620400	2.76046800	3.21350700
H	3.48230700	1.80304900	1.74488000
H	3.05089000	1.02378100	3.26267900
H	-4.37341800	-5.22314900	-0.50041000
H	-6.72370600	0.38890100	-0.98717800
H	-6.28263800	-0.41710000	0.51938800
H	-6.85851200	-1.36306800	-0.84593600
H	-3.85902100	-0.91211400	-3.04259100
H	-5.23284200	0.19175700	-3.05391500
H	-5.50594200	-1.54441400	-2.96185100
H	-2.22857600	-1.62303700	3.50715000
H	-0.83342900	-2.54456800	4.04917600
H	-2.35255200	-3.37240200	3.69319800
H	0.56662700	-3.83038500	2.45685300
H	0.00780000	-4.18146200	0.81949800
H	-0.80288700	-4.88828500	2.21618500
H	6.41230000	0.68200500	1.56822700
H	2.25064400	2.40164800	-2.70154600
H	3.27997800	2.78310000	-1.31920100
H	1.84048700	1.80354900	-1.09338500
H	5.24685700	1.85104400	-2.71589900
H	4.17330500	1.34798700	-4.01000900
H	5.23481700	0.16698800	-3.23565700
H	1.45120800	-0.90742200	2.64438800
H	2.80748700	-1.12325100	3.75272600
H	1.55486900	-2.35112500	3.65643200
H	4.43010100	-3.08168000	3.38632700
H	4.41088500	-3.97935200	1.87206800
H	3.13710500	-4.22636200	3.06799100
N	0.41525500	-0.54132200	-0.46059400

Cartesian coordinates of the optimized geometry for **6**$^{\bullet+}$ at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	-1.35169100	0.42832800	-0.40959000
C	1.56189700	-1.66005500	-0.75047500
Cl	-1.56364900	0.65997800	-2.58042400
N	-1.57181600	2.19019400	0.41084200
N	-2.93397400	-0.42486000	0.33747300
N	2.87143500	-1.59798900	-0.78633300
C	1.05009800	-2.80995500	-1.60196000
C	-2.77128100	2.55967500	0.85801700
C	-0.45970800	3.10629300	0.43971700
C	-3.95015800	0.32803700	0.76937600
C	-3.00945100	-1.85970100	0.41386200
C	3.52203000	-2.66822000	-1.65877600
C	3.61708500	-0.57234200	-0.08200000
C	2.33845500	-3.62599100	-1.84094800

C	-0.01146900	-3.63373400	-0.87472200
C	0.47008900	-2.25488400	-2.91251800
C	-3.87891400	1.70893900	0.94071500
C	-3.00817700	3.97478200	1.31506300
C	-0.31483100	4.08442900	-0.55863400
C	0.47040100	2.97919400	1.48952200
C	-5.27125900	-0.31811300	1.08979500
C	-3.57942600	-2.60295700	-0.63233800
C	-2.48988100	-2.48412700	1.56589400
C	4.70067600	-3.32587400	-0.95642400
C	4.02498300	-2.06654700	-2.97074200
C	3.80110000	0.67359100	-0.70646800
C	4.09654900	-0.84136000	1.21500000
H	2.40299000	-4.42244200	-1.09894100
H	2.34441000	-4.08875600	-2.82588600
H	-0.91721600	-3.05853800	-0.70014200
H	0.35358900	-3.99772700	0.08549700
H	-0.28145000	-4.49546400	-1.48564700
H	1.19522100	-1.66759300	-3.47185900
H	-0.38832700	-1.61828400	-2.72758500
H	0.15380600	-3.09123100	-3.53674800
H	-4.78820900	2.17744100	1.28384100
H	-3.52886700	4.51868400	0.52526600
H	-2.08812600	4.50418500	1.53821000
H	-3.65077800	3.98083900	2.19318600
C	0.79690200	4.92406800	-0.48909000
C	-1.32293400	4.30190700	-1.67519200
C	1.57238300	3.83004000	1.49806100
C	0.24226400	2.01181400	2.63913400
H	-5.87951700	-0.33857100	0.18350600
H	-5.80853400	0.25903600	1.83809800
H	-5.16183100	-1.34219200	1.43378900
C	-3.61210400	-3.99196600	-0.50399300
C	-4.18481700	-1.96435900	-1.86985400
C	-2.55170100	-3.87261400	1.64371900
C	-1.92458200	-1.67851600	2.72486300
H	5.47420900	-2.59964900	-0.71026300
H	5.13577800	-4.05676800	-1.63801400
H	4.40158300	-3.85005100	-0.05430000
H	4.81038800	-1.33671800	-2.78739600
H	3.23861600	-1.59611700	-3.55311300
H	4.45121200	-2.86992200	-3.57105900
C	4.50830500	1.64894200	-0.00719200
C	3.24464600	1.01705200	-2.07404300
C	4.80659900	0.17018200	1.85593400
C	3.83312800	-2.13055500	1.97564200
H	0.92590700	5.68996300	-1.24187800
C	1.73573500	4.79763800	0.51879900
H	-2.12673900	3.57588100	-1.55891400
C	-1.93157400	5.71149800	-1.60633200
C	-0.70623700	4.07904500	-3.06118700
H	2.30354900	3.74922800	2.28898500
H	-0.30060900	1.14886600	2.25019300
C	-0.65072400	2.63784700	3.72036000
C	1.53687000	1.49408500	3.26270100
H	-4.05025600	-4.58494200	-1.29544600
C	-3.10655800	-4.62370900	0.61836900
H	-4.07414700	-0.88398600	-1.78479400
C	-5.68168800	-2.28604100	-1.99113400
C	-3.45661900	-2.40148700	-3.14591400
H	-2.16664100	-4.37643700	2.51875900
H	-1.54185200	-0.74030300	2.32079900
C	-3.01536300	-1.31177500	3.74129200
C	-0.76332600	-2.37856600	3.43233900
H	4.65501200	2.61907400	-0.46050000
C	5.01702500	1.39993100	1.25471600
H	2.77965900	0.12887200	-2.49132000
C	2.15452900	2.08290000	-1.96849800
C	4.34099000	1.47551900	-3.04409100

H	5.18477700	-0.00417200	2.85354600
H	3.28657900	-2.80992600	1.32301500
C	2.94479300	-1.88068800	3.20152800
C	5.13458700	-2.81733900	2.41174000
H	2.59183300	5.45924100	0.54880200
H	-1.18690600	6.47023400	-1.85193600
H	-2.32209200	5.94609600	-0.61726900
H	-2.74531400	5.80425500	-2.32725500
H	0.11570600	4.77404100	-3.24199000
H	-1.45865900	4.24442300	-3.83390400
H	-0.33360000	3.06462200	-3.16995300
H	-0.18841300	3.54128700	4.12220700
H	-0.79534900	1.93559100	4.54349400
H	-1.63219400	2.90521600	3.33479600
H	2.05619000	2.27524500	3.81983000
H	2.21965200	1.10478300	2.50972200
H	1.31264200	0.69296000	3.96720500
H	-3.14887100	-5.70202300	0.69932400
H	-6.12005200	-1.72758300	-2.81960200
H	-6.23021200	-2.03724000	-1.08349900
H	-5.83993100	-3.34760600	-2.18809800
H	-2.39793700	-2.16056800	-3.10175700
H	-3.87786700	-1.89110300	-4.01305600
H	-3.55802700	-3.47621800	-3.30786500
H	-3.79790200	-0.70018100	3.29724400
H	-2.58396000	-0.74931600	4.57130000
H	-3.47971200	-2.21254200	4.14697700
H	-0.28404700	-1.68993900	4.12918200
H	-0.01012500	-2.72005800	2.72302800
H	-1.10115100	-3.23915300	4.01121900
H	5.56817000	2.16985000	1.77839100
H	1.72286900	2.27628100	-2.94929100
H	2.54907200	3.02027600	-1.58106600
H	1.35290900	1.76881900	-1.30338300
H	4.76030600	2.43436600	-2.73725800
H	3.92496700	1.60443600	-4.04428000
H	5.16212700	0.76189200	-3.10566000
H	2.00498200	-1.41538800	2.91875200
H	3.44331100	-1.23046000	3.92139800
H	2.72459300	-2.82530700	3.70134500
H	5.65130500	-2.22414500	3.16696500
H	5.82346400	-2.96679900	1.58250000
H	4.91502600	-3.78985400	2.85503000
P	0.63719400	-0.66370100	0.42895700

Cartesian coordinates of the optimized geometry for **1**$^{+}$ at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

As	0.67090500	-0.54958000	0.49351400
Ga	-1.45084000	0.36637900	-0.45326300
C	1.73376100	-1.54513900	-0.79418600
Cl	-1.67926000	0.55383400	-2.63048100
N	-1.82581500	2.11054700	0.35180500
N	-2.96971800	-0.60154700	0.28980100
N	3.03037200	-1.40241500	-0.79105100
C	1.30440200	-2.69257600	-1.67881000
C	-3.06271800	2.39169100	0.75832200
C	-0.77850500	3.09821900	0.40548700
C	-4.05703700	0.07040000	0.67574800
C	-2.90456200	-2.03373900	0.40295800
C	3.76812100	-2.41951600	-1.66320300
C	3.69102900	-0.32788700	-0.07124800
C	2.64081600	-3.43092000	-1.91648200
C	0.27114500	-3.58526000	-0.99153400
C	0.71933200	-2.12537000	-2.98380200
C	-4.10285500	1.45670500	0.82023400
C	-3.41903800	3.79054000	1.18642500
C	-0.66061300	4.06750600	-0.60500400

C	0.12852800	3.04338000	1.48286500
C	-5.32855600	-0.67885000	0.97051000
C	-3.36423400	-2.85663700	-0.63741100
C	-2.34315500	-2.57505700	1.57810200
C	4.94657400	-3.03476900	-0.92455000
C	4.29017200	-1.75639700	-2.93630400
C	3.78381300	0.93152300	-0.69075500
C	4.16287400	-0.55937700	1.23540200
H	2.72915600	-4.25425900	-1.20712100
H	2.69758500	-3.84962200	-2.91931800
H	-0.66058600	-3.05416500	-0.80928600
H	0.64020500	-3.96364700	-0.03823300
H	0.04380000	-4.43797400	-1.63179500
H	1.43392800	-1.50411500	-3.52022200
H	-0.16196800	-1.52040600	-2.79495200
H	0.43747100	-2.95641500	-3.63117300
H	-5.05750200	1.85642600	1.12545600
H	-3.94021100	4.28900100	0.36730900
H	-2.54764600	4.38492200	1.44081800
H	-4.09798600	3.76189000	2.03623000
C	0.39647000	4.97373000	-0.51857000
C	-1.64460000	4.20433700	-1.75499800
C	1.17581900	3.96045000	1.50871500
C	-0.06656600	2.07826700	2.64075000
H	-5.91107900	-0.75361000	0.04997900
H	-5.92974700	-0.14457900	1.70202200
H	-5.14283300	-1.68891200	1.32364900
C	-3.24584900	-4.23808300	-0.47977300
C	-4.00175200	-2.31239600	-1.90311900
C	-2.24609700	-3.95986300	1.68196800
C	-1.91130800	-1.68984700	2.73629100
H	5.67936400	-2.27936000	-0.64438500
H	5.43613900	-3.74069800	-1.59556300
H	4.63611100	-3.57917800	-0.03788800
H	5.01771300	-0.98255100	-2.70065700
H	3.50131900	-1.32314300	-3.54391500
H	4.79404300	-2.51594300	-3.53352200
C	4.40601100	1.95579600	0.01920000
C	3.20287400	1.24496600	-2.05613300
C	4.78192400	0.50339500	1.88832600
C	3.97659900	-1.86040200	1.99908900
H	0.50198600	5.73341100	-1.28126000
C	1.31030500	4.92089700	0.51816900
H	-2.40303900	3.42927500	-1.65241400
C	-2.34488400	5.57197500	-1.72552300
C	-0.97043300	4.00229500	-3.11708400
H	1.88653700	3.93662400	2.32181400
H	-0.53875500	1.17560700	2.24938100
C	-1.03495900	2.65270800	3.68513100
C	1.24180100	1.66117400	3.31356200
H	-3.59901800	-4.89107300	-1.26650900
C	-2.69249800	-4.78792000	0.66276200
H	-4.00630900	-1.22491600	-1.84169900
C	-5.45332800	-2.79106200	-2.04955100
C	-3.19646100	-2.69716200	-3.14942600
H	-1.82457100	-4.40036500	2.57426700
H	-1.62141100	-0.72288700	2.32266600
C	-3.07387900	-1.42465900	3.70377800
C	-0.70995200	-2.24300900	3.50504900
H	4.48412100	2.93537200	-0.43079900
C	4.91155800	1.74501700	1.28932800
H	2.80658100	0.32875300	-2.48385400
C	2.03399800	2.22470900	-1.93803600
C	4.25886800	1.79661600	-3.02226900
H	5.15268600	0.35816200	2.89332500
H	3.47189500	-2.57338500	1.34811800
C	3.07654500	-1.65921700	3.22669800
C	5.31656700	-2.46651400	2.43876800
H	2.12380900	5.63352300	0.56158500

H	-1.64230000	6.37526600	-1.95308100
H	-2.78568600	5.78963900	-0.75374400
H	-3.13621100	5.60462600	-2.47603400
H	-0.19312000	4.74966600	-3.28608500
H	-1.70749400	4.10134800	-3.91548600
H	-0.52577100	3.01417800	-3.19484600
H	-0.65085600	3.59211900	4.08674000
H	-1.15496800	1.95276700	4.51419600
H	-2.02024400	2.84362000	3.26532100
H	1.67313900	2.47910400	3.89256000
H	1.98536500	1.33203100	2.58873500
H	1.05549500	0.84045900	4.00694300
H	-2.61396600	-5.86242000	0.76488300
H	-5.92475000	-2.30602800	-2.90569200
H	-6.04764700	-2.57214300	-1.16313200
H	-5.49670800	-3.86883800	-2.21493200
H	-2.16983100	-2.34674100	-3.08110400
H	-3.64183300	-2.24937200	-4.03878500
H	-3.18226600	-3.77956800	-3.29019800
H	-3.90189100	-0.91436700	3.21677100
H	-2.73914900	-0.79971600	4.53372200
H	-3.45027000	-2.36290000	4.11560700
H	-0.32979400	-1.48714100	4.19350400
H	0.10034700	-2.52764400	2.83461000
H	-0.97923000	-3.11550000	4.10185100
H	5.39444100	2.55392000	1.82154500
H	1.58595900	2.39316100	-2.91611200
H	2.35763700	3.18630800	-1.54382900
H	1.25949400	1.84654400	-1.27301000
H	4.60967500	2.77821600	-2.70188400
H	3.82964600	1.91112500	-4.01861900
H	5.12827400	1.14441400	-3.09859300
H	2.11473900	-1.23649700	2.94939100
H	3.54398900	-0.99060400	3.95050600
H	2.90199900	-2.61581900	3.72169400
H	5.79895900	-1.83575700	3.18627000
H	6.01163100	-2.58469900	1.60988000
H	5.15471400	-3.44542800	2.89265700

Cartesian coordinates of the optimized geometry for **2**$^{\cdot+}$ at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Sb	0.77984400	-0.08930300	0.55839800
Ga	-1.62919900	0.26027500	-0.52780400
C	1.98370400	-1.29691400	-0.79933900
Cl	-1.92555300	0.33353300	-2.71637700
N	-2.25809000	1.96573800	0.19846900
N	-3.05873100	-0.85461800	0.20448600
N	3.27800600	-1.17028400	-0.76377400
C	1.56310500	-2.42268300	-1.71157700
C	-3.55743600	2.13026000	0.43954000
C	-1.30411100	3.02896600	0.36045300
C	-4.24301600	-0.30309600	0.46763400
C	-2.82258500	-2.26211900	0.37636700
C	4.02565100	-2.16206400	-1.66217000
C	3.96453100	-0.13560500	-0.01002800
C	2.89871500	-3.15703600	-1.96872100
C	0.53400200	-3.33308000	-1.03920100
C	0.97501800	-1.82877400	-3.00354600
C	-4.47674100	1.07656800	0.48231800
C	-4.10508800	3.51190100	0.67509400
C	-1.05316800	3.93072200	-0.68612700
C	-0.58774600	3.09681300	1.57641500
C	-5.42630700	-1.18552100	0.76190400
C	-3.13923200	-3.17236600	-0.64500400
C	-2.21777900	-2.68817900	1.57670200
C	5.19255500	-2.81093600	-0.93558600
C	4.55821200	-1.43991600	-2.89739300

C	4.10227900	1.14221900	-0.58281600
C	4.43999100	-0.43367800	1.28137600
H	2.97835800	-4.01106400	-1.29563400
H	2.96408900	-3.53213100	-2.98809900
H	-0.40001500	-2.81098100	-0.84160200
H	0.90731900	-3.72987700	-0.09479700
H	0.30621000	-4.17402400	-1.69448800
H	1.68759100	-1.18931600	-3.52198700
H	0.08238500	-1.24170700	-2.80749400
H	0.70490700	-2.64596700	-3.67339900
H	-5.50000200	1.36669600	0.66427000
H	-4.46247100	3.91301000	-0.27566200
H	-3.35200100	4.19414300	1.05872700
H	-4.94926100	3.48165700	1.36008800
C	-0.06362200	4.89599800	-0.49674000
C	-1.82898700	3.92240600	-1.99119800
C	0.39511700	4.07434400	1.70766000
C	-0.91338600	2.17628500	2.74277500
H	-5.95965000	-1.38323200	-0.17010500
H	-6.11628800	-0.68911100	1.44012600
H	-5.13229500	-2.14320300	1.18173900
C	-2.84294700	-4.52003700	-0.43675100
C	-3.78800600	-2.75917400	-1.95347700
C	-1.93925100	-4.04296900	1.73113600
C	-1.92185100	-1.71224900	2.70221400
H	5.92688800	-2.07250800	-0.61702400
H	5.68526000	-3.49347200	-1.62837400
H	4.86754100	-3.38826100	-0.07516400
H	5.30040000	-0.69472600	-2.61897500
H	3.77485900	-0.95662200	-3.47424400
H	5.04656300	-2.17251200	-3.53948600
C	4.80689600	2.09971600	0.14449800
C	3.47044900	1.56380800	-1.89832100
C	5.13337400	0.56750400	1.95645500
C	4.16957700	-1.73796900	2.01514200
H	0.14109000	5.60258600	-1.28978200
C	0.65803800	4.96807600	0.68053500
H	-2.55075600	3.10821600	-1.95455000
C	-2.59888200	5.23668700	-2.18700600
C	-0.91565000	3.66506200	-3.19503800
H	0.95765700	4.14667000	2.62698500
H	-1.21755600	1.21293900	2.32727000
C	-2.11144400	2.69421700	3.55256900
C	0.26914200	1.92795100	3.68238700
H	-3.08519900	-5.23799700	-1.20873100
C	-2.24920700	-4.95577500	0.73386100
H	-3.94397100	-1.68181400	-1.93292200
C	-5.15121600	-3.43812700	-2.14645500
C	-2.87539100	-3.06479600	-3.14756100
H	-1.48190300	-4.39397900	2.64519600
H	-1.73347100	-0.73956600	2.24658200
C	-3.13480600	-1.53480000	3.62593200
C	-0.68439900	-2.08535300	3.52021400
H	4.93218300	3.08894800	-0.27285900
C	5.33317600	1.81554200	1.39156800
H	2.98705500	0.69938400	-2.34802600
C	2.38190100	2.61804300	-1.65931500
C	4.50218500	2.10168200	-2.89818200
H	5.51157900	0.36776100	2.94926700
H	3.63797000	-2.41029600	1.34228000
C	3.26012200	-1.50153700	3.23137600
C	5.46091600	-2.43052500	2.47152600
H	1.42206800	5.72452000	0.80418900
H	-1.91558200	6.07514300	-2.33204400
H	-3.22893500	5.47226700	-1.32981500
H	-3.23468100	5.17168100	-3.07138500
H	-0.17773500	4.46185500	-3.30671100
H	-1.50648300	3.62511800	-4.11117900
H	-0.39266400	2.71626200	-3.09753700

H	-1.90201900	3.69025200	3.94670200
H	-2.31124900	2.03053500	4.39566300
H	-3.01681000	2.75044100	2.95381800
H	0.50347000	2.81452900	4.27312200
H	1.16991900	1.63463500	3.14294900
H	0.01978900	1.13203300	4.38488500
H	-2.03140100	-6.00649800	0.87434000
H	-5.64200100	-3.04863300	-3.03972400
H	-5.81224800	-3.27574200	-1.29561200
H	-5.04026500	-4.51623100	-2.27405700
H	-1.90995900	-2.57549100	-3.04271500
H	-3.33047600	-2.70470600	-4.07116300
H	-2.71009400	-4.13898600	-3.25075000
H	-4.00033100	-1.15235000	3.08854400
H	-2.90181400	-0.83145800	4.42754400
H	-3.41277300	-2.48764500	4.08021400
H	-0.41758600	-1.26566600	4.18809400
H	0.17392600	-2.29130100	2.87975500
H	-0.85918300	-2.96422500	4.14216700
H	5.88114400	2.57421300	1.93451000
H	1.89784200	2.88008500	-2.59906500
H	2.79907600	3.52859900	-1.22974100
H	1.61104000	2.26452700	-0.97298200
H	4.93921200	3.03674500	-2.54620200
H	4.02237800	2.30473000	-3.85657300
H	5.31730800	1.39989000	-3.06793100
H	2.33299000	-1.00484100	2.95171800
H	3.75970500	-0.88152200	3.97677100
H	3.00993500	-2.45327000	3.70271600
H	5.96275100	-1.84572900	3.24308800
H	6.16650500	-2.57345600	1.65565500
H	5.23098700	-3.40688100	2.90079800

Cartesian coordinates of the optimized geometry for **3**$^{+}$ at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Bi	0.79701900	0.30219200	0.42854300
Ga	-1.73864700	0.23816700	-0.61869200
C	1.98484600	-1.31456000	-0.71870400
Cl	-2.01465500	0.16418700	-2.81872200
N	-2.41388800	1.97190000	-0.00317000
N	-3.19656400	-0.83732500	0.12844800
N	3.28144000	-1.30761000	-0.64784700
C	1.48631500	-2.47533800	-1.54185800
C	-3.72531100	2.15695200	0.13349000
C	-1.44883900	3.00301400	0.24774300
C	-4.38816400	-0.27325100	0.31851000
C	-2.97926100	-2.23752700	0.37189700
C	3.95964200	-2.45637000	-1.41006300
C	4.04853800	-0.28507900	0.04414600
C	2.74870300	-3.35637400	-1.68460500
C	0.35763900	-3.22688800	-0.83651100
C	0.99493200	-1.93922700	-2.89887400
C	-4.63824000	1.10268600	0.20683000
C	-4.27183300	3.55671400	0.19537100
C	-0.95707200	3.79148800	-0.80472000
C	-0.93238400	3.12231900	1.55805200
C	-5.56981700	-1.13608200	0.67239300
C	-3.32228900	-3.19470500	-0.59720600
C	-2.36298800	-2.61075100	1.58264900
C	5.01699100	-3.14338900	-0.56049700
C	4.61867300	-1.92391500	-2.67899900
C	4.37730700	0.90278500	-0.63472400
C	4.40749200	-0.50319200	1.38752500
H	2.71700400	-4.15686700	-0.94514300
H	2.81006800	-3.81824800	-2.66804100
H	-0.53492000	-2.61465500	-0.73530400
H	0.65574500	-3.55695100	0.15891000

H	0.08544800	-4.10815500	-1.41743200
H	1.78318600	-1.41960300	-3.44195000
H	0.15764800	-1.25556400	-2.78225300
H	0.66136200	-2.77944700	-3.50917300
H	-5.67290200	1.39094000	0.31003900
H	-4.47948200	3.89060400	-0.82442100
H	-3.56024800	4.25550600	0.62730600
H	-5.20292300	3.59337000	0.75573200
C	0.07540400	4.68818800	-0.52835000
C	-1.52614300	3.72058400	-2.20873800
C	0.09465400	4.03664300	1.77972300
C	-1.50014100	2.30987100	2.71205600
H	-6.07149000	-1.45086100	-0.24439900
H	-6.28627000	-0.57602200	1.26841000
H	-5.27552200	-2.03383100	1.20907100
C	-3.06394100	-4.53613200	-0.31290400
C	-3.93758500	-2.83937300	-1.93844700
C	-2.12818700	-3.96212000	1.81662400
C	-1.98404900	-1.57438300	2.62511900
H	5.81022600	-2.45474000	-0.27278900
H	5.46573100	-3.93909700	-1.15553700
H	4.59329200	-3.59501000	0.33171500
H	5.42577400	-1.23605600	-2.43802500
H	3.91619900	-1.42556300	-3.34139200
H	5.05030800	-2.76625100	-3.21916500
C	5.14707500	1.84186300	0.04990900
C	3.89414600	1.25868900	-2.03143200
C	5.17467600	0.47493700	2.01569600
C	3.94677000	-1.69287200	2.21549700
H	0.46780600	5.30319700	-1.32717100
C	0.60199700	4.80949900	0.74552400
H	-2.29895600	2.95445000	-2.22263400
C	-2.17500500	5.05317900	-2.60739000
C	-0.46297400	3.31037900	-3.23253300
H	0.50552100	4.14777300	2.77308600
H	-1.91801000	1.39361100	2.29356000
C	-2.65492300	3.05334000	3.39927200
C	-0.45241200	1.91268300	3.75546100
H	-3.32798400	-5.28909800	-1.04321300
C	-2.48019700	-4.92221600	0.87976300
H	-4.08494400	-1.76132400	-1.97468600
C	-5.29879900	-3.51856600	-2.14228100
C	-2.99026900	-3.20784800	-3.08811300
H	-1.66712800	-4.27289300	2.74315500
H	-1.74004900	-0.65596000	2.08918700
C	-3.16125800	-1.24748800	3.55268700
C	-0.74853500	-1.96212800	3.43842700
H	5.41877900	2.76184700	-0.44844400
C	5.55722200	1.62854500	1.35347300
H	3.32829400	0.41923700	-2.42936600
C	2.94628300	2.46568700	-1.99427200
C	5.05474600	1.55024300	-2.99234300
H	5.46713300	0.33300900	3.04669700
H	3.39006200	-2.37105500	1.56986600
C	2.99131000	-1.24338300	3.33102600
C	5.12130500	-2.46732700	2.82860200
H	1.40243100	5.51186400	0.93793300
H	-1.43275400	5.85047300	-2.67561600
H	-2.92864700	5.36553200	-1.88405000
H	-2.65536500	4.96122800	-3.58276600
H	0.33134800	4.05628400	-3.29800600
H	-0.91261700	3.20865200	-4.22090600
H	-0.01662400	2.35169800	-2.97290200
H	-2.30762900	4.00530300	3.80535600
H	-3.05260500	2.45718100	4.22235600
H	-3.47194800	3.25960400	2.71189900
H	-0.09212000	2.77581300	4.31629300
H	0.41392700	1.42434700	3.30634600
H	-0.89291700	1.22367100	4.47655100

H	-2.29633000	-5.96948800	1.08128600
H	-5.76207400	-3.16178900	-3.06341600
H	-5.98302300	-3.32040800	-1.31757000
H	-5.19194700	-4.60138600	-2.22531900
H	-2.02350600	-2.72233300	-2.97457700
H	-3.41197600	-2.88659500	-4.04143300
H	-2.83396600	-4.28737600	-3.13502200
H	-4.01319800	-0.85558400	2.99958400
H	-2.86977400	-0.49909900	4.29193700
H	-3.48744500	-2.14175700	4.08687500
H	-0.41920700	-1.11824300	4.04431600
H	0.07833800	-2.25686400	2.79063600
H	-0.95220300	-2.78902400	4.11996000
H	6.15873900	2.37084800	1.86114900
H	2.57384400	2.68042800	-2.99577500
H	3.45536800	3.35670600	-1.62499600
H	2.08452600	2.29332100	-1.34871300
H	5.57942000	2.46233300	-2.70577800
H	4.67494400	1.69499700	-4.00463200
H	5.78596300	0.74408500	-3.01566200
H	2.13344000	-0.70250700	2.93353800
H	3.49828900	-0.58723700	4.03954200
H	2.62044800	-2.10910400	3.88143800
H	5.63399200	-1.86648200	3.58040600
H	5.85750900	-2.76031900	2.08266100
H	4.75796200	-3.36891400	3.32412500

G) References

[1] J. Krüger, C. Wölper, G. Haberhauer, S. Schulz, Switching from Heteronuclear Allyl Cations to Vinyl Cations by Using a Chemical Charge Trap, *Inorg. Chem.* **2022**, *61*, 597–604

[2] A. R. O'Connor, C. Nataro, J. A. Golen, A. L. Rheingold, Synthesis and reactivity of $[N(C_6H_4Br)_3][B(C_6F_5)_4]$: The X-ray crystal structure of $[Fe(C_5H_5)_2][B(C_6F_5)_4]$, *J. Organomet. Chem.* **2004**, *689*, 2411–2414.

[3] S. Stoll, A. Schweiger, EasySpin, a comprehensive software package for spectral simulation and analysis in EPR, *J. Magn. Reson*. **2006**, *178*, 42–55.

[4] G. M. Sheldrick, Phase annealing in *SHELX*-90: direct methods for larger structures, *Acta Crystallogr.* **1990**, *A46*, 467–473.

[5] G. M. Sheldrick, SHELXL-2017, Program for the Refinement of Crystal Structures University of Göttingen, Göttingen (Germany) **2017**. See also: G. M. Sheldrick, Crystal structure refinement with SHELXL, *Acta Cryst.* **2015**, *C71*, 3–8.

[6] C. B. Hübschle, G. M. Sheldrick, B. Dittrich, ShelXle: *A Qt graphical user interface for SHELXL*, *J. Appl. Cryst.* **2011**, *44*, 1281–1284.

[7] P. van der Sluis, A. L. Spek, BYPASS: an effective method for the refinement of crystal structures containing disordered solvent regions, *Acta Crystallogr.* **1990**, *A46,* 194–201.

[8] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr.; , J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian 16, Revision C.01, Inc., Wallingford CT, **2016**.

[9] a) G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders, T. Ziegler, Chemistry with ADF, *J. Comput. Chem.* **2001**, *22*, 931−967. b) E.J. Baerends, T. Ziegler, A. J. Atkins, J. Autschbach, O. Baseggio, D. Bashford, A. Bérces, F. M. Bickelhaupt, C. Bo, P. M. Boerrigter, C. Cappelli, L. Cavallo, C. Daul, D. P. Chong, D. V. Chulhai, L. Deng, R. M. Dickson, J.M. Dieterich, F. Egidi, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, A. Förster, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S. J. A. van Gisbergen, A. Goez, A. W. Götz, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, S. Gusarov, F. E. Harris, P. van den Hoek, Z. Hu, C. R. Jacob, H. Jacobsen, L. Jensen, L. Joubert, J. W. Kaminski, G. van Kessel, C. König, F. Kootstra, A. Kovalenko, M. V. Krykunov, P. Lafiosca, E. van Lenthe, D. A. McCormack, M. Medves, A. Michalak, M. Mitoraj, S. M. Morton, J. Neugebauer, V. P. Nicu, L. Noodleman, V. P. Osinga, S. Patchkovskii, M. Pavanello, C. A. Peeples, P. H. T. Philipsen, D. Post, C. C. Pye, H. Ramanantoanina, P. Ramos, W. Ravenek, M. Reimann, J. I. Rodríguez, P. Ros, R. Rüger, P. R. T. Schipper, D. Schlüns, H. van Schoot, G. Schreckenbach, J. S. Seldenthuis, M. Seth, J. G. Snijders, M. Solà, M. Stener, M. Swart, D. Swerhone, V. Tognetti, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T. A. Wesolowski, E. M. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo, A. L. Yakovlev, ADF 2020.1, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com.

[10] a) A. D. Becke, Density-functional exchange-energy approximation with correct asymptotic behavior, *Phys. Rev. A* **1988**, *38*, 3098−3100. b) C. Lee, W. Yang, R. G. Parr, Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density, *Phys. Rev. B* **1988**, *37*, 785−789. c) B. Miehlich, A. Savin, H. Stoll, H. Preuss, Results obtained with the correlation energy density functionals of becke and Lee, Yang and Parr, *Chem. Phys. Lett.* **1989**, *157*, 200−206.

[11] S. Grimme, S. Ehrlich, L. Goerigk, Effect of the damping function in dispersion corrected density functional theory, *J. Comp. Chem.* **2011**, *32*, 1456−1465.

[12] A. E. Reed, L. A. Curtiss, F. Weinhold, Intermolecular interactions from a natural bond orbital, donor-acceptor viewpoint, *Chem. Rev.* **1988**, *88*, 899−926.

[13] F. M. Bickelhaupt, E. J. Baerends, *Rev. Comput. Chem.* **2000**, *15*, 1−86.

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Supporting Information

From π-Bonded Gallapnictenes to Nucleophilic, Redox-Active Metal-Coordinated Pnictanides

*Julia Krüger, Christoph Wölper, and Stephan Schulz**

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Supporting Information

Contents

General Synthetic methods

All manipulations were performed in an atmosphere of purified argon using standard Schlenk and glove-box techniques. Toluene, Et_2O and *n*-hexane were dried using an mBraun Solvent Purification System (SPS). Benzene and THF were carefully dried over K. Deuterated solvents were dried over activated molecular sieves (4 Å) and degassed prior to use. The anhydrous nature of the solvents was verified by Karl Fischer titration. LGa,[1] IPr,[2] $[H(OEt_2)_2][BArF_4]$,[3] $[H(OEt_2)_2][Al(OC(CF_3)_3)_4]$,[4] LGaEGa(Cl)L (E = As, Sb)[5] were prepared according to literature methods, whereas other chemicals were obtained from commercial sources and purified prior to use. Microanalyses were performed at the Elementaranalyselabor of the University of Duisburg-Essen. The melting points were measured using a Thermo Scientific 9300 apparatus. Cyclic voltammetry measurements were performed in a glovebox using a Metrohm Autolab PGSTAT 204 potentiostat with a three electrodes setup consisting of a Pt disc (*d* = 1 mm) working electrode, Pt wire counter electrode, and Ag wire pseudo-reference electrode using ferrocene as the internal standard.

Spectroscopic methods NMR Spectroscopy

^1H (300.1 MHz; 400 MHz) and $^{13}C\{^1H\}$ (75.5 MHz; 150 MHz) NMR spectra were recorded using a Bruker Avance DPX-300 spectrometer or Ascend™ 400 spectrometer. The spectra were referenced to internal C_6D_5H (^1H: δ = 7.16; ^{13}C: δ = 128.06), $CDHCl_2$ (^1H: δ = 5.32; ^{13}C: δ = 53.84 and C_4D_7HO (^1H: δ = 3.58, 1.72; ^{13}C: δ = 67.21, 25,31). IR spectra were recorded with an ALPHA-T FT-IR spectrometer equipped with a single reflection ATR sampling module. The IR spectrometer was placed in a glovebox to guarantee measurements under inert gas conditions.

Synthesis [IPrH][Cl]

IPr (500 mg, 2.66 mmol) was dissolved in 4 mL toluene and HCl in Et_2O (2.66 mmol; 1.33 mL 2 M) was added at ambient temperature. The reaction mixture was stirred for 1 h while a white precipitate was formed. The raw product was separated from the mother liquor and washed two times with 1 mL toluene. The white residue was dried in vacuum to yield analytically pure [IPrH][Cl] (yield 545 mg; 93 %). **^{1}H-NMR ($C\boldsymbol{D}_2Cl_2$, 300 MHz, 25 °C) δ [ppm]:** 10.84(s, 1 H, $C^+\boldsymbol{H}$), 4.49 (s, 2 H, $^3J_{HH}$ = 6.8 Hz, $C\boldsymbol{H}(CH_3)_2$), 2.23 (s, 6 H, $CC\boldsymbol{H}_3$), 1.68 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, $CH(C\boldsymbol{H}_3)_2$).

Synthesis $[[LGa(Cl)]_2E][IPrH]$

LGaEGa(Cl)L (E = As, Sb) is prepared in-situ from the reaction of 3 equivalents LGa with ECl_3 (E = As, Sb) as the purification of LGaEGa(Cl)L from $LGaCl_2$ results in a low yield of the starting compound LGaEGa(Cl)L. Since $LGaCl_2$ does not react with [IPrH][Cl] and $[LGa(Cl)Sb]_2$, which is always formed in small amount as by-product, can be separated by filtration before starting the reaction with [IPrH][Cl] due to it's low solubility in benzene, the in-situ synthesis generates significantly higher yields referred to ECl_3.

LGa (500 mg; 1.03 mmol) was dissolved in 2 mL benzene and $AsCl_3$ (62 mg; 28.7 µL; 0.34 mmol) in 0.5 mL benzene was added (*in-situ* synthesis of LGaAsGa(Cl)L). The solution was stirred for 3 days and then filtered in a Schlenk flask with [IPrH][Cl] (52 mg; 0.24 mmol). The suspension was stirred vigorously

for 2 h while a rose crystalline precipitate was formed. The raw product was separated from the mother liquor and washed three times with 0.3 mL benzene. The rose residue was dried in vacuum to yield analytically pure **1**.

1: Yield 234 mg (75 % referred to [IPrH][Cl]). M.p.: 198 °C (dec.). Anal. Calcd. for $C_{69}H_{103}N_6Cl_2Ga_2As$: C, 63.66; H, 7.97; N, 6.46. Found: C, 64.8; H, 7.87; N, 5.95 % **^{1}H-NMR (THF-d_8, 300 MHz, 25 °C) δ [ppm]:** 9.21 (s, 1 H, *H*C$^+$), 6.90-7.09 (m, 12 H, C$_6$*H*$_3$), 4.76 (s, 2 H, *γ*-C*H*), 4.67 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH$_3$)$_2$), 3.56 (sept (br), 4 H, C*H*(CH$_3$)$_2$), 3.28 (sept (br), 4 H, C*H*(CH$_3$)$_2$), 2.35 (s, 6 H, CC*H*$_3$), 1.60 (d, 12 H, $^3J_{HH}$ = 6.7 Hz, CH(C*H*$_3$)$_2$), 1.48 (s, 12 H, CC*H*$_3$), 1.03-1.06 (m, 24 H, CH(C*H*$_3$)$_2$), 0.82-0.86 (m, 24 H, CH(C*H*$_3$)$_2$). **^{13}C{^{1}H}-NMR (THF-d_8, 150 MHz, 25 °C) δ [ppm]:** 165.7 (NCCH$_3$), 145.7 (*C*$_6$H$_3$), 145.4 (*C*$_6$H$_3$), 144.4 (*C*$_6$H$_3$), 131.5 ($^+$*C*H), 127.9 (NCCH$_3$), 125.9 (*C*$_6$H$_3$), 123.9 (*C*$_6$H$_3$), 123.6 (*C*$_6$H$_3$), 96.8 (*γ*-*C*H), 58.1 (*C*H(CH$_3$)$_2$), 29.9 (*C*H(CH$_3$)$_2$), 29.2 (CH(*C*H$_3$)$_2$), 28.1 (*C*H(CH$_3$)$_2$), 25.5 (CH(*C*H$_3$)$_2$), 25.0 (CH(*C*H$_3$)$_2$), 24.7 (CH(*C*H$_3$)$_2$),23.1 (CH(*C*H$_3$)$_2$, 8.7 (NC*C*H$_3$). **IR *ν* [cm^{-1}]:** 3120, 3055, 2956, 2928, 2862, 1630, 1550, 1524, 1460, 1437, 1393, 1346, 1319, 1258, 1128, 1175, 1106, 1057, 1020, 937, 852, 793, 758, 638, 527, 498, 442, 395.

LGa (300 mg; 0.616 mmol) was dissolved in 2 mL benzene and $SbCl_3$ (47 mg; 0.201 mmol) in 0.5 mL benzene was added (*in-situ* synthesis of LGaSbGa(Cl)L). The solution was stirred overnight and then filtered in a Schlenk flask with [IPrH][Cl] (23 mg; 0.105 mmol). The suspension was stirred vigorously for 2 h while a purple crystalline precipitate of [[LGa(Cl)]$_2$Sb][IPrH] was formed. The raw product was separated from the mother liquor and washed three times with 0.3 mL benzene. The purple residue was dried in vacuum to yield analytically pure **2**.

2: Yield 102 mg (72 % referred to [IPrH][Cl]). M. p.: 196 °C (dec.). Anal. Calcd. for $C_{69}H_{103}N_6Cl_2Ga_2Sb$: C, 61.45; H, 7.70; N, 6.23. Found: C, 61.6; H, 7.62; N, 6.15 % **^{1}H-NMR (THF-d_8, 600 MHz, 25 °C) δ [ppm]:** 9.23 (s, 1 H, *H*C$^+$), 6.78-7.00 (m, 12 H, C$_6$*H*$_3$), 4.82 (s, 2 H, *γ*-C*H*), 4.67 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH$_3$)$_2$), 3.61 (sept (br), 4 H, C*H*(CH$_3$)$_2$), 3.17 (sept (br), 4 H, C*H*(CH$_3$)$_2$), 2.36 (s, 6 H, CC*H*$_3$), 1.61 (d, 12 H, $^3J_{HH}$ = 6.7 Hz, CH(C*H*$_3$)$_2$), 1.54 (s, 12 H, CC*H*$_3$), 1.10 (d, 12 H, $^3J_{HH}$ = 6.5 Hz, CH(C*H*$_3$)$_2$), 1.05 (d, 12 H, $^3J_{HH}$ = 6.5 Hz, CH(C*H*$_3$)$_2$), 0.85-0.87 (m (br), 24 H, CH(C*H*$_3$)$_2$). **^{13}C{^{1}H}-NMR (THF-d_8, 150 MHz, 25 °C) δ [ppm]:** 165.6 (NCCH$_3$), 146.1 (*C*$_6$H$_3$), 145.2 (*C*$_6$H$_3$), 144.2 (*C*$_6$H$_3$), 133.4 ($^+$*C*H), 127.2 (NCCH$_3$), 125.9 (*C*$_6$H$_3$), 124.0 (*C*$_6$H$_3$), 123.5 (*C*$_6$H$_3$), 97.2 (*γ*-*C*H), 51.7 (*C*H(CH$_3$)$_2$), 30.1 (*C*H(CH$_3$)$_2$), 29.4 (CH(*C*H$_3$)$_2$), 28.2 (*C*H(CH$_3$)$_2$), 25.5 (CH(*C*H$_3$)$_2$), 25.1 (CH(*C*H$_3$)$_2$), 24.8 (CH(*C*H$_3$)$_2$),23.2 (CH(*C*H$_3$)$_2$, 8.6 (NC*C*H$_3$). **IR *ν* [cm^{-1}]:** 3124, 3058, 2961, 2923, 2862, 1630, 1550, 1523, 1461, 1437, 1392, 1346, 1319, 1283, 1260, 1228, 1175, 1139, 1100, 1059, 1018, 937, 852, 792, 758, 638, 592, 527, 442.

Synthesis [LGa(Cl)]$_2$EH (E = As 5, Sb 6)

a) [LGa(Cl)]$_2$E[IPrH] (0.023 mmol) and [H(OEt$_2$)$_2$][BAr$^F_4$] (19 mg; 0.023 mmol) were weighed in a Schlenk flask, cooled to −78°C and 2 mL THF were added. The reaction mixture was slowly warmed to ambient temperature over a period of 2 h and stirred for an additional hour at room temperature. The solvent was removed in vacuum and 6 mL n-hexane were added to the residue. The filtrate was

separated from the white precipitate of [IPrH][BAr^F_4], which was formed immediately, concentrated and stored for 5 days at ambient temperature to yield colorless crystals of **5** and **6**.

b) LGaEGa(Cl)L (0.026 mmol) and [$H(OEt_2)_2$][BAr^F_4] (22 mg; 0.026 mmol) were weighed in a Schlenk flask, cooled to −78°C and 1 mL Et_2O were added (*in situ* synthesis of the supposed cationic species [LGaE(H)Ga(Cl)L]). The reaction mixture was stirred for 10 minutes at -78°C. IPrHCl (6 mg; 0.026 mmol), suspended in 2 mL Et_2O, was added to the colorless reaction solution and stirred for 10 minutes at -78°C. The reactions mixture was warmed up to ambient temperature and stirred for additional 30 minutes. The purification is carried out according to the procedure described before.

c) LGaEGa(Cl)L (0.017 mmol) was weighed in a Schlenk flask, cooled to −78°C and 2 mL THF were added. HCl (0.018 mmol) in Et_2O was added and the reaction mixture was stirred for 10 minutes at -78°C. The colorless solution was warmed up to ambient temperature and stirred for an additional hour at room temperature. The solvent was removed in vacuum and the residue was dissolved in 3 mL n-hexane and stored for 3 days at ambient temperature to yield colorless crystals of **5** and **6**.

5: Yield 19 mg (65 %). M.p.: 186 °C (dec.). Anal. Calcd. for $C_{58}H_{83}N_4Cl_2Ga_2As$: C, 62.11; H, 7.46; N, 5.00. Found: C, 62.3; H, 7.60; N, 5.21 % **^{1}H-NMR (C_6D_6, 300 MHz, 25 °C) δ [ppm]:** 6.96-7.13 (m, 12 H, C_6H_3), 4.81 (s, 2 H, γ-C*H*), 3.58 (sept, 4 H, $^3J_{HH}$ = 6.8 Hz, C*H*(CH_3)$_2$), 3.10 (sept (br), 4 H, C*H*(CH_3)$_2$), 1.48 (s, 12 H, CC*H*$_3$) 1.19 (d, 36 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3$)$_2$), 0.98 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3$)$_2$), −1.32 (s, 1 H, *AsH*).**^{13}C{^{1}H}-NMR (C_6D_6, 150 MHz, 25 °C) δ [ppm]:** 169.1 (N*C*CH$_3$), 146.7 (*C*$_6$H$_3$), 142.8 (*C*$_6$H$_3$), 141.3 (*C*$_6$H$_3$), 127.7 (*C*$_6$H$_3$), 125.7 (*C*$_6$H$_3$), 123.9 (*C*$_6$H$_3$), 98.0 (γ-*C*H), 29.9 (*C*H(CH_3)$_2$), 28.5 (CH(*C*H$_3$)$_2$), 28.2 (*C*H(CH_3)$_2$), 25.4 (CH(*C*H$_3$)$_2$), 24.6 (CH(*C*H$_3$)$_2$), 24.2 (CH(*C*H$_3$)$_2$). **IR ν [cm^{-1}]:** 3061, 2961, 2925, 2867, 2078, 1626, 1547, 1526, 1460, 1438, 1383,1345, 1317, 1257, 1178, 1100, 1059, 1020, 937, 865, 797, 757, 722, 638, 616, 535, 461, 394,

6: Yield 16 mg (53 %). M.p.: 181 °C (dec.). Anal. Calcd. for $C_{58}H_{83}N_4Cl_2Ga_2Sb$: C, 59.62; H, 7.16; N, 4.80. Found: C, 60.7; H, 7.08; N, 4.56 % **^{1}H-NMR (C_6D_6, 400 MHz, 25 °C) δ [ppm]:** 6.99-7.20 (m, 12 H, C_6H_3), 4.84 (s, 2 H, γ-C*H*), 3.63 (sept, 4 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 3.16 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 2.99 (sept, 2 H, C*H*(CH_3)$_2$), 1.55 (s, 6 H, CC*H*$_3$), 1.51 (s, 6 H, CC*H*$_3$), 1.28 (d, 6 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3$)$_2$), 1.26 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, CH(C*H*$_3$)$_2$), 1.23-1.18 (m, 18 H, CH(C*H*$_3$)$_2$), 1.16 (d, 6 H, $^3J_{HH}$ = 6.7 Hz, CH(C*H*$_3$)$_2$), 0.98 (d, 6 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3$)$_2$), 0.96 (d, 6 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3$)$_2$), −3.59 (s, 1 H, Sb*H*).**^{13}C{^{1}H}-NMR (C_6D_6, 150 MHz, 25 °C) δ [ppm]:** 168.7 (N*C*CH$_3$), 168.6 (N*C*CH$_3$), 146.4 (*C*$_6$H$_3$), 146.4 (*C*$_6$H$_3$), 142.5 (*C*$_6$H$_3$), 142.5 (*C*$_6$H$_3$), 141.2 (*C*$_6$H$_3$), 141.1 (*C*$_6$H$_3$), 127.5 (*C*$_6$H$_3$), 127.4 (*C*$_6$H$_3$), 125.5 (*C*$_6$H$_3$), 125.4 (*C*$_6$H$_3$) 123.7 (*C*$_6$H$_3$),) 123.5 (*C*$_6$H$_3$), 97.9 (γ-*C*H), 30.0 (*C*H(CH_3)$_2$), 29.8 (*C*H(CH_3)$_2$), 28.3 (CH(*C*H$_3$)$_2$), 28.2 (CH(*C*H$_3$)$_2$), 28.0 (*C*H(CH_3)$_2$), 28.0 (*C*H(CH_3)$_2$), 25.0 (CH(*C*H$_3$)$_2$), 25.0 (CH(*C*H$_3$)$_2$), 24.5 (CH(*C*H$_3$)$_2$), 24.3 (CH(*C*H$_3$)$_2$), 24.3 (CH(*C*H$_3$)$_2$), 24.0 (CH(*C*H$_3$)$_2$), 23.9 (CH(*C*H$_3$)$_2$), 23.7 (CH(*C*H$_3$)$_2$). **IR ν [cm^{-1}]:** 3061, 2959, 2925, 2867, 1858, 1621, 1547, 1521, 1460, 1437, 1382, 1316, 1257, 1175, 1099, 1057, 1018, 935, 863, 796, 757, 710, 634, 528, 436.

Synthesis LGa(Cl)E(Me)Ga(I)L (As 7, Sb 8)

LGaEGa(Cl)L (0.029 mmol) was dissolved in 2 mL toluene, cooled to −78°C and methyl iodide (4.2 mg; 1.84 µL; 0.029 mmol) in 0.5 mL toluene was added. The reaction mixture was warmed up to ambient temperature and the solvent was removed. The residue was dissolved in 3 mL n-hexane, concentrated until crystallization started and stored for 2 days at ambient temperature to yield colorless crystals of **7** and **8**.

7: Yield 18 mg (51 %). M.p.: 209 °C (dec.). Anal. Calcd. for $C_{59}H_{85}N_4ClGa_2IAs$: C, 57.75; H, 6.98; N, 4.57. Found: C, 57.6; H, 6.82; N, 4.51 %. **^{1}H-NMR (C_6D_6, 300 MHz, 25 °C) δ [ppm]:** .6.89-7.14 (m, 12 H, C_6H_3), 5.04 (s, 1 H, γ-C*H*), 4.87 (s, 1 H, γ-C*H*), 3.83 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 3.86 (sept, 2 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 3.14-3.24 (m, 4 H, C*H*(CH_3)$_2$), 1.50 (s, 6 H, CCH_3), 1.49 (s, 6 H, CCH_3), 1.37-1.41 (m, 9 H, CH(CH_3)$_2$), 1.16-1.23 (m, 27 H, CH(CH_3)$_2$), 0.95-0.99 (m, 12 H, CH(CH_3)$_2$), 0.04 (s, 3 H, CH_3). **^{13}C{^{1}H}-NMR (C_6D_6, 150 MHz, 25 °C) δ [ppm]:** 169.4 (NCCH$_3$), 169.0 (NCCH$_3$), 146.3 (C_6H_3), 145.9 (C_6H_3), 143.2 (C_6H_3), 142.7 (C_6H_3), 127.4 (C_6H_3), 127.4 (C_6H_3), 125.6 (C_6H_3), 125.5 (C_6H_3), 123.8 (C_6H_3), 123.5 (C_6H_3), 99.2 (γ-*C*H), 98.2 (γ-*C*H), 29.6 (*C*H(CH_3)$_2$), 29.5 (*C*H(CH_3)$_2$), 28.8 (*C*H(CH_3)$_2$), 28.2 (*C*H(CH_3)$_2$), 28.2 (CH(*C*H$_3$)$_2$), 25.2 (CH(*C*H$_3$)$_2$), 25.1 (CH(*C*H$_3$)$_2$), 24.7 (CH(*C*H$_3$)$_2$), 24.6 (C(*C*H$_3$)$_2$), 24.4 (C(*C*H$_3$)$_2$), 24.1 (CH(*C*H$_3$)$_2$), 24.0 (CH(*C*H$_3$)$_2$), 23.8 (CH(*C*H$_3$)$_2$), 23.8 (CH(*C*H$_3$)$_2$), −8.5 (As*C*H$_3$). **IR ν [cm^{-1}]:** 3041, 2961, 2926, 2867, 1523, 1458, 1437, 1386, 1316, 1206, 1177, 1095, 1056, 1018, 937, 862, 796, 757, 723, 707, 661, 636, 490, 442, 398.

8: Yield 15 mg (42 %). M.p.: 207 °C (dec.). Anal. Calcd. for $C_{59}H_{85}N_4ClGa_2ISb$: C, 55.63; H, 6.73; N, 4.40. Found: C, 55.7 H, 6.73; N, 4.38%. **^{1}H-NMR (C_6D_6, 400 MHz, 25 °C) δ [ppm]:** 6.93-7.14 (m, 12 H, C_6H_3), 5.06 (s, 1 H, γ-C*H*), 4.90 (s, 1 H, γ-C*H*), 4.05 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 3.86 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 3.71 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 3.54 (sept, 1 H, $^3J_{HH}$ = 6.7 Hz, C*H*(CH_3)$_2$), 3.14-3.31 (m, 4 H, C*H*(CH_3)$_2$), 1.56 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$), 1.51 (d, 3 H, $^3J_{HH}$ = 6.7 Hz, CH(CH_3)$_2$), 1.49 (s, 12 H, CCH_3), 1.18-1.32 (m, 30 H, CH(CH_3)$_2$), 0.94-0.98 (m, 12 H, CH(CH_3)$_2$), −0.35 (s, 3 H, CH_3). **^{13}C{^{1}H}-NMR (C_6D_6, 150 MHz, 25 °C) δ [ppm]:** 169.2 (NCCH$_3$), 168.9 (NCCH$_3$), 168.6 (NCCH$_3$), 146.7 (C_6H_3), 146.3 (C_6H_3), 146.3 (C_6H_3), 146.1 (C_6H_3), 143.5 (C_6H_3), 143.3 (C_6H_3), 143.2 (C_6H_3), 143.1 (C_6H_3), 142.5 (C_6H_3), 141.8 (C_6H_3), 141.6 (C_6H_3), 141.4 (C_6H_3), 127.6 (C_6H_3), 127.5 (C_6H_3), 127.5 (C_6H_3), 125.8 (C_6H_3), 125.6 (C_6H_3), 125.5 (C_6H_3), 123.8 (C_6H_3), 123.6 (C_6H_3), 99.3 (γ-*C*H), 98.5 (γ-*C*H), 31.1 (CH(*C*H$_3$)$_2$), 30.2 (*C*H(CH_3)$_2$), 30.2 (*C*H(CH_3)$_2$), 29.3 (*C*H(CH_3)$_2$), 29.2 (CH(*C*H$_3$)$_2$), 29.2 (CH(*C*H$_3$)$_2$), 28.9 (*C*H(CH_3)$_2$), 28.4 (*C*H(CH_3)$_2$), 28.3 (*C*H(CH_3)$_2$), 28.1 (CH(*C*H$_3$)$_2$), 28.0 (*C*H(CH_3)$_2$), 25.3 (CH(*C*H$_3$)$_2$), 25.1 (CH(*C*H$_3$)$_2$), 25.0 (CH(*C*H$_3$)$_2$), 24.9 (CH(*C*H$_3$)$_2$), 24.6 (CH(*C*H$_3$)$_2$), 24.5 (CH(*C*H$_3$)$_2$), 24.4 (CH(*C*H$_3$)$_2$), 24.4 (CH(*C*H$_3$)$_2$), 24.3 (CH(*C*H$_3$)$_2$), 24.3 (C(*C*H$_3$)$_2$), 24.1 (C(*C*H$_3$)$_2$), 24.1 (C(*C*H$_3$)$_2$), 24.1 (C(*C*H$_3$)$_2$), 23.9 (CH(*C*H$_3$)$_2$), 23.6 (CH(*C*H$_3$)$_2$), 23.6 (CH(*C*H$_3$)$_2$), −28.2 (Sb*C*H$_3$). **IR ν [cm^{-1}]:** 3060, 2961, 2925, 2866, 1551, 1521, 1460, 1435, 1383, 1314, 1287, 1258, 1195, 1175, 1098, 1057, 1017, 937, 859, 794, 758, 707, 638, 619, 529, 500, 437, 419.

Synthesis [LGa(Cl)]$_2$EMe (As 9, Sb 10)

[[LGa(Cl)]$_2$E[IPrH] (0.029 mmol) was dissolved in 2 mL THF, cooled to −78°C and methyl iodide (4.2 mg; 1.84 µL; 0.029 mmol) in 0.5 mL THF was added. The reaction mixture was warmed up to

ambient temperature and the solvent was removed. 2 mL toluene were added to the residue and white precipitate of [IPrH][I] was formed. The mother liquor was separated and the solvent was removed. The residue was dissolved in 5 mL n-hexane, concentrated until crystallization started and stored for 6 days at 0 °C to yield colorless crystals of **7** and **8**.

9: Yield 21 mg (64 %). M.p.: 195 °C (dec.). Anal. Calcd. for $C_{59}H_{85}N_4Cl_2Ga_2As$: C, 62.40; H, 7.54; N, 4.93. Found: C, 62.5; H, 7.56; N, 4.99 %. **^{1}H-NMR (C_6D_6, 400 MHz, 25 °C) δ [ppm]:** 6.96-7.14 (m, 12 H, C_6H_3), 4.88 (s, 2 H, γ-C*H*), 3.71 (sept (br), 4 H, C*H*$(CH_3)_2$), 3.18 (sept, 4 H, $^3J_{HH}$ = 6.8 Hz, C*H*$(CH_3)_2$), 1.48 (s, 12 H, CC*H*$_3$), 1.33 (d, 12 H, $^3J_{HH}$ = 6.6 Hz, CH(C*H*$_3)_2$), 1.22 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3)_2$), 1.20 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3)_2$), 0.98 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3)_2$), 0.04 (s, 3 H, *C*H$_3$). **^{13}C{^{1}H}-NMR (C_6D_6, 150 MHz, 25 °C) δ [ppm]:** 169.0 (N*C*CH$_3$), 146.1 (*C*$_6$H$_3$), 142.9 (*C*$_6$H$_3$), 142.6 (*C*$_6$H$_3$), 127.4 (*C*$_6$H$_3$), 125.3 (*C*$_6$H$_3$), 123.6 (*C*$_6$H$_3$), 98.5 (γ-*C*H), 29.5 (*C*H$(CH_3)_2$), 28.3 (*C*H$(CH_3)_2$), 27.8 (CH(*C*H$_3)_2$), 25.0 (CH(*C*H$_3)_2$), 24.5 (CH(*C*H$_3)_2$), 24.2 (C(*C*H$_3)_2$), 23.9 (CH(*C*H$_3)_2$), −10.2 (As*C*H$_3$). **IR ν [cm^{-1}]:** 3038, 2958, 2925, 2867, 1551, 1524, 1460, 1435, 1383, 1316, 1287, 1253, 1177, 1100, 1057, 1018, 935, 860, 794, 758, 707, 639, 532, 448.

10: Yield 16 mg (47 %). M.p.: 192 °C (dec.). Anal. Calcd. for $C_{59}H_{85}N_4Cl_2Ga_2Sb$: C, 59.93; H, 7.25; N, 4.74. Found: C, 60.8; H, 7.06; N, 4.47 %**^{1}H-NMR (C_6D_6, 400 MHz, 25 °C) δ [ppm]:** 6.93-7.15 (m, 12 H, C_6H_3), 4.91 (s, 2 H, γ-C*H*), 3.88 (sept, 2 H, $^3J_{HH}$ = 6.8 Hz, C*H*$(CH_3)_2$), 3.58 (sept, 2 H, $^3J_{HH}$ = 6.8 Hz, C*H*$(CH_3)_2$), 3.24 (sept, 2 H, $^3J_{HH}$ = 6.8 Hz, C*H*$(CH_3)_2$), 3.16 (sept, 2 H, $^3J_{HH}$ = 6.8 Hz, C*H*$(CH_3)_2$), 1.48-1.50 (m, 18 H, CC*H*$_3$, CH(C*H*$_3)_2$), 1.29 (d, 6 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3)_2$), 1.19-1.23 (m, 24 H, CH(C*H*$_3)_2$), 0.97 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, CH(C*H*$_3)_2$), −0.32 (s, 3 H, *C*H$_3$). **^{13}C{^{1}H}-NMR (C_6D_6, 150 MHz, 25 °C) δ [ppm]:** 168.9 (N*C*CH$_3$), 168.7 (N*C*CH$_3$), 146.4 (*C*$_6$H$_3$), 146.2 (*C*$_6$H$_3$), 143.1 (*C*$_6$H$_3$), 143.1 (*C*$_6$H$_3$), 142.1 (*C*$_6$H$_3$), 141.5 (*C*$_6$H$_3$), 127.6 (*C*$_6$H$_3$), 127.5 (*C*$_6$H$_3$), 125.5 (*C*$_6$H$_3$), 125.3 (*C*$_6$H$_3$), 123.7 (*C*$_6$H$_3$), 123.5 (*C*$_6$H$_3$), 98.7 (γ-*C*H), 30.1 (*C*H$(CH_3)_2$), 29.3 (*C*H$(CH_3)_2$), 28.8 (CH(*C*H$_3)_2$), 28.3 (*C*H$(CH_3)_2$), 28.0 (*C*H$(CH_3)_2$), 27.7 (CH(*C*H$_3)_2$), 25.2 (CH(*C*H$_3)_2$), 24.8 (CH(*C*H$_3)_2$), 24.6 (CH(*C*H$_3)_2$), 24.4 (CH(*C*H$_3)_2$), 24.1 (C(*C*H$_3)_2$), 24.1 (C(*C*H$_3)_2$), 23.9 (CH(*C*H$_3)_2$), 23.5 (CH(*C*H$_3)_2$), −30.0 (Sb*C*H$_3$),. **IR ν [cm^{-1}]:** 3059, 2961, 2928, 2867, 1551, 1523, 1460, 1435, 1382, 1316, 1287, 1258, 1195, 1177, 1093, 1016, 937, 862, 792, 757, 705, 638, 530, 500, 451, 401.

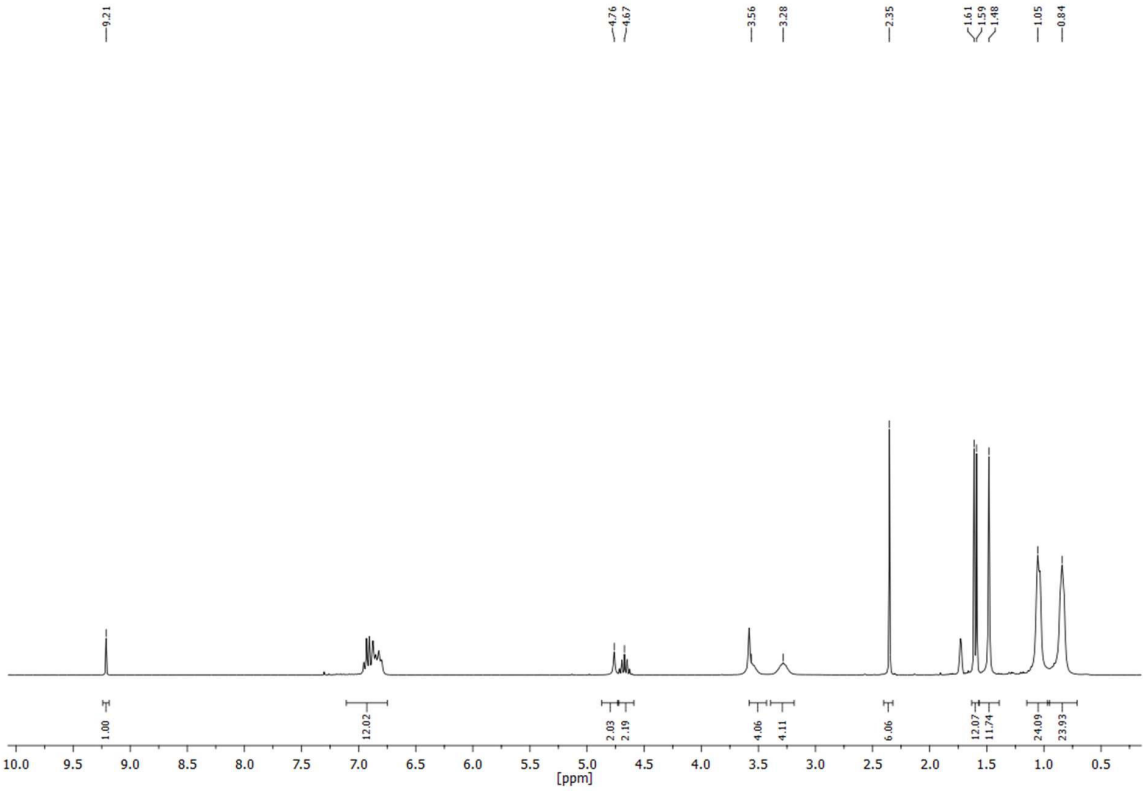

Fig. S1. ^{1}H NMR spectrum of [[LGa(Cl)]$_2$As][IPrH] (**1**) in THF-d_8.

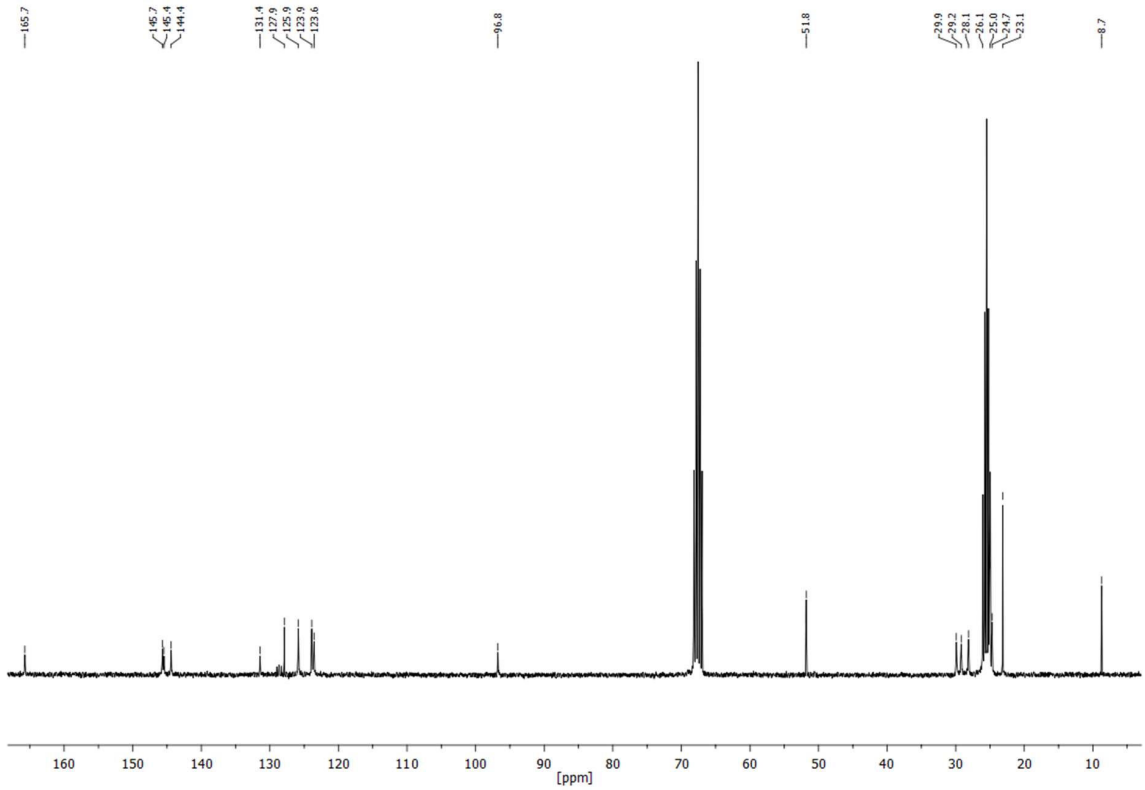

Fig. S2. ^{13}C NMR spectrum of [[LGa(Cl)]$_2$As][IPrH] (**1**) in THF-d_8.

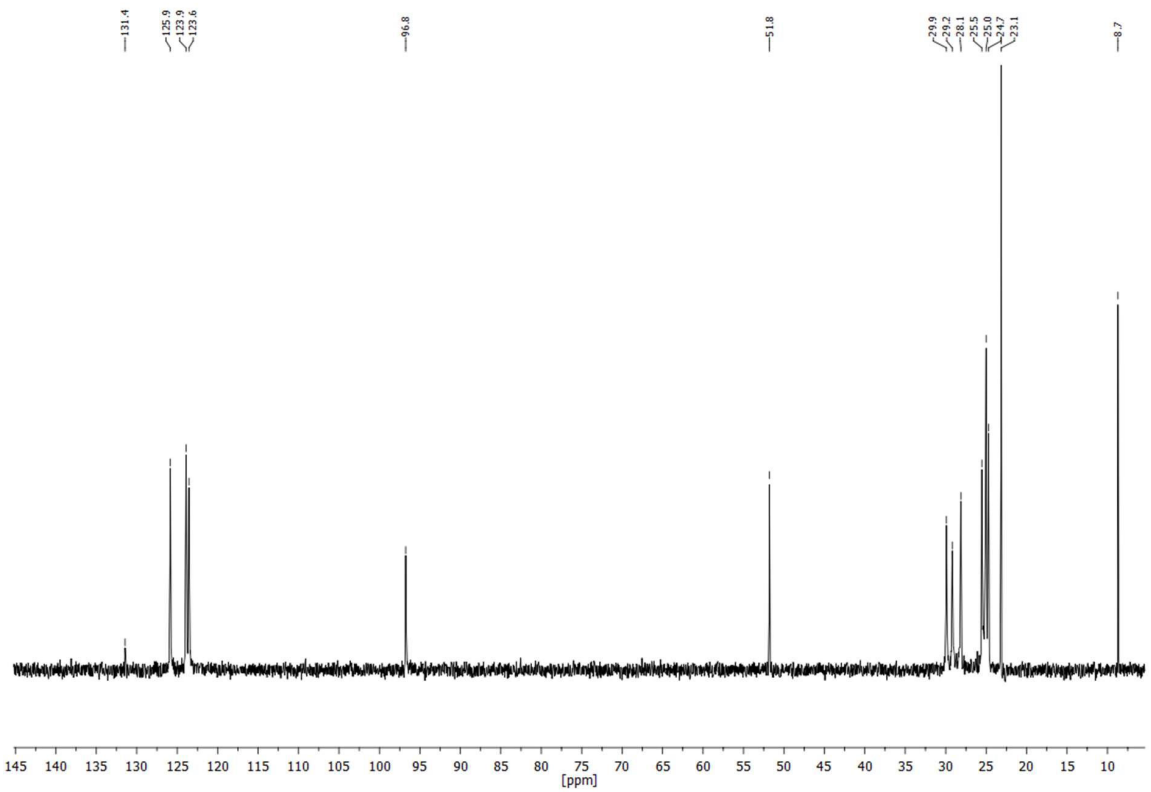

Fig. S3. DEPT135 spectrum of [[LGa(Cl)]$_2$As][IPrH] (**1**) in THF-d_8.

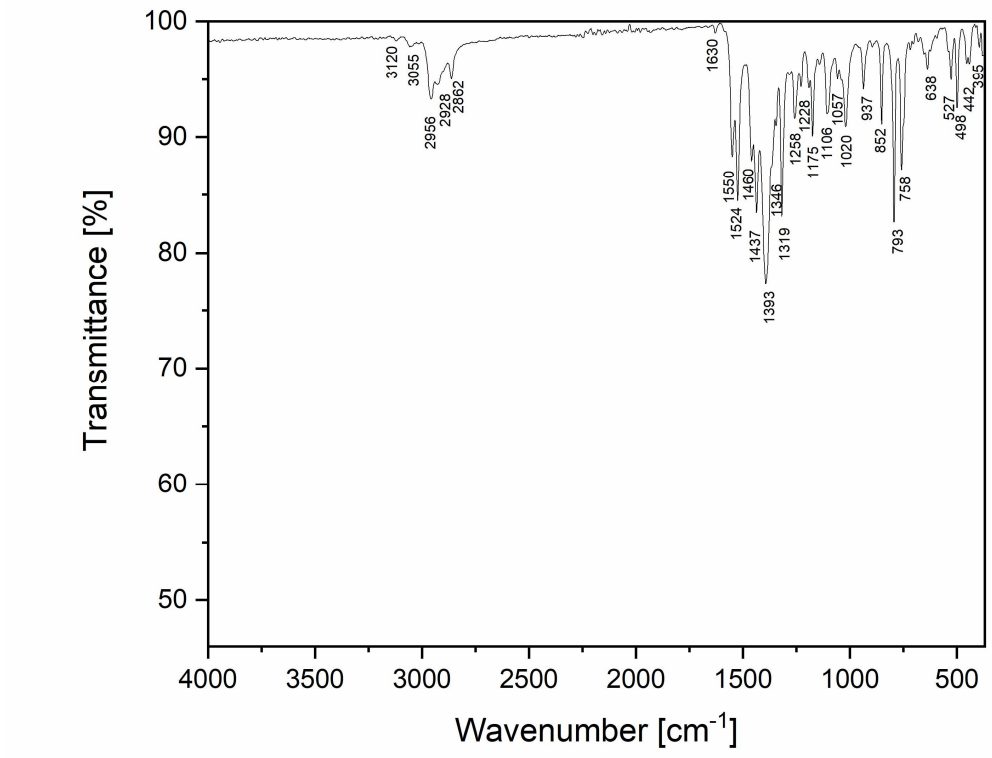

Fig. S4. ATR-IR spectrum of [[LGa(Cl)]$_2$As][IPrH] (**1**).

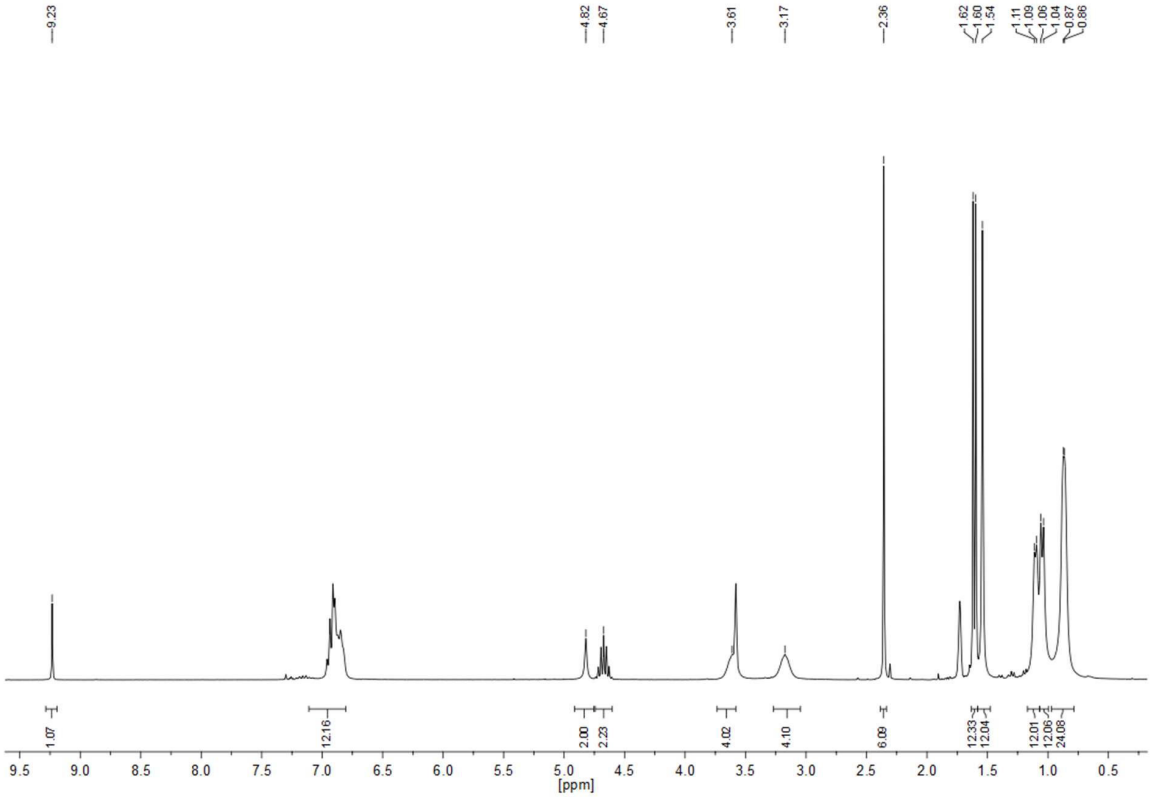

Fig. S5. ^{1}H NMR spectrum of [[LGa(Cl)]$_2$Sb][IPrH] (**2**) in THF-d_8.

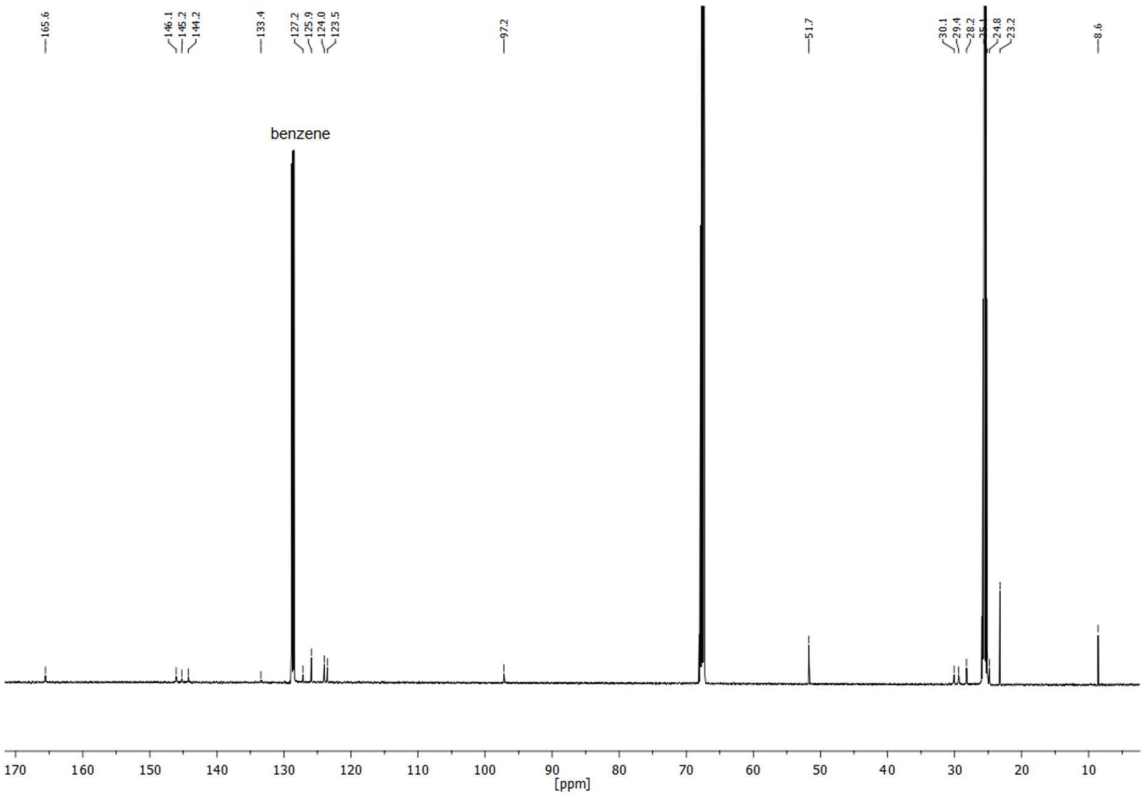

Fig. S6. ^{13}C NMR spectrum of [[LGa(Cl)]$_2$Sb][IPrH] (**2**) in THF-d_8.

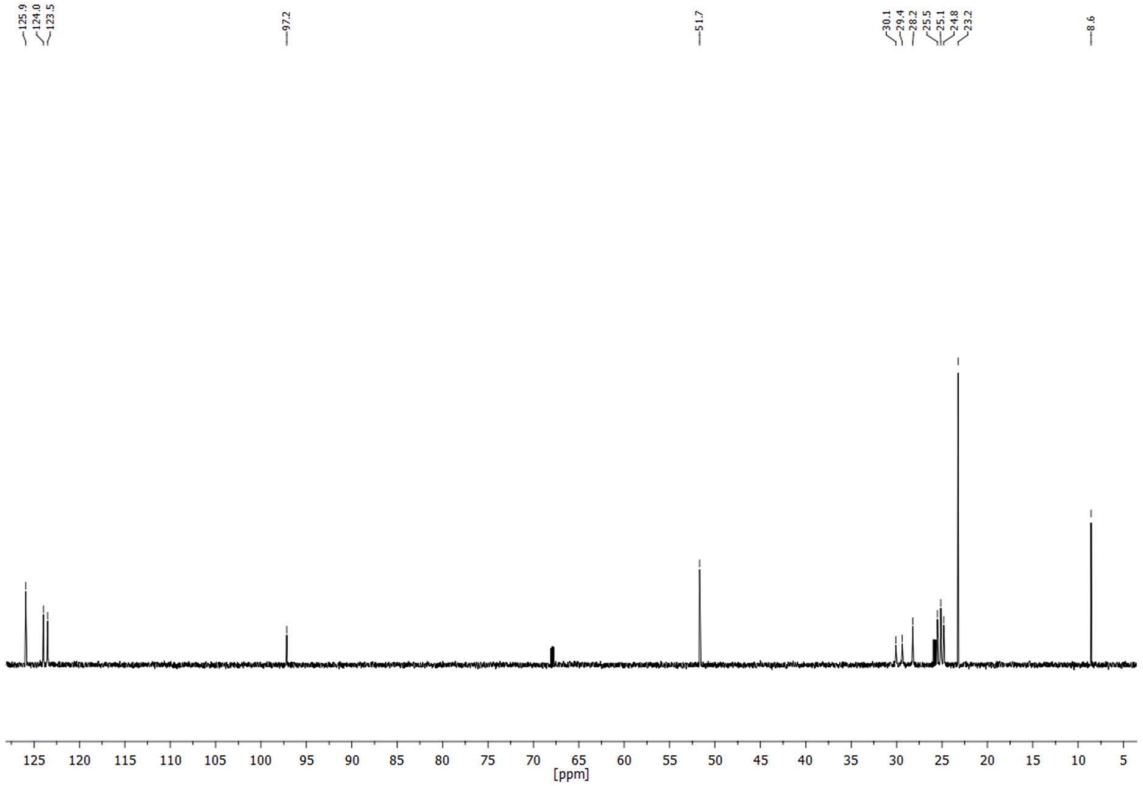

Fig. S7. DEPT135 spectrum of [[LGa(Cl)]$_2$Sb][IPrH] (**2**) in THF-d_8.

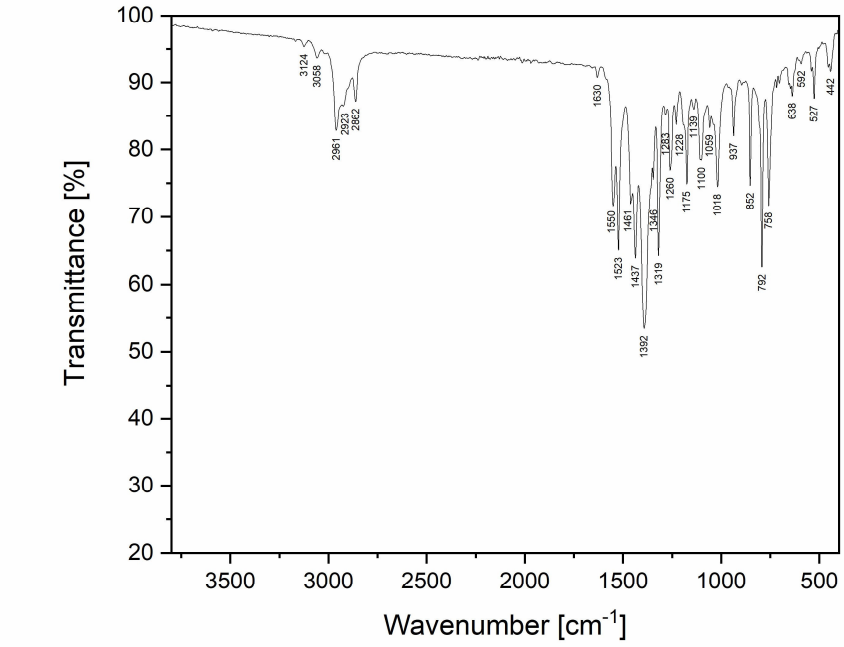

Fig. S8. ATR-IR spectrum of [[LGa(Cl)]$_2$Sb][IPrH] (**2**).

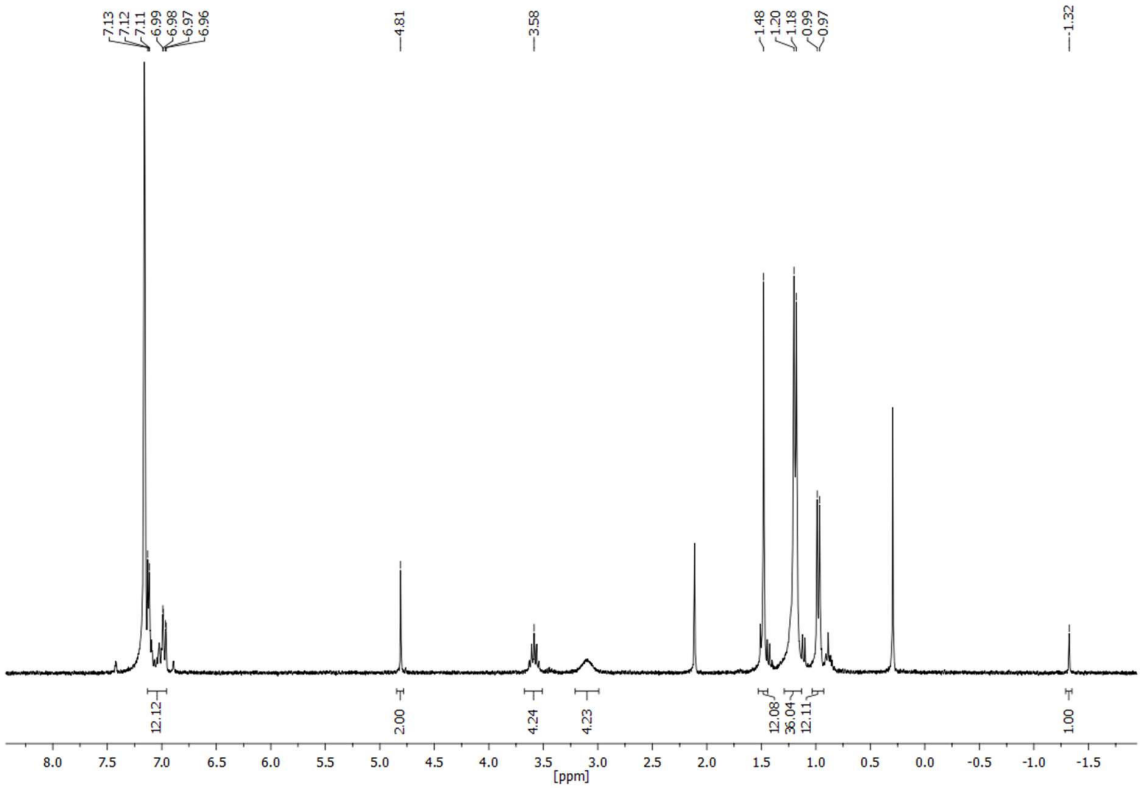

Fig. S9. ^{1}H NMR spectrum of [LGa(Cl)]$_2$AsH (**5**) in C_6D_6.

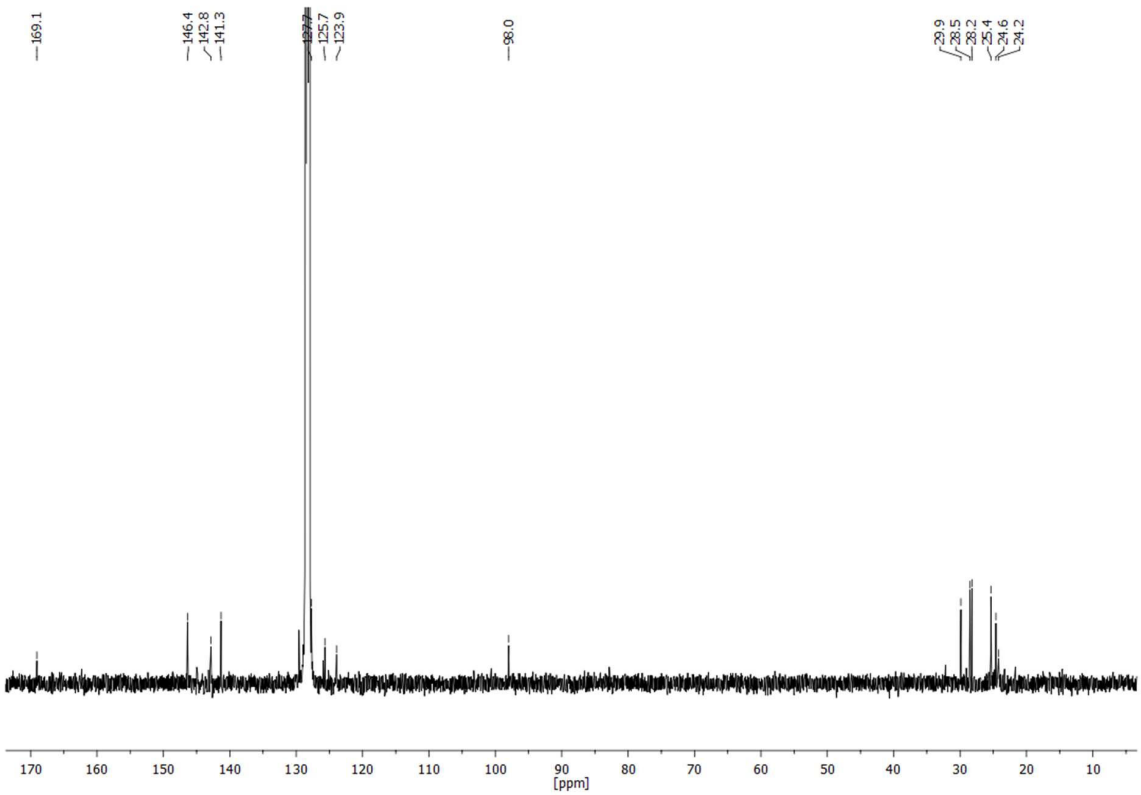

Fig. S10. ^{13}C NMR spectrum of [LGa(Cl)]$_2$AsH (**5**) in C_6D_6.

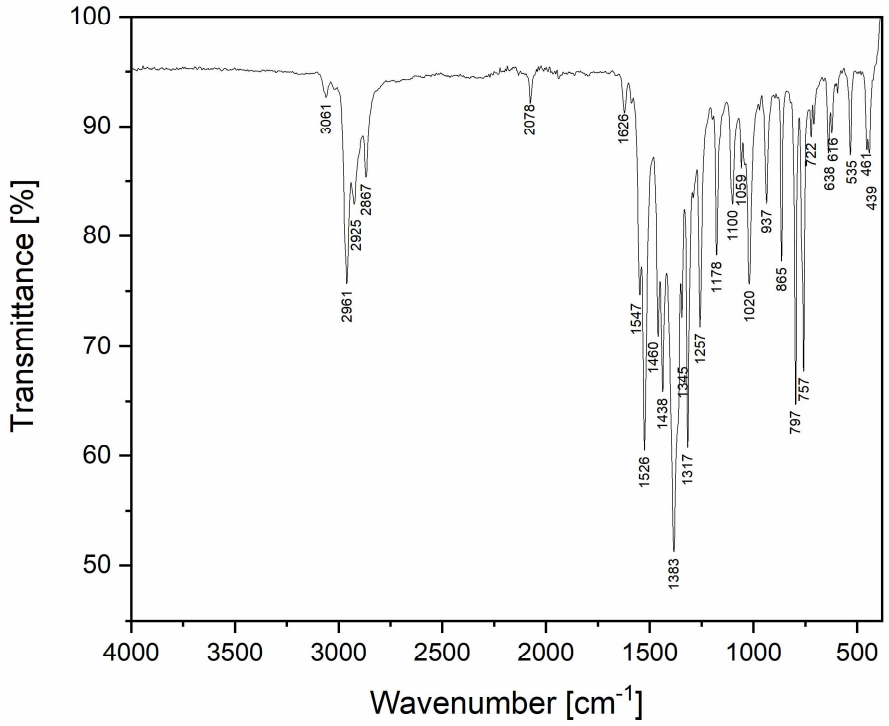

Fig. S11. ATR IR spectrum of $[LGa(Cl)]_2AsH$ (**5**).

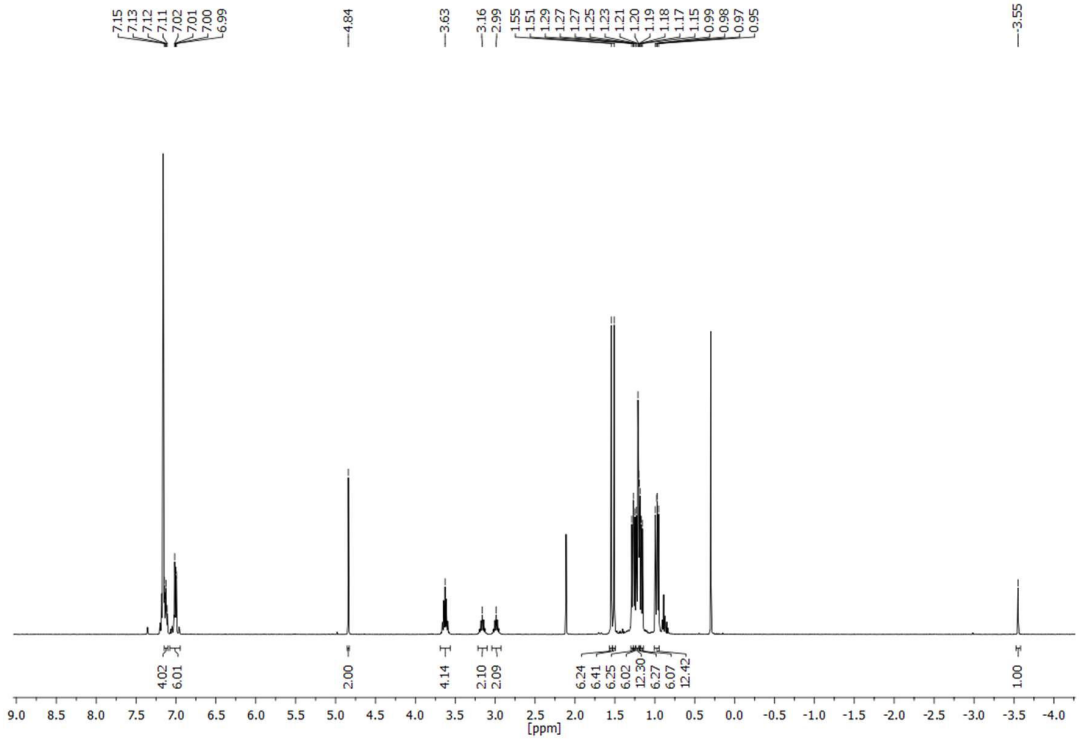

Fig. S12. ^1H NMR spectrum of $[LGa(Cl)]_2SbH$ (**6**) in C_6D_6.

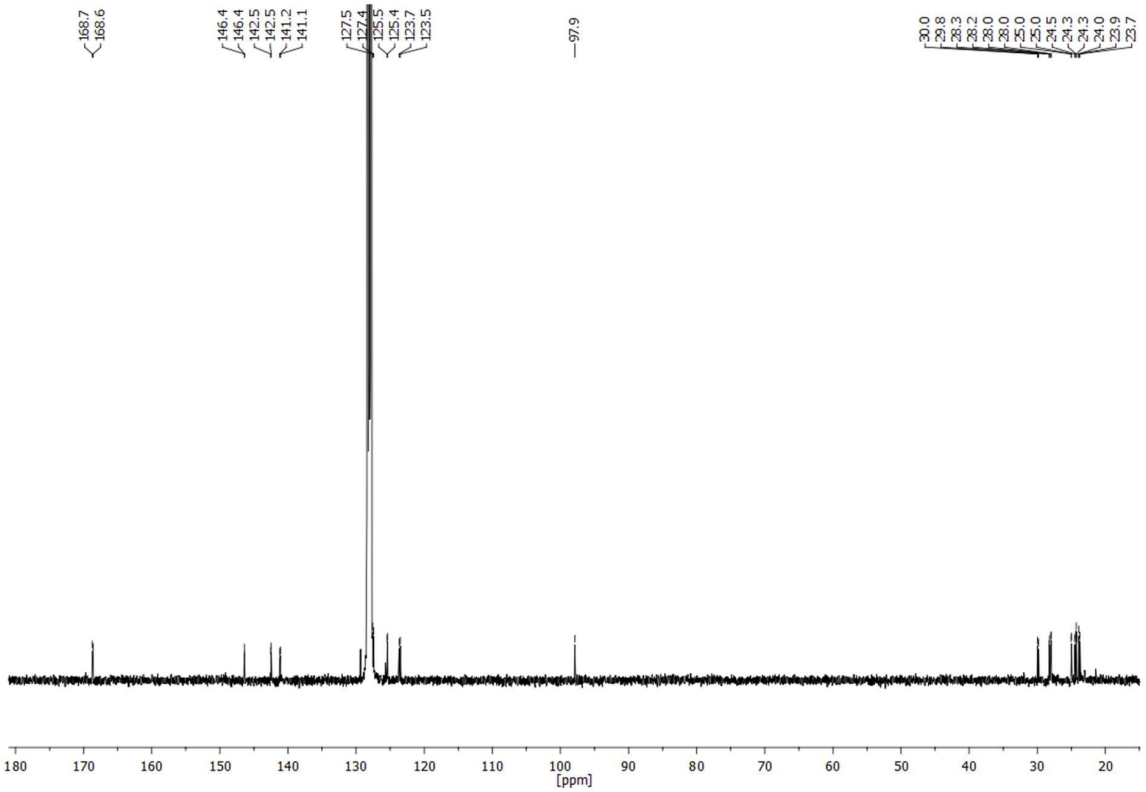

Fig. S13. ^{13}C NMR spectrum of $[LGa(Cl)]_2SbH$ (**6**) in C_6D_6.

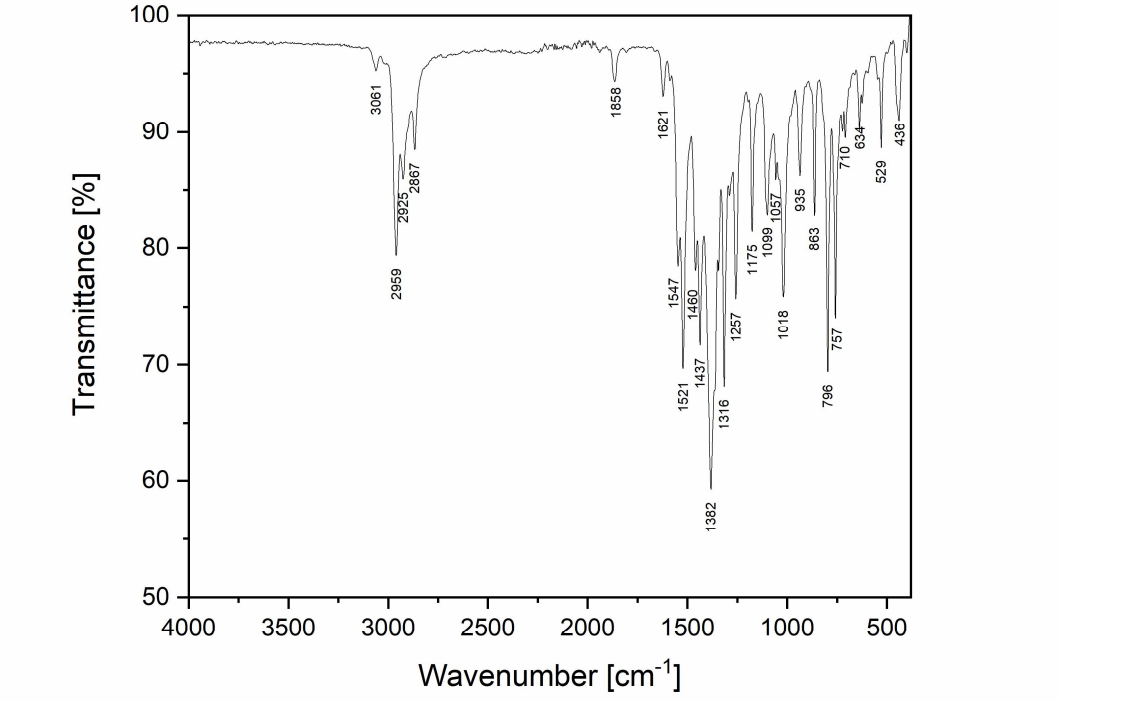

Fig. S14. ATR IR spectrum of $[LGa(Cl)]_2SbH$ (**6**).

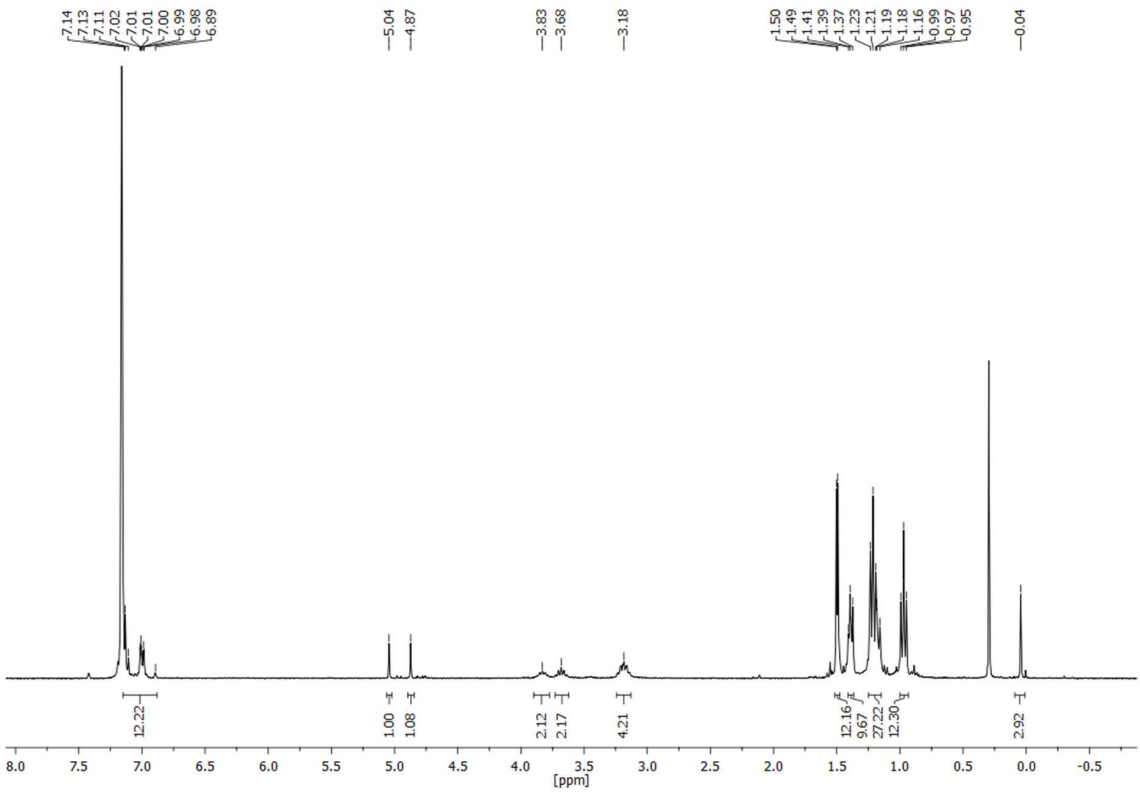

Fig. S15. ^{1}H NMR spectrum of LGa(Cl)As(Me)Ga(I)L (**7**) in C_6D_6.

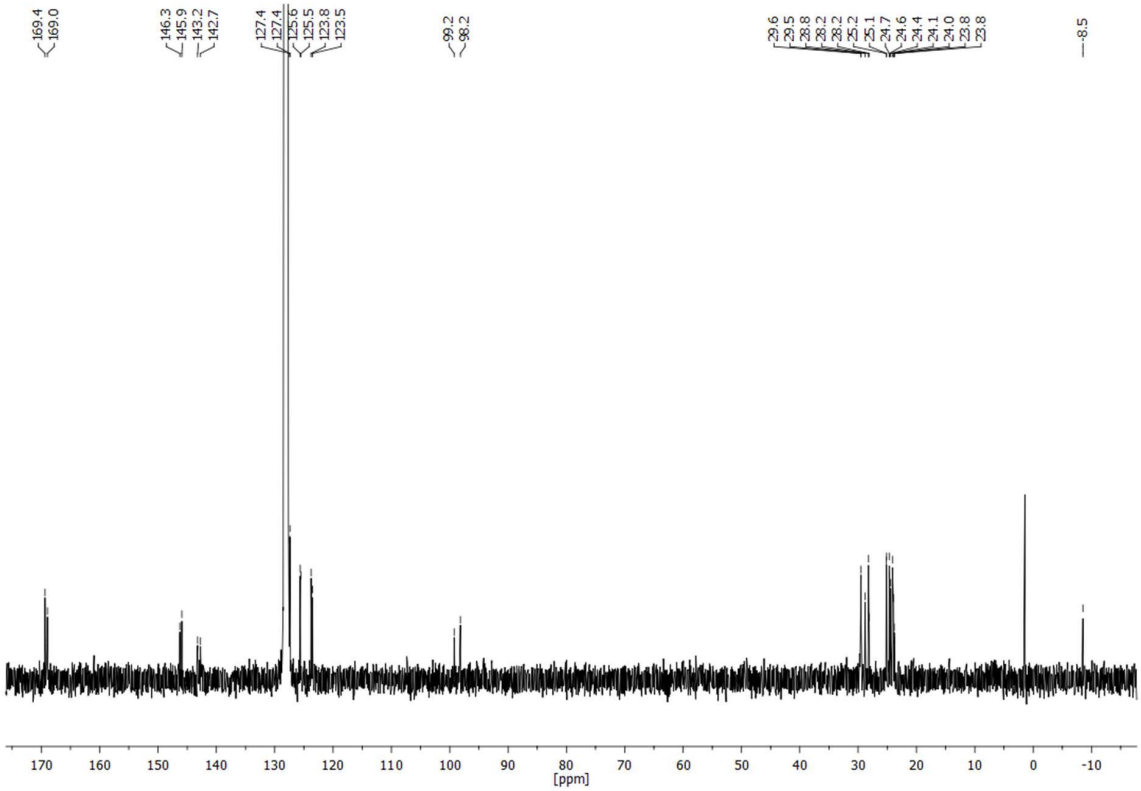

Fig. S16. ^{13}C NMR spectrum of LGa(Cl)As(Me)Ga(I)L (**7**) in C_6D_6.

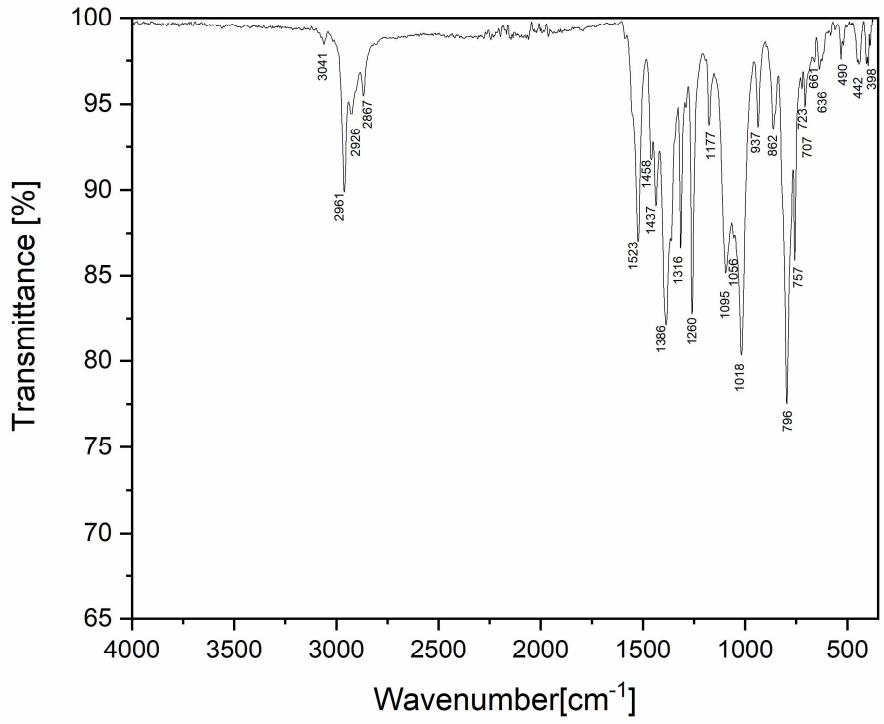

Fig. S17. ATR-IR spectrum of LGa(Cl)As(Me)Ga(I)L (**7**).

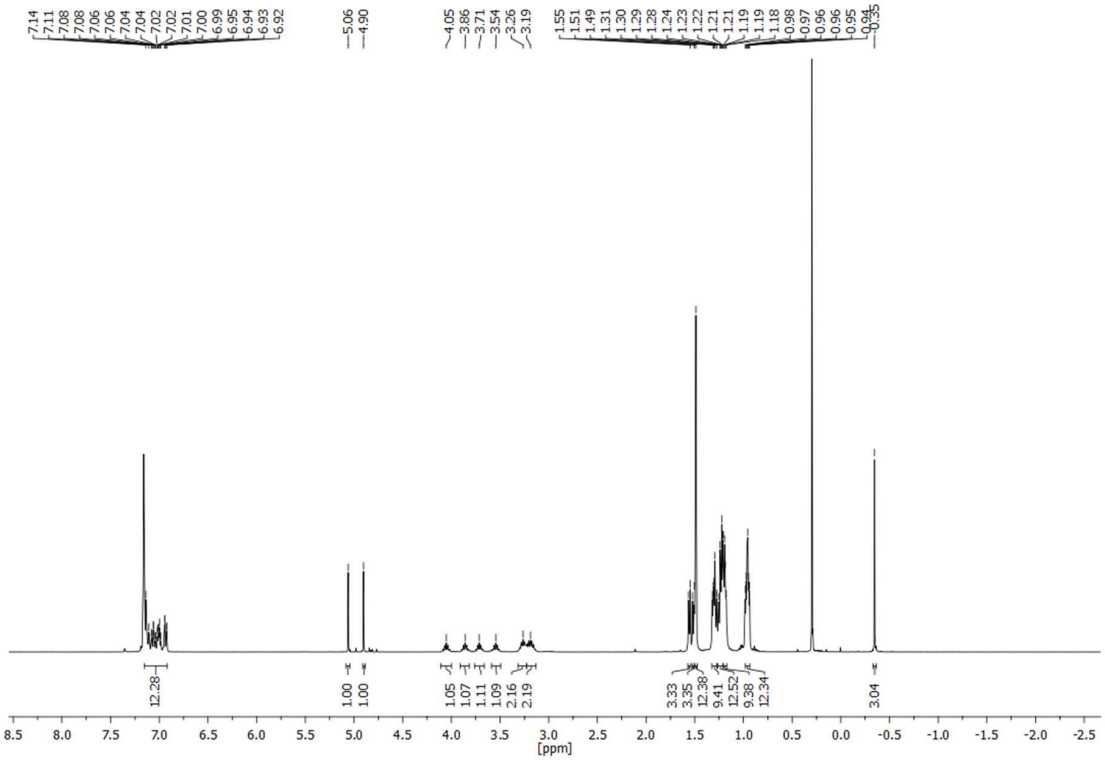

Fig. S18. ^{1}H NMR spectrum of LGa(Cl)Sb(Me)Ga(I)L (**8**) in C_6D_6.

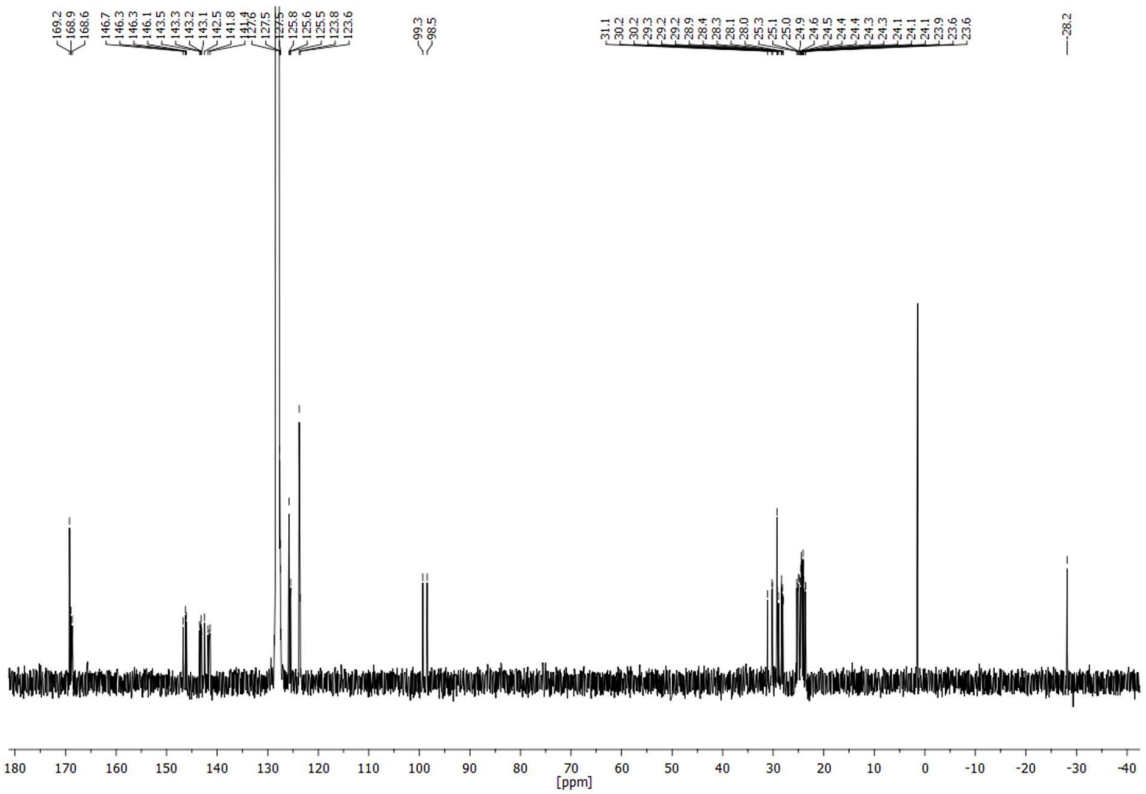

Fig. S19. ^{13}C NMR spectrum of LGa(Cl)Sb(Me)Ga(I)L (**8**) in C_6D_6.

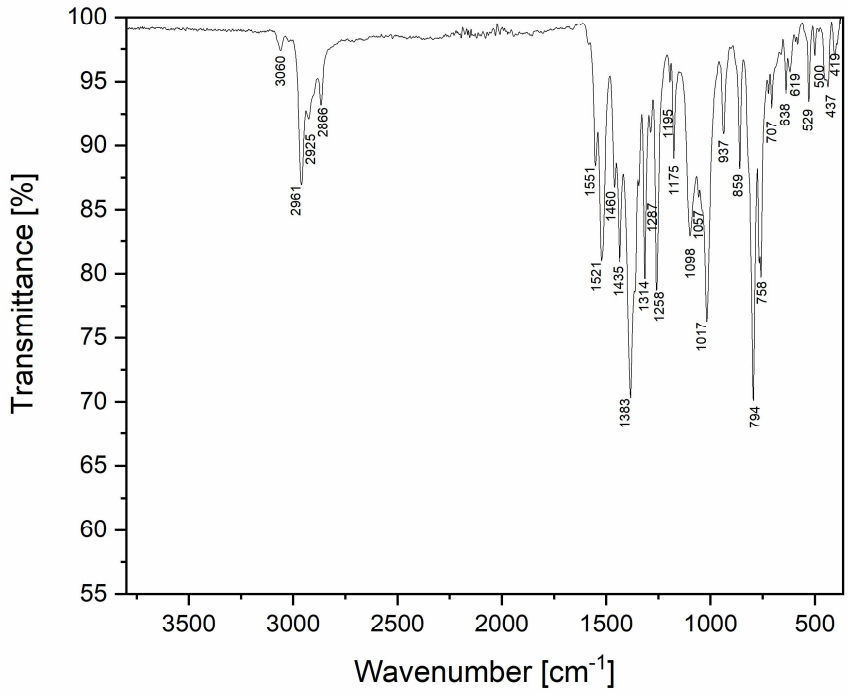

Fig. S20. ATR-IR spectrum of LGa(Cl)Sb(Me)Ga(I)L (**8**).

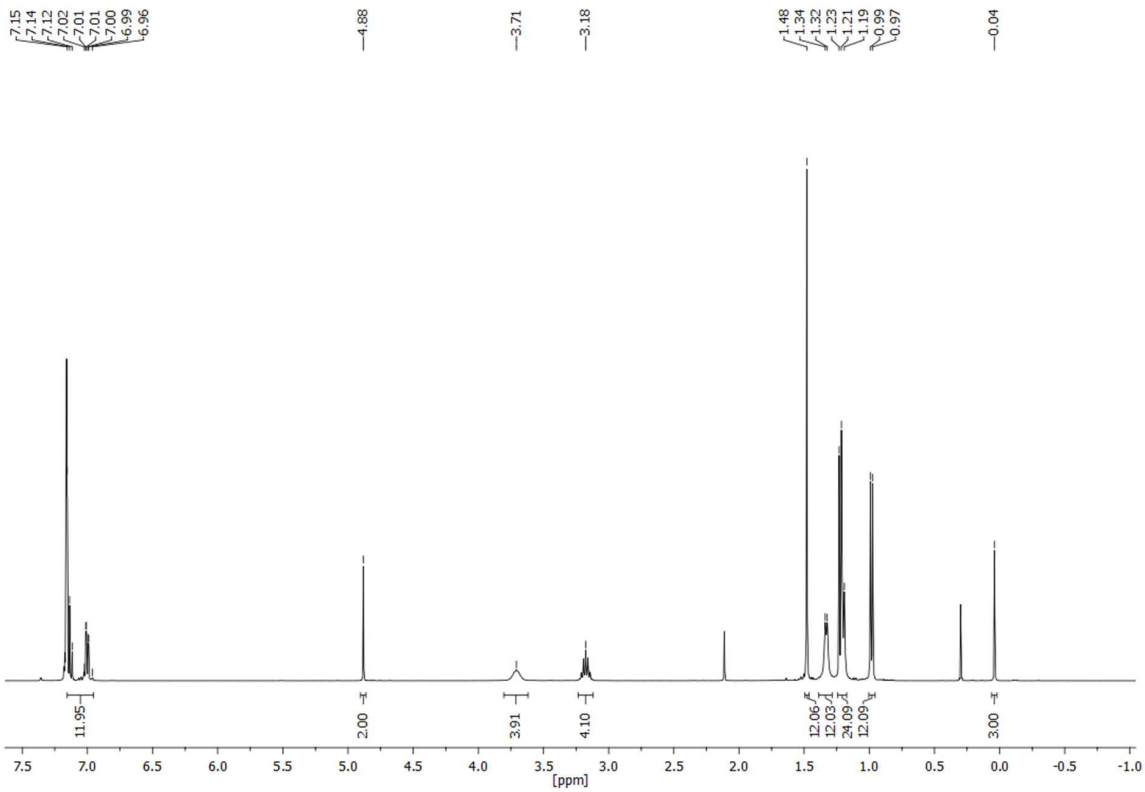

Fig. S21. ^{1}H NMR spectrum of [LGa(Cl)]$_2$AsMe (**9**) in C_6D_6.

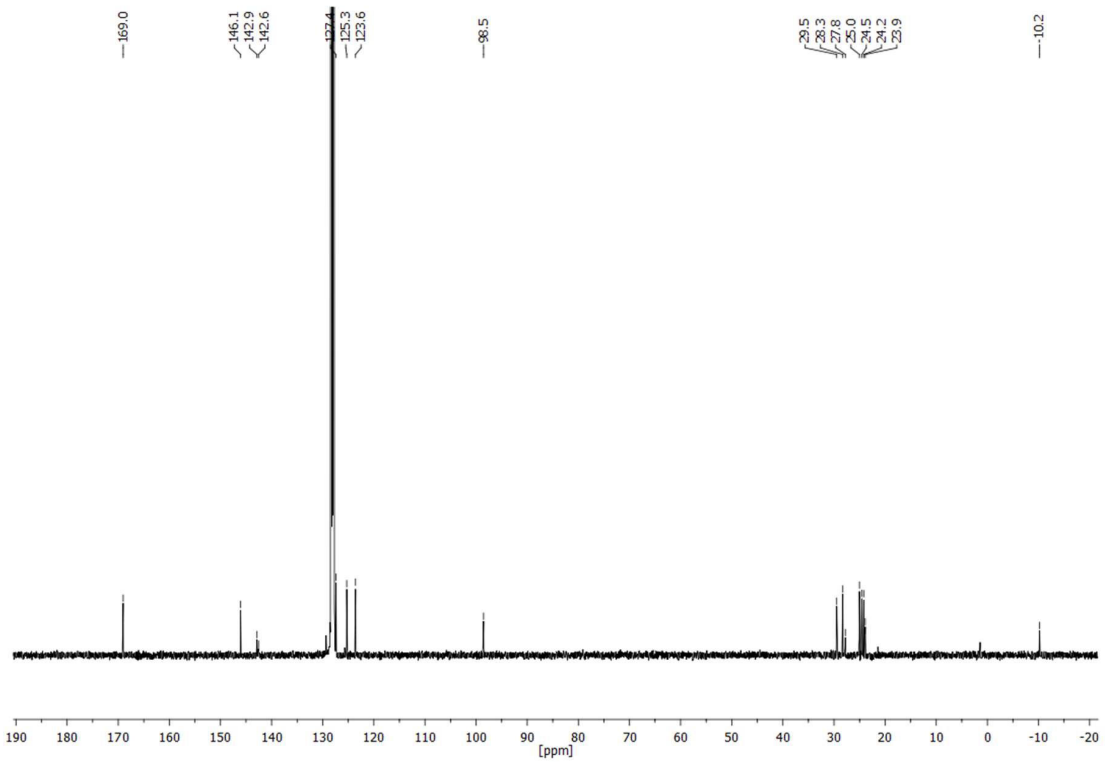

Fig. S22. ^{13}C NMR spectrum of [LGa(Cl)]$_2$AsMe (**9**) in C_6D_6.

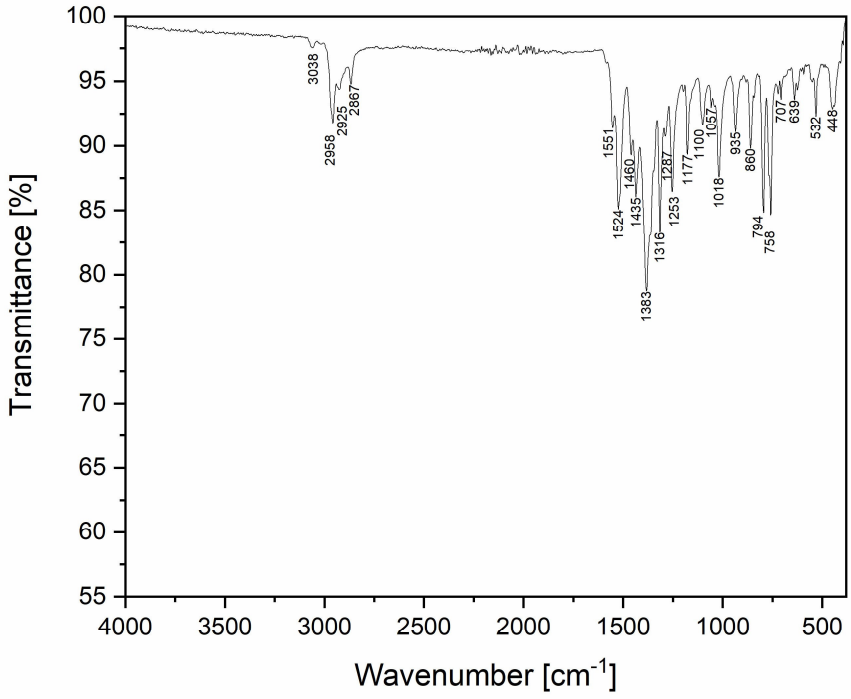

Fig. S23. ATR-IR spectrum of $[LGa(Cl)]_2AsMe$ (**9**).

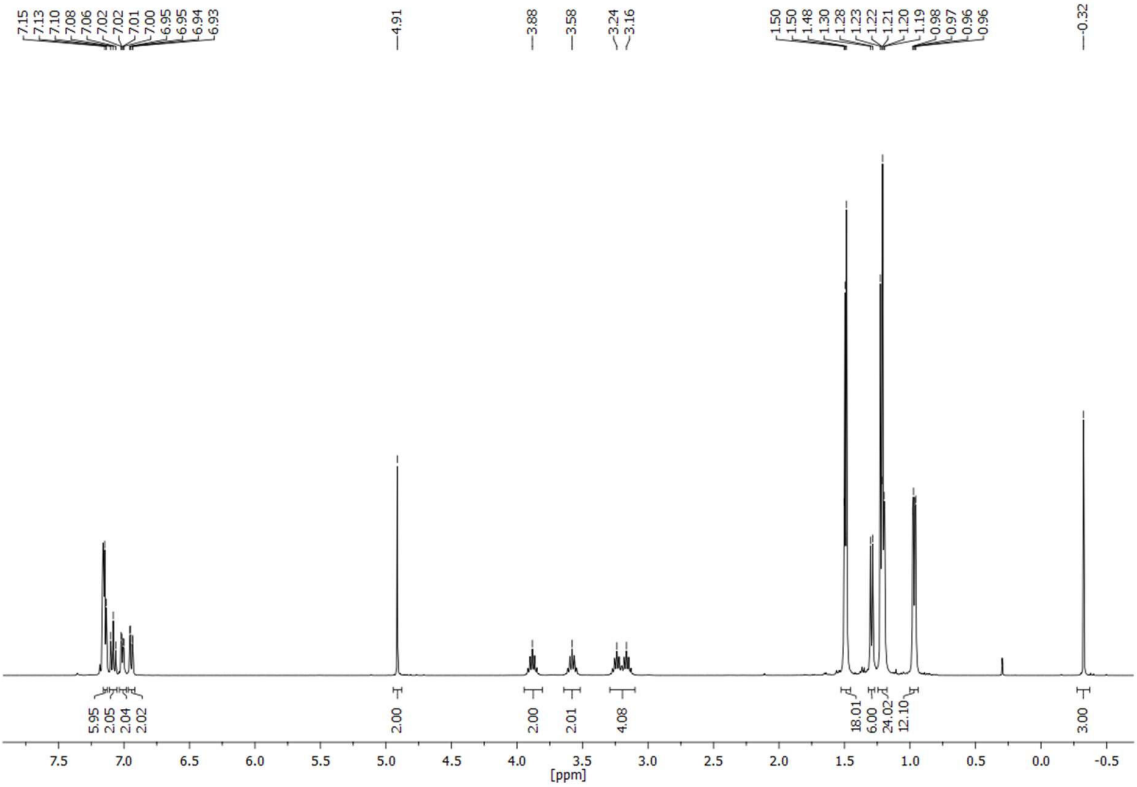

Fig. S24. ^1H NMR spectrum of $[LGa(Cl)]_2SbMe$ (**10**) in C_6D_6.

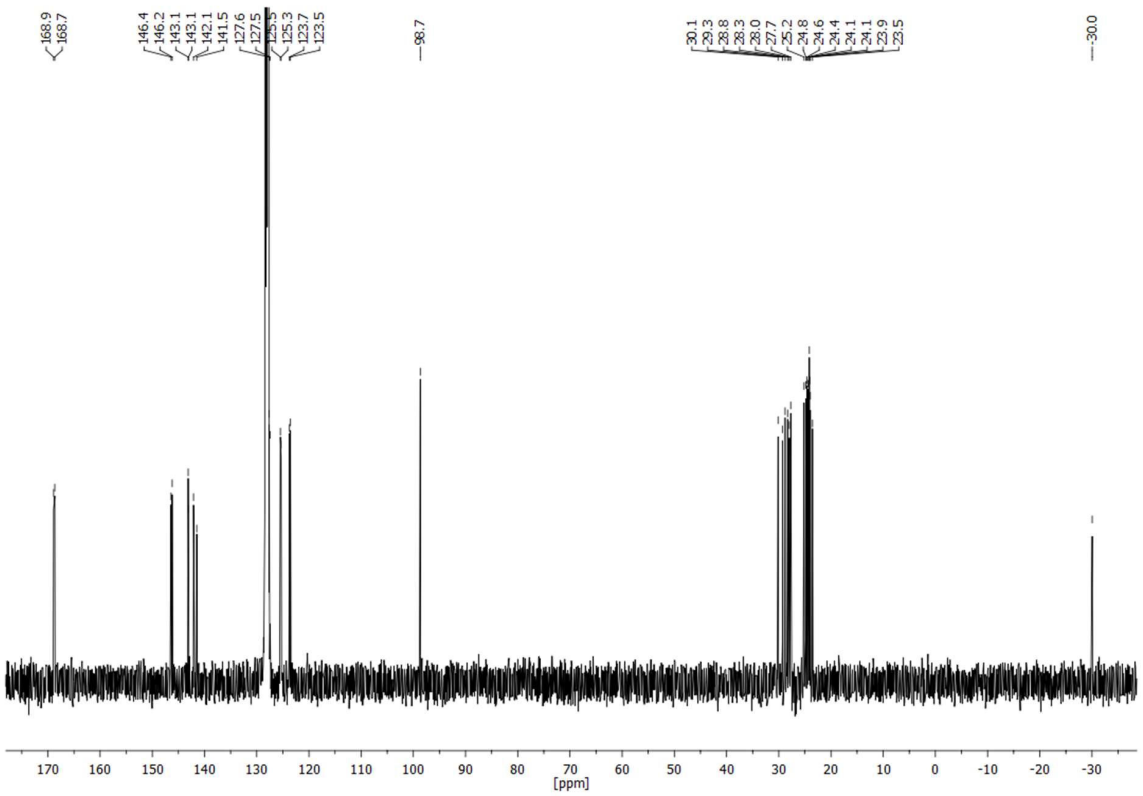

Fig. S25. ^{13}C NMR spectrum of $[LGa(Cl)]_2SbMe$ (**10**) in C_6D_6.

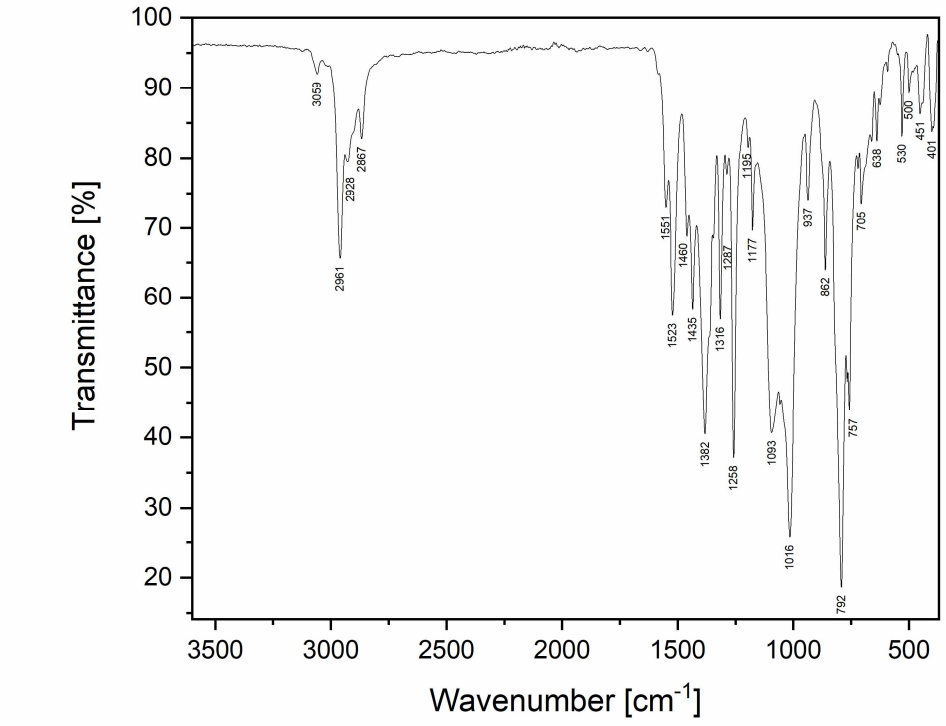

Fig. S26. ATR-IR spectrum of $[LGa(Cl)]_2SbMe$ (**10**).

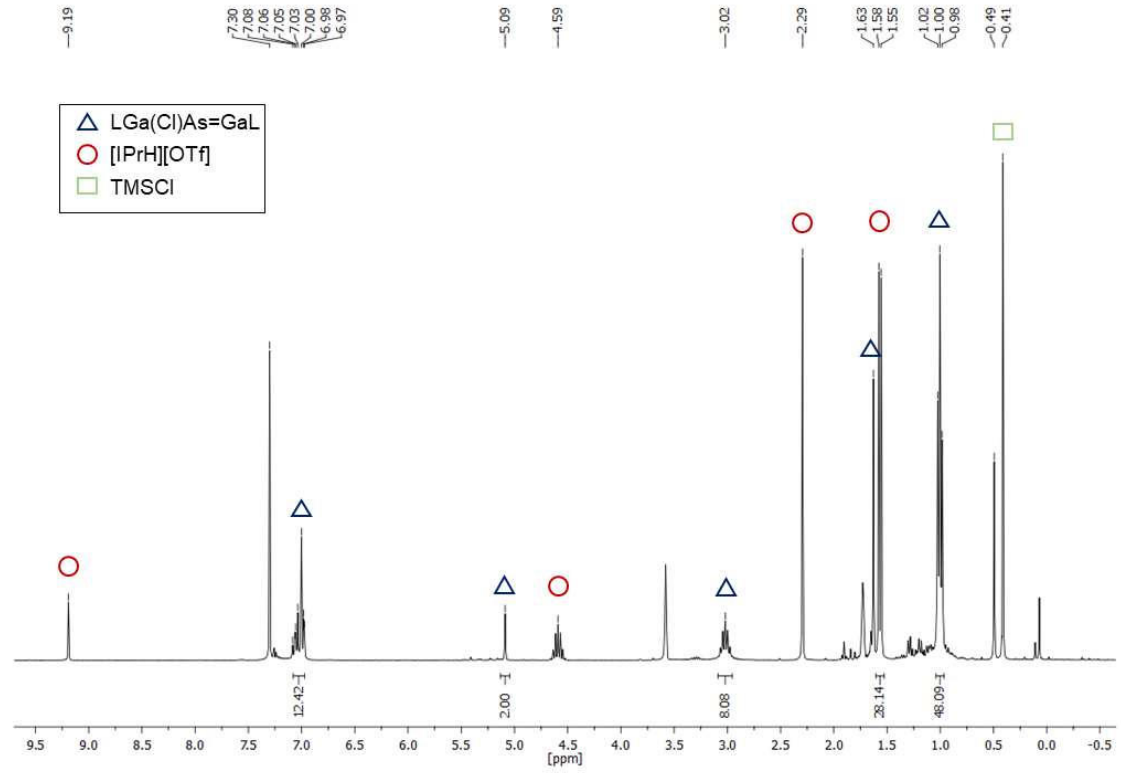

Fig. S27. ^{1}H NMR spectrum of the reaction of [[LGa(Cl)]$_2$As][IPrH] with TMSOTf in THF-d_8.

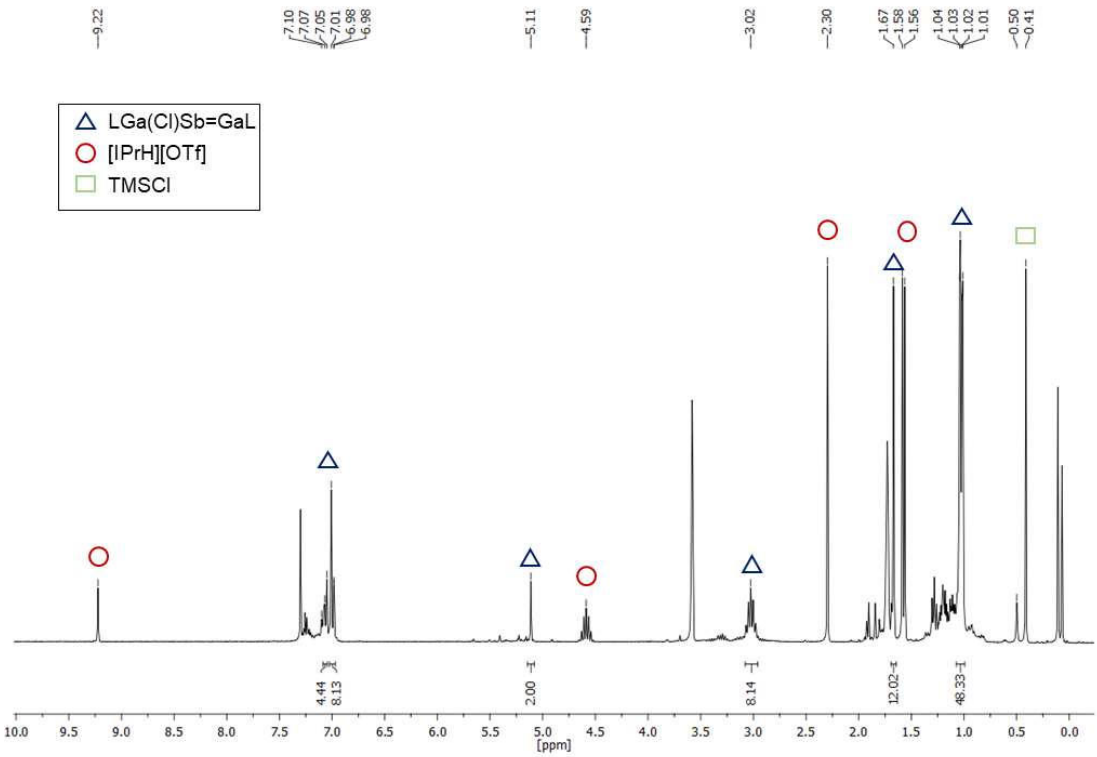

Fig. S28. ^{1}H NMR spectrum of the reaction of [[LGa(Cl)]$_2$Sb][IPrH] with TMSOTf in THF-d_8.

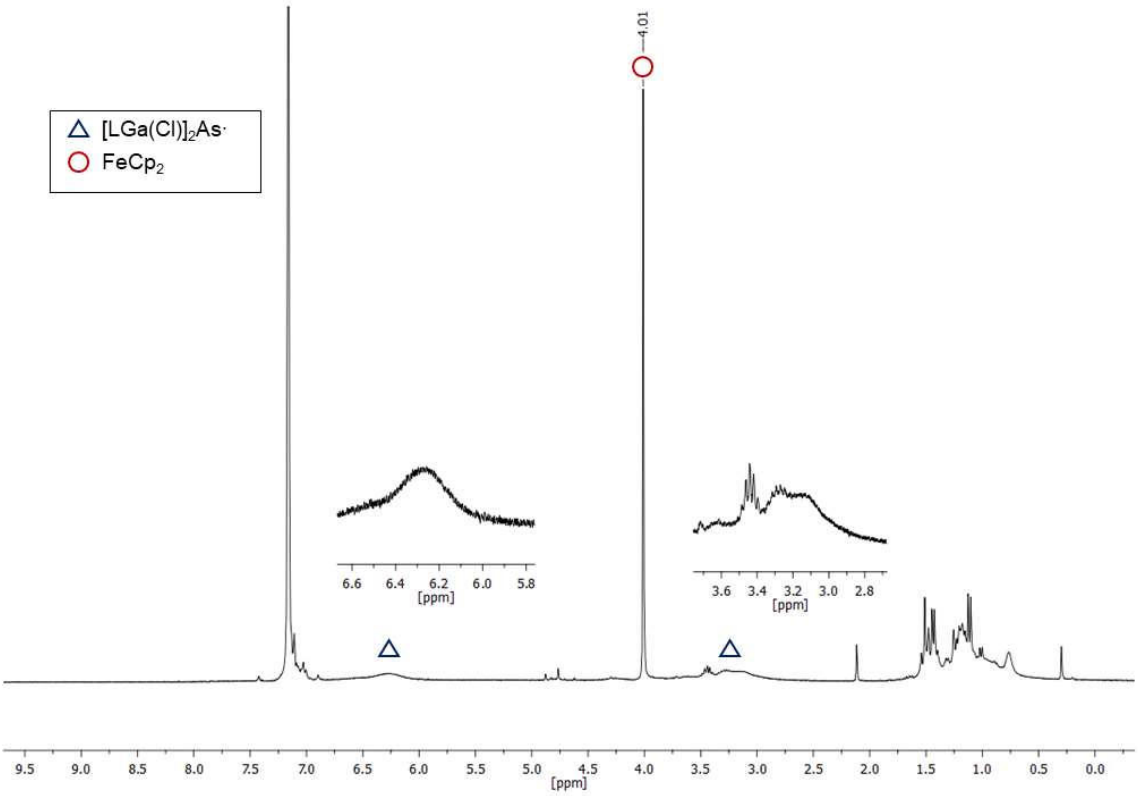

Fig. S29. ^{1}H NMR spectrum of the reaction of [[LGa(Cl)]$_2$As][IPrH] with [FeCp$_2$][BAr$^F{}_4$] in C_6D_6.

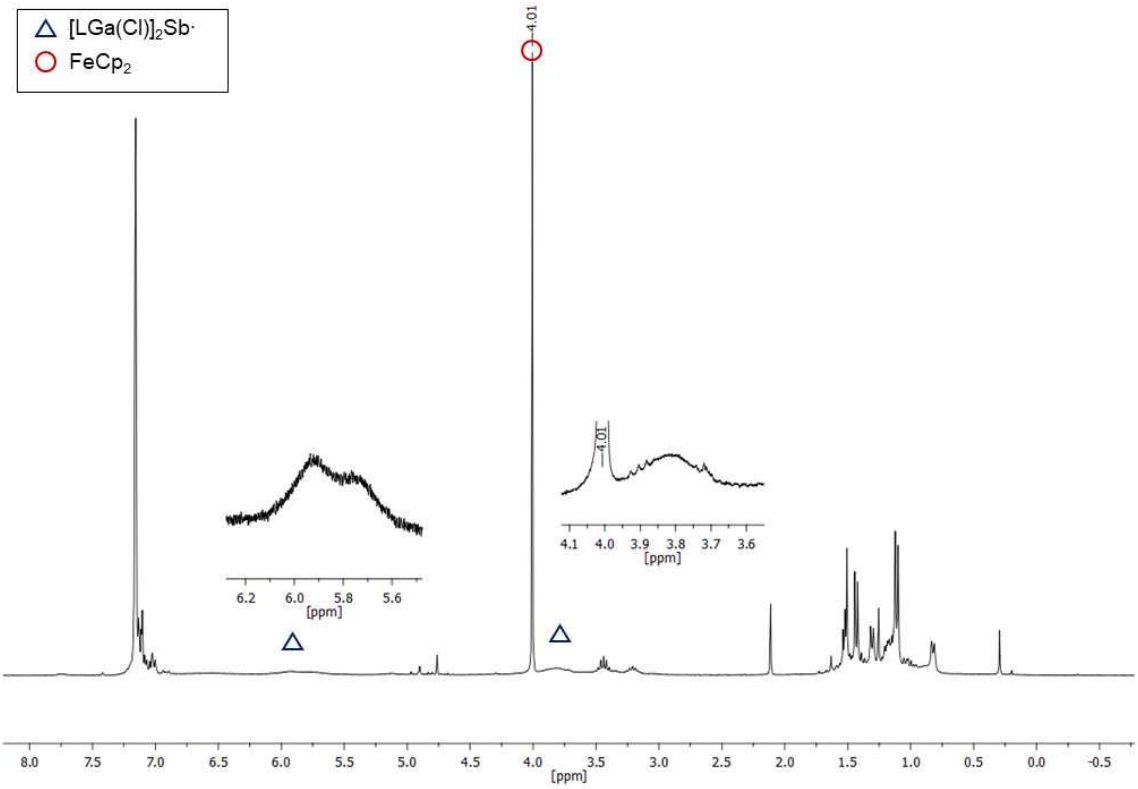

Fig. S30. ^{1}H NMR spectrum of the reaction of [[LGa(Cl)]$_2$Sb][IPrH] with [FeCp$_2$][BAr$^F{}_4$] in C_6D_6.

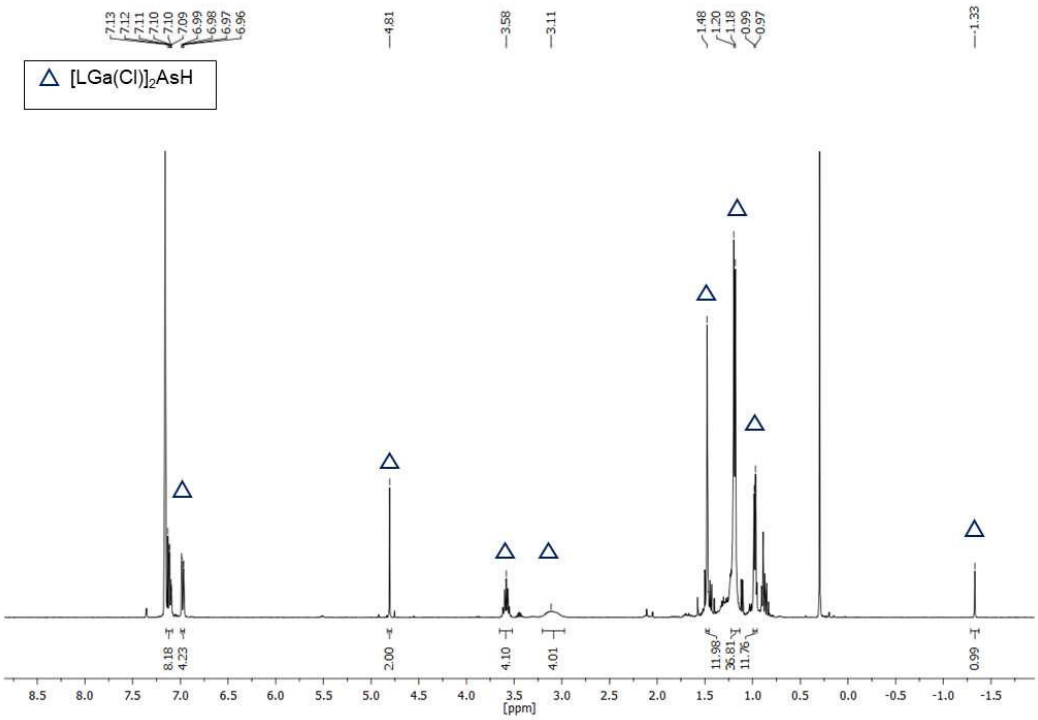

Fig. S31. ^{1}H NMR spectrum of the reaction of LGa(Cl)AsGaL with HCl in C_6D_6.

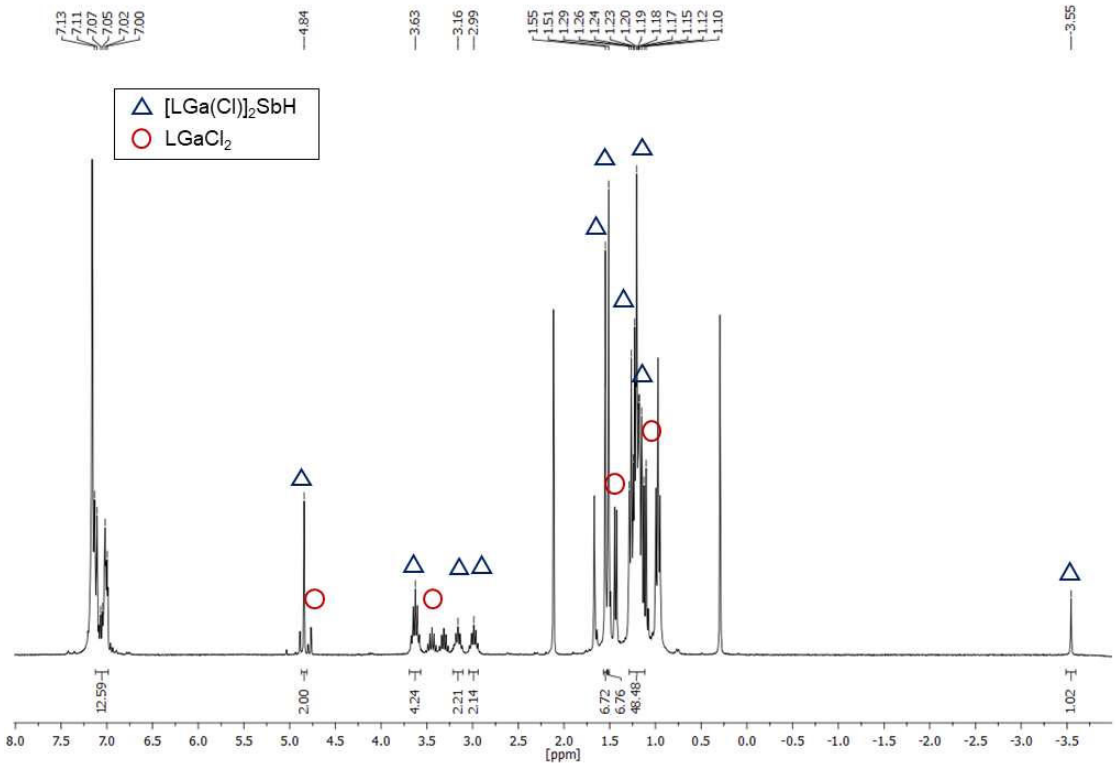

Fig. S32. In situ ^{1}H NMR spectrum of the reaction of LGa(Cl)SbGaL with HCl in C_6D_6.

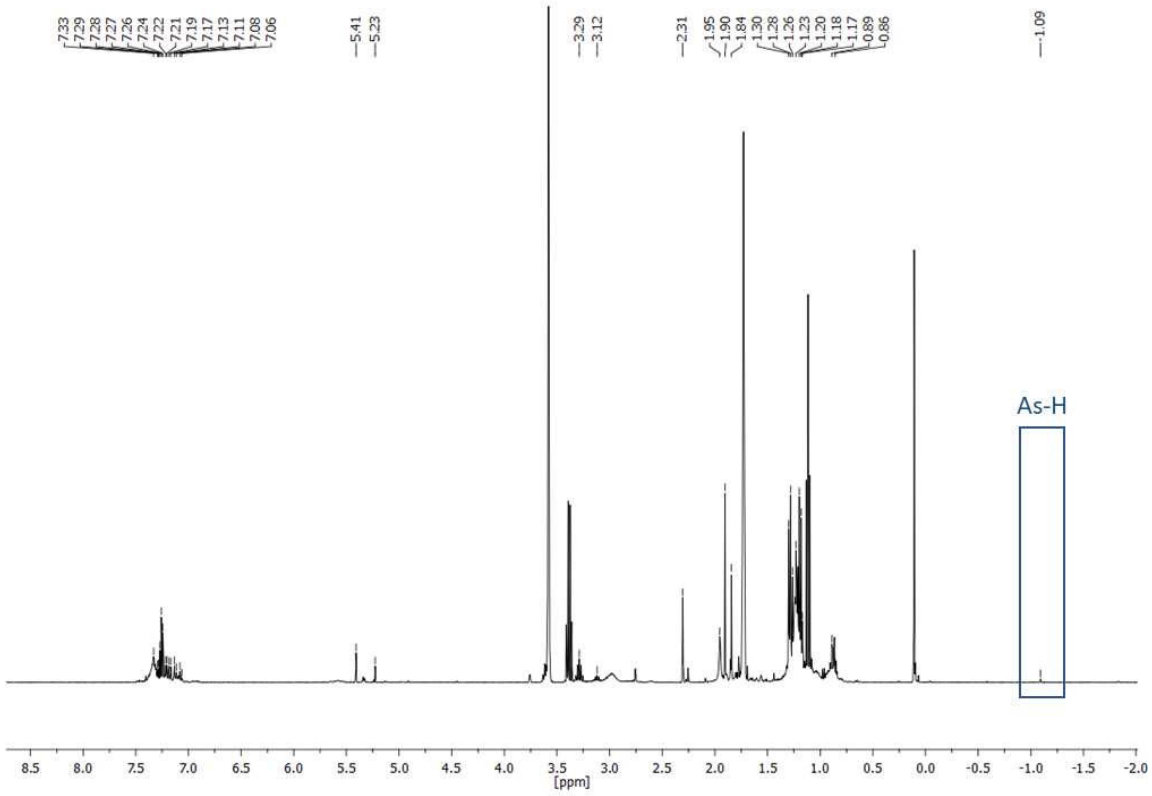

Fig. S33. *In-situ* ^{1}H NMR spectrum of the reaction of LGa(Cl)AsGaL with $[H(OEt_2)_2][BAr^F{}_4]$ in THF-d_8.

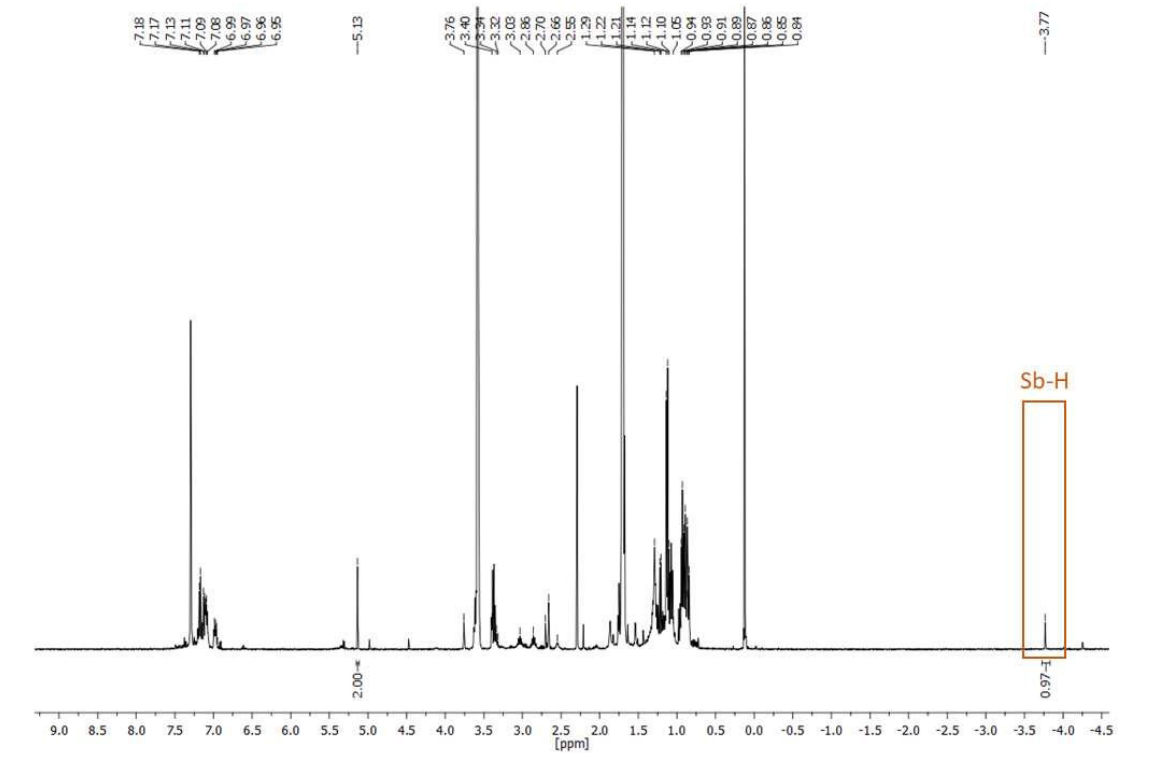

Fig. S34. *In-situ* ^{1}H NMR spectrum of the reaction of LGa(Cl)SbGaL with $[H(OEt_2)_2][Al(OC(CF_3)_3)_4]$ in THF-d_8.

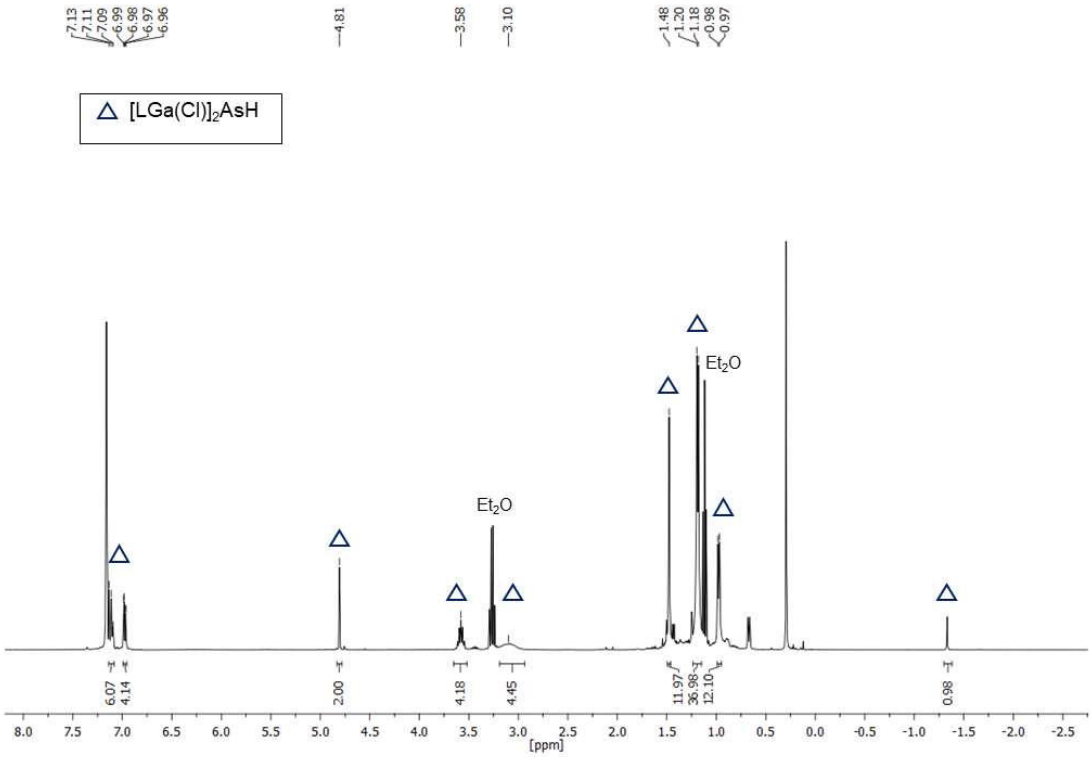

Fig. S35. ^{1}H NMR spectrum of the product from the stepwise reactions of LGa(Cl)AsGaL with $[H(OEt_2)_2][BArF_4]$ and IPrHCl in C_6D_6.

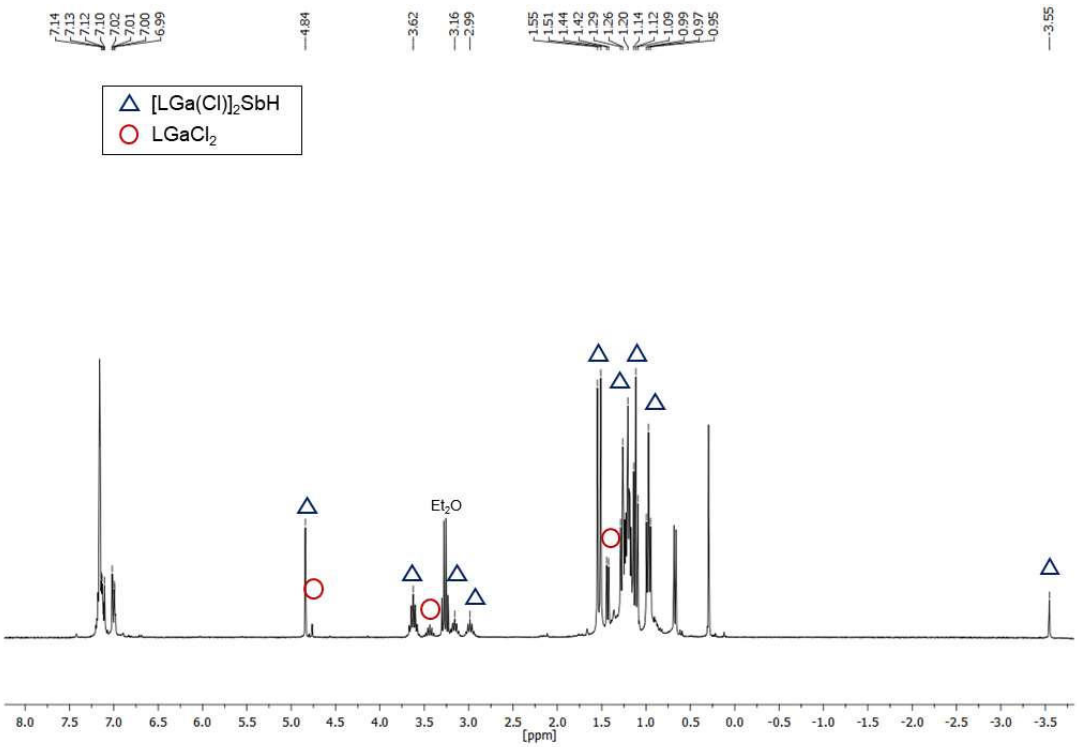

Fig. S36. ^{1}H NMR spectrum of the product from the stepwise reactions of LGa(Cl)SbGaL with $[H(OEt_2)_2][BArF_4]$ and IPrHCl in C_6D_6.

C) Cyclic voltammetry

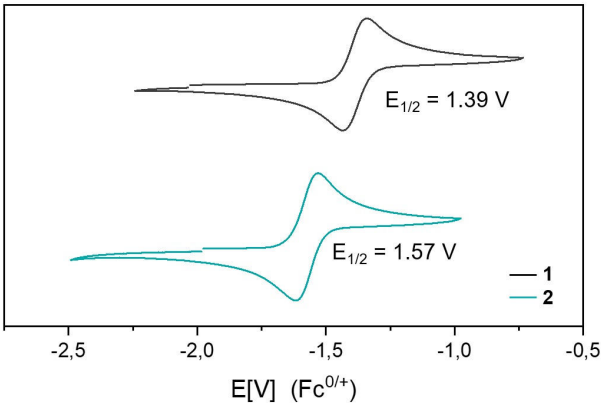

Fig. S37. Cyclic voltammograms of **1** and **2** in THF solution (1 mM) containing [n-Bu_4N][B(3,5-$(CF_3)_2$-$C_6H_3)_4$] (50 mM) as electrolyte at 100 mV s^{-1} scan rate.

D) Crystallographic Part

The crystals were mounted on nylon loops in inert oil. Data of **1** (jk_332_sq), **2** (jk_186), **5** (jk_460) and **9** (jk_347) were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) and data of **6** (jk_489), **7** (jk_577), **8** (jk_573) and **10** (jk_312) were collected on a Bruker AXS D8 Venture diffractometer with Photon II detector (mono-chromated $Cu_{K\alpha}$ radiation, λ = 1.54178 Å, micro-focus source) at 100(2) K and 120 K (**7**). The structures were solved by Direct Methods (SHELXS-97)[6] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2014).[7,8] Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX2/3). Hydrogen atoms were refined using a riding model or rigid methyl groups. In **1** (jk_332_sq) the i-Pr groups of the cation are disordered over two positions. The corresponding bond lengths were restrained to be equal (SADI). RIGU restraints were applied to the anisotropic displacement parameters of the disordered atoms. For the central C atoms additional SIMU restraints were used. The structure contains highly disordered molecules of benzene and THF. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run.[9] Missing atoms were included in the sum formula for completeness. In **2** (jk_186) an i-Pr group and a benzene molecule are disordered. The corresponding bond lengths and angles of the i-Pr groups were restrained to be equal (SADI) and its atoms' anisotropic displacement parameters were restrained with RIGU. The bond lengths of all benzene molecules were restrained to be equal to 1.39 Å (DFIX). The As-H atom of **5** (jk_460) was identified in a difference Fourier map calculated only from the low angle data. The orientation found was realistic but the distance of 1.27 Å was rather short thus the bond length restrained to be equal to 1.52 Å (DFIX). All other parameters were refined freely. To exclude a misinterpretation of Fourier truncation effects the existence of this H atom was confirmed by ^{1}H-NMR spectroscopy. Despite large detector distance and small scan width per frame the integration was hampered by overlapping reflections. The worst runs were discarded leading to a reduced redundancy and a completeness of only 94% at high angles. The Sb-H atom of **6** (jk_498) was refined freely with its bond length restrained to be equal to 1.7 Å (DFIX) and its displacement parameter constrained to 1.2 times the equivalent U_{ij} of the Sb atom. Since the original residual density peak was found (at realistic orientation) in the range of the fourier truncation peaks the existence of the H was additionally confirmed by H-NMR spectroscopic studies. I and Cl atoms in **7** (jk_577) are disordered. The Ga–Cl and Ga–I bond length of both components were restrained to be equal (SADI). Due to the proximity of the alternate positions the displacement parameters were constrained to be equal (EADP). A di-isopropyl phenyl ligand is disordered over two positions. All its corresponding bond length and angle were restrained to be equal (SADI). RIGU and SIMU restraints were applied to the anisotropic displacement parameters of these atoms. Attempts to refine the approx 4e- peak near As1 as alternate orientation of the AsMe unit failed. A suitable peak for the methyl group could be found but refining it did not yield reasonable results. Cl and I atoms in **8** (jk_573) are disordered. The bond lengths of both orientations were restrained to be equal (SADI) and the neighbouring atoms were refined with common anisotropic displacement parameters (EADP). The highest residual density peak approx. 0.8 Å near Sb1 is likely a result of Fourier truncation effects. Refining it as second orientation of Sb1 does reduce the R-values, but no suitable electron density peak for the methyl group can be found, thus this model was discarded.

CCDC-2034837 (**1**), -2034838 (**2**), -2034839 (**5**), -2034840 (**6**), -2043843 (**7**), -2042636 (**8**), -2034841 (**9**) and -2034842 (**10**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

Table S1. Crystallographic details of **1**, **2**, **5** and **6**

	1	**2**	**5**	**6**
Empirical formula	$C_{89}H_{131}AsCl_2Ga_2N_6O_2$	$C_{96}H_{130}Cl_2Ga_2N_6Sb$	$C_{61}H_{90}AsCl_2Ga_2N_4$	$C_{61}H_{90}Cl_2Ga_2N_4Sb$
M [g mol^{-1}]	1602.25	1700.14	1164.62	1211.45
Crystal size [mm]	0.395 × 0.251 × 0.115	0.371 × 0.137 × 0.130	0.310 × 0.282 × 0.205	0.147 × 0.139 × 0.068
T [K]	100(2)	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	monoclinic	monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$P2_1/n$
a [Å]	13.1432(14)	12.9336(10)	12.040(3)	12.2314(5)
b [Å]	18.927(2)	18.4527(16)	41.955(9)	41.5482(15)
c [Å]	19.015(2)	19.8000(16)	13.217(3)	13.1137(5)
α [°]	100.016(6)	93.287(5)	90	90
β [°]	101.582(6)	91.716(4)	112.218(11)	111.6273(17)
γ [°]	104.695(6)	102.306(4)	90	90
V [Å^3]	4354.5(8)	4605.0(7)	6181(2)	6195.1(4)
Z	2	2	4	4
D_{calcd} [g cm^{-3}]	1.222	1.226	1.252	1.299
μ(K_α [mm^{-1}])	1.105 (Mo)	0.976 (Mo)	1.528 (Mo)	5.527 (Cu)
Transmissions	0.75/0.66	0.75/0.59	0.75/0.63	0.75/0.61
F(000)	1704	1790	2452	2524
Index ranges	-18 ≤ h ≤ 16	-20 ≤ h ≤ 13	-15 ≤ h ≤ 18	-15 ≤ h ≤ 15
	-27 ≤ k ≤ 26	-26 ≤ k ≤ 28	-64 ≤ k ≤ 64	-53 ≤ k ≤ 52
	-27 ≤ l ≤ 27	-30 ≤ l ≤ 25	-20 ≤ l ≤ 16	-16 ≤ l ≤ 16
θ_{max} [°]	30.751	33.383	33.628	80.448
Reflections collected	150267	101351	84728	273138
Independent reflections	26307	32463	23017	13549
R_{int}	0.0350	0.0420	0.0265	0.0595
Refined parameters	861	1066	656	655
R_1 [$I > 2\sigma(I)$]	0.0432	0.0375	0.0423	0.0339
wR_2 [all data]	0.1278	0.0929	0.1052	0.0887
GooF	1.037	1.009	1.088	1.031
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	1.201/-0.520	1.661/-1.080	1.288/-0.992	0.970/-1.386

Table S2. Crystallographic details of **7**, **8**, **9** and **10**.

	7	**8**	**9**	**10**
Empirical formula	$C_{59}H_{85}AsClGa_2IN_4$	$C_{59}H_{85}ClGa_2IN_4Sb$	$C_{59}H_{85}AsCl_2Ga_2N_4$	$C_{59}H_{85}Cl_2Ga_2N_4Sb$
M [g mol^{-1}]	1227.02	1273.84	1135.56	1182.40
Crystal size [mm]	0.222 × 0.205 × 0.081	0.450 × 0.203 × 0.064	0.120 × 0.090 × 0.050	0.281 × 0.157 × 0.133
T [K]	100(2)	120(2)	100(2)	100(2)
Crystal system	triclinic	monoclinic	triclinic	triclinic
Space group	$P\bar{1}$	$P2_1/n$	$P\bar{1}$	$P\bar{1}$
a [Å]	12.0283(4)	13.143(3)	11.8191(11)	12.0390(17)
b [Å]	13.4279(4)	20.082(5)	13.5581(12)	13.6260(19)
c [Å]	20.1073(6)	22.477(5)	19.9868(18)	19.833(3)
α [°]	80.1899(17)	90	79.651(4)	79.981(4)
β [°]	85.0967(18)	101.298(7)	84.731(5)	84.097(4)
γ [°]	65.8065(17)	90	66.276(4)	66.850(4)
V [Å^3]	2918.62(16)	5818(2)	2883.7(5)	2943.8(7)
Z	2	4	2	2
D_{calcd} [g cm^{-3}]	1.396	1.454	1.308	1.334
μ(K_α [mm^{-1}])	6.624	1.997	1.636 (Mo)	5.803 (Cu)
Transmissions	0.75/0.38	0.75/0.50	0.75/0.68	0.75/0.62
F(000)	1264	2600	1192	1228
Index ranges	-15 ≤ h ≤ 15	-18 ≤ h ≤ 18	-16 ≤ h ≤ 16	-15 ≤ h ≤ 15
	-17 ≤ k ≤ 17	-28 ≤ k ≤ 28	-19 ≤ k ≤ 19	-17 ≤ k ≤ 17
	-23 ≤ l ≤ 25	-32 ≤ l ≤ 32	-28 ≤ l ≤ 28	-25 ≤ l ≤ 25
θ_{max} [°]	81.960	30.531	30.781	81.146
Reflections collected	143658	253879	146102	236084
Independent reflections	12743	17756	17914	12822
R_{int}	0.0717	0.0556	0.0887	0.0619
Refined parameters	755	641	634	634
R_1 [$I > 2\sigma(I)$]	0.0550	0.0329	0.0383	0.0599
wR_2 [all data]	0.1596	0.0771	0.0804	0.1392
GooF	1.079	1.123	1.015	1.038
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	3.299/-2.042	4.605/-1.911	1.541/-1.002	6.251/-4.221

Table S3. Selected bond lengths [Å] and angles [°] of pnictanides $[LGa(Cl)]_2E[IPrH]$ (E = As **1**, Sb **2**), pnictogen-centered radicals $[LGa(Cl)]_2E^{\bullet}$ (E = As **I**, Sb **II**) and gallapnictenes LGaEGa(Cl)L (E = As **III**, Sb **IV**).[5]

	1	**2**	**I**	**II**	**III**	**IV**
Ga1-E	2.3171(4)	2.5169(3)	2.3983(11)	2.5899(4)	2.2628(5);	2.4629(2)
Ga2-E	2.3197(4)	2.5186(3)	2.4085(14)	2.5909(3)	2.3503(4)	2.5528(2)
Ga1-Cl1	2.2943(6)	2.2611(5)	2.1967(10)	2.1623(9)	-	-
Ga2-Cl2	2.2548(7)	2.3012(5)	2.2069(10)	2.2028(7)	2.2783(9)	2.2409(5)
Ga1-E-Ga2	107.377(15)	104.534(9)	109.43(6)	104.89(1)	111.419(19	113.184(7)

Table S4. Central structural bond lengths [Å] and angles [°] of **1**, **2**, **5** and **6**.

	1 (E = As)	**2** (E = Sb)	**5**(E = As)	**6** (E = Sb)
Ga1–E	2.3171(4)	2.5169(3)	2.4156(5)	2.5669(3)
Ga2–E	2.3197(4)	2.5186(3)	2.4000(6)	2.5803(3)
Ga1–Cl1	2.2943(6)	2.2611(5)	2.2320(6)	2.2161(6)
Ga2–Cl2	2.2548(7)	2.3012(5)	2.2104(6)	2.2012(6)
Ga1–E–Ga2	107.377(15)	104.534(9)	110.566(13)	107.412(10)

Table S5. Central structural bond lengths [Å] and angles [°] of **7**–**10**.

	7 (E = As, X = I)	**8** (E = Sb X = I,)	**9** (E = As, X = Cl)	**10** (E = Sb, X = Cl)
E–C	1.939(6)	2.164(3)	1.990(2)	2.129(7)
Ga1–E	2.4232(6)	2.6118(6)	2.4044(4)	2.5837(7)
Ga2–E	2.3946(6)	2.6132(5)	2.4134(4)	2.6045(6)
Ga1–Cl1	2.193(5), 2.166(6)	2.228(8), 2.2300(14)	2.2045(6)	2.2084(12)
Ga2–X2	2.5169(7), 2.5197(19)	2.5973(6), 2.495(5)	2.2003(6)	2.2103(12)
Ga1–E–Ga2	110.14(2)	111.076(12)	108.431(12)	106.652(19)

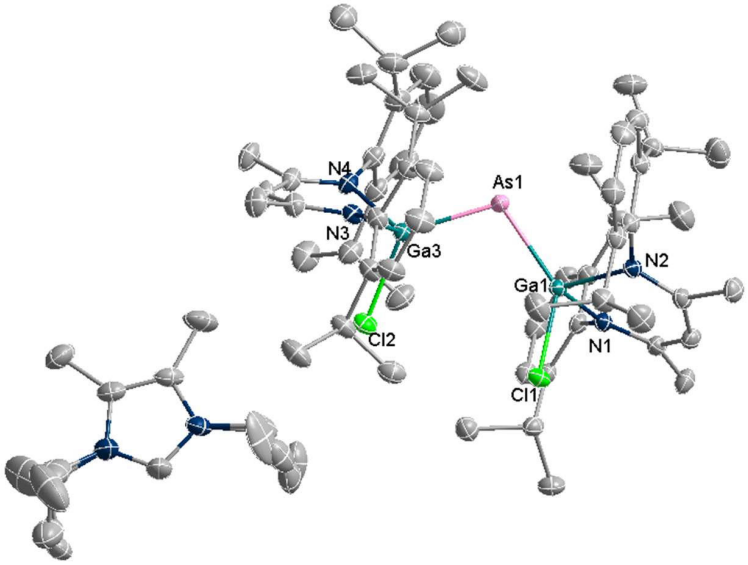

Fig. S38. Solid state structure of **1**. Hydrogen atoms and minor component of the disorder are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S6: Bond lengths [Å] for **1** (jk_332m).

As(1)-Ga(3)	2.3171(4)	C(9)-C(10)	1.378(4)	C(41)-C(42)	1.533(4)
As(1)-Ga(1)	2.3197(4)	C(10)-C(11)	1.397(3)	C(44)-C(45)	1.529(4)
Ga(1)-N(2)	2.0139(18)	C(11)-C(15)	1.521(3)	C(44)-C(46)	1.532(4)
Ga(1)-N(1)	2.0166(18)	C(12)-C(14)	1.532(3)	C(47)-C(52)	1.403(4)
Ga(1)-Cl(1)	2.2943(6)	C(12)-C(13)	1.538(3)	C(47)-C(48)	1.405(3)
Ga(3)-N(4)	2.0063(18)	C(15)-C(17)	1.521(4)	C(48)-C(49)	1.390(4)
Ga(3)-N(3)	2.0093(19)	C(15)-C(16)	1.552(4)	C(48)-C(53)	1.519(4)
Ga(3)-Cl(2)	2.2548(7)	C(18)-C(19)	1.402(3)	C(49)-C(50)	1.387(5)
N(1)-C(1)	1.336(3)	C(18)-C(23)	1.410(3)	C(50)-C(51)	1.384(5)
N(1)-C(6)	1.445(3)	C(19)-C(20)	1.403(3)	C(51)-C(52)	1.388(4)
N(2)-C(3)	1.328(3)	C(19)-C(24)	1.510(4)	C(52)-C(56)	1.520(4)
N(2)-C(18)	1.445(3)	C(20)-C(21)	1.376(4)	C(53)-C(54)	1.531(3)
N(3)-C(30)	1.336(3)	C(21)-C(22)	1.378(4)	C(53)-C(55)	1.535(4)
N(3)-C(35)	1.439(3)	C(22)-C(23)	1.393(3)	C(56)-C(58)	1.523(4)
N(4)-C(32)	1.326(3)	C(23)-C(27)	1.520(4)	C(56)-C(57)	1.525(4)
N(4)-C(47)	1.442(3)	C(24)-C(26)	1.525(4)	C(60)-C(61)	1.344(4)
N(5)-C(59)	1.328(3)	C(24)-C(25)	1.536(4)	C(60)-C(68)	1.488(4)
N(5)-C(60)	1.389(3)	C(27)-C(29)	1.521(4)	C(61)-C(69)	1.490(4)
N(5)-C(62')	1.476(13)	C(27)-C(28)	1.529(4)	C(62)-C(64)	1.509(8)
N(5)-C(62)	1.481(8)	C(30)-C(31)	1.404(3)	C(62)-C(63)	1.515(10)
N(6)-C(59)	1.336(4)	C(30)-C(33)	1.510(3)	C(62')-C(63')	1.513(13)
N(6)-C(61)	1.378(3)	C(31)-C(32)	1.400(3)	C(62')-C(64')	1.516(13)
N(6)-C(65)	1.488(5)	C(32)-C(34)	1.515(3)	C(65)-C(66)	1.511(6)
N(6)-C(65')	1.489(15)	C(35)-C(36)	1.400(3)	C(65)-C(67)	1.518(8)
C(1)-C(2)	1.406(3)	C(35)-C(40)	1.413(3)	C(65')-C(67')	1.511(15)

C(1)-C(4)	1.506(3)	C(36)-C(37)	1.398(3)	C(65')-C(66')	1.516(14)
C(2)-C(3)	1.402(3)	C(36)-C(41)	1.525(3)	C11-C21	1.377(4)
C(3)-C(5)	1.513(3)	C(37)-C(38)	1.384(4)	C11-C61	1.382(5)
C(6)-C(11)	1.402(3)	C(38)-C(39)	1.384(4)	C21-C31	1.382(4)
C(6)-C(7)	1.410(3)	C(39)-C(40)	1.387(3)	C31-C41	1.376(5)
C(7)-C(8)	1.398(3)	C(40)-C(44)	1.518(3)	C41-C51	1.380(4)
C(7)-C(12)	1.515(3)	C(41)-C(43)	1.521(4)	C51-C61	1.375(4)
C(8)-C(9)	1.384(4)				

Table S7: Bond angles [°] for **1** (jk_332m).

Ga(3)-As(1)-Ga(1)	107.377(15)	C(19)-C(24)-C(25)	111.6(2)
N(2)-Ga(1)-N(1)	92.78(7)	C(26)-C(24)-C(25)	109.9(2)
N(2)-Ga(1)-Cl(1)	98.11(6)	C(23)-C(27)-C(29)	112.8(2)
N(1)-Ga(1)-Cl(1)	95.58(6)	C(23)-C(27)-C(28)	112.3(2)
N(2)-Ga(1)-As(1)	108.27(5)	C(29)-C(27)-C(28)	110.1(2)
N(1)-Ga(1)-As(1)	123.38(5)	N(3)-C(30)-C(31)	123.9(2)
Cl(1)-Ga(1)-As(1)	130.34(2)	N(3)-C(30)-C(33)	120.6(2)
N(4)-Ga(3)-N(3)	91.42(8)	C(31)-C(30)-C(33)	115.5(2)
N(4)-Ga(3)-Cl(2)	99.86(6)	C(32)-C(31)-C(30)	126.9(2)
N(3)-Ga(3)-Cl(2)	97.59(6)	N(4)-C(32)-C(31)	123.9(2)
N(4)-Ga(3)-As(1)	112.19(6)	N(4)-C(32)-C(34)	120.1(2)
N(3)-Ga(3)-As(1)	122.03(5)	C(31)-C(32)-C(34)	116.0(2)
Cl(2)-Ga(3)-As(1)	126.56(2)	C(36)-C(35)-C(40)	120.9(2)
C(1)-N(1)-C(6)	117.19(18)	C(36)-C(35)-N(3)	120.7(2)
C(1)-N(1)-Ga(1)	120.73(15)	C(40)-C(35)-N(3)	118.4(2)
C(6)-N(1)-Ga(1)	122.05(13)	C(37)-C(36)-C(35)	118.5(2)
C(3)-N(2)-C(18)	119.15(18)	C(37)-C(36)-C(41)	118.6(2)
C(3)-N(2)-Ga(1)	121.57(15)	C(35)-C(36)-C(41)	122.8(2)
C(18)-N(2)-Ga(1)	119.05(14)	C(38)-C(37)-C(36)	120.9(2)
C(30)-N(3)-C(35)	117.60(19)	C(39)-C(38)-C(37)	119.8(2)
C(30)-N(3)-Ga(3)	121.19(15)	C(38)-C(39)-C(40)	121.3(2)
C(35)-N(3)-Ga(3)	120.80(15)	C(39)-C(40)-C(35)	118.3(2)
C(32)-N(4)-C(47)	120.61(19)	C(39)-C(40)-C(44)	120.7(2)
C(32)-N(4)-Ga(3)	121.26(16)	C(35)-C(40)-C(44)	120.9(2)
C(47)-N(4)-Ga(3)	117.91(14)	C(43)-C(41)-C(36)	109.8(2)
C(59)-N(5)-C(60)	108.4(2)	C(43)-C(41)-C(42)	109.5(2)
C(59)-N(5)-C(62')	126.9(10)	C(36)-C(41)-C(42)	113.1(2)
C(60)-N(5)-C(62')	124.3(10)	C(40)-C(44)-C(45)	111.0(2)
C(59)-N(5)-C(62)	124.8(6)	C(40)-C(44)-C(46)	112.8(2)
C(60)-N(5)-C(62)	126.8(6)	C(45)-C(44)-C(46)	110.5(2)
C(59)-N(6)-C(61)	108.4(2)	C(52)-C(47)-C(48)	121.0(2)
C(59)-N(6)-C(65)	125.4(3)	C(52)-C(47)-N(4)	118.8(2)
C(61)-N(6)-C(65)	126.2(3)	C(48)-C(47)-N(4)	120.1(2)

C(59)-N(6)-C(65')	119.0(14)	C(49)-C(48)-C(47)	118.3(3)
C(61)-N(6)-C(65')	124.8(11)	C(49)-C(48)-C(53)	119.3(2)
N(1)-C(1)-C(2)	124.1(2)	C(47)-C(48)-C(53)	122.4(2)
N(1)-C(1)-C(4)	120.0(2)	C(50)-C(49)-C(48)	121.1(3)
C(2)-C(1)-C(4)	115.9(2)	C(51)-C(50)-C(49)	119.9(3)
C(3)-C(2)-C(1)	128.1(2)	C(50)-C(51)-C(52)	120.8(3)
N(2)-C(3)-C(2)	123.7(2)	C(51)-C(52)-C(47)	118.8(2)
N(2)-C(3)-C(5)	119.8(2)	C(51)-C(52)-C(56)	119.5(3)
C(2)-C(3)-C(5)	116.4(2)	C(47)-C(52)-C(56)	121.6(2)
C(11)-C(6)-C(7)	120.5(2)	C(48)-C(53)-C(54)	111.7(2)
C(11)-C(6)-N(1)	118.58(19)	C(48)-C(53)-C(55)	110.1(2)
C(7)-C(6)-N(1)	120.9(2)	C(54)-C(53)-C(55)	109.7(2)
C(8)-C(7)-C(6)	118.4(2)	C(52)-C(56)-C(58)	112.5(3)
C(8)-C(7)-C(12)	118.6(2)	C(52)-C(56)-C(57)	110.6(2)
C(6)-C(7)-C(12)	123.1(2)	C(58)-C(56)-C(57)	110.7(2)
C(9)-C(8)-C(7)	121.5(2)	N(5)-C(59)-N(6)	108.7(2)
C(10)-C(9)-C(8)	119.4(2)	C(61)-C(60)-N(5)	107.0(2)
C(9)-C(10)-C(11)	121.4(2)	C(61)-C(60)-C(68)	130.8(3)
C(10)-C(11)-C(6)	118.8(2)	N(5)-C(60)-C(68)	122.2(3)
C(10)-C(11)-C(15)	119.2(2)	C(60)-C(61)-N(6)	107.5(2)
C(6)-C(11)-C(15)	122.1(2)	C(60)-C(61)-C(69)	130.4(3)
C(7)-C(12)-C(14)	110.83(19)	N(6)-C(61)-C(69)	122.2(3)
C(7)-C(12)-C(13)	112.3(2)	N(5)-C(62)-C(64)	114.7(9)
C(14)-C(12)-C(13)	109.3(2)	N(5)-C(62)-C(63)	112.9(8)
C(17)-C(15)-C(11)	111.2(2)	C(64)-C(62)-C(63)	112.6(7)
C(17)-C(15)-C(16)	109.9(2)	N(5)-C(62')-C(63')	105.4(13)
C(11)-C(15)-C(16)	110.4(2)	N(5)-C(62')-C(64')	104.7(13)
C(19)-C(18)-C(23)	121.0(2)	C(63')-C(62')-C(64')	111.9(15)
C(19)-C(18)-N(2)	120.6(2)	N(6)-C(65)-C(66)	111.8(4)
C(23)-C(18)-N(2)	118.3(2)	N(6)-C(65)-C(67)	107.4(5)
C(18)-C(19)-C(20)	118.0(2)	C(66)-C(65)-C(67)	111.9(5)
C(18)-C(19)-C(24)	123.1(2)	N(6)-C(65')-C(67')	124(3)
C(20)-C(19)-C(24)	118.9(2)	N(6)-C(65')-C(66')	100(2)
C(21)-C(20)-C(19)	121.5(2)	C(67')-C(65')-C(66')	105(3)
C(20)-C(21)-C(22)	119.7(2)	C21-C11-C61	120.3(3)
C(21)-C(22)-C(23)	121.4(2)	C11-C21-C31	119.7(3)
C(22)-C(23)-C(18)	118.3(2)	C41-C31-C21	120.2(3)
C(22)-C(23)-C(27)	120.5(2)	C31-C41-C51	119.8(3)
C(18)-C(23)-C(27)	121.2(2)	C61-C51-C41	120.3(3)
C(19)-C(24)-C(26)	110.7(2)	C51-C61-C11	119.7(3)

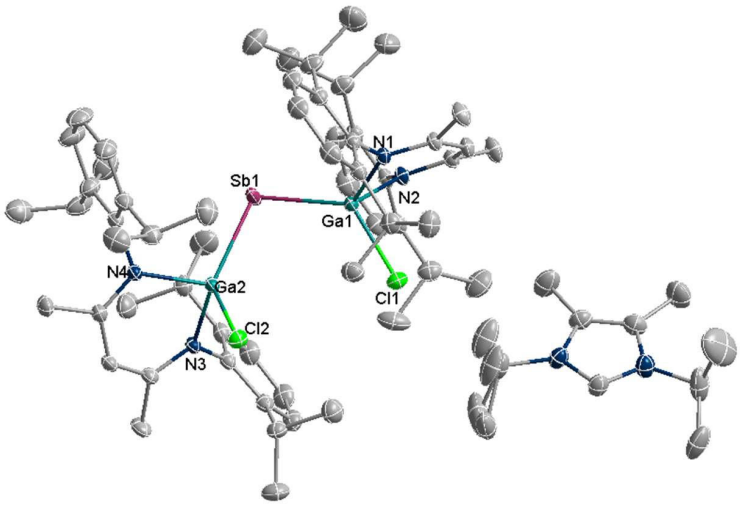

Fig. S39. Solid state structure of **2**. Hydrogen atoms and minor component of the disorder are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S8: Bond lengths [Å] for **2** (jk_186m).

Sb(1)-Ga(1)	2.5169(3)	C(19)-C(20)	1.402(2)	C(61)-C(66)	1.492(3)
Sb(1)-Ga(2)	2.5186(3)	C(19)-C(24)	1.511(3)	C(62)-C(63)	1.500(4)
Ga(1)-N(1)	2.0153(12)	C(20)-C(21)	1.374(3)	C(62)-C(64)	1.518(4)
Ga(1)-N(2)	2.0166(14)	C(21)-C(22)	1.383(3)	C(67)-C(69)	1.466(9)
Ga(1)-Cl(1)	2.2611(5)	C(22)-C(23)	1.393(3)	C(67)-C(68')	1.476(6)
Ga(2)-N(4)	1.9985(14)	C(23)-C(27)	1.521(3)	C(67)-C(69')	1.516(6)
Ga(2)-N(3)	2.0117(12)	C(24)-C(25)	1.522(3)	C(67)-C(68)	1.564(8)
Ga(2)-Cl(2)	2.3012(5)	C(24)-C(26)	1.539(3)	C11-C21	1.374(5)
N(1)-C(1)	1.326(2)	C(27)-C(29)	1.524(3)	C11-C61	1.375(5)
N(1)-C(6)	1.447(2)	C(27)-C(28)	1.524(3)	C21-C31	1.366(4)
N(2)-C(3)	1.329(2)	C(30)-C(31)	1.401(2)	C31-C41	1.353(4)
N(2)-C(18)	1.440(2)	C(30)-C(33)	1.512(2)	C41-C51	1.346(4)
N(3)-C(30)	1.330(2)	C(31)-C(32)	1.399(2)	C51-C61	1.358(5)
N(3)-C(35)	1.446(2)	C(32)-C(34)	1.508(2)	C12-C22	1.351(13)
N(4)-C(32)	1.329(2)	C(35)-C(36)	1.408(3)	C12-C62	1.386(12)
N(4)-C(47)	1.446(2)	C(35)-C(40)	1.409(3)	C22-C32	1.375(11)
N(5)-C(59)	1.326(3)	C(36)-C(37)	1.397(2)	C32-C42	1.376(10)
N(5)-C(60)	1.387(3)	C(36)-C(41)	1.519(3)	C42-C52	1.381(10)
N(5)-C(62)	1.483(3)	C(37)-C(38)	1.383(3)	C52-C62	1.382(12)
N(6)-C(59)	1.326(2)	C(38)-C(39)	1.377(3)	C13-C23	1.349(6)
N(6)-C(61)	1.381(3)	C(39)-C(40)	1.398(2)	C13-C63	1.366(6)
N(6)-C(67)	1.484(3)	C(40)-C(44)	1.514(3)	C23-C33	1.325(5)
C(1)-C(2)	1.404(2)	C(41)-C(42)	1.528(3)	C33-C43	1.336(5)
C(1)-C(4)	1.511(2)	C(41)-C(43)	1.533(3)	C43-C53	1.369(6)
C(2)-C(3)	1.401(2)	C(44)-C(45)	1.526(3)	C53-C63	1.360(6)
C(3)-C(5)	1.511(2)	C(44)-C(46)	1.528(3)	C14-C64	1.366(4)

C(6)-C(7)	1.404(3)	C(47)-C(52)	1.396(3)	C14-C24	1.369(4)
C(6)-C(11)	1.406(3)	C(47)-C(48)	1.408(2)	C24-C34	1.376(4)
C(7)-C(8)	1.402(2)	C(48)-C(49)	1.398(3)	C34-C44	1.364(5)
C(7)-C(12)	1.515(3)	C(48)-C(53)	1.511(3)	C44-C54	1.346(5)
C(8)-C(9)	1.379(3)	C(49)-C(50)	1.373(3)	C54-C64	1.351(4)
C(9)-C(10)	1.377(3)	C(50)-C(51)	1.377(3)	C15-C35#1	1.356(5)
C(10)-C(11)	1.402(2)	C(51)-C(52)	1.394(3)	C15-C25	1.373(5)
C(11)-C(15)	1.510(3)	C(52)-C(56)	1.527(3)	C25-C35	1.376(5)
C(12)-C(14)	1.527(3)	C(53)-C(54)	1.521(3)	C16-C26	1.361(11)
C(12)-C(13)	1.540(3)	C(53)-C(55)	1.531(3)	C16-C66	1.374(12)
C(15)-C(16)	1.517(3)	C(56)-C(57)	1.524(3)	C26-C36	1.376(13)
C(15)-C(17)	1.519(3)	C(56)-C(58)	1.527(3)	C36-C46	1.358(13)
C(18)-C(23)	1.401(3)	C(60)-C(61)	1.356(3)	C46-C56	1.352(14)
C(18)-C(19)	1.406(2)	C(60)-C(65)	1.484(3)	C56-C66	1.349(14

Table S9: Bond angles [°] for **2** (jk_186m).

Ga(1)-Sb(1)-Ga(2)	104.534(9)	C(40)-C(35)-N(3)	118.49(15)
N(1)-Ga(1)-N(2)	92.64(5)	C(37)-C(36)-C(35)	118.16(18)
N(1)-Ga(1)-Cl(1)	97.50(4)	C(37)-C(36)-C(41)	119.17(17)
N(2)-Ga(1)-Cl(1)	98.25(4)	C(35)-C(36)-C(41)	122.65(15)
N(1)-Ga(1)-Sb(1)	120.92(4)	C(38)-C(37)-C(36)	121.28(19)
N(2)-Ga(1)-Sb(1)	112.97(4)	C(39)-C(38)-C(37)	119.73(17)
Cl(1)-Ga(1)-Sb(1)	127.387(14)	C(38)-C(39)-C(40)	121.60(19)
N(4)-Ga(2)-N(3)	92.52(5)	C(39)-C(40)-C(35)	117.93(18)
N(4)-Ga(2)-Cl(2)	99.47(4)	C(39)-C(40)-C(44)	120.07(17)
N(3)-Ga(2)-Cl(2)	96.77(4)	C(35)-C(40)-C(44)	121.92(15)
N(4)-Ga(2)-Sb(1)	109.26(4)	C(36)-C(41)-C(42)	109.72(16)
N(3)-Ga(2)-Sb(1)	123.53(4)	C(36)-C(41)-C(43)	113.15(14)
Cl(2)-Ga(2)-Sb(1)	127.800(14)	C(42)-C(41)-C(43)	109.57(17)
C(1)-N(1)-C(6)	117.86(12)	C(40)-C(44)-C(45)	112.89(17)
C(1)-N(1)-Ga(1)	120.19(10)	C(40)-C(44)-C(46)	110.29(16)
C(6)-N(1)-Ga(1)	121.64(10)	C(45)-C(44)-C(46)	110.94(18)
C(3)-N(2)-C(18)	120.22(14)	C(52)-C(47)-C(48)	121.11(16)
C(3)-N(2)-Ga(1)	120.72(11)	C(52)-C(47)-N(4)	119.05(14)
C(18)-N(2)-Ga(1)	118.86(10)	C(48)-C(47)-N(4)	119.85(16)
C(30)-N(3)-C(35)	117.38(13)	C(49)-C(48)-C(47)	117.76(18)
C(30)-N(3)-Ga(2)	120.01(11)	C(49)-C(48)-C(53)	119.29(15)
C(35)-N(3)-Ga(2)	122.36(10)	C(47)-C(48)-C(53)	122.96(15)
C(32)-N(4)-C(47)	118.11(14)	C(50)-C(49)-C(48)	121.63(17)
C(32)-N(4)-Ga(2)	120.99(11)	C(49)-C(50)-C(51)	119.78(18)
C(47)-N(4)-Ga(2)	120.86(10)	C(50)-C(51)-C(52)	121.2(2)
C(59)-N(5)-C(60)	108.68(17)	C(51)-C(52)-C(47)	118.55(17)
C(59)-N(5)-C(62)	125.72(18)	C(51)-C(52)-C(56)	118.40(18)

C(60)-N(5)-C(62)	125.55(18)	C(47)-C(52)-C(56)	123.05(16)
C(59)-N(6)-C(61)	108.89(17)	C(48)-C(53)-C(54)	111.16(17)
C(59)-N(6)-C(67)	125.18(17)	C(48)-C(53)-C(55)	111.65(18)
C(61)-N(6)-C(67)	125.88(17)	C(54)-C(53)-C(55)	109.74(16)
N(1)-C(1)-C(2)	124.24(14)	C(57)-C(56)-C(58)	110.04(18)
N(1)-C(1)-C(4)	120.23(15)	C(57)-C(56)-C(52)	111.04(18)
C(2)-C(1)-C(4)	115.50(14)	C(58)-C(56)-C(52)	111.79(19)
C(3)-C(2)-C(1)	128.29(15)	N(6)-C(59)-N(5)	108.80(18)
N(2)-C(3)-C(2)	123.21(15)	C(61)-C(60)-N(5)	106.74(18)
N(2)-C(3)-C(5)	120.38(14)	C(61)-C(60)-C(65)	130.3(2)
C(2)-C(3)-C(5)	116.39(14)	N(5)-C(60)-C(65)	123.0(2)
C(7)-C(6)-C(11)	120.97(15)	C(60)-C(61)-N(6)	106.88(17)
C(7)-C(6)-N(1)	120.49(15)	C(60)-C(61)-C(66)	130.5(2)
C(11)-C(6)-N(1)	118.54(16)	N(6)-C(61)-C(66)	122.55(19)
C(8)-C(7)-C(6)	118.10(17)	N(5)-C(62)-C(63)	111.0(2)
C(8)-C(7)-C(12)	118.73(17)	N(5)-C(62)-C(64)	108.6(2)
C(6)-C(7)-C(12)	123.14(15)	C(63)-C(62)-C(64)	112.2(2)
C(9)-C(8)-C(7)	121.70(18)	C(69)-C(67)-N(6)	112.8(5)
C(10)-C(9)-C(8)	119.37(17)	C(68')-C(67)-N(6)	109.4(3)
C(9)-C(10)-C(11)	121.60(18)	C(68')-C(67)-C(69')	115.3(4)
C(10)-C(11)-C(6)	118.19(17)	N(6)-C(67)-C(69')	110.2(3)
C(10)-C(11)-C(15)	120.31(17)	C(69)-C(67)-C(68)	112.6(7)
C(6)-C(11)-C(15)	121.47(15)	N(6)-C(67)-C(68)	108.1(4)
C(7)-C(12)-C(14)	109.97(16)	C21-C11-C61	119.3(3)
C(7)-C(12)-C(13)	112.69(15)	C31-C21-C11	119.9(3)
C(14)-C(12)-C(13)	109.95(17)	C41-C31-C21	120.0(3)
C(11)-C(15)-C(16)	111.57(18)	C51-C41-C31	120.4(3)
C(11)-C(15)-C(17)	113.01(18)	C41-C51-C61	120.9(3)
C(16)-C(15)-C(17)	110.32(19)	C51-C61-C11	119.6(3)
C(23)-C(18)-C(19)	121.06(15)	C22-C12-C62	122.8(10)
C(23)-C(18)-N(2)	118.25(14)	C12-C22-C32	117.8(11)
C(19)-C(18)-N(2)	120.59(16)	C22-C32-C42	121.5(10)
C(20)-C(19)-C(18)	117.96(18)	C32-C42-C52	119.9(10)
C(20)-C(19)-C(24)	119.11(16)	C42-C52-C62	119.2(11)
C(18)-C(19)-C(24)	122.91(15)	C52-C62-C12	118.8(10)
C(21)-C(20)-C(19)	121.41(17)	C23-C13-C63	120.8(4)
C(20)-C(21)-C(22)	119.92(17)	C33-C23-C13	119.9(4)
C(21)-C(22)-C(23)	121.0(2)	C23-C33-C43	121.2(4)
C(22)-C(23)-C(18)	118.64(17)	C33-C43-C53	119.9(4)
C(22)-C(23)-C(27)	120.28(18)	C63-C53-C43	119.8(4)
C(18)-C(23)-C(27)	121.06(15)	C53-C63-C13	118.5(4)
C(19)-C(24)-C(25)	110.41(18)	C64-C14-C24	119.7(3)
C(19)-C(24)-C(26)	112.16(18)	C14-C24-C34	119.3(3)

C(25)-C(24)-C(26)	110.18(18)	C44-C34-C24	119.6(3)
C(23)-C(27)-C(29)	110.62(17)	C54-C44-C34	120.9(3)
C(23)-C(27)-C(28)	113.62(17)	C44-C54-C64	119.8(3)
C(29)-C(27)-C(28)	109.89(18)	C54-C64-C14	120.8(3)
N(3)-C(30)-C(31)	124.01(14)	C35#1-C15-C25	120.7(3)
N(3)-C(30)-C(33)	120.44(15)	C15-C25-C35	120.1(3)
C(31)-C(30)-C(33)	115.52(15)	C15#1-C35-C25	119.3(3)
C(32)-C(31)-C(30)	128.00(15)	C26-C16-C66	120.0(12)
N(4)-C(32)-C(31)	123.01(15)	C16-C26-C36	116.0(12)
N(4)-C(32)-C(34)	119.75(14)	C46-C36-C26	124.6(12)
C(31)-C(32)-C(34)	117.22(14)	C56-C46-C36	117.8(12)
C(36)-C(35)-C(40)	121.04(16)	C66-C56-C46	119.6(13)
C(36)-C(35)-N(3)	120.40(16)	C56-C66-C16	122.0(13)

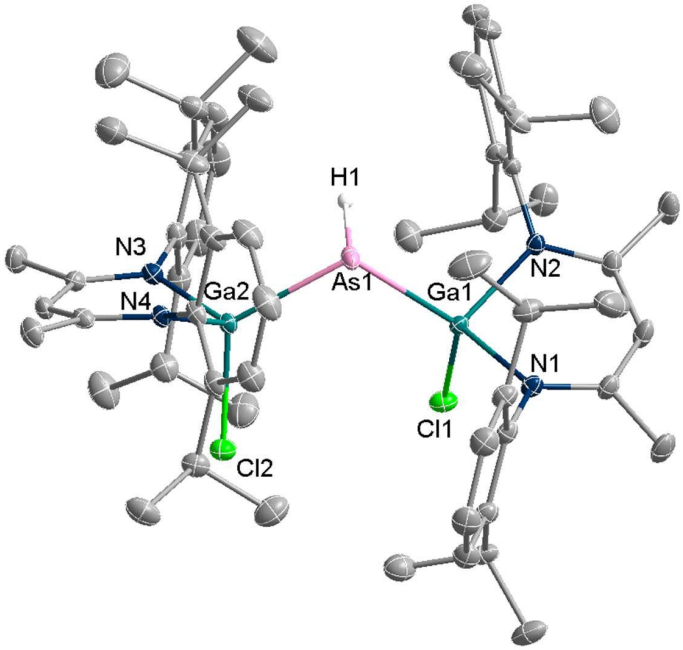

Fig. S40. Solid state structure of **5**. Hydrogen atoms except for As-H are omitted for clarity. H1 is displayed as sphere of arbitrary radius. Displacement ellipsoids drawn at 50% probability levels.

Table S10: Bond lengths [Å] for **5** (jk_460m).

As(1)-Ga(2)	2.4000(6)	C(9)-C(10)	1.385(3)	C(36)-C(37)	1.406(3)
As(1)-Ga(1)	2.4156(5)	C(10)-C(11)	1.400(3)	C(36)-C(41)	1.521(3)
Ga(1)-N(1)	1.9505(16)	C(11)-C(15)	1.524(3)	C(37)-C(38)	1.381(4)
Ga(1)-N(2)	1.9648(16)	C(12)-C(14)	1.527(3)	C(38)-C(39)	1.389(4)
Ga(1)-Cl(1)	2.2320(6)	C(12)-C(13)	1.534(3)	C(39)-C(40)	1.405(3)
Ga(2)-N(3)	1.9557(17)	C(15)-C(16)	1.531(4)	C(40)-C(44)	1.528(3)
Ga(2)-N(4)	1.9836(15)	C(15)-C(17)	1.537(3)	C(41)-C(43)	1.534(3)
Ga(2)-Cl(2)	2.2104(6)	C(18)-C(19)	1.406(3)	C(41)-C(42)	1.540(3)
N(1)-C(1)	1.339(2)	C(18)-C(23)	1.421(3)	C(44)-C(46)	1.523(3)
N(1)-C(6)	1.449(2)	C(19)-C(20)	1.394(3)	C(44)-C(45)	1.532(4)
N(2)-C(3)	1.332(2)	C(19)-C(24)	1.526(3)	C(47)-C(48)	1.404(3)
N(2)-C(18)	1.446(2)	C(20)-C(21)	1.393(3)	C(47)-C(52)	1.418(3)
N(3)-C(30)	1.337(2)	C(21)-C(22)	1.383(3)	C(48)-C(49)	1.401(3)
N(3)-C(35)	1.456(2)	C(22)-C(23)	1.396(3)	C(48)-C(53)	1.523(3)
N(4)-C(32)	1.327(2)	C(23)-C(27)	1.522(3)	C(49)-C(50)	1.397(3)
N(4)-C(47)	1.449(2)	C(24)-C(26)	1.536(3)	C(50)-C(51)	1.384(4)
C(1)-C(2)	1.402(3)	C(24)-C(25)	1.548(3)	C(51)-C(52)	1.400(3)
C(1)-C(4)	1.513(3)	C(27)-C(28)	1.525(3)	C(52)-C(56)	1.517(3)
C(2)-C(3)	1.401(3)	C(27)-C(29)	1.544(3)	C(53)-C(55)	1.532(3)
C(3)-C(5)	1.519(3)	C(30)-C(31)	1.411(3)	C(53)-C(54)	1.540(3)
C(6)-C(11)	1.412(3)	C(30)-C(33)	1.510(3)	C(56)-C(58)	1.531(3)
C(6)-C(7)	1.416(3)	C(31)-C(32)	1.402(3)	C(56)-C(57)	1.539(3)
C(7)-C(8)	1.397(3)	C(32)-C(34)	1.519(3)	C11-C11#1	1.524(9)
C(7)-C(12)	1.532(3)	C(35)-C(40)	1.414(3)	C11-C21	1.543(5)
C(8)-C(9)	1.399(3)	C(35)-C(36)	1.416(3)	C21-C31	1.542(6)

Table S11: Bond angles [°] for **5** (jk_460m).

Ga(2)-As(1)-Ga(1)	110.566(13)	C(22)-C(21)-C(20)	120.19(19)
N(1)-Ga(1)-N(2)	96.15(7)	C(21)-C(22)-C(23)	121.17(19)
N(1)-Ga(1)-Cl(1)	102.60(5)	C(22)-C(23)-C(18)	117.77(18)
N(2)-Ga(1)-Cl(1)	104.71(5)	C(22)-C(23)-C(27)	120.55(18)
N(1)-Ga(1)-As(1)	119.04(5)	C(18)-C(23)-C(27)	121.68(17)
N(2)-Ga(1)-As(1)	107.62(5)	C(19)-C(24)-C(26)	108.85(17)
Cl(1)-Ga(1)-As(1)	122.75(2)	C(19)-C(24)-C(25)	112.88(17)
N(3)-Ga(2)-N(4)	96.14(7)	C(26)-C(24)-C(25)	110.58(17)
N(3)-Ga(2)-Cl(2)	103.51(5)	C(23)-C(27)-C(28)	111.79(17)
N(4)-Ga(2)-Cl(2)	104.13(5)	C(23)-C(27)-C(29)	112.55(19)
N(3)-Ga(2)-As(1)	119.41(5)	C(28)-C(27)-C(29)	109.74(19)
N(4)-Ga(2)-As(1)	107.50(4)	N(3)-C(30)-C(31)	124.45(17)
Cl(2)-Ga(2)-As(1)	122.145(19)	N(3)-C(30)-C(33)	119.12(17)
C(1)-N(1)-C(6)	118.67(16)	C(31)-C(30)-C(33)	116.43(17)

C(1)-N(1)-Ga(1)	118.61(13)
C(6)-N(1)-Ga(1)	122.69(12)
C(3)-N(2)-C(18)	118.25(15)
C(3)-N(2)-Ga(1)	119.34(13)
C(18)-N(2)-Ga(1)	122.09(12)
C(30)-N(3)-C(35)	118.64(16)
C(30)-N(3)-Ga(2)	118.49(13)
C(35)-N(3)-Ga(2)	122.58(12)
C(32)-N(4)-C(47)	119.61(15)
C(32)-N(4)-Ga(2)	119.50(12)
C(47)-N(4)-Ga(2)	120.80(11)
N(1)-C(1)-C(2)	124.17(17)
N(1)-C(1)-C(4)	119.80(17)
C(2)-C(1)-C(4)	116.03(17)
C(3)-C(2)-C(1)	128.29(18)
N(2)-C(3)-C(2)	123.39(17)
N(2)-C(3)-C(5)	119.92(17)
C(2)-C(3)-C(5)	116.68(17)
C(11)-C(6)-C(7)	121.56(17)
C(11)-C(6)-N(1)	118.11(17)
C(7)-C(6)-N(1)	120.31(16)
C(8)-C(7)-C(6)	117.38(18)
C(8)-C(7)-C(12)	119.69(18)
C(6)-C(7)-C(12)	122.92(17)
C(7)-C(8)-C(9)	121.76(19)
C(10)-C(9)-C(8)	119.86(19)
C(9)-C(10)-C(11)	120.78(19)
C(10)-C(11)-C(6)	118.61(18)
C(10)-C(11)-C(15)	119.41(18)
C(6)-C(11)-C(15)	121.92(17)
C(14)-C(12)-C(7)	110.28(17)
C(14)-C(12)-C(13)	109.42(18)
C(7)-C(12)-C(13)	112.56(17)
C(11)-C(15)-C(16)	110.69(18)
C(11)-C(15)-C(17)	112.4(2)
C(16)-C(15)-C(17)	110.1(2)
C(19)-C(18)-C(23)	121.64(17)
C(19)-C(18)-N(2)	119.42(16)
C(23)-C(18)-N(2)	118.92(16)
C(20)-C(19)-C(18)	118.00(18)
C(20)-C(19)-C(24)	118.94(17)
C(18)-C(19)-C(24)	123.00(17)
C(21)-C(20)-C(19)	121.11(19)
C(32)-C(31)-C(30)	128.70(17)
N(4)-C(32)-C(31)	123.02(16)
N(4)-C(32)-C(34)	120.01(17)
C(31)-C(32)-C(34)	116.98(17)
C(40)-C(35)-C(36)	121.73(17)
C(40)-C(35)-N(3)	117.62(17)
C(36)-C(35)-N(3)	120.64(17)
C(37)-C(36)-C(35)	118.0(2)
C(37)-C(36)-C(41)	118.95(19)
C(35)-C(36)-C(41)	123.04(17)
C(38)-C(37)-C(36)	121.1(2)
C(37)-C(38)-C(39)	120.2(2)
C(38)-C(39)-C(40)	121.6(2)
C(39)-C(40)-C(35)	117.4(2)
C(39)-C(40)-C(44)	120.66(19)
C(35)-C(40)-C(44)	121.92(17)
C(36)-C(41)-C(43)	109.80(19)
C(36)-C(41)-C(42)	113.0(2)
C(43)-C(41)-C(42)	109.88(19)
C(46)-C(44)-C(40)	112.9(2)
C(46)-C(44)-C(45)	109.8(2)
C(40)-C(44)-C(45)	111.8(2)
C(48)-C(47)-C(52)	121.20(17)
C(48)-C(47)-N(4)	120.71(16)
C(52)-C(47)-N(4)	118.07(17)
C(49)-C(48)-C(47)	118.11(18)
C(49)-C(48)-C(53)	119.31(19)
C(47)-C(48)-C(53)	122.58(17)
C(50)-C(49)-C(48)	121.4(2)
C(51)-C(50)-C(49)	119.68(19)
C(50)-C(51)-C(52)	121.09(19)
C(51)-C(52)-C(47)	118.5(2)
C(51)-C(52)-C(56)	119.96(18)
C(47)-C(52)-C(56)	121.57(17)
C(48)-C(53)-C(55)	111.26(18)
C(48)-C(53)-C(54)	111.12(16)
C(55)-C(53)-C(54)	110.11(19)
C(52)-C(56)-C(58)	112.7(2)
C(52)-C(56)-C(57)	111.68(18)
C(58)-C(56)-C(57)	109.94(18)
C11#1-C11-C21	111.8(5)
C31-C21-C11	111.8(4)

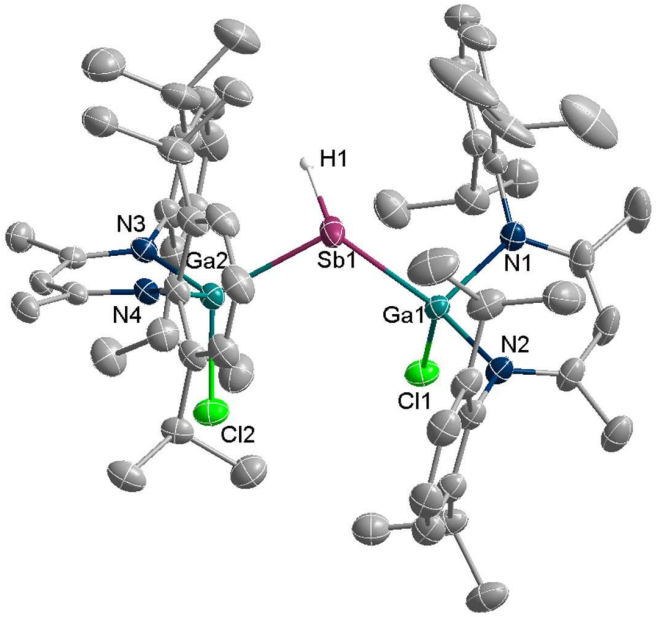

Fig. S41. Solid state structure of **6**. Hydrogen atoms except for Sb-H are omitted for clarity. H1 is displayed as sphere of arbitrary radius. Displacement ellipsoids drawn at 50% probability levels.

Table S12: Bond lengths [Å] for **6** (jk_489m).

Sb(1)-Ga(2)	2.5669(3)	C(9)-C(10)	1.369(5)	C(36)-C(37)	1.393(4)
Sb(1)-Ga(1)	2.5803(3)	C(10)-C(11)	1.390(4)	C(36)-C(41)	1.525(4)
Ga(1)-N(2)	1.9552(19)	C(11)-C(15)	1.515(4)	C(37)-C(38)	1.380(5)
Ga(1)-N(1)	1.9571(19)	C(12)-C(14)	1.526(4)	C(38)-C(39)	1.371(5)
Ga(1)-Cl(1)	2.2161(6)	C(12)-C(13)	1.538(4)	C(39)-C(40)	1.401(4)
Ga(2)-N(3)	1.9613(19)	C(15)-C(16)	1.504(7)	C(40)-C(44)	1.515(4)
Ga(2)-N(4)	1.9702(18)	C(15)-C(17)	1.530(6)	C(41)-C(43)	1.521(4)
Ga(2)-Cl(2)	2.2012(6)	C(18)-C(19)	1.407(4)	C(41)-C(42)	1.533(5)
N(1)-C(1)	1.328(3)	C(18)-C(23)	1.408(3)	C(44)-C(46)	1.533(4)
N(1)-C(6)	1.448(3)	C(19)-C(20)	1.401(3)	C(44)-C(45)	1.538(4)
N(2)-C(3)	1.338(3)	C(19)-C(24)	1.524(4)	C(47)-C(52)	1.402(3)
N(2)-C(18)	1.449(3)	C(20)-C(21)	1.384(4)	C(47)-C(48)	1.410(3)
N(3)-C(30)	1.331(3)	C(21)-C(22)	1.373(4)	C(48)-C(49)	1.397(4)
N(3)-C(35)	1.452(3)	C(22)-C(23)	1.397(3)	C(48)-C(53)	1.517(4)
N(4)-C(32)	1.328(3)	C(23)-C(27)	1.510(4)	C(49)-C(50)	1.381(4)
N(4)-C(47)	1.449(3)	C(24)-C(26)	1.530(4)	C(50)-C(51)	1.381(4)
C(1)-C(2)	1.397(4)	C(24)-C(25)	1.534(4)	C(51)-C(52)	1.398(3)
C(1)-C(4)	1.510(4)	C(27)-C(29)	1.522(4)	C(52)-C(56)	1.521(3)
C(2)-C(3)	1.402(4)	C(27)-C(28)	1.524(5)	C(53)-C(54)	1.530(4)
C(3)-C(5)	1.512(3)	C(30)-C(31)	1.407(3)	C(53)-C(55)	1.532(4)
C(6)-C(7)	1.397(3)	C(30)-C(33)	1.504(3)	C(56)-C(58)	1.528(4)
C(6)-C(11)	1.405(4)	C(31)-C(32)	1.396(3)	C(56)-C(57)	1.533(3)

C(7)-C(8)	1.395(4)	C(32)-C(34)	1.510(3)	C11-C11#1	1.516(10)
C(7)-C(12)	1.512(4)	C(35)-C(36)	1.405(3)	C11-C21	1.546(6)
C(8)-C(9)	1.371(5)	C(35)-C(40)	1.407(4)	C21-C31	1.533(7)

Table S13: Bond angles [°] for **6** (jk_489m).

Ga(2)-Sb(1)-Ga(1)	107.412(10)	C(22)-C(21)-C(20)	120.0(2)
N(2)-Ga(1)-N(1)	96.04(8)	C(21)-C(22)-C(23)	121.4(3)
N(2)-Ga(1)-Cl(1)	102.85(6)	C(22)-C(23)-C(18)	117.9(2)
N(1)-Ga(1)-Cl(1)	104.81(6)	C(22)-C(23)-C(27)	120.0(2)
N(2)-Ga(1)-Sb(1)	121.54(6)	C(18)-C(23)-C(27)	122.1(2)
N(1)-Ga(1)-Sb(1)	105.38(6)	C(19)-C(24)-C(26)	110.1(2)
Cl(1)-Ga(1)-Sb(1)	122.00(2)	C(19)-C(24)-C(25)	112.5(2)
N(3)-Ga(2)-N(4)	96.09(8)	C(26)-C(24)-C(25)	109.7(2)
N(3)-Ga(2)-Cl(2)	103.88(6)	C(23)-C(27)-C(29)	112.8(3)
N(4)-Ga(2)-Cl(2)	104.63(6)	C(23)-C(27)-C(28)	111.1(2)
N(3)-Ga(2)-Sb(1)	119.88(5)	C(29)-C(27)-C(28)	110.2(3)
N(4)-Ga(2)-Sb(1)	108.07(5)	N(3)-C(30)-C(31)	123.9(2)
Cl(2)-Ga(2)-Sb(1)	120.62(2)	N(3)-C(30)-C(33)	119.4(2)
C(1)-N(1)-C(6)	119.3(2)	C(31)-C(30)-C(33)	116.7(2)
C(1)-N(1)-Ga(1)	119.18(17)	C(32)-C(31)-C(30)	129.1(2)
C(6)-N(1)-Ga(1)	121.27(14)	N(4)-C(32)-C(31)	123.2(2)
C(3)-N(2)-C(18)	118.68(19)	N(4)-C(32)-C(34)	119.9(2)
C(3)-N(2)-Ga(1)	118.45(15)	C(31)-C(32)-C(34)	117.0(2)
C(18)-N(2)-Ga(1)	122.79(15)	C(36)-C(35)-C(40)	121.5(2)
C(30)-N(3)-C(35)	118.65(19)	C(36)-C(35)-N(3)	118.1(2)
C(30)-N(3)-Ga(2)	118.80(15)	C(40)-C(35)-N(3)	120.4(2)
C(35)-N(3)-Ga(2)	122.28(15)	C(37)-C(36)-C(35)	117.9(3)
C(32)-N(4)-C(47)	120.15(18)	C(37)-C(36)-C(41)	120.6(2)
C(32)-N(4)-Ga(2)	119.50(15)	C(35)-C(36)-C(41)	121.4(2)
C(47)-N(4)-Ga(2)	120.25(14)	C(38)-C(37)-C(36)	121.1(3)
N(1)-C(1)-C(2)	123.0(2)	C(39)-C(38)-C(37)	120.5(3)
N(1)-C(1)-C(4)	119.8(2)	C(38)-C(39)-C(40)	121.1(3)
C(2)-C(1)-C(4)	117.1(2)	C(39)-C(40)-C(35)	117.8(3)
C(1)-C(2)-C(3)	128.9(2)	C(39)-C(40)-C(44)	119.3(2)
N(2)-C(3)-C(2)	123.7(2)	C(35)-C(40)-C(44)	122.9(2)
N(2)-C(3)-C(5)	119.7(2)	C(43)-C(41)-C(36)	113.0(3)
C(2)-C(3)-C(5)	116.6(2)	C(43)-C(41)-C(42)	109.7(3)
C(7)-C(6)-C(11)	121.1(2)	C(36)-C(41)-C(42)	111.7(3)
C(7)-C(6)-N(1)	119.8(2)	C(40)-C(44)-C(46)	109.6(2)
C(11)-C(6)-N(1)	119.1(2)	C(40)-C(44)-C(45)	113.1(2)
C(8)-C(7)-C(6)	118.0(2)	C(46)-C(44)-C(45)	110.0(2)
C(8)-C(7)-C(12)	118.9(2)	C(52)-C(47)-C(48)	121.5(2)
C(6)-C(7)-C(12)	123.1(2)	C(52)-C(47)-N(4)	120.2(2)

C(9)-C(8)-C(7)	121.6(3)	C(48)-C(47)-N(4)	118.2(2)
C(10)-C(9)-C(8)	119.6(3)	C(49)-C(48)-C(47)	118.0(2)
C(9)-C(10)-C(11)	121.7(3)	C(49)-C(48)-C(53)	120.4(2)
C(10)-C(11)-C(6)	117.9(3)	C(47)-C(48)-C(53)	121.6(2)
C(10)-C(11)-C(15)	120.5(3)	C(50)-C(49)-C(48)	121.2(2)
C(6)-C(11)-C(15)	121.5(3)	C(49)-C(50)-C(51)	119.9(2)
C(7)-C(12)-C(14)	109.3(2)	C(50)-C(51)-C(52)	121.5(3)
C(7)-C(12)-C(13)	112.0(2)	C(51)-C(52)-C(47)	117.8(2)
C(14)-C(12)-C(13)	111.2(2)	C(51)-C(52)-C(56)	119.3(2)
C(16)-C(15)-C(11)	111.2(3)	C(47)-C(52)-C(56)	122.9(2)
C(16)-C(15)-C(17)	110.0(4)	C(48)-C(53)-C(54)	111.5(2)
C(11)-C(15)-C(17)	112.8(4)	C(48)-C(53)-C(55)	112.9(3)
C(19)-C(18)-C(23)	121.7(2)	C(54)-C(53)-C(55)	109.8(2)
C(19)-C(18)-N(2)	120.4(2)	C(52)-C(56)-C(58)	110.6(2)
C(23)-C(18)-N(2)	117.9(2)	C(52)-C(56)-C(57)	111.7(2)
C(20)-C(19)-C(18)	117.4(2)	C(58)-C(56)-C(57)	109.7(2)
C(20)-C(19)-C(24)	119.5(2)	C11#1-C11-C21	111.6(5)
C(18)-C(19)-C(24)	123.1(2)	C31-C21-C11	111.8(4)
C(21)-C(20)-C(19)	121.5(3)	C(22)-C(21)-C(20)	120.0(2)

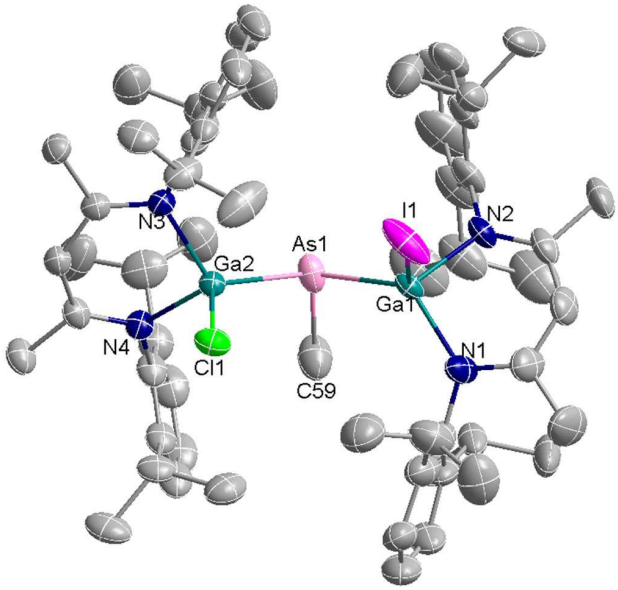

Fig. S42. Solid state structure of **7**. Hydrogen atoms and minor component of the disorder are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S14: Bond lengths [Å] for **7** (jk_577m).

I(1)-Ga(1)	2.5169(7)	C(10)-C(11)	1.397(10)	C(27)-C(29)	1.534(9)
Cl(1)-Ga(2)	2.193(5)	C(11)-C(15)	1.530(12)	C(30)-C(31)	1.402(5)
Cl(1')-Ga(1)	2.166(6)	C(12)-C(13)	1.540(10)	C(30)-C(33)	1.513(5)
I(1')-Ga(2)	2.5197(19)	C(12)-C(14)	1.548(10)	C(31)-C(32)	1.398(5)
As(1)-C(59)	1.939(6)	C(15)-C(16)	1.521(13)	C(32)-C(34)	1.510(5)
As(1)-Ga(2)	2.3946(6)	C(15)-C(17)	1.552(13)	C(35)-C(40)	1.400(6)
As(1)-Ga(1)	2.4232(6)	C(6')-C(7')	1.382(11)	C(35)-C(36)	1.413(6)
Ga(1)-N(1)	1.967(3)	C(6')-C(11')	1.393(10)	C(36)-C(37)	1.400(6)
Ga(1)-N(2)	1.975(3)	C(7')-C(8')	1.396(11)	C(36)-C(41)	1.505(7)
Ga(2)-N(3)	1.974(3)	C(7')-C(12')	1.510(12)	C(37)-C(38)	1.369(9)
Ga(2)-N(4)	1.976(3)	C(8')-C(9')	1.376(11)	C(38)-C(39)	1.377(9)
N(1)-C(1)	1.338(6)	C(9')-C(10')	1.381(11)	C(39)-C(40)	1.398(6)
N(1)-C(6')	1.418(16)	C(10')-C(11')	1.387(10)	C(40)-C(44)	1.529(7)
N(1)-C(6)	1.493(13)	C(11')-C(15')	1.501(13)	C(41)-C(43)	1.536(7)
N(2)-C(3)	1.321(5)	C(12')-C(14')	1.523(13)	C(41)-C(42)	1.544(6)
N(2)-C(18)	1.441(5)	C(12')-C(13')	1.544(12)	C(44)-C(45)	1.523(7)
N(3)-C(30)	1.323(5)	C(15')-C(16')	1.530(10)	C(44)-C(46)	1.539(7)
N(3)-C(35)	1.449(5)	C(15')-C(17')	1.534(11)	C(47)-C(52)	1.403(6)
N(4)-C(32)	1.333(5)	C(18)-C(19)	1.387(7)	C(47)-C(48)	1.405(6)
N(4)-C(47)	1.442(4)	C(18)-C(23)	1.414(7)	C(48)-C(49)	1.403(5)
C(1)-C(2)	1.389(7)	C(19)-C(20)	1.403(7)	C(48)-C(53)	1.509(6)
C(1)-C(4)	1.514(7)	C(19)-C(24)	1.515(7)	C(49)-C(50)	1.375(8)
C(2)-C(3)	1.401(7)	C(20)-C(21)	1.390(10)	C(50)-C(51)	1.382(8)
C(3)-C(5)	1.506(6)	C(21)-C(22)	1.329(11)	C(51)-C(52)	1.403(6)
C(6)-C(7)	1.390(10)	C(22)-C(23)	1.385(9)	C(52)-C(56)	1.514(7)
C(6)-C(11)	1.400(10)	C(23)-C(27)	1.522(9)	C(53)-C(55)	1.518(7)
C(7)-C(8)	1.397(9)	C(24)-C(26)	1.521(7)	C(53)-C(54)	1.532(6)
C(7)-C(12)	1.521(11)	C(24)-C(25)	1.536(6)	C(56)-C(58)	1.514(9)
C(8)-C(9)	1.372(10)	C(27)-C(28)	1.524(11)	C(56)-C(57)	1.520(9)
C(9)-C(10)	1.379(10)				

Table S15: Bond angles [°] for **7** (jk_577m).

C(59)-As(1)-Ga(2)	102.30(18)	C(10')-C(11')-C(15')	118.4(12)
C(59)-As(1)-Ga(1)	99.36(18)	C(6')-C(11')-C(15')	121.7(12)
Ga(2)-As(1)-Ga(1)	110.14(2)	C(7')-C(12')-C(14')	109.2(11)
N(1)-Ga(1)-N(2)	95.15(15)	C(7')-C(12')-C(13')	111.0(11)
N(1)-Ga(1)-Cl(1')	103.9(3)	C(14')-C(12')-C(13')	109.3(9)
N(2)-Ga(1)-Cl(1')	104.4(2)	C(11')-C(15')-C(16')	110.1(14)
N(1)-Ga(1)-As(1)	122.38(10)	C(11')-C(15')-C(17')	108.2(11)
N(2)-Ga(1)-As(1)	107.93(10)	C(16')-C(15')-C(17')	109.9(8)
Cl(1')-Ga(1)-As(1)	119.2(3)	C(19)-C(18)-C(23)	121.3(5)

N(1)-Ga(1)-I(1)	106.25(11)	C(19)-C(18)-N(2)	121.1(4)
N(2)-Ga(1)-I(1)	101.40(9)	C(23)-C(18)-N(2)	117.5(4)
As(1)-Ga(1)-I(1)	118.99(3)	C(18)-C(19)-C(20)	116.9(5)
N(3)-Ga(2)-N(4)	95.57(12)	C(18)-C(19)-C(24)	123.6(4)
N(3)-Ga(2)-Cl(1)	103.12(19)	C(20)-C(19)-C(24)	119.5(5)
N(4)-Ga(2)-Cl(1)	104.0(2)	C(21)-C(20)-C(19)	121.3(6)
N(3)-Ga(2)-As(1)	118.83(9)	C(22)-C(21)-C(20)	120.6(5)
N(4)-Ga(2)-As(1)	110.91(9)	C(21)-C(22)-C(23)	121.3(6)
Cl(1)-Ga(2)-As(1)	120.70(19)	C(22)-C(23)-C(18)	118.5(6)
N(3)-Ga(2)-I(1')	99.97(11)	C(22)-C(23)-C(27)	120.6(5)
N(4)-Ga(2)-I(1')	105.55(12)	C(18)-C(23)-C(27)	120.9(5)
As(1)-Ga(2)-I(1')	122.15(8)	C(19)-C(24)-C(26)	110.2(4)
C(1)-N(1)-C(6')	110.1(10)	C(19)-C(24)-C(25)	112.5(5)
C(1)-N(1)-C(6)	120.7(8)	C(26)-C(24)-C(25)	109.6(5)
C(1)-N(1)-Ga(1)	117.5(3)	C(23)-C(27)-C(28)	112.5(5)
C(6')-N(1)-Ga(1)	132.4(10)	C(23)-C(27)-C(29)	113.9(7)
C(6)-N(1)-Ga(1)	121.3(7)	C(28)-C(27)-C(29)	110.4(6)
C(3)-N(2)-C(18)	119.8(3)	N(3)-C(30)-C(31)	124.2(3)
C(3)-N(2)-Ga(1)	119.1(3)	N(3)-C(30)-C(33)	120.3(3)
C(18)-N(2)-Ga(1)	120.9(3)	C(31)-C(30)-C(33)	115.5(3)
C(30)-N(3)-C(35)	118.4(3)	C(32)-C(31)-C(30)	128.8(3)
C(30)-N(3)-Ga(2)	118.9(2)	N(4)-C(32)-C(31)	123.2(3)
C(35)-N(3)-Ga(2)	122.3(2)	N(4)-C(32)-C(34)	119.6(3)
C(32)-N(4)-C(47)	118.1(3)	C(31)-C(32)-C(34)	117.2(3)
C(32)-N(4)-Ga(2)	118.9(2)	C(40)-C(35)-C(36)	121.6(4)
C(47)-N(4)-Ga(2)	122.9(2)	C(40)-C(35)-N(3)	118.4(3)
N(1)-C(1)-C(2)	125.0(4)	C(36)-C(35)-N(3)	120.0(4)
N(1)-C(1)-C(4)	119.8(5)	C(37)-C(36)-C(35)	117.4(5)
C(2)-C(1)-C(4)	115.1(5)	C(37)-C(36)-C(41)	118.6(4)
C(1)-C(2)-C(3)	127.7(4)	C(35)-C(36)-C(41)	124.1(4)
N(2)-C(3)-C(2)	123.2(4)	C(38)-C(37)-C(36)	121.5(5)
N(2)-C(3)-C(5)	120.7(4)	C(37)-C(38)-C(39)	120.4(4)
C(2)-C(3)-C(5)	116.1(4)	C(38)-C(39)-C(40)	121.1(5)
C(7)-C(6)-C(11)	120.5(7)	C(39)-C(40)-C(35)	118.0(5)
C(7)-C(6)-N(1)	122.7(10)	C(39)-C(40)-C(44)	120.8(4)
C(11)-C(6)-N(1)	116.4(10)	C(35)-C(40)-C(44)	121.2(4)
C(6)-C(7)-C(8)	119.2(7)	C(36)-C(41)-C(43)	113.1(5)
C(6)-C(7)-C(12)	123.4(9)	C(36)-C(41)-C(42)	111.3(4)
C(8)-C(7)-C(12)	117.4(9)	C(43)-C(41)-C(42)	108.0(4)
C(9)-C(8)-C(7)	120.2(8)	C(45)-C(44)-C(40)	110.5(4)
C(8)-C(9)-C(10)	120.1(8)	C(45)-C(44)-C(46)	112.3(5)
C(9)-C(10)-C(11)	120.6(8)	C(40)-C(44)-C(46)	111.9(4)
C(10)-C(11)-C(6)	118.4(8)	C(52)-C(47)-C(48)	121.6(4)

C(10)-C(11)-C(15)	117.0(12)	C(52)-C(47)-N(4)	118.5(4)
C(6)-C(11)-C(15)	124.3(12)	C(48)-C(47)-N(4)	119.9(3)
C(7)-C(12)-C(13)	114.2(10)	C(49)-C(48)-C(47)	117.9(4)
C(7)-C(12)-C(14)	111.8(8)	C(49)-C(48)-C(53)	119.2(4)
C(13)-C(12)-C(14)	108.3(7)	C(47)-C(48)-C(53)	122.9(3)
C(16)-C(15)-C(11)	115.8(15)	C(50)-C(49)-C(48)	121.3(5)
C(16)-C(15)-C(17)	109.4(12)	C(49)-C(50)-C(51)	120.2(4)
C(11)-C(15)-C(17)	115.1(15)	C(50)-C(51)-C(52)	121.0(5)
C(7')-C(6')-C(11')	119.9(9)	C(51)-C(52)-C(47)	118.0(5)
C(7')-C(6')-N(1)	118.2(12)	C(51)-C(52)-C(56)	119.5(4)
C(11')-C(6')-N(1)	121.9(12)	C(47)-C(52)-C(56)	122.5(4)
C(6')-C(7')-C(8')	119.9(8)	C(48)-C(53)-C(55)	110.9(4)
C(6')-C(7')-C(12')	120.3(12)	C(48)-C(53)-C(54)	111.1(4)
C(8')-C(7')-C(12')	119.6(13)	C(55)-C(53)-C(54)	111.3(4)
C(9')-C(8')-C(7')	119.9(9)	C(52)-C(56)-C(58)	113.3(5)
C(8')-C(9')-C(10')	120.0(9)	C(52)-C(56)-C(57)	111.5(5)
C(9')-C(10')-C(11')	120.4(9)	C(58)-C(56)-C(57)	109.8(5)
C(10')-C(11')-C(6')	119.4(9)		

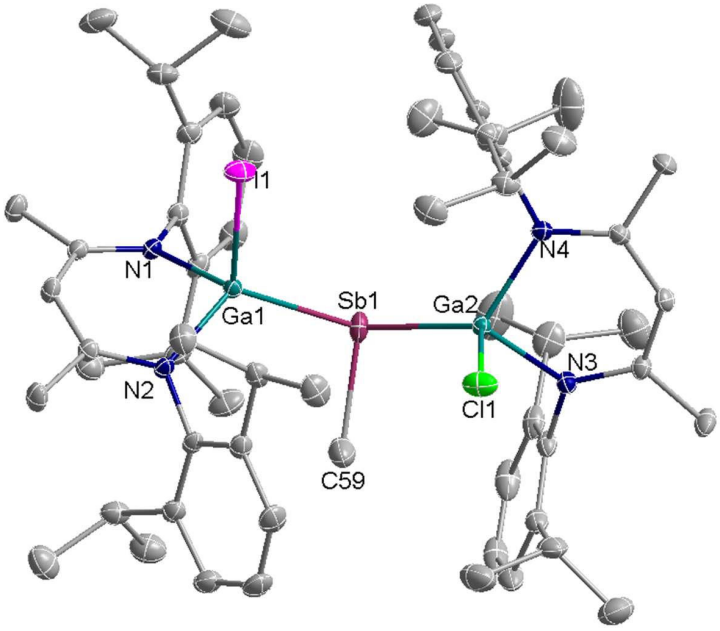

Fig. S43. Solid state structure of **8**. Hydrogen atoms and minor component of the disorder are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S16: Bond lengths [Å] for **8** (jk_573m).

I(1)-Ga(1)	2.5973(6)	C(7)-C(8)	1.402(3)	C(32)-C(34)	1.507(3)
Cl(1)-Ga(2)	2.2300(14)	C(7)-C(12)	1.524(3)	C(35)-C(36)	1.408(3)
I(1')-Ga(2)	2.495(5)	C(8)-C(9)	1.381(4)	C(35)-C(40)	1.411(3)
Cl(1')-Ga(1)	2.228(8)	C(9)-C(10)	1.390(4)	C(36)-C(37)	1.401(3)
Sb(1)-C(59)	2.164(3)	C(10)-C(11)	1.393(3)	C(36)-C(41)	1.526(4)
Sb(1)-Ga(1)	2.6118(6)	C(11)-C(15)	1.524(3)	C(37)-C(38)	1.384(4)
Sb(1)-Ga(2)	2.6132(5)	C(12)-C(14)	1.534(4)	C(38)-C(39)	1.387(5)
Ga(1)-N(2)	1.9700(17)	C(12)-C(13)	1.546(4)	C(39)-C(40)	1.397(3)
Ga(1)-N(1)	1.9942(17)	C(15)-C(17)	1.532(3)	C(40)-C(44)	1.522(4)
Ga(2)-N(4)	1.9544(18)	C(15)-C(16)	1.544(3)	C(41)-C(43)	1.535(4)
Ga(2)-N(3)	1.9759(18)	C(18)-C(19)	1.416(3)	C(41)-C(42)	1.540(4)
N(1)-C(1)	1.329(3)	C(18)-C(23)	1.418(3)	C(44)-C(45)	1.530(4)
N(1)-C(6)	1.449(3)	C(19)-C(20)	1.399(3)	C(44)-C(46)	1.537(4)
N(2)-C(3)	1.341(3)	C(19)-C(24)	1.528(3)	C(47)-C(48)	1.410(3)
N(2)-C(18)	1.451(3)	C(20)-C(21)	1.385(4)	C(47)-C(52)	1.414(3)
N(3)-C(30)	1.330(3)	C(21)-C(22)	1.380(4)	C(48)-C(49)	1.402(3)
N(3)-C(35)	1.443(3)	C(22)-C(23)	1.400(3)	C(48)-C(53)	1.525(3)
N(4)-C(32)	1.335(3)	C(23)-C(27)	1.530(3)	C(49)-C(50)	1.392(4)
N(4)-C(47)	1.452(3)	C(24)-C(26)	1.536(3)	C(50)-C(51)	1.379(4)
C(1)-C(2)	1.411(3)	C(24)-C(25)	1.537(3)	C(51)-C(52)	1.395(3)
C(1)-C(4)	1.513(3)	C(27)-C(29)	1.533(4)	C(52)-C(56)	1.521(3)
C(2)-C(3)	1.403(3)	C(27)-C(28)	1.538(4)	C(53)-C(55)	1.531(3)
C(3)-C(5)	1.510(3)	C(30)-C(31)	1.404(3)	C(53)-C(54)	1.539(3)
C(6)-C(7)	1.410(3)	C(30)-C(33)	1.510(3)	C(56)-C(57)	1.513(4)
C(6)-C(11)	1.415(3)	C(31)-C(32)	1.404(3)	C(56)-C(58)	1.530(4)

Table S17: Bond angles [°] for **8** (jk_573m).

C(59)-Sb(1)-Ga(1)	96.54(8)	C(23)-C(18)-N(2)	118.77(18)
C(59)-Sb(1)-Ga(2)	94.69(9)	C(20)-C(19)-C(18)	117.7(2)
Ga(1)-Sb(1)-Ga(2)	111.076(12)	C(20)-C(19)-C(24)	120.1(2)
N(2)-Ga(1)-N(1)	94.89(7)	C(18)-C(19)-C(24)	122.26(19)
N(2)-Ga(1)-Cl(1')	107.1(3)	C(21)-C(20)-C(19)	121.6(2)
N(1)-Ga(1)-Cl(1')	102.0(3)	C(22)-C(21)-C(20)	120.0(2)
N(2)-Ga(1)-I(1)	107.53(5)	C(21)-C(22)-C(23)	121.5(2)
N(1)-Ga(1)-I(1)	100.66(5)	C(22)-C(23)-C(18)	117.7(2)
N(2)-Ga(1)-Sb(1)	121.26(5)	C(22)-C(23)-C(27)	118.0(2)
N(1)-Ga(1)-Sb(1)	109.41(5)	C(18)-C(23)-C(27)	124.19(19)
Cl(1')-Ga(1)-Sb(1)	118.1(3)	C(19)-C(24)-C(26)	113.22(19)
I(1)-Ga(1)-Sb(1)	118.477(16)	C(19)-C(24)-C(25)	113.43(18)
N(4)-Ga(2)-N(3)	95.48(7)	C(26)-C(24)-C(25)	107.4(2)
N(4)-Ga(2)-Cl(1)	102.89(8)	C(23)-C(27)-C(29)	114.1(2)

N(3)-Ga(2)-Cl(1)	101.54(9)	C(23)-C(27)-C(28)	109.8(2)
N(4)-Ga(2)-I(1')	103.93(19)	C(29)-C(27)-C(28)	107.0(2)
N(3)-Ga(2)-I(1')	101.96(19)	N(3)-C(30)-C(31)	122.63(19)
N(4)-Ga(2)-Sb(1)	122.12(5)	N(3)-C(30)-C(33)	120.53(19)
N(3)-Ga(2)-Sb(1)	108.23(5)	C(31)-C(30)-C(33)	116.83(18)
Cl(1)-Ga(2)-Sb(1)	121.70(7)	C(32)-C(31)-C(30)	128.37(19)
I(1')-Ga(2)-Sb(1)	120.5(2)	N(4)-C(32)-C(31)	124.64(19)
C(1)-N(1)-C(6)	122.38(17)	N(4)-C(32)-C(34)	119.60(18)
C(1)-N(1)-Ga(1)	118.52(14)	C(31)-C(32)-C(34)	115.75(18)
C(6)-N(1)-Ga(1)	118.86(13)	C(36)-C(35)-C(40)	122.4(2)
C(3)-N(2)-C(18)	119.50(17)	C(36)-C(35)-N(3)	120.1(2)
C(3)-N(2)-Ga(1)	117.42(14)	C(40)-C(35)-N(3)	117.3(2)
C(18)-N(2)-Ga(1)	123.06(13)	C(37)-C(36)-C(35)	117.4(2)
C(30)-N(3)-C(35)	120.35(17)	C(37)-C(36)-C(41)	118.6(2)
C(30)-N(3)-Ga(2)	121.01(14)	C(35)-C(36)-C(41)	124.0(2)
C(35)-N(3)-Ga(2)	118.59(13)	C(38)-C(37)-C(36)	121.2(3)
C(32)-N(4)-C(47)	119.80(17)	C(37)-C(38)-C(39)	120.3(2)
C(32)-N(4)-Ga(2)	120.07(14)	C(38)-C(39)-C(40)	121.2(3)
C(47)-N(4)-Ga(2)	119.98(13)	C(39)-C(40)-C(35)	117.4(3)
N(1)-C(1)-C(2)	123.08(18)	C(39)-C(40)-C(44)	120.3(2)
N(1)-C(1)-C(4)	120.96(19)	C(35)-C(40)-C(44)	122.3(2)
C(2)-C(1)-C(4)	115.94(18)	C(36)-C(41)-C(43)	112.1(2)
C(3)-C(2)-C(1)	128.00(19)	C(36)-C(41)-C(42)	111.1(2)
N(2)-C(3)-C(2)	123.87(18)	C(43)-C(41)-C(42)	109.3(2)
N(2)-C(3)-C(5)	120.31(18)	C(40)-C(44)-C(45)	111.2(2)
C(2)-C(3)-C(5)	115.81(18)	C(40)-C(44)-C(46)	113.6(3)
C(7)-C(6)-C(11)	120.64(19)	C(45)-C(44)-C(46)	109.8(2)
C(7)-C(6)-N(1)	121.41(19)	C(48)-C(47)-C(52)	121.18(19)
C(11)-C(6)-N(1)	117.73(18)	C(48)-C(47)-N(4)	120.37(18)
C(8)-C(7)-C(6)	118.1(2)	C(52)-C(47)-N(4)	118.44(19)
C(8)-C(7)-C(12)	118.2(2)	C(49)-C(48)-C(47)	117.8(2)
C(6)-C(7)-C(12)	123.7(2)	C(49)-C(48)-C(53)	118.6(2)
C(9)-C(8)-C(7)	121.7(2)	C(47)-C(48)-C(53)	123.59(19)
C(8)-C(9)-C(10)	119.6(2)	C(50)-C(49)-C(48)	121.3(2)
C(9)-C(10)-C(11)	121.2(2)	C(51)-C(50)-C(49)	119.9(2)
C(10)-C(11)-C(6)	118.7(2)	C(50)-C(51)-C(52)	121.2(2)
C(10)-C(11)-C(15)	120.3(2)	C(51)-C(52)-C(47)	118.5(2)
C(6)-C(11)-C(15)	120.96(19)	C(51)-C(52)-C(56)	119.8(2)
C(7)-C(12)-C(14)	111.8(2)	C(47)-C(52)-C(56)	121.8(2)
C(7)-C(12)-C(13)	110.4(2)	C(48)-C(53)-C(55)	110.2(2)
C(14)-C(12)-C(13)	109.4(2)	C(48)-C(53)-C(54)	113.2(2)
C(11)-C(15)-C(17)	113.5(2)	C(55)-C(53)-C(54)	109.7(2)
C(11)-C(15)-C(16)	110.53(18)	C(57)-C(56)-C(52)	111.4(2)

C(17)-C(15)-C(16)	109.5(2)	C(57)-C(56)-C(58)	110.4(2)
C(19)-C(18)-C(23)	121.36(19)	C(52)-C(56)-C(58)	113.2(2)
C(19)-C(18)-N(2)	119.84(19)		

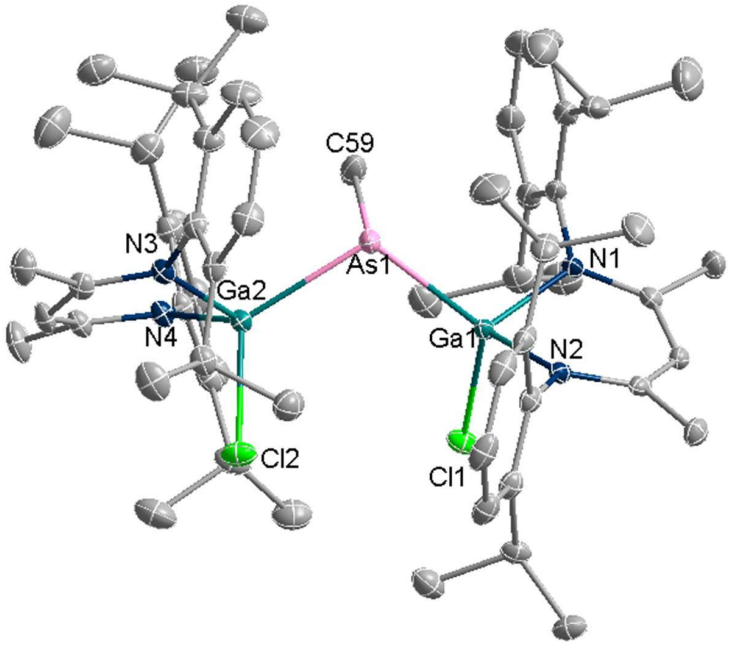

Fig. S44. Solid state structure of **9**. Hydrogen atoms are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S18: Bond lengths [Å] for **9** (jk_347m).

As(1)-C(59)	1.990(2)	C(8)-C(9)	1.381(4)	C(35)-C(36)	1.403(3)
As(1)-Ga(1)	2.4044(4)	C(9)-C(10)	1.373(4)	C(35)-C(40)	1.408(3)
As(1)-Ga(2)	2.4134(4)	C(10)-C(11)	1.401(3)	C(36)-C(37)	1.397(3)
Ga(1)-N(1)	1.9702(16)	C(11)-C(15)	1.517(3)	C(36)-C(41)	1.513(3)
Ga(1)-N(2)	1.9726(16)	C(12)-C(13)	1.531(3)	C(37)-C(38)	1.380(3)
Ga(1)-Cl(1)	2.2045(6)	C(12)-C(14)	1.534(3)	C(38)-C(39)	1.374(3)
Ga(2)-N(4)	1.9668(16)	C(15)-C(16)	1.526(4)	C(39)-C(40)	1.387(3)
Ga(2)-N(3)	1.9726(16)	C(15)-C(17)	1.531(3)	C(40)-C(44)	1.519(3)
Ga(2)-Cl(2)	2.2003(6)	C(18)-C(19)	1.404(3)	C(41)-C(42)	1.528(3)
N(1)-C(1)	1.334(3)	C(18)-C(23)	1.404(3)	C(41)-C(43)	1.532(3)
N(1)-C(6)	1.449(2)	C(19)-C(20)	1.398(3)	C(44)-C(45)	1.530(3)
N(2)-C(3)	1.325(2)	C(19)-C(24)	1.521(3)	C(44)-C(46)	1.531(3)
N(2)-C(18)	1.456(2)	C(20)-C(21)	1.382(3)	C(47)-C(48)	1.402(3)
N(3)-C(30)	1.322(3)	C(21)-C(22)	1.379(3)	C(47)-C(52)	1.412(3)
N(3)-C(35)	1.446(3)	C(22)-C(23)	1.397(3)	C(48)-C(49)	1.396(3)
N(4)-C(32)	1.346(3)	C(23)-C(27)	1.519(3)	C(48)-C(53)	1.532(3)
N(4)-C(47)	1.452(2)	C(24)-C(26)	1.526(3)	C(49)-C(50)	1.377(3)
C(1)-C(2)	1.389(3)	C(24)-C(25)	1.538(3)	C(50)-C(51)	1.376(3)

C(1)-C(4)	1.509(3)	C(27)-C(28)	1.527(3)	C(51)-C(52)	1.395(3)
C(2)-C(3)	1.407(3)	C(27)-C(29)	1.532(3)	C(52)-C(56)	1.519(3)
C(3)-C(5)	1.504(3)	C(30)-C(31)	1.404(3)	C(53)-C(54)	1.527(3)
C(6)-C(7)	1.401(3)	C(30)-C(33)	1.510(3)	C(53)-C(55)	1.534(3)
C(6)-C(11)	1.406(3)	C(31)-C(32)	1.388(3)	C(56)-C(57)	1.536(3)
C(7)-C(8)	1.396(3)	C(32)-C(34)	1.516(3)	C(56)-C(58)	1.539(3)
C(7)-C(12)	1.517(3)				

Table S19: Bond angles [°] for **9** (jk_347m).

C(59)-As(1)-Ga(1)	100.86(7)	C(18)-C(19)-C(24)	123.72(17)
C(59)-As(1)-Ga(2)	97.46(7)	C(21)-C(20)-C(19)	121.3(2)
Ga(1)-As(1)-Ga(2)	108.431(12)	C(22)-C(21)-C(20)	119.9(2)
N(1)-Ga(1)-N(2)	95.20(7)	C(21)-C(22)-C(23)	121.4(2)
N(1)-Ga(1)-Cl(1)	103.96(5)	C(22)-C(23)-C(18)	117.8(2)
N(2)-Ga(1)-Cl(1)	102.44(5)	C(22)-C(23)-C(27)	120.40(19)
N(1)-Ga(1)-As(1)	113.17(5)	C(18)-C(23)-C(27)	121.78(19)
N(2)-Ga(1)-As(1)	116.73(5)	C(19)-C(24)-C(26)	110.74(18)
Cl(1)-Ga(1)-As(1)	121.479(18)	C(19)-C(24)-C(25)	112.40(17)
N(4)-Ga(2)-N(3)	95.16(7)	C(26)-C(24)-C(25)	109.05(17)
N(4)-Ga(2)-Cl(2)	104.33(5)	C(23)-C(27)-C(28)	111.33(19)
N(3)-Ga(2)-Cl(2)	101.17(5)	C(23)-C(27)-C(29)	112.5(2)
N(4)-Ga(2)-As(1)	124.31(5)	C(28)-C(27)-C(29)	110.8(2)
N(3)-Ga(2)-As(1)	106.23(5)	N(3)-C(30)-C(31)	122.76(18)
Cl(2)-Ga(2)-As(1)	120.195(19)	N(3)-C(30)-C(33)	120.10(18)
C(1)-N(1)-C(6)	118.32(16)	C(31)-C(30)-C(33)	117.14(18)
C(1)-N(1)-Ga(1)	118.88(13)	C(32)-C(31)-C(30)	128.15(19)
C(6)-N(1)-Ga(1)	122.76(13)	N(4)-C(32)-C(31)	124.97(18)
C(3)-N(2)-C(18)	117.62(16)	N(4)-C(32)-C(34)	119.30(18)
C(3)-N(2)-Ga(1)	118.82(13)	C(31)-C(32)-C(34)	115.73(18)
C(18)-N(2)-Ga(1)	123.15(12)	C(36)-C(35)-C(40)	121.76(19)
C(30)-N(3)-C(35)	120.00(17)	C(36)-C(35)-N(3)	120.71(18)
C(30)-N(3)-Ga(2)	119.45(14)	C(40)-C(35)-N(3)	117.50(18)
C(35)-N(3)-Ga(2)	120.37(13)	C(37)-C(36)-C(35)	117.5(2)
C(32)-N(4)-C(47)	115.66(16)	C(37)-C(36)-C(41)	119.62(19)
C(32)-N(4)-Ga(2)	117.04(13)	C(35)-C(36)-C(41)	122.86(18)
C(47)-N(4)-Ga(2)	127.08(13)	C(38)-C(37)-C(36)	121.3(2)
N(1)-C(1)-C(2)	123.47(18)	C(39)-C(38)-C(37)	120.1(2)
N(1)-C(1)-C(4)	119.37(17)	C(38)-C(39)-C(40)	121.4(2)
C(2)-C(1)-C(4)	117.14(18)	C(39)-C(40)-C(35)	117.9(2)
C(1)-C(2)-C(3)	128.15(19)	C(39)-C(40)-C(44)	121.2(2)
N(2)-C(3)-C(2)	124.25(18)	C(35)-C(40)-C(44)	120.92(19)
N(2)-C(3)-C(5)	119.83(17)	C(36)-C(41)-C(42)	110.56(17)
C(2)-C(3)-C(5)	115.91(17)	C(36)-C(41)-C(43)	111.86(18)

C(7)-C(6)-C(11)	121.83(19)	C(42)-C(41)-C(43)	109.34(18)
C(7)-C(6)-N(1)	120.20(18)	C(40)-C(44)-C(45)	112.42(18)
C(11)-C(6)-N(1)	117.95(19)	C(40)-C(44)-C(46)	112.7(2)
C(8)-C(7)-C(6)	117.8(2)	C(45)-C(44)-C(46)	110.9(2)
C(8)-C(7)-C(12)	119.5(2)	C(48)-C(47)-C(52)	121.31(18)
C(6)-C(7)-C(12)	122.68(18)	C(48)-C(47)-N(4)	120.31(17)
C(9)-C(8)-C(7)	121.2(2)	C(52)-C(47)-N(4)	118.17(18)
C(10)-C(9)-C(8)	120.2(2)	C(49)-C(48)-C(47)	117.67(19)
C(9)-C(10)-C(11)	121.2(2)	C(49)-C(48)-C(53)	119.9(2)
C(10)-C(11)-C(6)	117.6(2)	C(47)-C(48)-C(53)	122.44(18)
C(10)-C(11)-C(15)	119.9(2)	C(50)-C(49)-C(48)	121.8(2)
C(6)-C(11)-C(15)	122.48(19)	C(51)-C(50)-C(49)	119.7(2)
C(7)-C(12)-C(13)	110.96(19)	C(50)-C(51)-C(52)	121.5(2)
C(7)-C(12)-C(14)	111.76(17)	C(51)-C(52)-C(47)	117.7(2)
C(13)-C(12)-C(14)	110.08(19)	C(51)-C(52)-C(56)	119.14(19)
C(11)-C(15)-C(16)	112.7(2)	C(47)-C(52)-C(56)	123.10(18)
C(11)-C(15)-C(17)	111.4(2)	C(54)-C(53)-C(48)	113.16(18)
C(16)-C(15)-C(17)	110.0(2)	C(54)-C(53)-C(55)	109.08(19)
C(19)-C(18)-C(23)	121.78(18)	C(48)-C(53)-C(55)	113.1(2)
C(19)-C(18)-N(2)	119.86(17)	C(52)-C(56)-C(57)	111.94(19)
C(23)-C(18)-N(2)	118.33(17)	C(52)-C(56)-C(58)	113.4(2)
C(20)-C(19)-C(18)	117.79(19)	C(57)-C(56)-C(58)	108.3(2)
C(20)-C(19)-C(24)	118.49(18)		

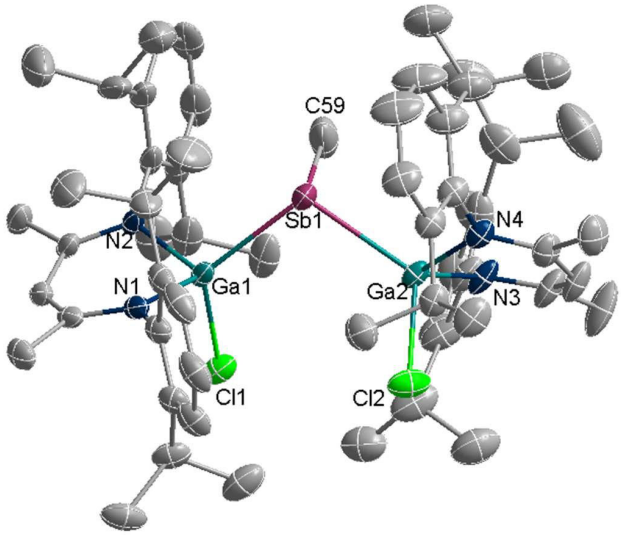

Fig. S45. Solid state structure of **10**. Hydrogen atoms are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S20: Bond lengths [Å] for **10** (jk_312m).

Sb(1)-C(59)	2.129(7)	C(8)-C(9)	1.378(7)	C(35)-C(36)	1.409(7)
Sb(1)-Ga(1)	2.5837(7)	C(9)-C(10)	1.373(8)	C(35)-C(40)	1.417(8)
Sb(1)-Ga(2)	2.6045(6)	C(10)-C(11)	1.398(8)	C(36)-C(37)	1.403(6)
Ga(1)-N(2)	1.963(3)	C(11)-C(15)	1.527(7)	C(36)-C(41)	1.523(8)
Ga(1)-N(1)	1.975(3)	C(12)-C(13)	1.517(7)	C(37)-C(38)	1.376(8)
Ga(1)-Cl(1)	2.2084(12)	C(12)-C(14)	1.542(7)	C(38)-C(39)	1.372(8)
Ga(2)-N(3)	1.960(3)	C(15)-C(17)	1.527(8)	C(39)-C(40)	1.401(6)
Ga(2)-N(4)	1.975(4)	C(15)-C(16)	1.536(8)	C(40)-C(44)	1.600(8)
Ga(2)-Cl(2)	2.2103(12)	C(18)-C(19)	1.396(8)	C(41)-C(43)	1.512(9)
N(1)-C(1)	1.331(5)	C(18)-C(23)	1.409(8)	C(41)-C(42)	1.544(9)
N(1)-C(6)	1.445(5)	C(19)-C(20)	1.410(6)	C(44)-C(46)	1.488(9)
N(2)-C(3)	1.335(5)	C(19)-C(24)	1.511(9)	C(44)-C(45)	1.513(9)
N(2)-C(18)	1.449(5)	C(20)-C(21)	1.373(12)	C(47)-C(52)	1.404(6)
N(3)-C(30)	1.341(6)	C(21)-C(22)	1.372(12)	C(47)-C(48)	1.408(7)
N(3)-C(35)	1.454(5)	C(22)-C(23)	1.399(7)	C(48)-C(49)	1.394(8)
N(4)-C(32)	1.319(6)	C(23)-C(27)	1.514(10)	C(48)-C(53)	1.526(7)
N(4)-C(47)	1.445(5)	C(24)-C(26)	1.533(7)	C(49)-C(50)	1.373(9)
C(1)-C(2)	1.408(6)	C(24)-C(25)	1.539(8)	C(50)-C(51)	1.378(8)
C(1)-C(4)	1.509(5)	C(27)-C(29)	1.529(10)	C(51)-C(52)	1.397(6)
C(2)-C(3)	1.395(6)	C(27)-C(28)	1.532(9)	C(52)-C(56)	1.513(6)
C(3)-C(5)	1.507(6)	C(30)-C(31)	1.394(7)	C(53)-C(54)	1.525(9)
C(6)-C(7)	1.405(6)	C(30)-C(33)	1.519(6)	C(53)-C(55)	1.534(8)
C(6)-C(11)	1.413(6)	C(31)-C(32)	1.405(7)	C(56)-C(58)	1.520(7)
C(7)-C(8)	1.405(6)	C(32)-C(34)	1.505(6)	C(56)-C(57)	1.537(6)
C(7)-C(12)	1.517(6)				

Table S21: Bond angles [°] for **10** (jk_312m).

C(59)-Sb(1)-Ga(1)	101.0(2)	C(20)-C(19)-C(24)	119.4(6)
C(59)-Sb(1)-Ga(2)	97.95(18)	C(21)-C(20)-C(19)	121.1(7)
Ga(1)-Sb(1)-Ga(2)	106.652(19)	C(22)-C(21)-C(20)	120.5(5)
N(2)-Ga(1)-N(1)	95.42(14)	C(21)-C(22)-C(23)	121.4(7)
N(2)-Ga(1)-Cl(1)	103.69(13)	C(22)-C(23)-C(18)	117.4(7)
N(1)-Ga(1)-Cl(1)	102.24(10)	C(22)-C(23)-C(27)	120.1(6)
N(2)-Ga(1)-Sb(1)	112.33(11)	C(18)-C(23)-C(27)	122.4(4)
N(1)-Ga(1)-Sb(1)	117.55(11)	C(19)-C(24)-C(26)	110.8(5)
Cl(1)-Ga(1)-Sb(1)	121.69(4)	C(19)-C(24)-C(25)	112.7(5)
N(3)-Ga(2)-N(4)	95.43(15)	C(26)-C(24)-C(25)	110.1(5)
N(3)-Ga(2)-Cl(2)	103.79(12)	C(23)-C(27)-C(29)	113.5(5)
N(4)-Ga(2)-Cl(2)	101.96(10)	C(23)-C(27)-C(28)	111.1(7)
N(3)-Ga(2)-Sb(1)	125.48(10)	C(29)-C(27)-C(28)	109.9(6)
N(4)-Ga(2)-Sb(1)	105.89(10)	N(3)-C(30)-C(31)	124.9(4)

Cl(2)-Ga(2)-Sb(1)	119.19(4)	N(3)-C(30)-C(33)	119.2(4)
C(1)-N(1)-C(6)	118.6(3)	C(31)-C(30)-C(33)	115.9(4)
C(1)-N(1)-Ga(1)	118.3(3)	C(30)-C(31)-C(32)	128.2(4)
C(6)-N(1)-Ga(1)	122.6(3)	N(4)-C(32)-C(31)	122.6(4)
C(3)-N(2)-C(18)	118.6(4)	N(4)-C(32)-C(34)	120.0(4)
C(3)-N(2)-Ga(1)	119.2(3)	C(31)-C(32)-C(34)	117.5(4)
C(18)-N(2)-Ga(1)	122.1(3)	C(36)-C(35)-C(40)	121.7(4)
C(30)-N(3)-C(35)	116.6(3)	C(36)-C(35)-N(3)	117.8(4)
C(30)-N(3)-Ga(2)	117.1(3)	C(40)-C(35)-N(3)	120.4(4)
C(35)-N(3)-Ga(2)	126.1(3)	C(37)-C(36)-C(35)	117.2(5)
C(32)-N(4)-C(47)	120.7(4)	C(37)-C(36)-C(41)	119.5(5)
C(32)-N(4)-Ga(2)	119.4(3)	C(35)-C(36)-C(41)	123.3(4)
C(47)-N(4)-Ga(2)	119.7(3)	C(38)-C(37)-C(36)	121.5(5)
N(1)-C(1)-C(2)	124.4(4)	C(39)-C(38)-C(37)	120.4(4)
N(1)-C(1)-C(4)	119.8(4)	C(38)-C(39)-C(40)	121.4(5)
C(2)-C(1)-C(4)	115.8(4)	C(39)-C(40)-C(35)	117.3(5)
C(3)-C(2)-C(1)	128.4(4)	C(39)-C(40)-C(44)	117.9(5)
N(2)-C(3)-C(2)	122.8(4)	C(35)-C(40)-C(44)	124.7(4)
N(2)-C(3)-C(5)	120.0(4)	C(43)-C(41)-C(36)	112.9(5)
C(2)-C(3)-C(5)	117.2(4)	C(43)-C(41)-C(42)	108.1(6)
C(7)-C(6)-C(11)	121.3(4)	C(36)-C(41)-C(42)	112.9(6)
C(7)-C(6)-N(1)	120.0(4)	C(46)-C(44)-C(45)	111.5(5)
C(11)-C(6)-N(1)	118.8(4)	C(46)-C(44)-C(40)	114.7(4)
C(6)-C(7)-C(8)	118.0(4)	C(45)-C(44)-C(40)	108.9(6)
C(6)-C(7)-C(12)	123.3(4)	C(52)-C(47)-C(48)	121.9(4)
C(8)-C(7)-C(12)	118.7(4)	C(52)-C(47)-N(4)	120.4(4)
C(9)-C(8)-C(7)	121.0(5)	C(48)-C(47)-N(4)	117.6(4)
C(10)-C(9)-C(8)	120.4(5)	C(49)-C(48)-C(47)	118.0(5)
C(9)-C(10)-C(11)	121.3(5)	C(49)-C(48)-C(53)	120.6(5)
C(10)-C(11)-C(6)	117.9(5)	C(47)-C(48)-C(53)	121.3(4)
C(10)-C(11)-C(15)	120.6(5)	C(50)-C(49)-C(48)	120.7(5)
C(6)-C(11)-C(15)	121.5(5)	C(49)-C(50)-C(51)	120.9(5)
C(7)-C(12)-C(13)	111.1(5)	C(50)-C(51)-C(52)	121.1(5)
C(7)-C(12)-C(14)	112.0(4)	C(51)-C(52)-C(47)	117.5(4)
C(13)-C(12)-C(14)	109.5(4)	C(51)-C(52)-C(56)	119.7(4)
C(17)-C(15)-C(11)	110.9(5)	C(47)-C(52)-C(56)	122.8(4)
C(17)-C(15)-C(16)	110.7(5)	C(54)-C(53)-C(48)	112.5(5)
C(11)-C(15)-C(16)	112.7(5)	C(54)-C(53)-C(55)	109.9(5)
C(19)-C(18)-C(23)	122.2(4)	C(48)-C(53)-C(55)	113.1(5)
C(19)-C(18)-N(2)	119.8(5)	C(52)-C(56)-C(58)	110.8(4)
C(23)-C(18)-N(2)	118.0(5)	C(52)-C(56)-C(57)	111.3(4)
C(18)-C(19)-C(20)	117.4(6)	C(58)-C(56)-C(57)	109.6(4)
C(18)-C(19)-C(24)	123.2(4)		

C) Computational methods

All quantum chemical calculations were employed with the ORCA quantum chemistry package (version 4.12).[10] Geometry optimizations of the anionic model systems were calculated with a PBE0 density functional, def2-TZVP[11] and atom-pairwise dispersion correction with Becke-Johnson damping Scheme (D3BJ).[12] The quantum chemical calculations of **1** and **2** were carried out without the counter cation $IPrH^+$ (**1'** and **2'**)and the ground-state geometry optimizations of **1'** and **2'** as well as **5**-**6** and **9**-**10** and LGaEGa(Cl)L (E = As **III**, Sb **IV**) were performed with a PBE0 density functional, def2-SVP basis sets for C, H and N atoms and def2-TZVP basis set for Cl, Ga, As and Sb atoms basis set and atom-pairwise dispersion correction with Becke-Johnson damping Scheme.[13] Additionally, effective core potentials (ECP) were employed for Sb atoms to accelerate geometry optimizations.[14] The RIJCOSX approximation was employed to accelerate the calculations in conjunction with the appropriate auxiliary basis sets.[15] Frequency calculations were carried out to determine the optimized structures as minima on the potential energy surface. Natural bond orbital analysis was performed using the NBO version 6.0.[16]

Table S22. Calculated bond lengths, Mayer bond order, natural charge (e) and Wiberg bond index of anionic model system $[ER_2]^-$ (E = As, Sb; R = Me, NMe_2, OMe, $SiMe_3$, $GaMe_2$) (PBE0-D3BJ/def2-TZVP).

	$[As(OMe)_2]^-$	**$[Sb(OMe)_2]^-$**
bond lengths E-O1/2	1.864	2.037
Mayer bond order E-O1/2	0.83	0.73
Wiberg bond index E-O1/2	0.63	0.55
Mulliken atomic charge (E;O)	-0.15; -0.45	-0.06; -0.54
Natural charge (E; O)	0.29; -0.80	0.37; -0.84
	$[As(NMe_2)_2]^-$	**$[Sb(NMe_2)_2]^-$**
bond lengths E-N1/2	1.910	2.098
Mayer bond order E-N1/2	0.95	0.86
Wiberg bond index E-N1/2	0.72	0.64
Mulliken atomic charge (E; N)	-0.34; -0.26	-0.26; -0.38
Natural charge (E; N)	0.16; -0.71	0.23; -0.75
	$[As(CMe_3)_2]^-$	**$[Sb(CMe_3)_2]^-$**
bond lengths E-C1/2	2.0089	2.212
Mayer bond order E-C1/2	1.08	0.88
Wiberg bond index As-C1/2	0.92	0.87
Mulliken atomic charge (E; C)	-0.42; -0.53	-0.31; -0.62
Natural charge (E; C)	-0.19; -0.93	-0.16; -0.98
	$[As(SiMe_3)_2]^-$	**$[Sb(SiMe_3)_2]^-$**
bond lengths E-Si1/2	2.292	2.519
Mayer bond order E-Si1/2	1.49	1.26
Wiberg bond index E-Si1/2	1.15	1.10
Mulliken atomic charge (E; Si)	-0.58; 0.22	-0.47; 0.23
Natural charge (E; Si)	-0.86; 1.33	-0.72; 1.25
	$[As(GaMe_2)_2]^-$	**$[Sb(GaMe_2)_2]^-$**
bond lengths E-Ga1/2	2.330	2.528
Mayer bond order E-Ga1/2	1.48	1.39
Wiberg bond index E-Ga1/2	1.24	1.26
Mulliken atomic charge (E; Ga)	-0.48; 0.25	-0.52; 0.23
Natural charge (E; Ga)	-1.06; 1.19	-0.89; 1.10

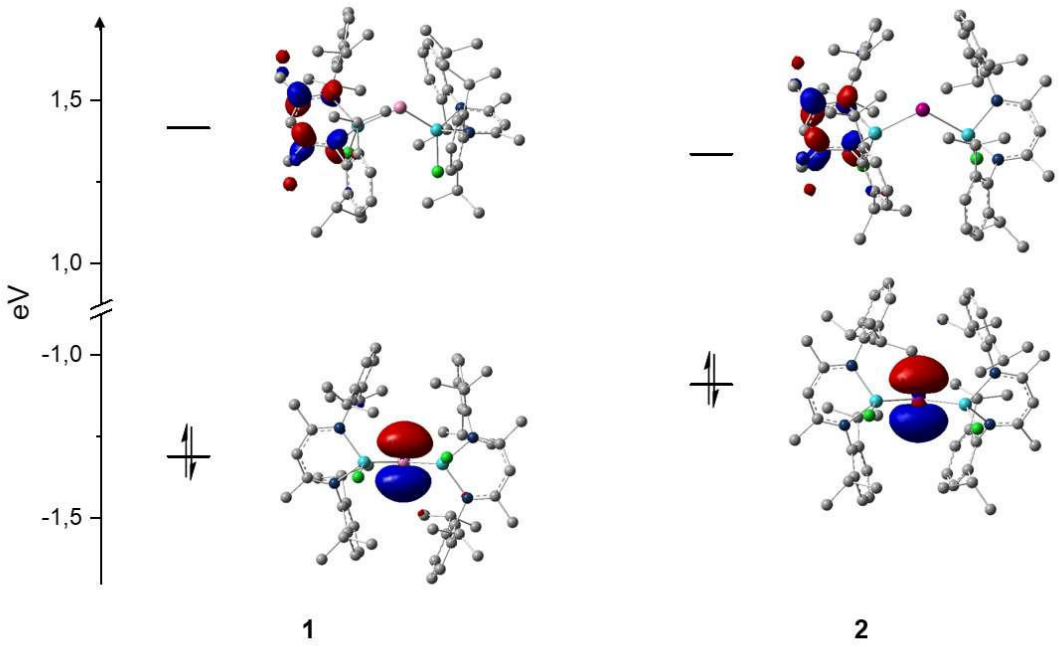

Fig. S46. Calculated HOMO's and LUMO's with their corresponding orbital energy in eV of **1'** (left) and **2'** (right) (PBE0-D3BJ/def2-TZVP).

Table S23. Mayer bond order of LGaEGa(Cl)L (E = As **III**, Sb **IV**), **1'**, **2'**, **5**, **6**, **9** and **10** (PBE0-D3BJ/def2-SVP; def2-TZVP E, Ga, Cl).

X-Y	III'	IV'	1	2	5	6	9	10
E-Ga(1)	1.65	1.62	1.28	1.22	0.97	0.95	0.95	0.94
E-Ga(2)	1.09	1.06	1.30	1.23	0.97	0.96	0.95	0.95
Ga(1)-Cl(1)	-	-	0.78	0.78	0.90	0.89	0.86	0.85
Ga(2)-Cl(1)	0.81	0.81	0.78	0.78	0.90	0.89	0.87	0.87
E-H	-	-	-	-	0.88	0.92	-	-
E-C	-	-	-	-	-	-	1.08	1.10

Table S24. Wiberg bond index of LGaEGa(Cl)L (E = As **III**, Sb **IV**), **1'**, **2'**, **5**, **6**, **9** and **10** (PBE0-D3BJ/def2-SVP; def2-TZVP E, Ga, Cl).

X-Y	III'	IV'	1	2	5	6	9	10
E-Ga(1)	1.49	1.54	1.12	1.17	0.85	0.92	0.86	0.93
E-Ga(2)	0.98	1.04	1.11	1.17	0.85	0.93	0.86	0.94
Ga(1)-Cl(1)	-	-	0.63	0.63	0.69	0.69	0.66	0.67
Ga(2)-Cl(1)	0.66	0.65	0.63	0.63	0.69	0.69	0.68	0.66
E-H	-	-	-	-	0.95	0.94	-	-
E-C	-	-	-	-	-	-	0.95	0.90

Table S25. Natural Charge of LGaEGa(Cl)L (E = As **III**, Sb **IV**), **1'**, **2'**, **5**, **6**, **9** and **10** (PBE0-D3BJ/def2-SVP; def2-TZVP E, Ga, Cl).

X	III'	IV'	1	2	5	6	9	10
E	-1.00	-0.71	-1.21	-0.93	-0.69	-0.33	-0.38	-0.03
Ga(1)	1.27	1.12	1.29	1.17	1.40	1.28	1.39	1.26
Ga(2)	1.33	1.21	1.29	1.16	1.39	1.27	1.38	1.25
Cl1	-	-	-0.57	-0.57	-0.53	-0.53	-0.55	-0.55
Cl2	-0.55	-0.56	-0.57	-0.58	-0.53	-0.53	-0.54	-0.55
H	-	-	-	-	0.04	-0.07	-	-
C	-	-	-	-	-	-	-0.94	-1.02

Table S26. Bond polarization P(X; Y) of LGaEGa(Cl)L (E = As **III**, Sb **IV**), **1'**, **2'**, **5**, **6**, **9** and **10** in % (PBE0-D3BJ/def2-SVP; def2-TZVP E, Ga, Cl).

X-Y	III'	IV'	1	2	5	6	9	10
E-Ga(1)	63; 37 84; 16	55; 45 83; 17	69; 32	59; 41	71; 29	64; 36	70; 30	62; 38
E-Ga(2)	69; 31	61; 39	69; 31	59; 41	71; 29	64; 37	69; 31	62; 38
E-H	-	-	-	-	51; 49	46; 54	-	-
E-C	-	-	-	-	-	-	39; 61	35; 65

Table S27. Cartesian coordinates (x,y,z) for the optimized geometry of **1'**.

As	5,23323	10,22928	14,48519	C	6,36326	10,57134	18,04366
Ga	5,00833	7,92103	14,4338	H	7,4441	10,64282	18,24857
Ga	4,45483	11,07741	12,47432	H	5,85845	11,32198	18,67243
Cl	3,69071	6,60802	13,15898	H	6,18511	10,83147	16,98946
Cl	3,97972	10,0473	10,52602	C	2,76804	13,43895	11,90011
N	6,66017	6,74122	14,37855	C	3,821	13,96125	11,12738
N	4,59478	7,35011	16,34753	H	3,57461	14,8316	10,52178
N	2,85414	12,33784	12,63349	C	5,18162	13,61864	11,17015
N	5,66655	12,57724	11,83647	C	1,48521	14,22839	11,89396
C	6,75005	5,64121	15,11239	H	1,58967	15,14017	11,29391
C	5,88209	5,32059	16,17174	H	1,18914	14,5017	12,91718
H	6,05856	4,35847	16,64977	H	0,66345	13,62471	11,48637
C	4,95845	6,16202	16,81172	C	6,12906	14,54569	10,45164
C	7,8757	4,67314	14,86413	H	6,78042	13,98274	9,76997
H	7,77357	4,21122	13,87292	H	6,79786	15,04861	11,16627
H	7,88682	3,88048	15,62175	H	5,57604	15,3048	9,88483
H	8,84399	5,19523	14,87186	C	1,77038	12,00294	13,50083
C	4,40395	5,68314	18,12768	C	0,63408	11,32524	13,00291
H	3,30557	5,72235	18,12879	C	-0,42348	11,05505	13,87646
H	4,73647	6,34311	18,94151	H	-1,29855	10,52261	13,49588
H	4,73386	4,66021	18,34739	C	-0,37364	11,42521	15,21288
C	7,71654	7,06635	13,47902	H	-1,20806	11,19936	15,88158
C	7,82257	6,46076	12,20718	C	0,75789	12,06625	15,6978
C	8,92559	6,78803	11,40974	H	0,81166	12,33982	16,75372
H	9,02152	6,32834	10,42298	C	1,83733	12,37161	14,8646
C	9,87849	7,70579	11,82895	C	0,51046	10,85883	11,56465
H	10,71935	7,96259	11,17911	H	1,3521	11,27858	10,99329
C	9,73343	8,33287	13,06142	C	-0,79921	11,32632	10,9253
H	10,45884	9,08845	13,36579	H	-0,9416	12,41534	11,01078
C	8,66465	8,0257	13,90686	H	-1,66911	10,84334	11,39825
C	6,77463	5,51167	11,65002	H	-0,82327	11,06045	9,85652
H	6,04902	5,30454	12,45021	C	0,62186	9,33732	11,47711
C	7,37432	4,1867	11,1704	H	0,51099	9,00294	10,43349
H	6,57988	3,51621	10,80641	H	-0,164	8,85158	12,07717
H	7,92546	3,65961	11,96477	H	1,59611	8,98136	11,83855
H	8,0767	4,33837	10,33487	C	3,00965	13,13888	15,44689
C	5,99782	6,1724	10,50954	H	3,83247	13,07084	14,71977
H	6,65734	6,36028	9,64648	C	2,65079	14,61445	15,64144
H	5,55075	7,12742	10,81973	H	2,34167	15,09621	14,70145
H	5,17653	5,51887	10,17663	H	3,50912	15,17546	16,04555
C	8,52597	8,69591	15,26076	H	1,81876	14,72276	16,35703
H	7,44531	8,84155	15,4189	C	3,49939	12,52469	16,75265
C	9,05764	7,82684	16,40136	H	3,73901	11,46301	16,60343

H	8,485	6,89536	16,51402	H	2,75291	12,61072	17,55865
H	8,98311	8,37312	17,35572	H	4,41445	13,03111	17,09781
H	10,11728	7,56122	16,24553	C	7,0805	12,5069	12,01009
C	9,13908	10,0865	15,29626	C	7,89256	11,89228	11,03462
H	10,23961	10,07164	15,22519	C	9,28231	11,95037	11,19002
H	8,88204	10,57732	16,24671	H	9,92144	11,47622	10,43986
H	8,74085	10,70452	14,47957	C	9,85777	12,59189	12,27974
C	3,77427	8,18833	17,16133	H	10,94509	12,64013	12,3847
C	2,37259	8,14906	17,0008	C	9,04337	13,14546	13,26275
C	1,57624	8,98343	17,78936	H	9,50213	13,60593	14,13971
H	0,49287	8,97102	17,64444	C	7,65106	13,09913	13,16111
C	2,1337	9,82593	18,74146	C	7,29198	11,13318	9,86807
H	1,49655	10,47444	19,34802	H	6,20223	11,2631	9,91671
C	3,51288	9,84968	18,90017	C	7,75644	11,62487	8,49818
H	3,95833	10,52608	19,63415	H	7,26509	11,03831	7,70636
C	4,35394	9,05339	18,11775	H	8,84559	11,50778	8,36704
C	1,70682	7,23278	15,99651	H	7,50591	12,68355	8,32617
H	2,49018	6,64048	15,50554	C	7,56719	9,63841	10,0176
C	0,74259	6,2556	16,66879	H	6,95522	9,06042	9,30912
H	0,29082	5,58497	15,92045	H	7,32448	9,2863	11,03041
H	-0,07672	6,78281	17,18449	H	8,62739	9,40585	9,82541
H	1,25471	5,62924	17,41635	C	6,77597	13,6461	14,27463
C	1,01037	8,03925	14,90588	H	5,87571	13,01142	14,28151
H	1,7015	8,76302	14,44999	C	6,33495	15,09157	14,03944
H	0,15507	8,60493	15,3062	H	5,71422	15,19882	13,13955
H	0,64834	7,37336	14,10847	H	7,20877	15,75803	13,94432
C	5,85055	9,16241	18,34556	H	5,73232	15,44627	14,88989
H	6,34434	8,47049	17,64757	C	7,41679	13,51249	15,65235
C	6,22742	8,7635	19,77438	H	7,78051	12,4914	15,82587
H	5,89825	7,74328	20,02576	H	6,67412	13,7432	16,43095
H	5,7665	9,44523	20,50676	H	8,25924	14,21053	15,78988
H	7,31885	8,8199	19,91596				

Table S28. Cartesian coordinates (x,y,z) for the optimized geometry of **2'**.

Sb	0,69145	4,34393	14,60856	C	0,55077	-1,63867	13,80965
Ga	1,13915	3,72109	12,20478	H	-0,52025	-1,88816	13,87848
Ga	2,09981	6,31232	15,37077	H	1,06449	-2,20573	14,60177
Cl	2,18834	4,72691	10,47436	H	0,93148	-2,0077	12,84465
Cl	2,929	8,10895	14,28183	C	3,67609	7,08643	17,74341
N	-0,59394	3,31307	11,22638	C	2,66395	8,01351	18,06501
N	1,77387	1,80126	11,98976	H	2,91013	8,72968	18,84795
N	3,61344	6,21508	16,74513	C	1,3282	8,02234	17,63407
N	0,85738	7,20327	16,70454	C	4,8946	7,10963	18,62994
C	-0,62641	2,40663	10,26271	H	5,21104	6,09103	18,89604
C	0,39908	1,46905	10,033	H	4,69464	7,67849	19,5461

H	0,27607	0,83732	9,15444	H	5,74171	7,57654	18,10865
C	1,45302	1,12125	10,89341	C	0,3895	8,9884	18,30741
C	-1,84254	2,31441	9,38054	H	0,92866	9,63502	19,01105
H	-2,7437	2,15827	9,99204	H	-0,40521	8,45292	18,84678
H	-1,74742	1,48988	8,66362	H	-0,1156	9,61239	17,55692
H	-1,99844	3,25133	8,82879	C	4,66472	5,27125	16,55502
C	2,21907	-0,13052	10,55636	C	5,90166	5,64917	15,98421
H	2,00794	-0,92046	11,29168	C	6,89269	4,67257	15,83473
H	3,30191	0,0574	10,59851	H	7,84825	4,95667	15,3867
H	1,95107	-0,50267	9,55967	C	6,68077	3,35582	16,21717
C	-1,74324	4,10085	11,51609	H	7,46837	2,60986	16,08346
C	-2,02935	5,27216	10,78105	C	5,45292	2,99057	16,75589
C	-3,15049	6,02646	11,14679	H	5,27244	1,95293	17,04011
H	-3,37776	6,94063	10,59208	C	4,43522	3,92835	16,93631
C	-3,96383	5,6483	12,20585	C	6,21144	7,05435	15,50025
H	-4,82391	6,26089	12,48865	H	5,39092	7,71616	15,81439
C	-3,66135	4,49948	12,92889	C	6,25601	7,1017	13,97386
H	-4,28478	4,22793	13,78126	H	5,28557	6,82436	13,54417
C	-2,55504	3,71056	12,60835	H	7,02178	6,41384	13,58053
C	-1,15426	5,77226	9,64381	H	6,4964	8,11861	13,62515
H	-0,38601	5,01002	9,44716	C	7,52728	7,58153	16,07895
C	-1,94691	6,00987	8,35608	H	7,57259	7,49228	17,17567
H	-2,7176	6,78522	8,49357	H	7,66719	8,64165	15,81428
H	-2,4585	5,10089	8,00074	H	8,3892	7,02921	15,67158
H	-1,276	6,35842	7,55494	C	3,13666	3,51648	17,59615
C	-0,41369	7,05154	10,0356	H	2,35948	4,19326	17,21135
H	0,16147	6,91349	10,95945	C	2,70033	2,10775	17,22523
H	-1,11863	7,88523	10,18639	H	1,68556	1,91523	17,60401
H	0,29583	7,34069	9,24518	H	3,36501	1,33579	17,64713
C	-2,21406	2,48531	13,44052	H	2,66967	1,99254	16,13399
H	-1,11457	2,46957	13,51955	C	3,21865	3,69445	19,11111
C	-2,63177	1,16553	12,78902	H	4,02995	3,07876	19,53308
H	-2,39991	0,32637	13,46434	H	2,27637	3,38059	19,58844
H	-2,09889	0,98102	11,8458	H	3,40667	4,74068	19,39349
H	-3,71585	1,14328	12,5879	C	-0,54879	7,05001	16,53727
C	-2,75115	2,57182	14,86302	C	-1,25612	7,84668	15,61546
H	-2,49828	3,54229	15,31341	C	-2,62357	7,61211	15,44162
H	-2,29523	1,78655	15,482	H	-3,17557	8,20507	14,70752
H	-3,84432	2,43001	14,90531	C	-3,27893	6,61269	16,14689
C	2,68253	1,22307	12,92576	H	-4,33979	6,4174	15,96764
C	4,04023	1,61369	12,93529	C	-2,56848	5,82625	17,04791
C	4,90818	1,01894	13,85569	H	-3,08221	5,02137	17,57676
H	5,9518	1,34063	13,8797	C	-1,20181	6,01946	17,25437
C	4,47346	0,03989	14,73794	C	-0,55422	8,8651	14,73973
H	5,17051	-0,41585	15,44588	H	0,50936	8,86292	15,01606
C	3,13573	-0,33103	14,72979	C	-0,62921	8,4453	13,27437

H	2,77958	-1,07614	15,44582	H	-1,65114	8,56206	12,87609
C	2,22116	0,25926	13,85349	H	-0,33676	7,39068	13,15959
C	4,58693	2,66589	11,99448	H	0,05061	9,05654	12,66196
H	3,80466	2,90698	11,26233	C	-1,07132	10,28971	14,92198
C	4,9125	3,95294	12,75242	H	-0,94889	10,64617	15,95688
H	5,70069	3,79093	13,50376	H	-2,13889	10,37384	14,65626
H	4,02643	4,33738	13,28098	H	-0,51506	10,97901	14,26839
H	5,25308	4,73185	12,05404	C	-0,42779	5,10215	18,18471
C	5,80193	2,16833	11,21165	H	0,58708	5,03157	17,76357
H	6,6538	1,94711	11,87447	C	-0,98934	3,68455	18,23403
H	6,13215	2,93684	10,49555	H	-1,9498	3,63172	18,77336
H	5,57376	1,25284	10,64278	H	-0,28696	3,02392	18,76526
C	0,76217	-0,1352	13,98091	H	-1,1318	3,2796	17,22192
H	0,20369	0,38656	13,19064	C	-0,29505	5,67403	19,59794
C	0,20373	0,32291	15,32971	H	0,21355	4,95282	20,25698
H	0,28208	1,41646	15,43568	H	-1,28558	5,89148	20,0311
H	0,75914	-0,13839	16,16153	H	0,29655	6,59866	19,61527
H	-0,85321	0,02845	15,43212				

Table S29. Cartesian coordinates (x,y,z) for the optimized geometry of **5**.

As	2,30322	15,99906	5,09862	H	7,66114	16,40607	6,58695
H	2,56577	15,18711	3,83353	C	5,92437	17,3264	4,71657
Ga	2,84227	14,03226	6,3852	H	4,93651	17,50148	4,26649
Ga	-0,06534	15,96539	4,67873	H	6,69554	17,58189	3,97302
Cl	1,63802	12,18758	6,37285	H	6,04322	18,02682	5,55731
Cl	-1,42458	14,61674	5,76746	C	-1,64179	16,36545	2,31649
N	3,31169	14,27392	8,2787	C	-2,3565	17,34788	3,0216
N	4,63837	13,45832	5,80059	H	-3,26624	17,70346	2,54139
N	-0,54599	15,76657	2,77948	C	-1,9605	18,0536	4,16723
N	-0,88884	17,74211	4,8943	C	-2,15443	16,00673	0,95009
C	4,3232	13,57903	8,79859	H	-1,34244	16,00395	0,20948
C	5,23178	12,8169	8,04506	H	-2,9367	16,70449	0,63048
H	5,95989	12,25073	8,6234	H	-2,57371	14,99045	0,95838
C	5,43635	12,82624	6,65731	C	-2,8015	19,23138	4,56931
C	4,54401	13,61009	10,28515	H	-2,18418	20,11183	4,79276
H	5,50602	13,15502	10,54712	H	-3,34667	18,99005	5,49437
H	3,74337	13,06129	10,80068	H	-3,52968	19,48396	3,79016
H	4,51099	14,63907	10,66888	C	0,19043	14,89425	1,92009
C	6,63247	12,0812	6,13552	C	-0,23232	13,56351	1,72139
H	7,14292	12,63683	5,33799	C	0,48455	12,77335	0,81734
H	6,29764	11,12923	5,69443	H	0,1673	11,74197	0,64665
H	7,3431	11,85791	6,93971	C	1,59908	13,26513	0,15234
C	2,5455	15,11698	9,14391	H	2,14688	12,62749	-0,54607
C	1,5356	14,57248	9,96682	C	2,03139	14,56395	0,39521
C	0,91429	15,41844	10,8901	H	2,92415	14,9351	-0,10997

H	0,13926	15,01224	11,54419	C	1,34007	15,40212	1,27353
C	1,2489	16,76351	10,98078	C	-1,40416	12,95565	2,46881
H	0,75153	17,40447	11,71283	H	-1,91387	13,76214	3,01656
C	2,19479	17,29877	10,11523	C	-2,41784	12,29533	1,53381
H	2,42815	18,36397	10,16349	H	-1,99624	11,40195	1,04673
C	2,85948	16,49223	9,18728	H	-2,75899	12,9712	0,73478
C	1,08281	13,12837	9,86268	H	-3,30172	11,96853	2,10237
H	1,78212	12,59976	9,19811	C	-0,91288	11,95236	3,5116
C	1,07073	12,41054	11,21229	H	-0,2103	12,4085	4,22111
H	0,82761	11,3461	11,0729	H	-0,40818	11,09944	3,03046
H	0,31194	12,83155	11,8905	H	-1,76055	11,5634	4,0959
H	2,04048	12,46998	11,72958	C	1,79713	16,83272	1,49353
C	-0,29865	13,05214	9,20982	H	1,53777	17,09115	2,53257
H	-0,60189	12,00212	9,07946	C	1,05069	17,81399	0,58833
H	-0,30958	13,52349	8,21794	H	1,19218	17,55419	-0,47306
H	-1,05545	13,5525	9,83558	H	1,42859	18,8375	0,73808
C	3,92665	17,0845	8,28842	H	-0,02809	17,83031	0,7962
H	4,01488	16,42045	7,41607	C	3,30471	17,00652	1,3533
C	5,29287	17,1106	8,97468	H	3,63707	16,89468	0,30892
H	6,04716	17,56547	8,31318	H	3,85615	16,27893	1,96514
H	5,64341	16,09959	9,22893	H	3,60053	18,01495	1,67849
H	5,25655	17,70282	9,90324	C	-0,41407	18,66482	5,8762
C	3,54071	18,45923	7,75798	C	-0,91069	18,63127	7,19472
H	2,54005	18,44509	7,30531	C	-0,42524	19,57162	8,11015
H	4,25362	18,78242	6,98492	H	-0,79447	19,55091	9,13813
H	3,54161	19,22813	8,54686	C	0,50411	20,53249	7,734
C	5,05687	13,66337	4,45084	H	0,86169	21,26527	8,46119
C	4,78037	12,70448	3,45723	C	0,98649	20,55173	6,4298
C	5,19559	12,96757	2,14708	H	1,72471	21,30275	6,14079
H	4,97859	12,23707	1,36418	C	0,55411	19,61723	5,48575
C	5,87847	14,13275	1,8275	C	-1,94071	17,61572	7,64386
H	6,19925	14,3168	0,79932	H	-2,25805	17,04465	6,75988
C	6,14629	15,07018	2,82026	C	-3,17887	18,27208	8,25535
H	6,67909	15,98725	2,56209	H	-3,63341	19,01653	7,58393
C	5,73658	14,86338	4,13916	H	-2,93949	18,78662	9,19937
C	4,04629	11,41496	3,75922	H	-3,93956	17,50929	8,48211
H	3,86588	11,37577	4,84314	C	-1,32336	16,62486	8,6259
C	4,85929	10,18174	3,3641	H	-0,40964	16,16625	8,2229
H	4,99657	10,12203	2,27278	H	-2,02859	15,81218	8,85467
H	4,33868	9,26465	3,68072	H	-1,05381	17,12234	9,56879
H	5,86036	10,17971	3,82058	C	1,08972	19,66541	4,06756
C	2,68365	11,40075	3,07418	H	0,86297	18,69201	3,60834
H	2,79111	11,35848	1,97972	C	0,37788	20,7353	3,23786
H	2,10214	12,30078	3,31373	H	0,77868	20,7617	2,21278
H	2,09622	10,52841	3,39805	H	0,51667	21,73443	3,6814
C	6,0566	15,88957	5,21044	H	-0,70241	20,54591	3,16581

H	5,31917	15,74953	6,0154	C	2,60318	19,84955	4,02013
C	7,44185	15,6514	5,81558	H	2,95948	19,7914	2,98043
H	8,22336	15,7179	5,04126	H	3,11215	19,06639	4,60018
H	7,52042	14,66351	6,28957	H	2,91531	20,83019	4,41215

Table S30. Cartesian coordinates (x,y,z) for the optimized geometry of **6**.

Sb	8,70709	15,96944	5,04287	H	11,61017	17,312	10,13538
H	8,94851	15,00265	3,65438	C	9,9628	18,22397	7,99156
Ga	9,19546	13,84391	6,45382	H	8,96629	18,26952	7,52979
Ga	6,14947	15,87981	4,63822	H	10,69546	18,5508	7,23894
Cl	7,9782	12,00619	6,36214	H	9,98574	18,95888	8,81179
Cl	4,81639	14,53447	5,77	C	4,48988	16,2704	2,33587
N	11,00113	13,26779	5,89675	C	3,80163	17,25594	3,06345
N	9,62969	14,01262	8,36346	H	2,87246	17,60606	2,61725
N	5,60587	15,67516	2,75551	C	4,23576	17,96666	4,19358
N	5,33421	17,65857	4,87767	C	3,92303	15,90071	0,99374
C	11,7454	12,55524	6,7356	H	4,7009	15,91945	0,21733
C	11,4968	12,4878	8,1156	H	3,11061	16,57961	0,71079
H	12,18053	11,86192	8,68706	H	3,53149	14,87361	1,0179
C	10,59945	13,2559	8,87816	C	3,3973	19,13254	4,63336
C	12,91362	11,77535	6,20261	H	2,71703	19,45683	3,83732
H	13,40971	12,29841	5,37479	H	4,01529	19,97985	4,95807
H	12,54312	10,81797	5,80155	H	2,79316	18,82877	5,50255
H	13,6432	11,5559	6,99124	C	6,30745	14,79876	1,86996
C	10,78004	13,219	10,36982	C	7,42184	15,30525	1,16317
H	11,71078	12,70695	10,63945	C	8,06615	14,4674	0,24966
H	9,93891	12,6936	10,84361	H	8,92652	14,8421	-0,30675
H	10,7872	14,23416	10,79064	C	7,6282	13,16513	0,03655
C	11,44628	13,57015	4,57516	H	8,13768	12,52751	-0,69021
C	11,10803	12,73423	3,49396	C	6,55839	12,66997	0,76899
C	11,48915	13,12661	2,2062	H	6,23991	11,63499	0,6246
H	11,21959	12,49482	1,3567	C	5,88691	13,46273	1,70536
C	12,19399	14,30243	1,98992	C	7,89484	16,73292	1,36245
H	12,479	14,59348	0,97601	H	7,67899	16,98881	2,41251
C	12,53084	15,11397	3,06867	C	7,11406	17,71961	0,4928
H	13,08231	16,0386	2,89047	H	7,20546	17,4587	-0,57374
C	12,16314	14,77314	4,37204	H	7,50473	18,74073	0,62451
C	10,33888	11,44336	3,67911	H	6,04595	17,7421	0,7496
H	10,13993	11,32006	4,75333	C	9,39647	16,90234	1,15706
C	11,14076	10,232	3,20135	H	9,67975	16,80298	0,09712
H	11,31599	10,26958	2,11437	H	9,97235	16,16638	1,73668
H	10,59169	9,30182	3,41548	H	9,70954	17,90634	1,48052
H	12,124	10,16828	3,69104	C	4,77134	12,84886	2,52883
C	8,98806	11,51038	2,97369	H	4,28501	13,65413	3,09888
H	9,1091	11,55447	1,88084	C	3,70939	12,16463	1,66827
H	8,417	12,39825	3,27787	H	4,11353	11,2794	1,15241

H	8,3808	10,62554	3,21604	H	3,29753	12,83245	0,89605
C	12,554	15,66345	5,53784	H	2,87544	11,82098	2,29882
H	11,80912	15,49309	6,33076	C	5,34668	11,8661	3,54864
C	13,91955	15,27005	6,10655	H	5,83598	11,01717	3,04469
H	14,70388	15,36884	5,33878	H	4,54702	11,46876	4,19182
H	13,93302	14,23346	6,4684	H	6,08558	12,34284	4,20597
H	14,18737	15,92109	6,95341	C	5,8616	18,55687	5,85394
C	12,53102	17,14911	5,19274	C	6,85696	19,47573	5,44677
H	11,56211	17,44643	4,76401	C	7,37388	20,36013	6,39605
H	13,32306	17,41783	4,4764	H	8,13758	21,08059	6,09743
H	12,70197	17,7504	6,09849	C	6,94043	20,33114	7,71762
C	8,86057	14,84625	9,23486	H	7,36273	21,02598	8,44733
C	7,81011	14,30239	10,00625	C	5,98059	19,40728	8,10723
C	7,17273	15,13602	10,92999	H	5,65168	19,37678	9,14862
H	6,36585	14,72869	11,54349	C	5,41968	18,5102	7,1911
C	7,53015	16,47068	11,07037	C	7,32501	19,53765	4,00548
H	7,02031	17,10157	11,80263	H	7,14682	18,54105	3,57335
C	8,51522	17,00932	10,25192	C	6,49761	20,53561	3,19305
H	8,76674	18,06803	10,33673	H	6,85382	20,57785	2,15226
C	9,19451	16,21521	9,32393	H	6,57651	21,54809	3,62049
C	7,32257	12,8757	9,83822	H	5,43396	20,2622	3,16641
H	8,03268	12,34704	9,18534	C	8,8148	19,83582	3,87244
C	7,23327	12,11567	11,16135	H	9,12464	19,74382	2,82046
H	6,96047	11,06537	10,97687	H	9,41723	19,13326	4,46745
H	6,46251	12,5402	11,82367	H	9,06231	20,86088	4,19004
H	8,18353	12,12463	11,71692	C	4,37526	17,52175	7,66577
C	5,96833	12,86481	9,12642	H	4,01432	16,96461	6,78963
H	5,64015	11,83028	8,94361	C	3,17764	18,21443	8,31679
H	6,01307	13,37191	8,15339	H	2,72684	18,97293	7,65899
H	5,20025	13,36571	9,73772	H	3,46338	18,7212	9,25214
C	10,29369	16,81475	8,46975	H	2,40125	17,4756	8,56829
H	10,37853	16,18443	7,57163	C	4,99449	16,50778	8,62351
C	11,64702	16,76497	9,17962	H	5,87531	16,01876	8,18446
H	12,42886	17,22665	8,55617	H	4,27098	15,71841	8,87605
H	11,95876	15,73141	9,38993	H	5,31594	16,99123	9,5575

Table S31. Cartesian coordinates (x,y,z) for the optimized geometry of **9**.

As	7,81128	3,40181	5,20603	H	6,33419	0,00169	3,82827
Ga	10,17437	2,9719	4,91998	H	6,36584	-0,0161	2,05631
Ga	7,26864	5,40744	3,98195	C	4,72162	6,58261	3,30429
Cl	11,69864	4,56978	4,86433	C	5,3225	7,83801	3,52208
Cl	8,1415	5,58878	1,96061	H	4,74842	8,697	3,17851
N	10,83969	1,84327	6,39767	C	6,45287	8,13359	4,29055
N	10,7655	1,77358	3,47924	C	3,32666	6,60276	2,74474
N	5,31812	5,4309	3,57443	H	3,37773	6,61142	1,64509
N	7,2911	7,20884	4,78211	H	2,79513	7,50843	3,06244

C	11,89022	1,05011	6,20591	H	2,75214	5,71582	3,0396
C	12,36775	0,69296	4,93804	C	6,70855	9,5893	4,58259
H	13,236	0,03569	4,92998	H	7,66818	9,89433	4,14486
C	11,78041	0,93611	3,68467	H	6,78902	9,78351	5,65916
C	12,62374	0,49239	7,39307	H	5,91092	10,21492	4,16556
H	13,14684	-0,43664	7,13629	C	4,62066	4,1922	3,44687
H	11,95571	0,3154	8,24541	C	4,43276	3,59368	2,18436
H	13,37725	1,22806	7,71776	C	3,7731	2,36015	2,13078
C	12,35098	0,1731	2,52184	H	3,62239	1,88111	1,16039
H	11,55575	-0,24517	1,88973	C	3,32069	1,72964	3,2809
H	13,00375	-0,63534	2,87067	H	2,81714	0,76257	3,21517
H	12,9395	0,84461	1,88026	C	3,51364	2,33289	4,51951
C	10,21466	1,92695	7,67585	H	3,15566	1,83283	5,4208
C	10,62361	2,88649	8,62369	C	4,15767	3,56623	4,62645
C	9,92814	2,95461	9,836	C	4,92585	4,21799	0,89309
H	10,22906	3,69631	10,57994	H	5,36063	5,19929	1,13259
C	8,86382	2,10466	10,10807	C	6,04511	3,38058	0,28193
H	8,33314	2,1778	11,06014	H	5,68472	2,3775	0,00178
C	8,47478	1,15939	9,16329	H	6,88199	3,26208	0,98021
H	7,63766	0,4932	9,38216	H	6,44242	3,8641	-0,62389
C	9,13412	1,05252	7,93648	C	3,79451	4,42032	-0,11659
C	11,78057	3,83576	8,37886	H	4,16301	4,96639	-0,99884
H	12,2083	3,59514	7,3948	H	2,94999	4,98432	0,30613
C	11,31313	5,28951	8,31575	H	3,39765	3,45582	-0,47137
H	12,16535	5,95887	8,1244	C	4,30816	4,24957	5,97035
H	10,83932	5,60655	9,2589	H	5,23903	4,83641	5,92061
H	10,59318	5,44982	7,50255	C	3,17235	5,24522	6,21458
C	12,87905	3,66439	9,42987	H	3,14778	6,0353	5,45136
H	13,21937	2,62063	9,50348	H	3,29123	5,73448	7,19412
H	12,53358	3,96846	10,43092	H	2,1967	4,73387	6,20552
H	13,74942	4,28985	9,1779	C	4,43714	3,27934	7,13747
C	8,72199	-0,00744	6,93136	H	3,4982	2,73483	7,32377
H	9,09896	0,317	5,95007	H	4,6794	3,82769	8,06052
C	7,21059	-0,16447	6,80518	H	5,23431	2,54287	6,95886
H	6,73444	0,79133	6,54013	C	8,19671	7,63396	5,8049
H	6,75155	-0,5417	7,73253	C	9,53255	7,9766	5,49111
H	6,97307	-0,88871	6,0113	C	10,31936	8,51201	6,51781
C	9,38759	-1,34779	7,25304	H	11,34951	8,79634	6,30656
H	9,11637	-2,10657	6,50248	C	9,8265	8,68458	7,8053
H	9,06632	-1,71601	8,24096	H	10,46624	9,10959	8,58234
H	10,4837	-1,26777	7,26667	C	8,53206	8,28569	8,10795
C	10,19086	1,8595	2,17193	H	8,16249	8,38774	9,12987
C	10,81064	2,6265	1,16216	C	7,69694	7,74886	7,1242
C	10,24492	2,60777	-0,11678	C	10,13703	7,74867	4,1101
H	10,70741	3,19979	-0,90989	H	9,90057	6,70494	3,84089
C	9,11723	1,84976	-0,39993	C	11,65711	7,87475	4,09872

H	8,70248	1,8389	-1,41045	H	12,0438	7,52846	3,1298
C	8,50255	1,12479	0,61418	H	12,13228	7,26542	4,87797
H	7,60095	0,54979	0,39516	H	11,97584	8,92265	4,22483
C	9,00772	1,13275	1,91553	C	9,57156	8,63647	2,99935
C	12,04862	3,47048	1,40493	H	10,11399	8,43314	2,06407
H	12,41162	3,25584	2,42103	H	9,70775	9,70427	3,23811
C	13,17336	3,15863	0,4149	H	8,51372	8,44065	2,79126
H	12,9076	3,46817	-0,60806	C	6,29464	7,29388	7,50468
H	13,41997	2,08673	0,37469	H	6,00176	6,53068	6,76789
H	14,08692	3,70665	0,69283	C	6,2525	6,65127	8,89251
C	11,71083	4,96091	1,35767	H	5,29077	6,13529	9,03892
H	11,36881	5,25708	0,35298	H	6,33268	7,40561	9,69092
H	12,60044	5,55981	1,60646	H	7,05884	5,91876	9,03706
H	10,91567	5,2155	2,0687	C	5,24339	8,40618	7,43693
C	8,31186	0,34079	3,00627	H	5,04274	8,73432	6,40973
H	8,62908	0,77118	3,96807	H	5,55779	9,28218	8,0271
C	8,75033	-1,12366	3,00322	H	4,28902	8,04903	7,85432
H	8,48595	-1,61181	2,05125	C	7,85047	4,20558	7,01462
H	8,25579	-1,67873	3,81634	H	8,5719	5,02189	7,12014
H	9,83671	-1,22475	3,14331	H	8,06306	3,42528	7,75164
C	6,7936	0,47162	2,94643	H	6,84763	4,59311	7,21401
H	6,48008	1,52474	2,94039				

Table S32. Cartesian coordinates (x,y,z) for the optimized geometry of **10**.

Sb	7,93711	4,40713	4,4874	H	8,54362	8,80353	3,74758
Ga	5,39263	4,8233	4,87936	H	8,68686	8,52349	2,00625
Ga	8,50802	2,22192	5,77591	C	9,34053	-0,49234	5,47673
Cl	3,8423	3,24908	4,97202	C	10,45146	-0,19173	6,27211
Cl	7,6199	1,98165	7,79134	H	11,01705	-1,04807	6,6364
N	4,86161	6,00872	6,35957	C	11,04873	1,06614	6,49167
N	4,70053	5,99472	3,44866	C	9,08686	-1,94785	5,18401
N	8,51877	0,43195	4,95837	H	9,02889	-2,14388	4,10606
N	10,4545	2,21433	6,20423	H	8,1163	-2,24659	5,60265
C	3,83428	6,84099	6,20324	H	9,87271	-2,57587	5,61945
C	3,20561	7,10183	4,9728	C	12,43518	1,05216	7,07204
H	2,3299	7,74751	5,02021	H	12,98623	0,16456	6,73635
C	3,64703	6,77216	3,6842	H	12,36794	1,00939	8,17002
C	3,2938	7,57297	7,39989	H	12,99911	1,95623	6,81073
H	4,10506	7,99028	8,01211	C	7,65627	0,02732	3,89273
H	2,73894	6,87904	8,04791	C	8,21513	-0,08479	2,59666
H	2,61751	8,3785	7,09133	C	7,41749	-0,59782	1,57028
C	2,86874	7,33451	2,52825	H	7,833	-0,69982	0,56625
H	3,50565	7,52513	1,6553	C	6,09973	-0,96562	1,80589
H	2,34505	8,25582	2,81077	H	5,48922	-1,37093	0,99557
H	2,11217	6,59349	2,22283	C	5,54711	-0,78389	3,06755
C	5,48223	5,89674	7,64325	H	4,49972	-1,03858	3,22535

C	4,90795	5,09467	8,65276	C	6,29681	-0,2764	4,13554
C	5,5205	5,08108	9,91015	C	9,6351	0,36893	2,28561
H	5,09195	4,46243	10,70194	H	9,87682	1,15288	3,02006
C	6,65504	5,83602	10,17178	C	10,68886	-0,73296	2,43654
H	7,11001	5,81812	11,16469	H	10,4096	-1,6256	1,85372
C	7,22851	6,59188	9,1559	H	10,84044	-1,03276	3,48044
H	8,138	7,16072	9,35644	H	11,66085	-0,38016	2,05814
C	6,6711	6,62335	7,87639	C	9,75502	0,98002	0,88828
C	3,67606	4,23798	8,4272	H	9,73505	0,20686	0,10404
H	3,27607	4,47459	7,43035	H	10,71746	1,50604	0,7901
C	4,04471	2,75379	8,41922	H	8,94952	1,69684	0,67732
H	3,16522	2,14431	8,16031	C	5,63105	-0,0339	5,48487
H	4,40673	2,43087	9,40851	H	5,88909	0,99953	5,7769
H	4,83601	2,53915	7,69029	C	6,11375	-0,95232	6,60947
C	2,57838	4,50204	9,45996	H	5,95679	-2,01154	6,34655
H	2,3082	5,56687	9,52923	H	5,53516	-0,74458	7,52176
H	2,88408	4,1786	10,46737	H	7,16647	-0,79247	6,86821
H	1,6692	3,93843	9,19966	C	4,1091	-0,10678	5,41872
C	7,32045	7,44929	6,78197	H	3,69543	0,52173	4,61983
H	7,01084	7,00573	5,82306	H	3,68549	0,25204	6,36738
C	8,84404	7,391	6,82637	H	3,76198	-1,14289	5,272
H	9,21044	6,35559	6,87262	C	11,1261	3,46427	6,3512
H	9,25575	7,93513	7,69095	C	11,58518	4,11802	5,18398
H	9,26985	7,84691	5,92055	C	12,18783	5,37008	5,3137
C	6,81922	8,89338	6,78796	H	12,54187	5,89171	4,42361
H	7,29397	9,4718	5,97942	C	12,34172	5,96789	6,56026
H	7,05917	9,38787	7,7431	H	12,81218	6,95024	6,64212
H	5,73077	8,94931	6,64146	C	11,89045	5,31306	7,69691
C	5,29667	5,93621	2,1556	H	12,00854	5,7878	8,67394
C	4,86957	4,9904	1,20202	C	11,27307	4,05899	7,62155
C	5,52236	4,95749	-0,0353	C	11,46584	3,45221	3,82705
H	5,20379	4,22915	-0,78493	H	10,51591	2,89177	3,83351
C	6,5713	5,8216	-0,32181	C	12,58478	2,43052	3,61264
H	7,07114	5,77469	-1,29197	H	12,49936	1,9659	2,61803
C	6,98764	6,74464	0,63318	H	12,55308	1,62375	4,35755
H	7,81366	7,42059	0,403	H	13,57137	2,91598	3,67775
C	6,36445	6,82294	1,88098	C	11,407	4,43659	2,66522
C	3,74543	4,01143	1,47602	H	11,18127	3,9032	1,7295
H	3,33537	4,24234	2,46967	H	12,36811	4,9532	2,51624
C	2,61426	4,14476	0,45581	H	10,62768	5,19793	2,82145
H	2,24072	5,17787	0,39063	C	10,77636	3,41134	8,89978
H	1,77061	3,49472	0,73492	H	10,36089	2,42571	8,64518
H	2,93875	3,84793	-0,55436	C	11,90081	3,2174	9,91887
C	4,26563	2,57504	1,53538	H	12,75783	2,67035	9,49917
H	4,71439	2,26532	0,57754	H	11,53254	2,65788	10,79277
H	3,44592	1,87854	1,76805	H	12,27929	4,18496	10,28537

H	5,02413	2,45381	2,32027	C	9,63651	4,22336	9,50814
C	6,78757	7,87647	2,88875	H	9,97986	5,22444	9,81544
H	6,47069	7,51774	3,87989	H	9,22987	3,71688	10,39701
C	6,05855	9,19701	2,62883	H	8,80981	4,34688	8,79815
H	6,32008	9,59588	1,63524	C	7,82272	3,49871	2,52537
H	6,33794	9,95012	3,38206	H	7,41237	4,22712	1,81798
H	4,96696	9,07764	2,66434	H	7,22286	2,58306	2,5131
C	8,29544	8,09548	2,94236	H	8,85112	3,26378	2,23025
H	8,82799	7,15441	3,14622				

Table S33. Cartesian coordinates (x,y,z) for the optimized geometry of **III**.

As	7,38934	3,65609	4,20298	H	4,81583	-1,89994	3,22763
Ga	8,19579	2,12829	5,81941	H	6,77542	-0,73993	6,20233
Ga	5,65114	4,87603	4,98362	C	5,69215	-2,54005	5,795
Cl	7,23451	1,54449	7,73787	C	4,75611	-0,20294	5,81088
N	10,10727	2,28273	6,37476	H	7,45452	6,97912	9,78122
N	8,46376	0,38765	4,88364	C	5,95464	5,54449	10,34282
N	4,64103	5,78622	6,35889	H	6,53413	7,19218	6,13476
N	4,71342	5,76303	3,49835	C	8,43873	6,98149	7,05811
C	10,84084	1,19054	6,56564	C	6,75879	8,82251	7,48033
C	10,65375	3,56521	6,67873	H	4,39582	4,09412	10,63066
C	9,40614	-0,45668	5,30081	H	2,77044	4,50034	7,3196
C	7,60404	-0,04068	3,82488	C	3,79224	2,64622	7,49924
C	3,62483	6,63025	6,12648	C	2,24871	3,66507	9,20463
C	5,11371	5,66254	7,70354	H	7,61851	6,78125	0,09096
C	3,66404	6,56271	3,615	C	6,54184	4,94137	-0,19464
C	5,29026	5,51153	2,21638	H	5,91749	7,80655	3,28848
C	10,45184	-0,09738	6,16256	C	6,52656	8,92442	1,5776
C	12,18188	1,29545	7,23998	C	8,02067	7,55906	3,08262
C	11,15181	4,34912	5,61381	H	5,34717	3,1522	-0,22699
C	10,70122	4,03338	8,00823	H	3,66597	3,68027	3,09575
C	9,39336	-1,87848	4,80977	C	2,62312	3,42751	1,24695
C	7,95696	0,2792	2,49514	C	4,43529	1,93173	2,1522
C	6,45275	-0,80576	4,10007	H	12,20724	7,04588	7,42339
C	3,12718	6,93741	4,85829	H	10,85628	4,4106	2,14712
C	2,9835	7,32618	7,29462	H	11,79782	5,58787	3,0793
C	6,2153	6,44116	8,10363	H	10,03201	5,44495	3,33149
C	4,44413	4,80006	8,59532	H	12,46319	2,63537	2,9019
C	3,0462	7,15415	2,3826	H	12,55698	2,16468	4,61044
C	6,24653	6,41453	1,7114	H	13,33956	3,66628	4,06151
C	4,95188	4,32643	1,53392	H	8,12179	4,03532	8,90363
H	11,1352	-0,90008	6,43444	H	9,09513	4,91061	10,11109
H	12,81481	0,43802	6,98177	H	8,40721	3,31168	10,49449
H	12,04522	1,30103	8,33191	H	12,09693	2,62404	9,94828
H	12,70123	2,2258	6,97651	H	10,73957	2,39754	11,0802
C	11,69903	5,60049	5,90503	H	11,39558	4,01836	10,78726

C	11,16922	3,81074	4,19787	H	5,48734	-1,44879	0,886
C	11,27343	5,28702	8,24888	H	8,77274	1,60524	0,07523
C	10,1362	3,24476	9,17352	H	9,7522	2,80818	0,92778
H	9,36167	-1,92039	3,71189	H	8,00428	2,72607	1,23622
H	8,48826	-2,39257	5,16372	H	10,24609	-0,39241	1,0794
H	10,27372	-2,42546	5,16676	H	10,69737	-0,29099	2,79966
C	7,18562	-0,24581	1,45562	H	11,26442	0,94775	1,66224
C	9,16229	1,14431	2,18352	H	4,83424	-2,90856	5,21039
C	5,70625	-1,29963	3,02548	H	5,44955	-2,68392	6,85927
C	5,98116	-1,06656	5,51554	H	6,55295	-3,18371	5,55694
H	2,27136	7,60966	4,82827	H	4,97155	0,85605	5,61337
H	2,20752	8,02014	6,95223	H	4,45804	-0,29601	6,86611
H	3,73613	7,88327	7,87116	H	3,90202	-0,50054	5,18023
H	2,53593	6,60486	7,99344	H	6,2835	5,49931	11,38347
C	6,60917	6,37526	9,44326	H	8,57908	5,93426	6,75077
C	6,95994	7,34592	7,13944	H	8,94721	7,12072	8,02377
C	4,89176	4,75355	9,91671	H	8,95246	7,61471	6,31902
C	3,28394	3,94471	8,12053	H	7,28119	9,46078	6,75076
H	3,68907	7,95923	1,99391	H	7,15872	9,061	8,47875
H	2,05787	7,57573	2,60166	H	5,69403	9,10148	7,47232
H	2,96245	6,40805	1,58175	H	4,50637	2,83453	6,68256
C	6,86458	6,10305	0,49786	H	2,95853	2,05346	7,09197
C	6,62965	7,67967	2,45879	H	4,32844	2,03531	8,23988
C	5,59055	4,06663	0,31881	H	1,37512	3,15694	8,76911
C	3,91151	3,36133	2,07083	H	1,89999	4,59161	9,6872
H	12,08755	6,21714	5,09259	H	2,64506	3,00365	9,99038
C	11,76937	6,06722	7,21318	H	7,04025	4,71396	-1,13972
H	10,32835	3,10619	4,11828	H	7,26893	8,90842	0,7644
C	10,95442	4,88115	3,13696	H	6,71182	9,83263	2,17201
C	12,45372	3,02352	3,93231	H	5,53221	9,01769	1,11413
H	11,32298	5,66013	9,27496	H	8,79651	7,47272	2,30528
H	9,84186	2,25197	8,80301	H	8,09165	6,66677	3,72367
C	8,86936	3,91455	9,6976	H	8,2509	8,44792	3,69189
C	11,1507	3,05979	10,30266	H	2,19867	4,44224	1,21827
H	7,45666	-0,01836	0,42274	H	1,8591	2,75514	1,66761
C	6,07655	-1,04382	1,71225	H	2,80639	3,11633	0,2061
H	9,35778	1,74519	3,0838	H	4,6384	1,51537	1,15413
C	8,90069	2,12008	1,04083	H	3,69361	1,2761	2,63373
C	10,41035	0,30182	1,91943	H	5,36581	1,88481	2,7367

Table S34. Cartesian coordinates (x,y,z) for the optimized geometry of **IV**.

Sb	4,20185	5,06923	9,78872	C	3,20612	11,53362	9,69624
Ga	2,01586	6,39224	9,68637	H	4,18313	12,04134	9,66
Ga	4,78057	4,3849	7,5133	H	2,73261	11,80084	10,65327
Cl	1,26937	7,52335	7,91486	H	2,58875	11,95055	8,88549
N	0,31425	5,68565	10,44989	C	5,2871	3,40396	4,82989

N	2,23125	7,79095	11,09444	C	6,56637	2,9768	5,1952
N	4,43	4,03244	5,64973	H	7,1454	2,48707	4,41418
N	6,63355	3,7124	7,47464	C	7,21841	3,1472	6,43057
C	-0,47903	6,47512	11,16892	C	4,86805	3,15142	3,40837
C	-0,1126	7,74803	11,64071	H	4,50692	4,07623	2,93655
H	-0,89629	8,29906	12,15852	H	4,03122	2,43847	3,36987
C	1,16473	8,32524	11,68214	H	5,70311	2,74778	2,82426
C	-1,86417	6,01158	11,53087	C	8,62624	2,64159	6,54902
H	-2,55093	6,21016	10,69412	H	9,08476	2,51897	5,56046
H	-2,23618	6,55125	12,41011	H	8,62684	1,66202	7,05236
H	-1,89613	4,93125	11,72371	H	9,24173	3,31217	7,16307
C	1,31592	9,6078	12,45213	C	3,18351	4,47725	5,1069
H	1,52291	10,43206	11,75287	C	2,13647	3,5496	4,93837
H	2,16912	9,565	13,14272	C	0,97782	3,98364	4,2911
H	0,40467	9,8436	13,01433	H	0,1558	3,28403	4,13159
C	-0,1059	4,3609	10,12028	C	0,84865	5,29973	3,86329
C	0,41837	3,28363	10,87115	H	-0,06665	5,62299	3,36238
C	0,00189	1,98711	10,5609	C	1,86371	6,21695	4,10808
H	0,39972	1,14668	11,13204	H	1,72582	7,25607	3,8092
C	-0,9142	1,74955	9,54196	C	3,0517	5,83138	4,73658
H	-1,23372	0,72891	9,31775	C	2,23808	2,14303	5,4998
C	-1,41075	2,81537	8,80451	H	3,3034	1,86437	5,52339
H	-2,11927	2,62523	7,99414	C	1,73296	2,12199	6,94478
C	-1,01441	4,1319	9,06552	H	0,67371	2,41314	6,99651
C	1,37337	3,53046	12,0216	H	2,28911	2,81907	7,5923
H	1,96789	4,41508	11,74519	H	1,82695	1,11475	7,38012
C	2,35968	2,39098	12,24151	C	1,51589	1,09794	4,65531
H	1,87222	1,4886	12,64404	H	1,82394	1,13627	3,59858
H	3,12976	2,69529	12,96569	H	0,42317	1,22815	4,69094
H	2,8712	2,12769	11,30495	H	1,73042	0,0882	5,0369
C	0,62277	3,86473	13,31116	C	4,15343	6,8391	5,02791
H	0,00927	4,77059	13,20743	H	4,49188	6,63827	6,06405
H	1,3325	4,03994	14,13491	C	3,66241	8,28049	5,00481
H	-0,04126	3,03593	13,6052	H	3,39695	8,59975	3,9842
C	-1,54495	5,24249	8,18001	H	4,4609	8,95	5,35513
H	-1,19697	6,20202	8,58947	H	2,79082	8,41791	5,65927
C	-0,95642	5,11967	6,77664	C	5,3675	6,69674	4,10666
H	-1,29692	4,19348	6,28555	H	5,0783	6,86077	3,05604
H	0,14054	5,11216	6,79972	H	5,85231	5,71462	4,17919
H	-1,26321	5,96965	6,14834	H	6,12561	7,45226	4,36636
C	-3,07233	5,26631	8,11686	C	7,32938	3,90424	8,70701
H	-3,41719	6,14169	7,54504	C	7,40966	2,8508	9,63859
H	-3,53246	5,3084	9,11535	C	8,00453	3,1131	10,8764
H	-3,4702	4,3712	7,61292	H	8,06795	2,31358	11,61845
C	3,53234	8,29005	11,4044	C	8,50102	4,37345	11,18383
C	4,27063	7,65433	12,42962	H	8,95663	4,55863	12,15933

C	5,54394	8,14071	12,73367	C	8,40814	5,40261	10,2532
H	6,12708	7,66003	13,52101	H	8,78292	6,39493	10,50958
C	6,08584	9,22107	12,04605	C	7,81388	5,19675	9,00707
H	7,0837	9,58805	12,29832	C	6,8395	1,47182	9,36089
C	5,35801	9,82187	11,0284	H	6,52627	1,44318	8,30609
H	5,7932	10,65869	10,4765	C	7,8799	0,37004	9,56629
C	4,07958	9,37021	10,68482	H	7,47067	-0,60818	9,27018
C	3,698	6,48008	13,2019	H	8,17992	0,29168	10,62285
H	2,97616	5,98463	12,53345	H	8,79364	0,55121	8,97954
C	4,75295	5,44678	13,58572	C	5,59104	1,21323	10,20601
H	5,3486	5,13789	12,71367	H	4,83321	1,9924	10,03489
H	4,26813	4,55004	14,00048	H	5,83229	1,21849	11,28096
H	5,43956	5,82715	14,35845	H	5,15158	0,23287	9,96244
C	2,922	6,93765	14,43871	C	7,70959	6,33559	8,00966
H	2,05698	7,56221	14,17658	H	6,88847	6,08643	7,31663
H	3,57137	7,51779	15,11405	C	8,98421	6,45537	7,17197
H	2,54353	6,06783	14,99816	H	9,20326	5,52751	6,62321
C	3,34935	10,0217	9,52908	H	9,85272	6,67885	7,81225
H	2,34076	9,58677	9,47759	H	8,88972	7,26725	6,43366
C	4,04384	9,68642	8,21146	C	7,341	7,66251	8,66279
H	3,46926	10,08684	7,36376	H	7,15126	8,42368	7,89049
H	4,13164	8,59841	8,07738	H	8,14625	8,04777	9,30769
H	5,057	10,11937	8,17683	H	6,43125	7,55881	9,27282

Table S35. Cartesian coordinates (x,y,z) for the optimized geometry of $[AsMe_2]^-$.

As	-5,51506	5,23683	-0,43843	C	-4,19048	3,81246	0,06397
C	-7,10284	4,05297	-0,10201	H	-3,18063	4,22529	-0,0389
H	-7,10954	3,16384	-0,74722	H	-4,25644	2,9282	-0,58461
H	-8,01346	4,62436	-0,31438	H	-4,30827	3,47551	1,10296
H	-7,15976	3,71098	0,94045				

Table S36. Cartesian coordinates (x,y,z) for the optimized geometry of $[SbMe_2]^-$.

Sb	-5,50473	5,37586	-0,46537	C	-4,06716	3,78103	0,06645
C	-7,23029	4,04344	-0,09126	H	-3,0531	4,17878	-0,03423
H	-7,20639	3,17271	-0,75209	H	-4,16825	2,92073	-0,60072
H	-8,15021	4,60154	-0,28859	H	-4,20781	3,45198	1,0996
H	-7,24853	3,70438	0,94804				

Table S37. Cartesian coordinates (x,y,z) for the optimized geometry of $[As(NMe_2)_2]^-$.

As	0,28331	0,95981	1,876	H	-1,1191	-1,31988	0,73539
N	-1,16525	0,7466	0,64899	C	2,13626	2,02109	-0,08852
N	1,83623	0,9107	0,76443	H	1,80516	2,94496	0,3891
C	-1,52049	1,82294	-0,22619	H	1,64339	1,96239	-1,08168
H	-1,33212	2,77435	0,27442	H	3,22344	2,09663	-0,28863
H	-2,59069	1,77865	-0,50971	C	2,2559	-0,32866	0,18271

H	-0,94926	1,82691	-1,17826	H	3,34744	-0,33825	-0,0074
C	-1,39874	-0,52763	0,03866	H	1,77127	-0,54702	-0,79211
H	-0,81979	-0,68374	-0,89574	H	2,01346	-1,14821	0,86157
H	-2,46469	-0,65735	-0,23454				

Table S38. Cartesian coordinates (x,y,z) for the optimized geometry of $[Sb(NMe_2)_2]^-$.

Sb	0,32995	1,10742	2,02844	H	-1,24664	-1,26214	0,90145
N	-1,25995	0,80504	0,69379	C	2,23841	1,98903	-0,21262
N	1,96847	0,9434	0,72879	H	1,95829	2,95549	0,21083
C	-1,59276	1,8207	-0,26014	H	1,68876	1,8735	-1,17004
H	-1,40127	2,80874	0,16288	H	3,31361	2,02505	-0,47828
H	-2,66119	1,76816	-0,5494	C	2,32876	-0,33614	0,19468
H	-1,01447	1,74546	-1,20463	H	3,40693	-0,37895	-0,05769
C	-1,50596	-0,50218	0,16184	H	1,78431	-0,59442	-0,73757
H	-0,9245	-0,72132	-0,75801	H	2,11706	-1,11961	0,92487
H	-2,57209	-0,63293	-0,11069				

Table S39. Cartesian coordinates (x,y,z) for the optimized geometry of $[As(OMe)_2]^-$.

As	0,41465	-0,28936	-1,56487	H	-2,40316	0,83289	0,56913
O	-1,06156	-0,348	-0,42678	C	2,26463	0,29011	0,45625
O	1,76487	-0,72111	-0,35325	H	2,20914	1,27496	-0,03619
C	-1,31984	0,76279	0,36513	H	3,31932	0,08039	0,70883
H	-0,99095	1,69719	-0,11889	H	1,71322	0,37414	1,40964
H	-0,80842	0,70824	1,34264	H	-2,40316	0,83289	0,56913

Table S40. Cartesian coordinates (x,y,z) for the optimized geometry of $[Sb(OMe)_2]^-$.

Sb	0,43119	-0,10931	-1,7954	H	-2,4574	0,81911	0,64067
O	-1,16117	-0,24445	-0,5318	C	2,32281	0,24583	0,47285
O	1,87226	-0,66708	-0,46776	H	2,30026	1,28514	0,10265
C	-1,38207	0,76174	0,39562	H	3,36294	0,00973	0,75937
H	-1,06327	1,75365	0,03199	H	1,7216	0,22478	1,39919
H	-0,84525	0,5831	1,34426				

Table S41. Cartesian coordinates (x,y,z) for the optimized geometry of $[As(SiMe_3)_2]^-$.

As	4,73125	9,42346	4,18903	H	2,73441	10,16726	1,07793
Si	5,0184	9,56749	1,91939	C	1,6111	8,11985	2,96121
Si	3,0506	7,86456	4,17727	H	0,8194	7,37933	3,1277
C	5,11727	7,94479	0,93301	H	1,94721	8,0255	1,92496
H	4,16535	7,40736	0,9589	H	1,18566	9,11945	3,08138
H	5,87975	7,28794	1,35943	C	2,24354	7,85049	5,89676
H	5,36753	8,13722	-0,11733	H	1,4759	7,07209	5,97589
C	6,66921	10,44577	1,58512	H	1,78115	8,81852	6,10727
H	7,50051	9,85489	1,97883	H	2,99811	7,66916	6,66758
H	6,68839	11,41865	2,08469	C	3,59131	6,06325	3,89262
H	6,83137	10,60559	0,51291	H	4,34882	5,78494	4,63047

C	3,73	10,60799	0,98382	H	4,04096	5,94563	2,9035
H	3,97163	10,69496	-0,08299	H	2,74844	5,36562	3,97581
H	3,68431	11,61217	1,41421				

Table S42. Cartesian coordinates (x,y,z) for the optimized geometry of $[Sb(SiMe_3)_2]^-$.

Sb	4,82801	9,53542	4,36021	H	2,77755	10,20416	1,09043
Si	5,09218	9,63351	1,85686	C	1,60193	8,12209	3,00393
Si	2,9889	7,81614	4,26494	H	0,80548	7,37483	3,10612
C	5,16051	7,97025	0,94234	H	1,98285	8,071	1,98049
H	4,2102	7,43628	1,02558	H	1,17078	9,11586	3,14728
H	5,93699	7,33262	1,37191	C	2,1262	7,74978	5,95488
H	5,37445	8,11589	-0,12358	H	1,3549	6,97111	5,97954
C	6,73175	10,49907	1,44786	H	1,65778	8,71091	6,18173
H	7,57473	9,9235	1,83871	H	2,8516	7,53914	6,74571
H	6,76508	11,4907	1,9078	C	3,55613	6,03295	3,93694
H	6,86169	10,61744	0,36576	H	4,28311	5,72952	4,69486
C	3,76846	10,63805	0,9361	H	4,04846	5,95686	2,96438
H	3,96678	10,67775	-0,14247	H	2,71404	5,3296	3,95651
H	3,74103	11,65952	1,32453				

Table S43. Cartesian coordinates (x,y,z) for the optimized geometry of $[As(GaMe_2)_2]^-$.

As	-0,68676	2,64078	-1,36344	H	-4,3385	2,93928	-0,71538
Ga	1,22977	1,50847	-0,67553	H	-4,5299	2,27105	0,91892
C	1,51286	0,08137	0,71579	H	-4,80432	1,24203	-0,48482
C	3,00823	1,95798	-1,51904	H	0,84075	0,19496	1,56786
Ga	-2,24054	1,4882	-0,06492	H	2,54808	0,09556	1,07187
C	-4,1785	2,05384	-0,09634	H	1,32438	-0,90629	0,28089
C	-2,04686	-0,09902	1,15807	H	2,91079	2,70195	-2,31265
H	-1,28175	-0,79647	0,8134	H	3,46974	1,0577	-1,94085
H	-3,00036	-0,62943	1,24854	H	3,69918	2,34733	-0,76233
H	-1,7562	0,2354	2,15998				

Table S44. Cartesian coordinates (x,y,z) for the optimized geometry of $[Sb(GaMe_2)_2]^-$.

Sb	-0,70439	2,79821	-1,46401	H	-4,50205	2,92039	-0,63988
Ga	1,34425	1,52675	-0,70436	H	-4,63722	2,23001	0,99069
C	1,53997	0,07613	0,67417	H	-4,91911	1,20925	-0,41857
C	3,15048	1,94031	-1,50077	H	0,82654	0,18653	1,4919
Ga	-2,358	1,50986	-0,05073	H	2,55596	0,06882	1,08193
C	-4,30581	2,03277	-0,03518	H	1,35979	-0,90014	0,21098
C	-2,08609	-0,08658	1,14135	H	3,09367	2,6933	-2,28935
H	-1,30775	-0,75155	0,76433	H	3,59805	1,03131	-1,91851
H	-3,01889	-0,64955	1,24829	H	3,83	2,30474	-0,72183
H	-1,77928	0,24413	2,13955				

[1] N. J. Hardman, B. E. Eichler, P. P. Power, *Chem. Commun*. **2000**, 1991-1992.

[2] N. Kuhn, T. Kratz, *Synthesis* **1993**, 561-562.

[3] P. Jutzi, C. Müller, A. Stammler, H.-G. Stammler, *Organomet.* **2000**, *19*, 1442-1444.

[4] I. Krossing, A. Reisinger, *Eur. J. Inorg. Chem.* **2005**, 1979-1989.

[5] a) C. Ganesamoorthy, C. Helling, C. Wölper, W. Frank, E. Bill, G. E. Cutsail III, S. Schulz, *Nat. Commun*. **2018**, *9*, 87–95; b) J. Krüger, C. Ganesamoorthy, L. John, C. Wölper, S. Schulz, *Chem. Eur. J*. **2018**, *24*, 9157–9164; c) J. Schoening, L. John, C. Wölper, S. Schulz, *Dalton Transaction*, **2019**, *48*, 17729–17734.

[6] G. M. Sheldrick, *Acta Crystallogr.* 1990, **A46**, 467.

[7] G. M. Sheldrick, SHELXL-2017, Program for the Refinement of Crystal Structures University of Göttingen, Göttingen (Germany) **2017**. (see also: Sheldrick, G. M. Acta Crystallogr. 2008, **A64**, 112).

[8] shelXle, *A Qt GUI for SHELXL*, C. B. Hübschle, G. M. Sheldrick, B. Dittrich, *J. Appl. Cryst.* **2011**, *44*, 1281-1284.

[9] PLATON/SQUEEZE, P. van der Sluis, A. L. Spek, *Acta Crystallogr.* **1990**, *A46,* 194-201.

[10] F. Neese, The ORCA program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science* **2012**, *2*, 73.

[11] a) F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

[12] a) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456–1465; b) S. Grimme, J. Antony, S. Ehrlich; H. Krieg, *J. Chem. Phys*. **2010**, *132*, 154104.

[13] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

[14] B. Metz, H. Stoll, M. Dolg, *J. Chem. Phys*. **2000**, *113*, 2563-2569.

[15] S. Kossmann, F. Neese, *Chem. Phys. Lett*. **2009**, *481*, 240-243.

[16] NBO 6.0: E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, F. Weinhold (Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, 2013); http://nbo6.chem.wisc.edu/]

-Supporting Information-

Stepwise Bi−Bi Bond Formation: From a Bi-centered Radical to Bi_4 Butterfly and Bi_8 Cuneane-Type Clusters

*Julia Krüger,[a] Christoph Wölper,[a] Stephan Schulz[a]**

[a] Faculty of Chemistry, University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen (Cenide), Universitätsstr. 5-7, S07 S03 C30, D-45117 Essen.

E-mail: stephan.schulz@uni-due.de.

Content

A) Experimental Details

General Synthetic methods

All manipulations were performed in an atmosphere of purified argon using standard Schlenk and glove-box techniques. Toluene and *n*-hexane were dried using an mBraun Solvent Purification System (SPS). Benzene was carefully dried over Na. Deuterated solvents were dried over activated molecular sieves (4 Å) and degassed prior to use. The anhydrous nature of the solvents was verified by Karl Fischer titration. L^1Ga[1] $[L^{1,2}Mg]_2$[2] Cp^*_2BiCl,[3] and Bi_2Ph_4[4] were prepared according to literature methods, whereas other chemicals were obtained from commercial sources and purified prior to use. Microanalyses were performed at the Elementaranalyselabor of the University of Duisburg-Essen. The melting points were measured using a Thermo Scientific 9300 apparatus.

Spectroscopic methods NMR Spectroscopy

^1H (300.1 MHz; 600 MHz) and $^{13}C\{^1H\}$ (75.5 MHz; 150 MHz) NMR spectra were recorded using a Bruker Avance DPX-300 spectrometer or Avance III HD 600 spectrometer. The spectra were referenced to internal C_6D_5H (^1H: δ = 7.154; ^{13}C: δ = 128.39) and $C_6D_5CHD_2$ (^1H: δ = 2.09; ^{13}C: δ = 20.40). IR spectra were recorded with an ALPHA-T FT-IR spectrometer equipped with a single reflection ATR sampling module. The IR spectrometer was placed in a glovebox to guarantee measurements under inert gas conditions.

Synthetic procedures

Synthesis of $[(L^1GaCl)_2Bi\cdot)]$ (1). L^1Ga (100 mg, 0.21 mmol) and $BiCl_3$ (32 mg, 0.10 mmol) were weighed in a Schlenk flask, cooled to −78 °C and 2 mL of toluene were added. The reaction mixture was slowly warmed to ambient temperature over a period of 5 h and stirred for additional 30 min. The solvent was removed in vacuum and 6 mL of *n*-hexane were added to the residue. The orange solution was separated from metallic bismuth particle, which were formed during the reaction, and stored at 0 °C for 2 h to afford orange crystals of **1**. The mother liquor was stored at −30 °C for 24 h to yield a second crop of **1**.

Yield 31 mg (28%). M.p. 128 °C (dec.). Anal. Calcd. for $C_{58}H_{82}N_4Cl_2Ga_2Bi$: C, 55.52; H, 6.59; N, 4.47. Found: C, 55.0; H, 6.97; N, 4.60 %. **IR ν [cm^{-1}]:** 3060, 2962, 2925, 2866, 1520, 1461, 1438, 1382, 1316, 1260, 1175, 1105, 1056, 1020, 935, 876, 860, 797, 758, 727, 636, 532, 442.

Synthesis of $[(L^1GaCl)_2(\mu,\eta^{1:1}\text{-}Bi_4)]$ (3). L^1Ga (30 mg, 0.062 mmol) and Cp^*_2BiCl (32 mg, 0.062 mmol) were weighed in a Schlenk flask, cooled to −78 °C and 2 mL of THF were added. The reaction mixture was stirred at −78 °C for 5 h, slowly warmed to ambient temperature over a period of 2 h and stirred for additional 30 min. The solvent was removed in vacuum and 1.5 mL of *n*-hexane were added to the residue. A dark orange precipitate formed immediately, which was separated from the mother liquor by filtration. The orange solid was washed two times with 0.3 mL of *n*-hexane and dried in vacuum to yield analytically pure powder of **3**.

Yield 12 mg (42%). M.p. 48 °C (dec.). Anal. Calcd. for $C_{58}H_{82}N_4Cl_2Ga_2Bi_4$·hexane: C, 39.06; H, 4.92; N, 2.85. Found: C, 39.1; H, 4.90; N, 3.16 %. **^{1}H-NMR (C_6D_6, 300 MHz, 25 °C) δ [ppm]:** 7.09-7.28 (m, 12 H, C_6H_3), 4.83 (s, 2 H, γ-C*H*), 3.71 (sept, $^3J_{HH}$ = 6.8 Hz, 4 H, C*H*(CH_3)$_2$), 3.03 (sept, $^3J_{HH}$ = 6.8 Hz, 4 H, C*H*(CH_3)$_2$), 1.57 (s, 12 H, CCH_3), 1.49 (d, 12 H, $^3J_{HH}$ = 6.6 Hz, CH(CH_3)$_2$), 1.41 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 1.18 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$), 1.00 (d, 12 H, $^3J_{HH}$ = 6.8 Hz, CH(CH_3)$_2$). **^{13}C{^{1}H}-NMR (C_6D_6, 150 MHz, 25 °C) *δ* [ppm]:** 168.0 (N*C*CH_3), 146.1 (C_6H_3), 143.0 (C_6H_3), 141.5 (C_6H_3), 126.2 (C_6H_3), 124.5 (C_6H_3), 97.5 (γ-*C*H), 30.0 (*C*H(CH_3)$_2$), 28.4 (CH(*C*H_3)$_2$), 28.1 (*C*H(CH_3)$_2$), 26.2 (CH(*C*H_3)$_2$), 24.7 (CH(*C*H_3)$_2$), 24.5 (CH(*C*H_3)$_2$), 24.1 (N*C*(CH_3)). **IR *ν* [cm^{-1}]:** 3038, 2958, 2922, 2864, 1523, 1458, 1437, 1382, 1317, 1261, 1177, 1099, 1018, 935, 862, 794, 757, 728, 636, 527, 438.

Synthesis of [(L^{2}Mg)$_4$Bi$_8$] (4). [L^{2}Mg]$_2$ (50 mg, 0.069 mmol) was suspended in 2 mL of benzene and a solution of Bi_2Ph_4 (20 mg, 0.027 mmol) in 0.5 mL of benzene was added. The solution was stirred for 5 h at ambient temperature with exclusion of light. The solvent was removed in vacuum and 1 mL of *n*-hexane was added to the residue. The orange-brown solution was directly separated from metallic bismuth particles, which were formed during the reaction, by filtration. The filtrate was stored at −30 °C for 12 h to yield black crystals of **4**.

Yield 9 mg (0.0029 mmol; 43%). M.p. 54 °C (dec.). Anal. Calcd. for $C_{92}H_{116}N_8Mg_4Bi_8$: C, 35.61; H, 3.77; N, 3.61. Found: C, 35.9; H, 3.95; N, 3.51 %. **^{1}H-NMR (C_6D_6, 300 MHz, 25 °C) δ [ppm]:** 7.09 (s, 8 H, C_6H_2), 7.06 (s, 8 H, C_6H_2), 4.83 (s, 4 H, γ-C*H*), 2.59 (s, 12 H, *p*-CH_3), 2.57 (s, 12 H, *p*-CH_3), 2.26 (s, 24 H, *o*-CH_3), 2.20 (s, 24 H, *o*-CH_3), 1.70 (s, 12 H, ArNCCH_3), 1.69 (s, 12 H, ArNCCH_3). **^{13}C{^{1}H}-NMR (C_6D_6, 150 MHz, 25 °C) *δ* [ppm]:** 168.9 (ArN*C*CH_3), 167.8 (ArN*C*CH_3), 145.2 (C_6H_2), 143.9 (C_6H_2), 134.0 (C_6H_2), 133.5 (C_6H_2), 132.6 (C_6H_2), 131.7 (C_6H_2), 131.1 (C_6H_2), 130.4 (*m*-C_6H_2), 130.2 (*m*-C_6H_2), 94.5 (γ-*C*H), 24.1 (ArNC*C*H_3), 23.7 (ArNC*C*H_3), 23.0 (*p*-*C*H_3), 22.9 (*p*-*C*H_3), 22.0 (*o*-*C*H_3), 21.7 (*o*-*C*H_3). **IR *ν* [cm^{-1}]:** 2964, 2912, 2844, 1622, 1544, 1518, 1437, 1388, 1372, 1258, 1194, 1145, 1092, 1010, 957, 925, 852, 796, 740, 721, 626, 596, 565, 543, 498, 421.

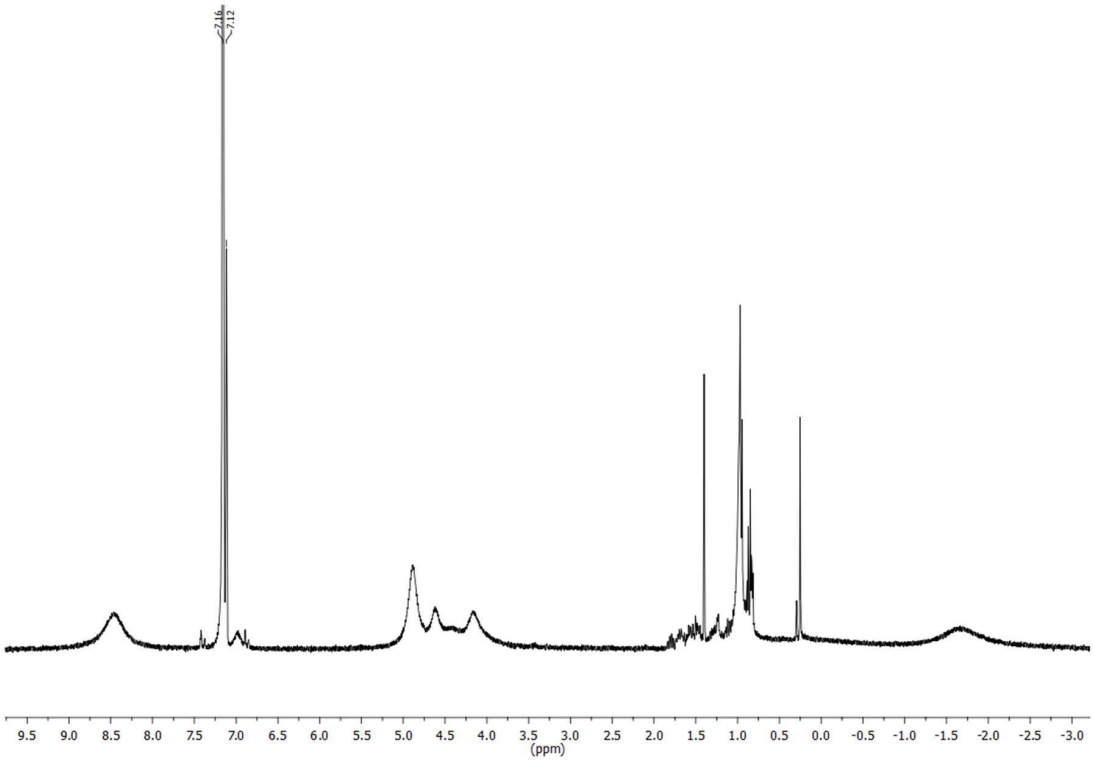

Figure S1. ^{1}H NMR spectrum of [(L^{1}GaCl)$_2$Bi·] (**1**) in C_6D_6.

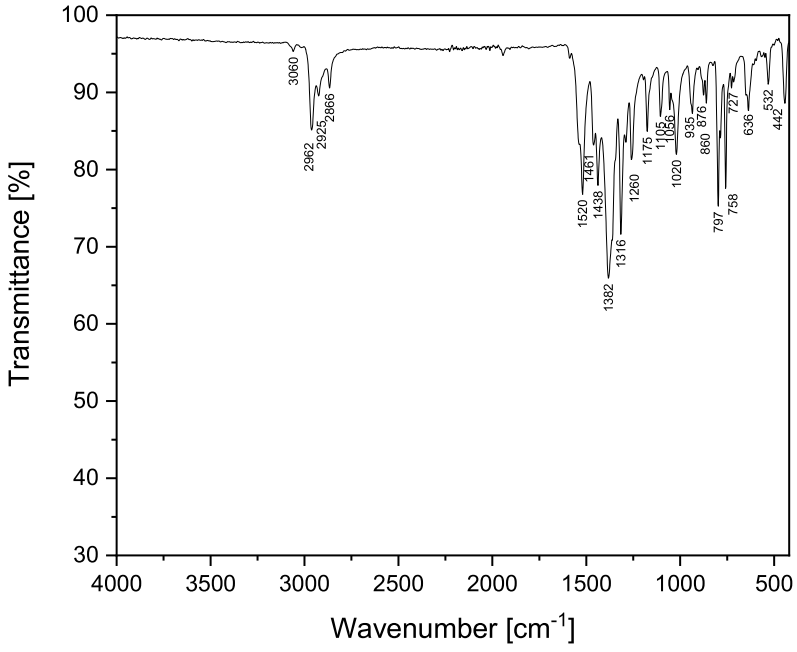

Figure S2. ATR-IR spectrum of [(L^{1}GaCl)$_2$Bi·] (**1**).

Comment to EPR Spectroscopy

We have previously collected both X- and Q-band frequency EPR spectra of the similar iodine-substituted ([L(I)Ga]$_2$Bi) radical (*Nat. Commun.* **2018**, *9*, 87) and given our recent results with comparable Sb radicals ([L(X)Ga]$_2$Sb) (X = Cl, Br, I) that the halide substituent "X" does not influence the EPR spectrum of the Sb radicals (*Chem. Eur. J.*, DOI: 10.1002/chem.202001739), the radical structure of ([L(Cl)Ga]$_2$Bi) should be identical with that of [L(I)Ga]$_2$Bi.

The EPR of ([L(I)Ga]$_2$Bi) exhibits a S = 1/2 signal that is split by the ^{209}Bi hyperfine coupling. The X-band spectrum of ([L(I)Ga]$_2$Bi) exhibits a complex pattern of transitions from 0 to 8000 G with inconsistent line widths. The Q-band spectrum of ([L(I)Ga]$_2$Bi) begins at ~7500 G and exceeds slightly beyond the upper limit of the magnet at 14400 G. This width of ~8000 G in both spectra constrains the hyperfine to a very small ^{209}Bi isotropic coupling. Unfortunately, the complex spectrum, including refinement of the g-tensor, ^{209}Bi hyperfine the Ga superhyperfine (that is partially observed at lower field of the X-band spectrum) has eluded satisfactory simulation, even though the EPR spectrum of ([L(I)Ga]$_2$Bi) undoubtedly exhibits a Bi centered radical.

We are currently employing additional EPR experiments in close cooperation with Dr. G. Cutsail III (MPI CEC, Mülheim), including additional microwave frequencies to further refine the EPR parameters, and advanced techniques such as Echo-Detected NMR to elucidate the Ga hyperfine couplings. We believe that these advanced EPR characterization of ([L(I)Ga]$_2$Bi) and ([L(Cl)Ga]$_2$Bi) can be published in the future.

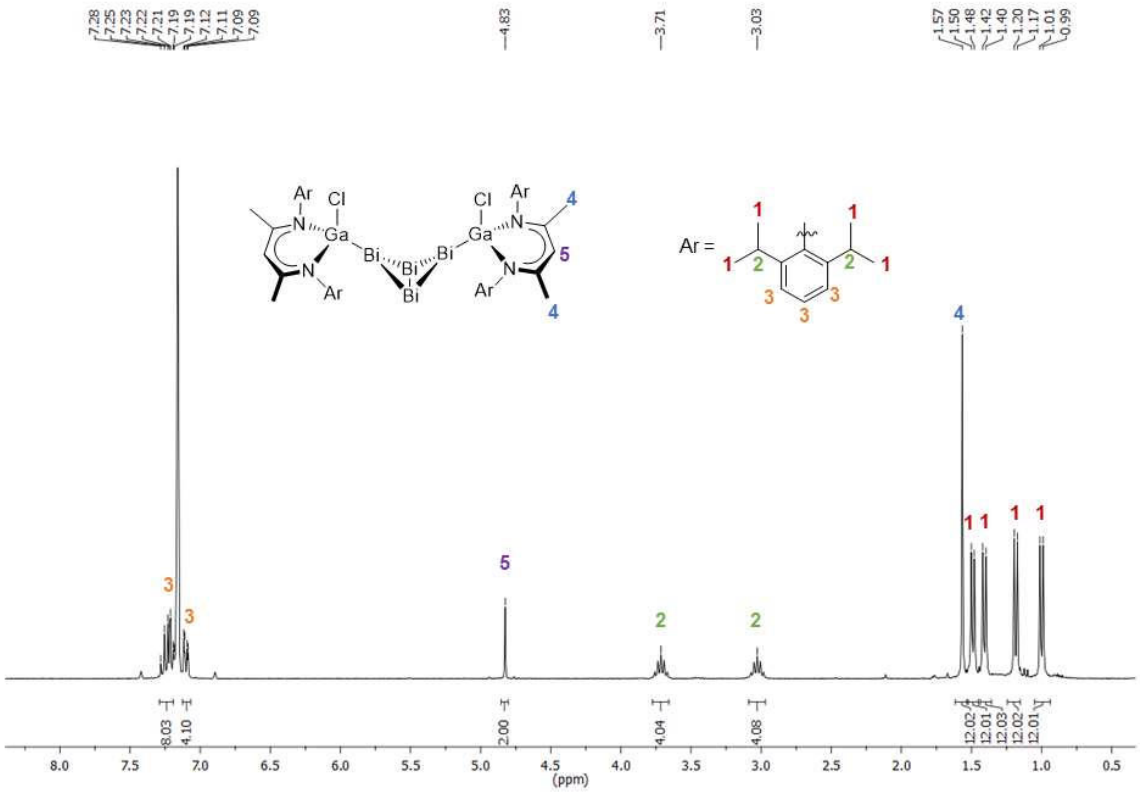

Figure S3. ^{1}H NMR spectrum of [(L^{1}GaCl)$_2$(μ,η$^{1:1}$-Bi$_4$)] (**3**) in C_6D_6.

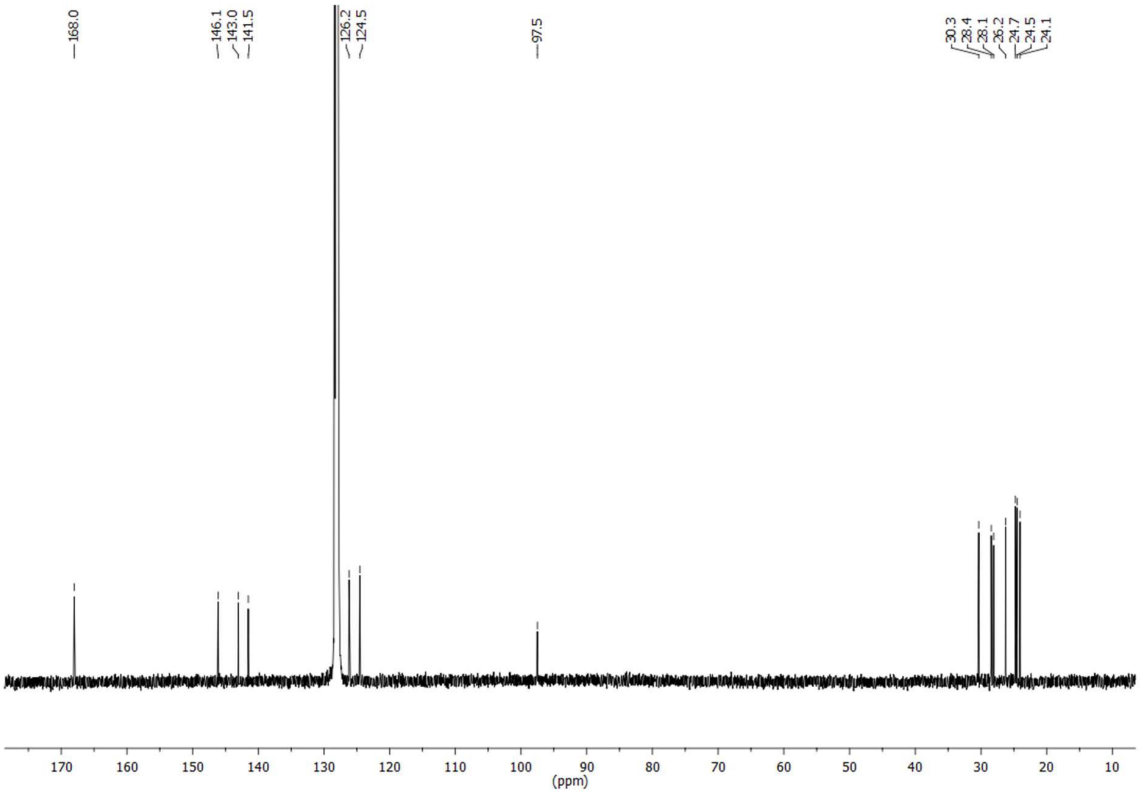

Figure S4. ^{13}C NMR spectrum of [(L^{1}GaCl)$_2$(μ,η$^{1:1}$-Bi$_4$)] (**3**) in C_6D_6.

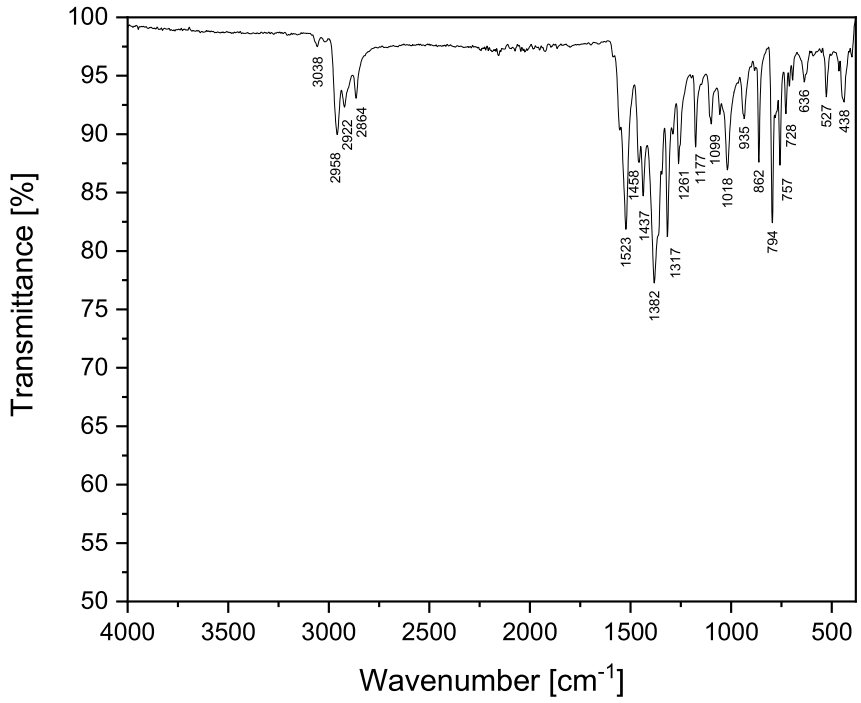

Figure S5. ATR-IR spectrum of $[(L^1GaCl)_2(\mu,\eta^{1:1}\text{-}Bi_4)]$ (**3**).

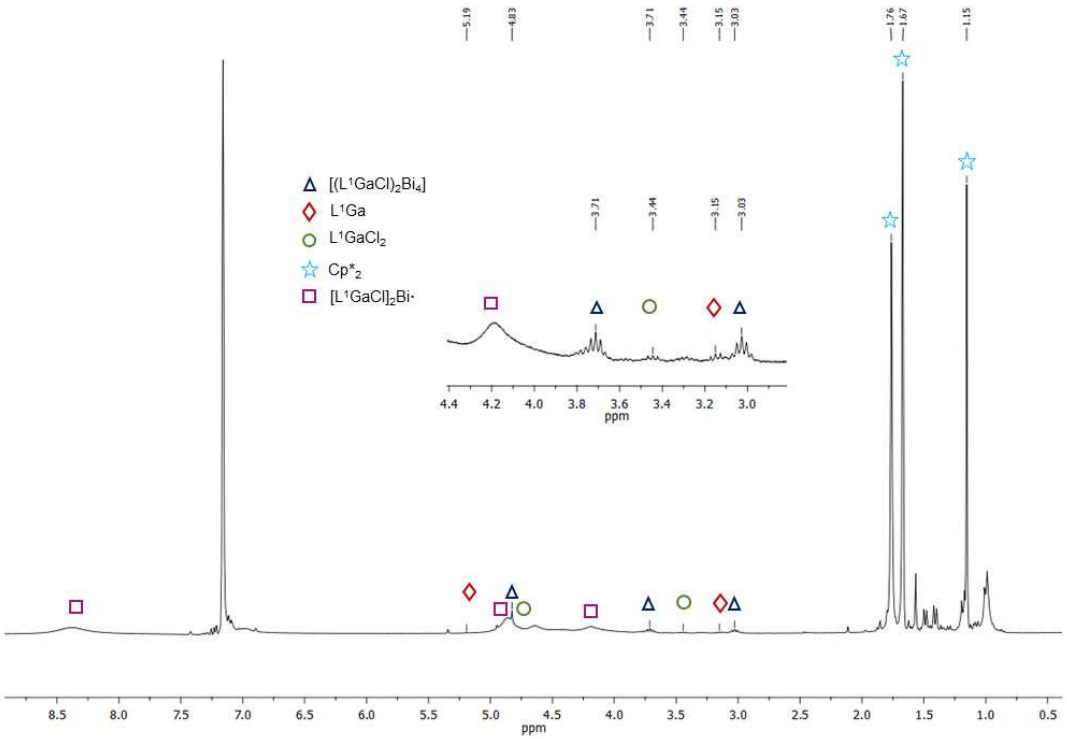

Figure S6. ^{1}H NMR spectrum of the equimolar reaction of Cp^*_2BiCl and L^1Ga at ambient temperature in C_6D_6.

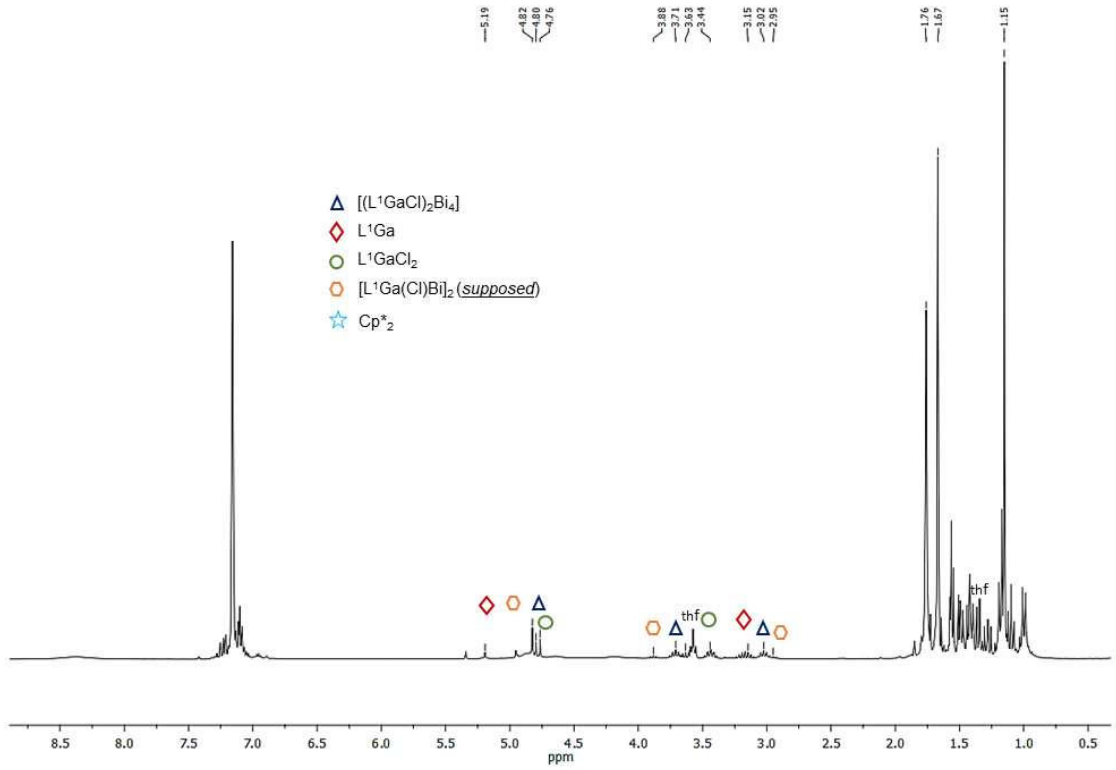

Figure S7. ^{1}H NMR spectrum of the reaction of Cp^*_2BiCl and L^1Ga after 5 h at −78 °C in C_6D_6.

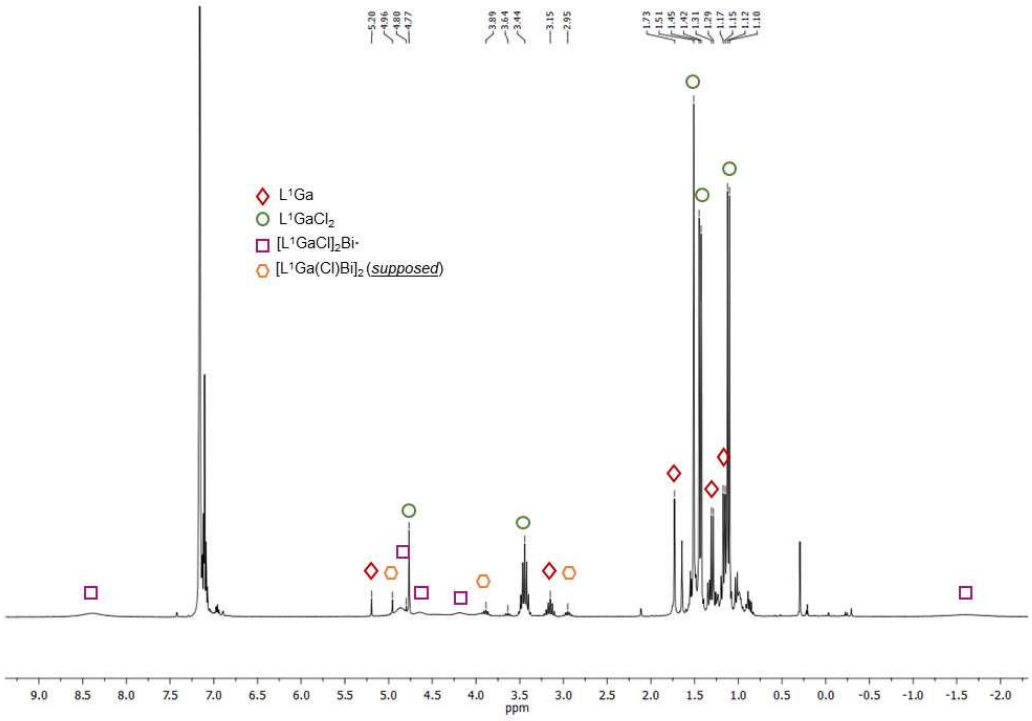

Figure S8. ^{1}H NMR spectrum of the reaction of $BiCl_3$ and two equivalent of L^1Ga after warming up the reaction mixture from −80 °C to ambient temperature in C_6D_6.

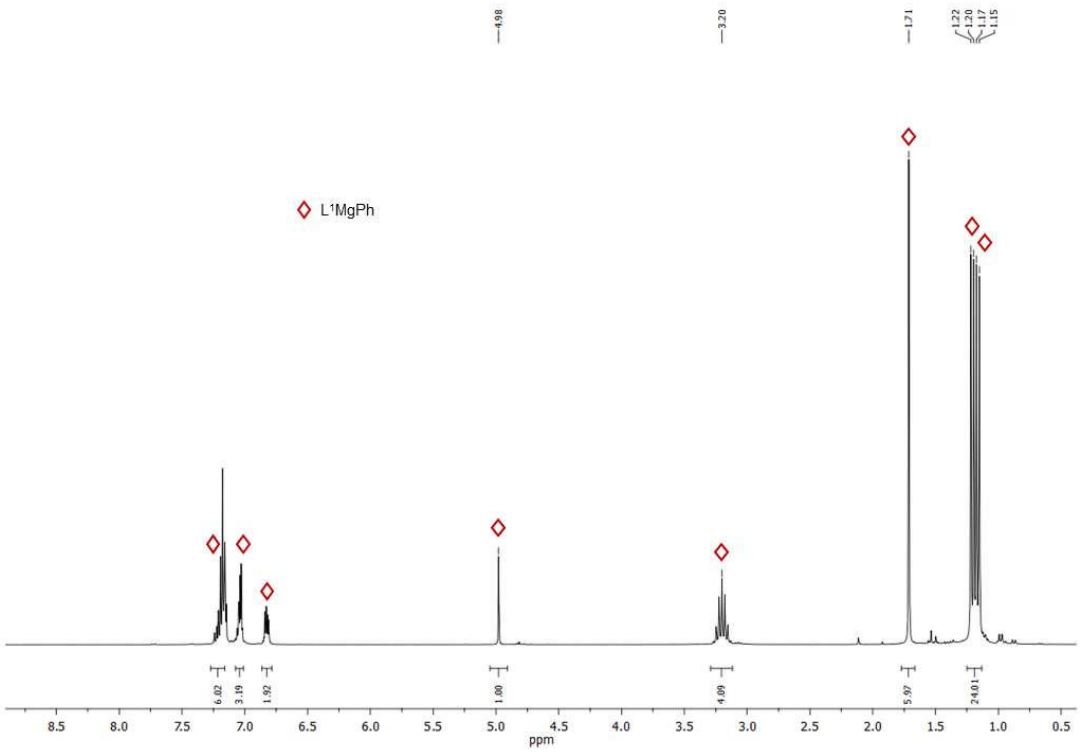

Figure S9. ^{1}H NMR spectrum of the reaction of 2.5 equivalents of $[L^{1}Mg]_2$ and Bi_2Ph_4 in C_6D_6 at ambient temperature, yielding $L^{1}MgPh$ and elemental bismuth.

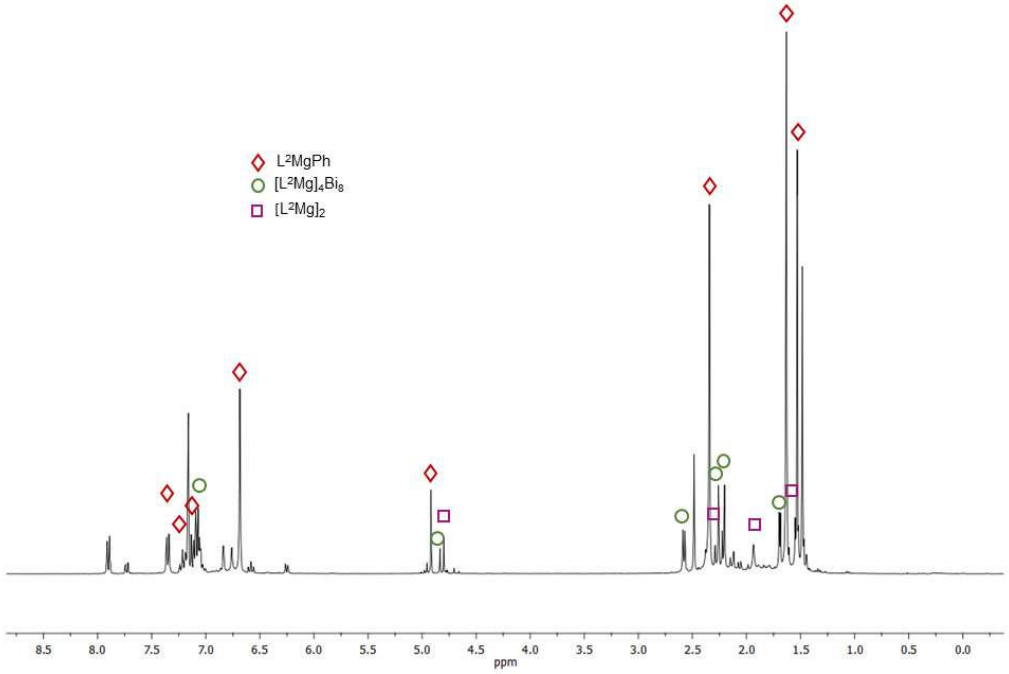

Figure S10. ^{1}H NMR spectrum of the reaction of $[L^{2}Mg]_2$ and Bi_2Ph_4 after 3 h at ambient temperature in C_6D_6.

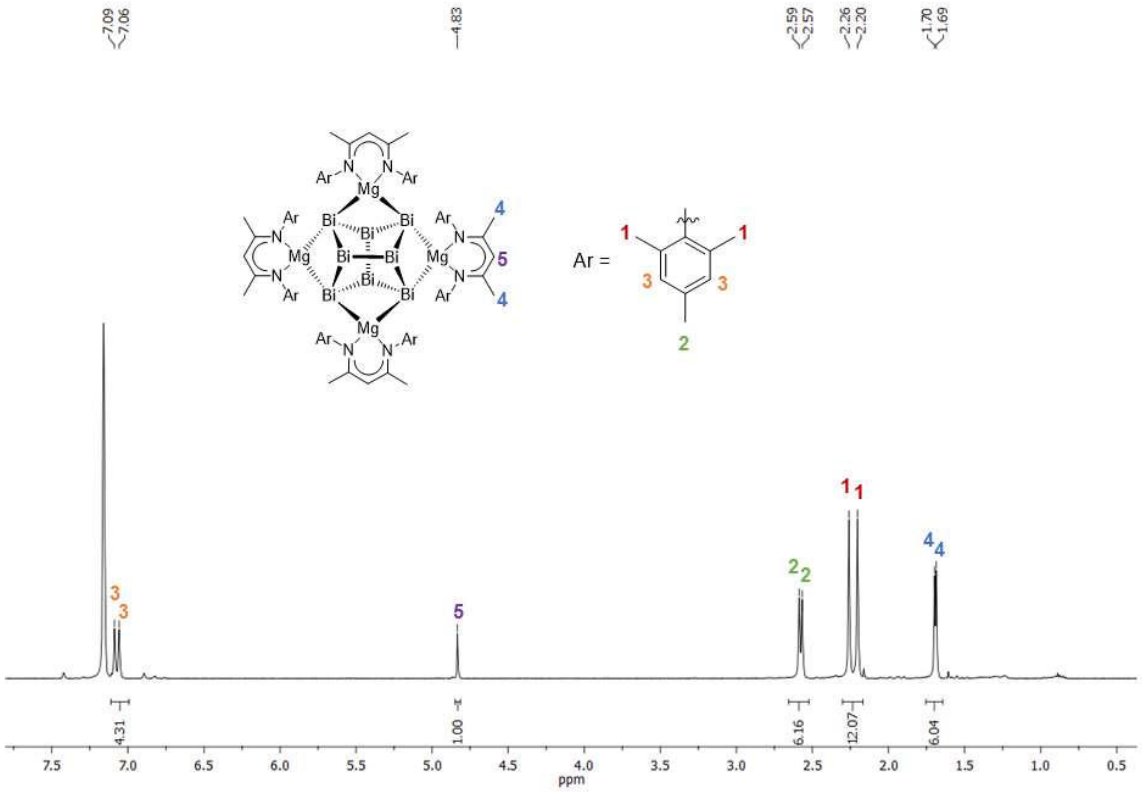

Figure S11. ^{1}H NMR spectrum of [(L^{2}Mg)$_4$Bi$_8$] (**4**) in C_6D_6.

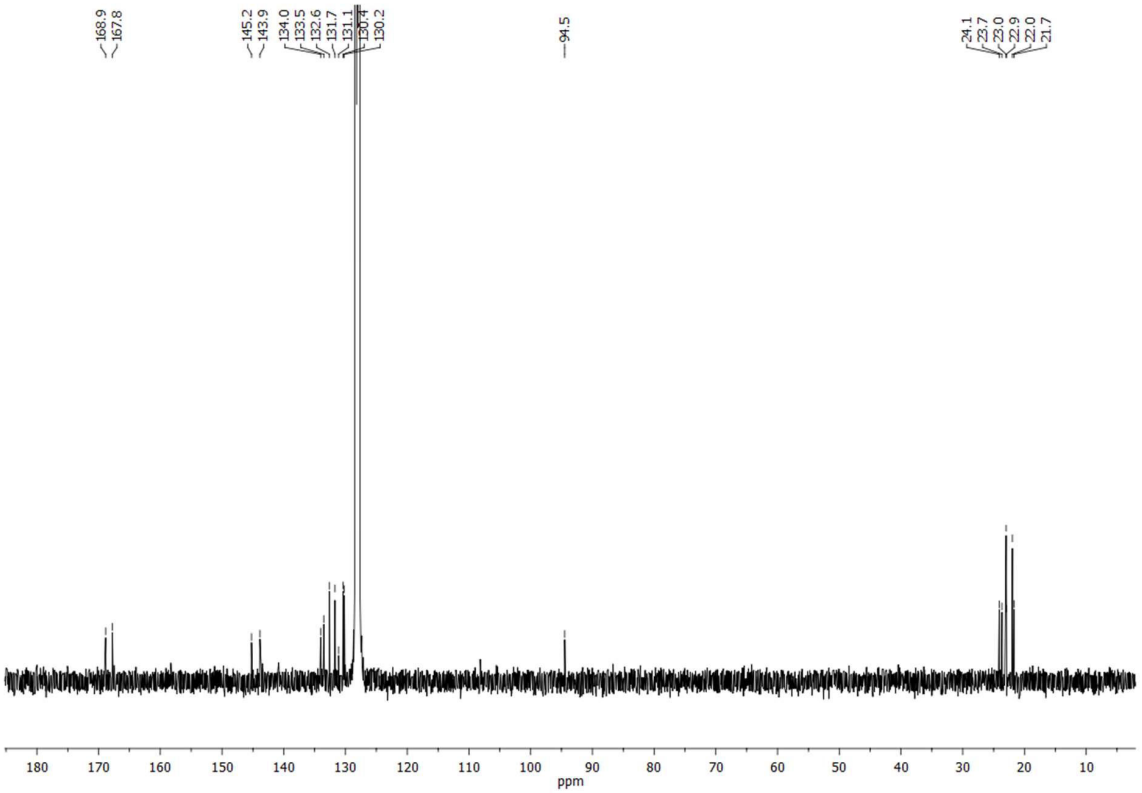

Figure S12. ^{13}C NMR spectrum of [(L^{2}Mg)$_4$Bi$_8$] (**4**) in C_6D_6.

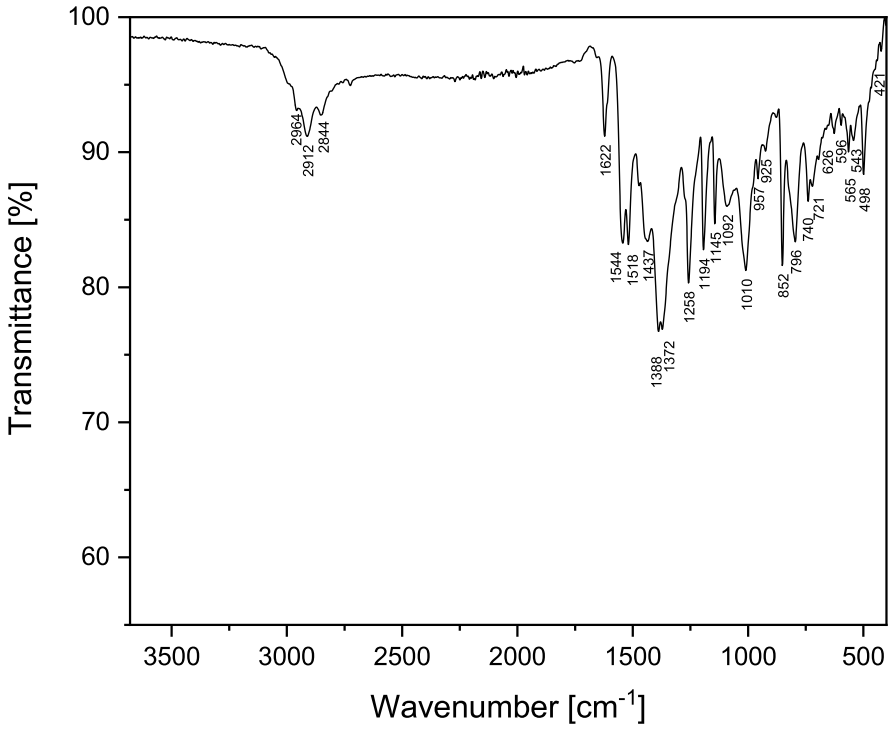

Figure S13. ATR-IR spectrum of $[(L^2Mg)_4Bi_8]$ (**4**).

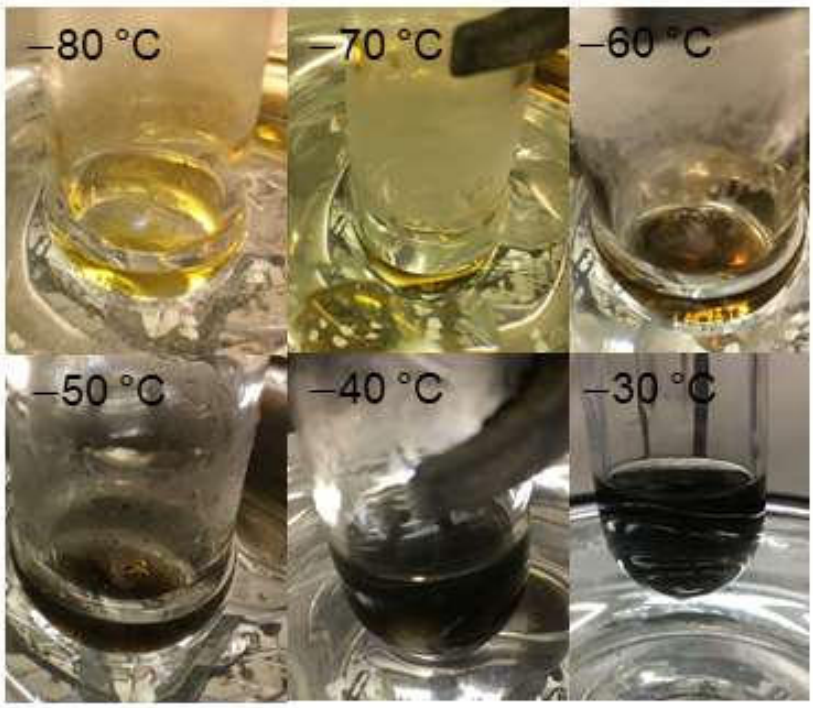

Fig. S14. Reaction of Ph_4Bi_2 with $[L^1Mg]_2$ yielding bismuth metal.

B) Crystallographic Details

Single crystals were mounted on a nylon loop in inert oil. Data were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (monochromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å). The structures were solved by Direct Methods[5] and refined anisotropically by full-matrix least-squares on F^2.[6] Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (**1**, **2**, **4**) and numerical from crystal faces (**3**), respectively (Bruker AXS APEX2). Hydrogen atoms were refined using a riding model or rigid methyl groups. **1** contains a highly disordered n-hexane molecule. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run.[7] The *n*-hexane molecule is included in the sum formula for completeness. In **3** a Dipp group is disordered over two positions. All corresponding bond lengths were restrained to be equal (SADI) and RIGU and SIMU restraints were applied to the anisotropic displacement parameters. The anisotropic displacement parameters of the solvent atoms suggest disorder, but a refinement of two separate positions of the molecule failed. The C–C bond lengths were restrained to be equal to 1.54 Å(DFIX). The crystals of **3** quickly oxidized even under inert oil and quickly degraded from loss of solvent even under cooling during preparation, resulting in a loss of quality of the dataset. A particular flaw of the model are the displacement parameters of Ga1. Their small values and the residual density in its vicinity suggest the presence of an atom with higher atomic number. Refining Ga1's occupancy yields 1.19 with reasonable values for the displacement parameters. However, by other analytical means the presence of any elements except for those listed in the sum formula can be excluded. We thus consider the unusual displacement parameters of Ga1 to be a result of the poor data quality. The combination of disorder, low data quality and the presence of many heavy atoms leads to a low precision of the parameters of the light atoms (CheckCIF Alert level B). In **4** a mesityl group is disordered over two positions. All corresponding bond lengths were restrained to be equal (SADI). RIGU restraints were applied to all anisotropic displacement parameters of the disordered atoms. Where the alternate positions are in close proximity further SIMU restraints and EADP constraints were applied to avoid correlations of parameters. The R_{int} values of the later runs were significantly higher. The crystals degraded rapidly during preparation even under inert oil and are also light sensitive, decomposition during the measurement cannot be excluded. Bond length criteria are to some extent arbitrary. The Bi-Bi bonds are simply longer than the maximum bond length assumed by checkcif. The novel nature of the compounds does not render CheckCIF a suitable tool to access the Bi-Bi bond lengths thus the Level A alerts can be ignored.[i]

1: $[C_{64}H_{96}BiCl_2Ga_2N_4]$, M = 1340.76, orange crystal, (0.356 × 0.196 × 0.190 mm); monoclinic, space group $P2_1/n$; a = 13.6015(11) Å, b = 25.492(2) Å, c = 18.3534(15) Å; α = 90°, β = 93.094(4)°, γ = 90°, V = 6354.4(9) Å^3; Z = 4; μ = 3.728 mm^{-1}; ρ_{calc} = 1.401 g·cm^{-3}; 186246 reflections (θ_{max} = 33.295°), 23293

[i] CheckCIF routines have been updated during the publication procedure (thanks to A. L. Spek) and should no longer produce comparable A alerts.

unique (R_{int} = 0.0409); 624 parameters; largest max./min in the final difference Fourier synthesis 2.475 e·Å^{-3}/ -2.005 e·Å^{-3}; max./min. transmission 0.75/0.51; R_1 = 0.0396 (I > 2σ(I)), wR_2 = 0.0908 (all data).

2: [$C_{58}H_{82}Bi_2Cl_2Ga_2N_4$], M = 1463.57, orange crystal, (0.302 × 0.153 × 0.119 mm); monoclinic, space group $P2_1/n$; a = 13.811(3) Å, b = 10.503(2) Å, c = 21.145(4) Å; α = 90°, β = 97.567(9)°, γ = 90°, V = 3040.5(10) Å^3; Z = 2; μ = 6.772 mm^{-1}; ρ_{calc} = 1.599 g·cm^{-3}; 106423 reflections (θ_{max} = 32.031°), 10589 unique (R_{int} = 0.0592); 317 parameters; largest max./min in the final difference Fourier synthesis 2.936 e·Å^{-3}/ -2.470 e·Å^{-3}; max./min. transmission 0.75/0.55; R_1 = 0.0374 (I > 2σ(I)), wR_2 = 0.1078 (all data).

3: [$C_{61}H_{89}Bi_4Cl_2Ga_2N_4$], M = 1924.62, red crystal, (0.274 × 0.126 × 0.079 mm); monoclinic, space group $P2_1/c$; a = 19.428(2) Å, b = 16.8828(19) Å, c = 20.473(2) Å; α = 90°, β = 104.697(6)°, γ = 90°, V = 6495.2(12) Å^3; Z = 4; μ = 11.737 mm^{-1}; ρ_{calc} = 1.968 g·cm^{-3}; 98193 reflections (θ_{max} = 26.565°), 13392 unique (R_{int} = 0.0864); 792 parameters; largest max./min in the final difference Fourier synthesis 3.213 e·Å^{-3}/ -1.830 e·Å^{-3}; max./min. transmission 0.54/0.16; R_1 = 0.0575 (I > 2σ(I)), wR_2 = 0.1756 (all data).

4: [$C_{92}H_{116}Bi_8Mg_4N_8$], M = 3103.00, black crystal, (0.217 × 0.071 × 0.049 mm); triclinic, space group P-1; a = 15.475(6) Å, b = 15.731(6) Å, c = 21.669(4) Å; α = 79.673(6)°, β = 85.162(5)°, γ = 73.302(8)°, V = 4968(3) Å^3; Z = 2; μ = 14.185 mm^{-1}; ρ_{calc} = 2.074 g·cm^{-3}; 423122 reflections (θ_{max} = 33.203°), 37802 unique (R_{int} = 0.1315); 1114 parameters; largest max./min in the final difference Fourier synthesis 2.145 e·Å^{-3}/ -1.974 e·Å^{-3}; max./min. transmission 0.26/0.17; R_1 = 0.0432 (I > 2σ(I)), wR_2 = 0.0796 (all data).

The crystallographic data (without structure factors) was deposited as „supplementary publication no. CCDC-1983875 (**1**), CCDC-1983873 (**2**), CCDC-1983874 (**3**), and CCDC-1983876 (**4**) at the Cambridge Crystallographic Data Centre. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.: CCDC, 12 Union Road, Cambridge, CB21EZ (Fax: (+44)1223/336033; E-mail: deposit@ccdc.cam-ak.uk).

Table S1. Single crystal X-ray diffraction data of **1** - **4**.

Identification code	**1 (jk_321m_sq)**	**2 (jk_183m)**	**3 (jk_340m)**	**4 (jk_383am)**
Empirical formula	$C_{64}H_{96}BiCl_2Ga_2N_4$	$C_{58}H_{82}Bi_2Cl_2Ga_2N_4$	$C_{61}H_{89}Bi_4Cl_2Ga_2N_4$	$C_{92}H_{116}Bi_8Mg_4N_8$
M	1340.76	1463.57	1924.62	3103.00
Crystal size [mm]	0.356×0.196×0.190	0.302×0.153×0.119	0.274×0.126×0.079	0.217×0.071×0.049
T [K]	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/c$	P-1
a [Å]	13.6015(11)	13.811(3)	19.428(2)	15.475(6)
b [Å]	25.492(2)	10.503(2)	16.8828(19)	15.731(6)
c [Å]	18.3534(15)	21.145(4)	20.473(2)	21.669(4)
α [°]	90	90	90	79.673(6)
β [°]	93.094(4)	97.567(9)	104.697(6)	85.162(5)
γ [°]	90	90	90	73.302(8)
V [Å^3]	6354.4(9)	3040.5(10)	6495.2(12)	4968(3)
Z	4	2	4	2
D_{calc} [g·cm^{-3}]	1.401	1.599	1.968	2.074
μ(MoK_α [mm^{-1}])	3.728	6.772	11.737	14.185
Transmissions	0.75/0.51	0.75/0.55	0.54/0.16	0.26/0.17
F(000)	2748	1440	3644	2872
Index ranges	$-20 \le h \le 19$	$-18 \le h \le 20$	$-24 \le h \le 24$	$-23 \le h \le 23$
	$-39 \le k \le 37$	$-15 \le k \le 15$	$-21 \le k \le 18$	$-24 \le k \le 24$
	$-28 \le l \le 26$	$-31 \le l \le 31$	$-25 \le l \le 25$	$-33 \le l \le 33$
θ_{max} [°]	33.295	32.031	26.565	33.203
Reflections collected	186246	106423	98193	423122
Independent reflections	23293	10589	13392	37802
R_{int}	0.0409	0.0592	0.0864	0.1315
Refined parameters	624	317	792	1114
R_1 [$I > 2\sigma(I)$]	0.0396	0.0374	0.0575	0.0432
wR_2 [all data]	0.0908	0.1078	0.1756	0.0796
GooF	1.089	1.018	1.063	1.030
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	2.475/-2.005	2.936/-2.470	3.213/-1.830	2.145/-1.974

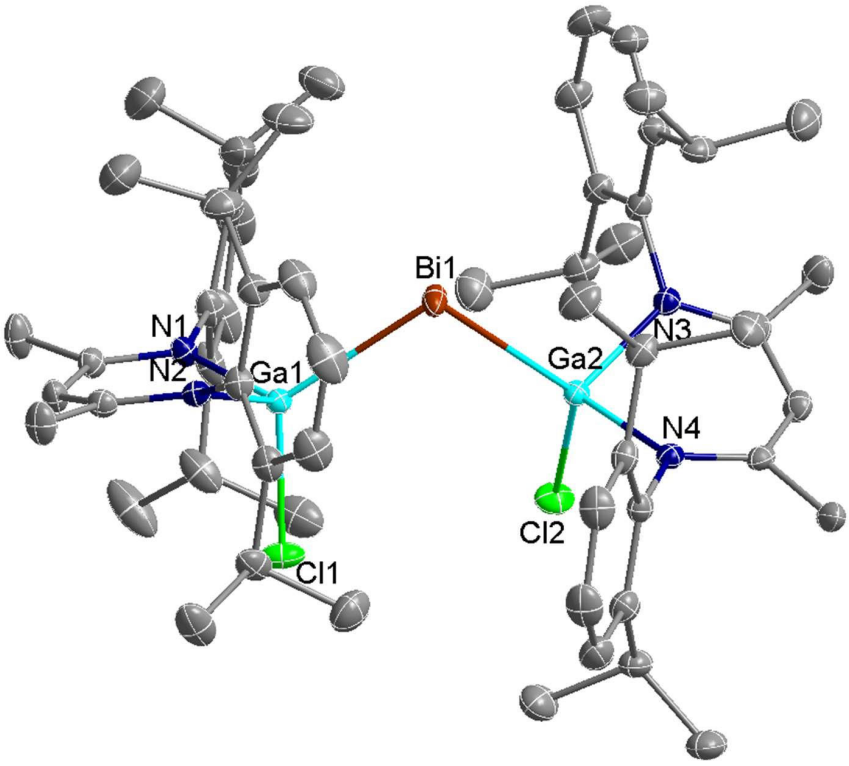

Fig. S15. Solid state structure of **1**. Hydrogen atoms are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S2: Bond lengths [Å] for **1** (jk_321m_sq).

Bi(1)-Ga(2)	2.6485(3)	C(8)-C(9)	1.368(6)	C(35)-C(36)	1.398(4)
Bi(1)-Ga(1)	2.6619(4)	C(9)-C(10)	1.375(6)	C(35)-C(40)	1.410(4)
Ga(1)-N(1)	1.955(2)	C(10)-C(11)	1.392(5)	C(36)-C(37)	1.394(4)
Ga(1)-N(2)	1.964(2)	C(11)-C(15)	1.519(5)	C(36)-C(41)	1.518(4)
Ga(1)-Cl(1)	2.2113(8)	C(12)-C(14)	1.531(6)	C(37)-C(38)	1.387(5)
Ga(2)-N(3)	1.956(2)	C(12)-C(13)	1.533(5)	C(38)-C(39)	1.388(5)
Ga(2)-N(4)	1.968(2)	C(15)-C(16)	1.523(5)	C(39)-C(40)	1.388(4)
Ga(2)-Cl(2)	2.2084(7)	C(15)-C(17)	1.526(5)	C(40)-C(44)	1.521(4)
N(1)-C(1)	1.335(4)	C(18)-C(19)	1.400(4)	C(41)-C(43)	1.531(5)
N(1)-C(6)	1.450(4)	C(18)-C(23)	1.405(4)	C(41)-C(42)	1.531(5)
N(2)-C(3)	1.334(4)	C(19)-C(20)	1.398(4)	C(44)-C(46)	1.527(5)
N(2)-C(18)	1.443(3)	C(19)-C(24)	1.517(4)	C(44)-C(45)	1.532(5)
N(3)-C(30)	1.329(4)	C(20)-C(21)	1.386(5)	C(47)-C(48)	1.406(4)
N(3)-C(35)	1.448(4)	C(21)-C(22)	1.374(6)	C(47)-C(52)	1.414(4)
N(4)-C(32)	1.330(4)	C(22)-C(23)	1.399(4)	C(48)-C(49)	1.399(5)
N(4)-C(47)	1.442(4)	C(23)-C(27)	1.512(5)	C(48)-C(53)	1.518(4)
C(1)-C(2)	1.399(4)	C(24)-C(26)	1.525(5)	C(49)-C(50)	1.376(5)
C(1)-C(4)	1.513(4)	C(24)-C(25)	1.529(5)	C(50)-C(51)	1.378(5)

C(2)-C(3)	1.399(4)	C(27)-C(29)	1.522(5)	C(51)-C(52)	1.390(4)
C(3)-C(5)	1.505(4)	C(27)-C(28)	1.525(6)	C(52)-C(56)	1.516(4)
C(6)-C(7)	1.405(4)	C(30)-C(31)	1.401(4)	C(53)-C(54)	1.526(5)
C(6)-C(11)	1.407(5)	C(30)-C(33)	1.506(4)	C(53)-C(55)	1.534(5)
C(7)-C(8)	1.397(4)	C(31)-C(32)	1.397(4)	C(56)-C(58)	1.531(4)
C(7)-C(12)	1.512(5)	C(32)-C(34)	1.490(4)	C(56)-C(57)	1.533(5)

Table S3: Bond angles [°] **1** for (jk_321m_sq).

Ga(2)-Bi(1)-Ga(1)	105.459(11)	C(21)-C(20)-C(19)	121.2(3)
N(1)-Ga(1)-N(2)	95.74(10)	C(22)-C(21)-C(20)	120.0(3)
N(1)-Ga(1)-Cl(1)	103.48(7)	C(21)-C(22)-C(23)	121.3(3)
N(2)-Ga(1)-Cl(1)	103.37(7)	C(22)-C(23)-C(18)	117.9(3)
N(1)-Ga(1)-Bi(1)	119.93(7)	C(22)-C(23)-C(27)	120.2(3)
N(2)-Ga(1)-Bi(1)	106.86(7)	C(18)-C(23)-C(27)	121.8(3)
Cl(1)-Ga(1)-Bi(1)	122.92(3)	C(19)-C(24)-C(26)	109.8(3)
N(3)-Ga(2)-N(4)	95.23(10)	C(19)-C(24)-C(25)	111.8(3)
N(3)-Ga(2)-Cl(2)	104.60(7)	C(26)-C(24)-C(25)	110.4(3)
N(4)-Ga(2)-Cl(2)	103.14(7)	C(23)-C(27)-C(29)	114.0(3)
N(3)-Ga(2)-Bi(1)	109.35(7)	C(23)-C(27)-C(28)	111.4(3)
N(4)-Ga(2)-Bi(1)	117.32(7)	C(29)-C(27)-C(28)	110.0(3)
Cl(2)-Ga(2)-Bi(1)	123.08(2)	N(3)-C(30)-C(31)	122.9(3)
C(1)-N(1)-C(6)	117.6(2)	N(3)-C(30)-C(33)	119.5(3)
C(1)-N(1)-Ga(1)	119.34(19)	C(31)-C(30)-C(33)	117.6(3)
C(6)-N(1)-Ga(1)	122.92(19)	C(32)-C(31)-C(30)	128.2(3)
C(3)-N(2)-C(18)	120.5(2)	N(4)-C(32)-C(31)	124.1(3)
C(3)-N(2)-Ga(1)	119.82(19)	N(4)-C(32)-C(34)	120.1(3)
C(18)-N(2)-Ga(1)	119.57(18)	C(31)-C(32)-C(34)	115.8(3)
C(30)-N(3)-C(35)	118.8(2)	C(36)-C(35)-C(40)	121.4(3)
C(30)-N(3)-Ga(2)	118.7(2)	C(36)-C(35)-N(3)	120.7(3)
C(35)-N(3)-Ga(2)	122.54(18)	C(40)-C(35)-N(3)	117.9(2)
C(32)-N(4)-C(47)	119.9(2)	C(37)-C(36)-C(35)	118.1(3)
C(32)-N(4)-Ga(2)	118.70(19)	C(37)-C(36)-C(41)	119.7(3)
C(47)-N(4)-Ga(2)	121.10(18)	C(35)-C(36)-C(41)	122.2(3)
N(1)-C(1)-C(2)	124.6(3)	C(38)-C(37)-C(36)	121.3(3)
N(1)-C(1)-C(4)	119.2(3)	C(37)-C(38)-C(39)	119.7(3)
C(2)-C(1)-C(4)	116.1(3)	C(40)-C(39)-C(38)	121.0(3)
C(1)-C(2)-C(3)	128.0(3)	C(39)-C(40)-C(35)	118.5(3)
N(2)-C(3)-C(2)	123.1(3)	C(39)-C(40)-C(44)	119.5(3)
N(2)-C(3)-C(5)	120.3(3)	C(35)-C(40)-C(44)	122.0(3)
C(2)-C(3)-C(5)	116.6(3)	C(36)-C(41)-C(43)	110.3(3)
C(7)-C(6)-C(11)	121.4(3)	C(36)-C(41)-C(42)	112.2(3)

C(7)-C(6)-N(1)	119.8(3)	C(43)-C(41)-C(42)	110.1(3)
C(11)-C(6)-N(1)	118.7(3)	C(40)-C(44)-C(46)	112.1(3)
C(8)-C(7)-C(6)	117.3(3)	C(40)-C(44)-C(45)	111.0(3)
C(8)-C(7)-C(12)	119.9(3)	C(46)-C(44)-C(45)	110.1(3)
C(6)-C(7)-C(12)	122.8(3)	C(48)-C(47)-C(52)	121.2(3)
C(9)-C(8)-C(7)	121.8(4)	C(48)-C(47)-N(4)	119.9(2)
C(8)-C(9)-C(10)	120.2(3)	C(52)-C(47)-N(4)	118.9(2)
C(9)-C(10)-C(11)	121.0(4)	C(49)-C(48)-C(47)	117.6(3)
C(10)-C(11)-C(6)	118.0(3)	C(49)-C(48)-C(53)	119.3(3)
C(10)-C(11)-C(15)	120.2(3)	C(47)-C(48)-C(53)	123.1(3)
C(6)-C(11)-C(15)	121.8(3)	C(50)-C(49)-C(48)	121.7(3)
C(7)-C(12)-C(14)	109.6(3)	C(49)-C(50)-C(51)	119.9(3)
C(7)-C(12)-C(13)	112.9(3)	C(50)-C(51)-C(52)	121.4(3)
C(14)-C(12)-C(13)	109.7(3)	C(51)-C(52)-C(47)	118.1(3)
C(11)-C(15)-C(16)	112.0(3)	C(51)-C(52)-C(56)	120.8(3)
C(11)-C(15)-C(17)	111.6(3)	C(47)-C(52)-C(56)	121.0(3)
C(16)-C(15)-C(17)	111.1(3)	C(48)-C(53)-C(54)	111.4(3)
C(19)-C(18)-C(23)	121.7(3)	C(48)-C(53)-C(55)	110.1(3)
C(19)-C(18)-N(2)	120.1(3)	C(54)-C(53)-C(55)	110.0(3)
C(23)-C(18)-N(2)	118.2(3)	C(52)-C(56)-C(58)	113.2(3)
C(20)-C(19)-C(18)	117.9(3)	C(52)-C(56)-C(57)	110.8(3)
C(20)-C(19)-C(24)	119.1(3)	C(58)-C(56)-C(57)	110.4(3)
C(18)-C(19)-C(24)	123.0(3)		

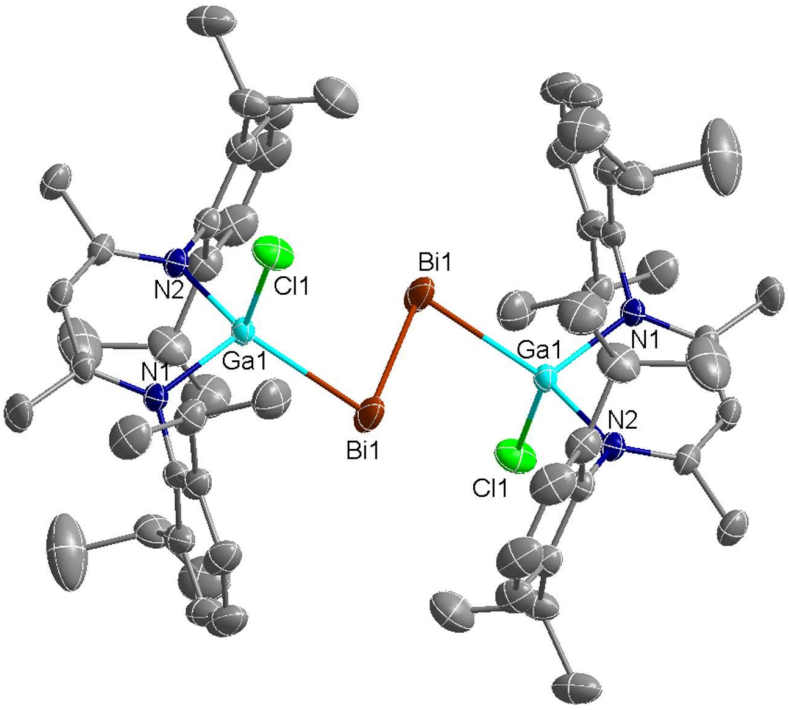

Fig. S16. Solid state structure of **2**. Hydrogen atoms are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S4: Bond lengths [Å] for **2** (jk_183m).

Bi(1)-Ga(1)	2.6793(5)	C(6)-C(11)	1.399(5)	C(18)-C(23)	1.397(5)
Bi(1)-Bi(1)#1	2.8031(5)	C(6)-C(7)	1.408(5)	C(18)-C(19)	1.414(5)
Ga(1)-N(2)	1.950(3)	C(7)-C(8)	1.397(6)	C(19)-C(20)	1.394(6)
Ga(1)-N(1)	1.966(3)	C(7)-C(12)	1.511(6)	C(19)-C(24)	1.516(6)
Ga(1)-Cl(1)	2.2408(11)	C(8)-C(9)	1.368(7)	C(20)-C(21)	1.363(7)
N(1)-C(1)	1.329(4)	C(9)-C(10)	1.371(7)	C(21)-C(22)	1.383(7)
N(1)-C(6)	1.447(4)	C(10)-C(11)	1.396(5)	C(22)-C(23)	1.401(5)
N(2)-C(3)	1.338(4)	C(11)-C(15)	1.513(5)	C(23)-C(27)	1.515(5)
N(2)-C(18)	1.436(4)	C(12)-C(14)	1.515(8)	C(24)-C(26)	1.515(8)
C(1)-C(2)	1.396(5)	C(12)-C(13)	1.521(7)	C(24)-C(25)	1.518(6)
C(1)-C(4)	1.507(5)	C(15)-C(16)	1.527(6)	C(27)-C(29)	1.524(7)
C(2)-C(3)	1.392(5)	C(15)-C(17)	1.535(6)	C(27)-C(28)	1.540(6)
C(3)-C(5)	1.507(5)				

#1 -x+1,-y+1,-z+1

Table S5: Bond angles [°] for **2** (jk_183m).

Ga(1)-Bi(1)-Bi(1)#1	93.029(17)	C(9)-C(10)-C(11)	120.9(4)
N(2)-Ga(1)-N(1)	95.57(11)	C(10)-C(11)-C(6)	118.4(4)
N(2)-Ga(1)-Cl(1)	102.74(9)	C(10)-C(11)-C(15)	118.5(4)
N(1)-Ga(1)-Cl(1)	103.35(9)	C(6)-C(11)-C(15)	123.1(3)
N(2)-Ga(1)-Bi(1)	126.53(8)	C(7)-C(12)-C(14)	111.2(4)
N(1)-Ga(1)-Bi(1)	113.75(8)	C(7)-C(12)-C(13)	113.4(4)
Cl(1)-Ga(1)-Bi(1)	111.73(3)	C(14)-C(12)-C(13)	110.4(5)
C(1)-N(1)-C(6)	122.2(3)	C(11)-C(15)-C(16)	111.0(4)
C(1)-N(1)-Ga(1)	120.3(2)	C(11)-C(15)-C(17)	111.5(3)
C(6)-N(1)-Ga(1)	117.2(2)	C(16)-C(15)-C(17)	109.9(4)
C(3)-N(2)-C(18)	120.1(3)	C(23)-C(18)-C(19)	121.2(3)
C(3)-N(2)-Ga(1)	119.0(2)	C(23)-C(18)-N(2)	120.8(3)
C(18)-N(2)-Ga(1)	120.8(2)	C(19)-C(18)-N(2)	117.9(3)
N(1)-C(1)-C(2)	123.4(3)	C(20)-C(19)-C(18)	117.7(4)
N(1)-C(1)-C(4)	120.6(3)	C(20)-C(19)-C(24)	121.2(4)
C(2)-C(1)-C(4)	116.0(3)	C(18)-C(19)-C(24)	121.1(3)
C(3)-C(2)-C(1)	128.1(3)	C(21)-C(20)-C(19)	121.6(4)
N(2)-C(3)-C(2)	124.5(3)	C(20)-C(21)-C(22)	120.5(4)
N(2)-C(3)-C(5)	119.3(3)	C(21)-C(22)-C(23)	120.5(4)
C(2)-C(3)-C(5)	116.3(3)	C(18)-C(23)-C(22)	118.5(3)
C(11)-C(6)-C(7)	121.3(3)	C(18)-C(23)-C(27)	123.2(3)
C(11)-C(6)-N(1)	120.1(3)	C(22)-C(23)-C(27)	118.3(3)
C(7)-C(6)-N(1)	118.5(3)	C(26)-C(24)-C(19)	112.6(4)
C(8)-C(7)-C(6)	117.5(4)	C(26)-C(24)-C(25)	110.5(4)
C(8)-C(7)-C(12)	120.6(4)	C(19)-C(24)-C(25)	113.6(4)
C(6)-C(7)-C(12)	121.9(3)	C(23)-C(27)-C(29)	110.7(4)
C(9)-C(8)-C(7)	121.6(4)	C(23)-C(27)-C(28)	111.5(4)
C(8)-C(9)-C(10)	120.4(4)	C(29)-C(27)-C(28)	110.5(4)

#1 -x+1,-y+1,-z+1

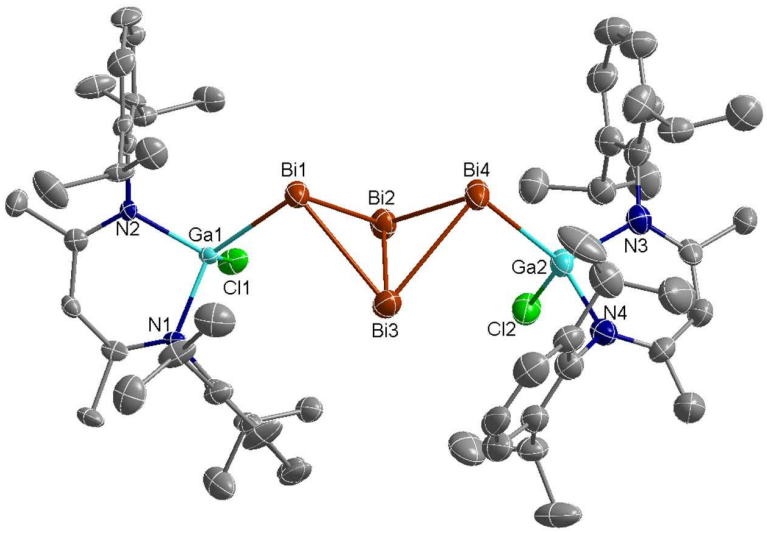

Fig. S17. Solid state structure of **3**. Hydrogen atoms are omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S6: Bond lengths [Å] for **3** (jk_340m).

Bi(1)-Ga(1)	2.6682(14)	C(9)-C(10)	1.39(2)	C(41)-C(42)	1.509(17)
Bi(1)-Bi(2)	2.9957(9)	C(10)-C(11)	1.40(2)	C(41)-C(43)	1.511(18)
Bi(1)-Bi(3)	3.0186(9)	C(11)-C(15)	1.54(2)	C(44)-C(45)	1.507(18)
Bi(2)-Bi(3)	2.9391(9)	C(12)-C(14)	1.493(19)	C(44)-C(46)	1.511(17)
Bi(2)-Bi(4)	2.9814(9)	C(12)-C(13)	1.55(2)	C(35')-C(36')	1.390(17)
Bi(3)-Bi(4)	3.0274(9)	C(15)-C(17)	1.47(2)	C(35')-C(40')	1.395(17)
Bi(4)-Ga(2)	2.6692(17)	C(15)-C(16)	1.50(2)	C(36')-C(37')	1.390(17)
Ga(1)-N(2)	1.953(10)	C(18)-C(23)	1.402(17)	C(36')-C(41')	1.55(3)
Ga(1)-N(1)	1.955(9)	C(18)-C(19)	1.415(17)	C(37')-C(38')	1.392(17)
Ga(1)-Cl(1)	2.244(4)	C(19)-C(20)	1.390(17)	C(38')-C(39')	1.390(17)
Ga(2)-N(4)	1.940(13)	C(19)-C(24)	1.527(18)	C(39')-C(40')	1.394(17)
Ga(2)-N(3)	1.956(12)	C(20)-C(21)	1.386(19)	C(40')-C(44')	1.55(3)
Ga(2)-Cl(2)	2.238(4)	C(21)-C(22)	1.39(2)	C(41')-C(42')	1.506(19)
N(1)-C(1)	1.333(16)	C(22)-C(23)	1.369(19)	C(41')-C(43')	1.514(19)
N(1)-C(6)	1.436(16)	C(23)-C(27)	1.533(18)	C(44')-C(45')	1.509(19)
N(2)-C(3)	1.310(16)	C(24)-C(26)	1.49(2)	C(44')-C(46')	1.511(19)
N(2)-C(18)	1.421(16)	C(24)-C(25)	1.51(2)	C(47)-C(48)	1.39(2)
N(3)-C(30)	1.314(18)	C(27)-C(28)	1.49(2)	C(47)-C(52)	1.41(2)
N(3)-C(35')	1.49(2)	C(27)-C(29)	1.54(2)	C(48)-C(49)	1.39(2)
N(3)-C(35)	1.50(2)	C(30)-C(31)	1.38(2)	C(48)-C(53)	1.51(2)
N(4)-C(32)	1.344(19)	C(30)-C(33)	1.51(2)	C(49)-C(50)	1.41(3)
N(4)-C(47)	1.426(19)	C(31)-C(32)	1.43(2)	C(50)-C(51)	1.36(3)
C(1)-C(2)	1.380(18)	C(32)-C(34)	1.46(2)	C(51)-C(52)	1.40(2)
C(1)-C(4)	1.510(17)	C(35)-C(36)	1.398(15)	C(52)-C(56)	1.55(2)

C(2)-C(3)	1.422(18)	C(35)-C(40)	1.400(15)	C(53)-C(54)	1.49(3)
C(3)-C(5)	1.512(19)	C(36)-C(37)	1.395(16)	C(53)-C(55)	1.51(2)
C(6)-C(11)	1.403(19)	C(36)-C(41)	1.54(2)	C(56)-C(57)	1.41(3)
C(6)-C(7)	1.418(18)	C(37)-C(38)	1.390(16)	C(56)-C(58)	1.56(3)
C(7)-C(8)	1.37(2)	C(38)-C(39)	1.396(16)	C11-C11#1	1.49(6)
C(7)-C(12)	1.51(2)	C(39)-C(40)	1.391(15)	C11-C21	1.521(19)
C(8)-C(9)	1.33(2)	C(40)-C(44)	1.55(2)	C21-C31	1.506(19)

#1 -x+1,-y+2,-z

Table S7: Bond angles [°] for **3** (jk_340m).

Ga(1)-Bi(1)-Bi(2)	86.50(3)	C(22)-C(23)-C(18)	120.6(12)
Ga(1)-Bi(1)-Bi(3)	95.20(3)	C(22)-C(23)-C(27)	117.9(11)
Bi(2)-Bi(1)-Bi(3)	58.51(2)	C(18)-C(23)-C(27)	121.5(11)
Bi(3)-Bi(2)-Bi(4)	61.50(2)	C(26)-C(24)-C(25)	111.2(13)
Bi(3)-Bi(2)-Bi(1)	61.14(2)	C(26)-C(24)-C(19)	112.9(11)
Bi(4)-Bi(2)-Bi(1)	79.79(2)	C(25)-C(24)-C(19)	109.9(11)
Bi(2)-Bi(3)-Bi(1)	60.36(2)	C(28)-C(27)-C(23)	115.3(12)
Bi(2)-Bi(3)-Bi(4)	59.94(2)	C(28)-C(27)-C(29)	109.3(12)
Bi(1)-Bi(3)-Bi(4)	78.70(2)	C(23)-C(27)-C(29)	110.8(12)
Ga(2)-Bi(4)-Bi(2)	88.96(4)	N(3)-C(30)-C(31)	124.2(14)
Ga(2)-Bi(4)-Bi(3)	93.06(4)	N(3)-C(30)-C(33)	118.7(14)
Bi(2)-Bi(4)-Bi(3)	58.56(2)	C(31)-C(30)-C(33)	117.0(13)
N(2)-Ga(1)-N(1)	96.8(4)	C(30)-C(31)-C(32)	128.8(14)
N(2)-Ga(1)-Cl(1)	105.8(3)	N(4)-C(32)-C(31)	121.8(14)
N(1)-Ga(1)-Cl(1)	103.1(3)	N(4)-C(32)-C(34)	121.1(15)
N(2)-Ga(1)-Bi(1)	110.8(3)	C(31)-C(32)-C(34)	117.0(14)
N(1)-Ga(1)-Bi(1)	126.9(3)	C(36)-C(35)-C(40)	123(2)
Cl(1)-Ga(1)-Bi(1)	111.09(11)	C(36)-C(35)-N(3)	120.8(19)
N(4)-Ga(2)-N(3)	95.7(5)	C(40)-C(35)-N(3)	116.2(19)
N(4)-Ga(2)-Cl(2)	102.3(4)	C(37)-C(36)-C(35)	120(2)
N(3)-Ga(2)-Cl(2)	104.8(4)	C(37)-C(36)-C(41)	118(2)
N(4)-Ga(2)-Bi(4)	119.2(4)	C(35)-C(36)-C(41)	122(2)
N(3)-Ga(2)-Bi(4)	116.7(4)	C(38)-C(37)-C(36)	117(2)
Cl(2)-Ga(2)-Bi(4)	115.28(12)	C(37)-C(38)-C(39)	123(2)
C(1)-N(1)-C(6)	122.2(10)	C(40)-C(39)-C(38)	121(2)
C(1)-N(1)-Ga(1)	118.6(8)	C(39)-C(40)-C(35)	116(2)
C(6)-N(1)-Ga(1)	119.2(8)	C(39)-C(40)-C(44)	117(2)
C(3)-N(2)-C(18)	120.6(10)	C(35)-C(40)-C(44)	126(2)
C(3)-N(2)-Ga(1)	119.4(8)	C(42)-C(41)-C(43)	113(2)
C(18)-N(2)-Ga(1)	119.9(7)	C(42)-C(41)-C(36)	114(2)
C(30)-N(3)-C(35')	119(4)	C(43)-C(41)-C(36)	108(2)

C(30)-N(3)-C(35)	123(2)	C(45)-C(44)-C(46)	110(3)
C(30)-N(3)-Ga(2)	120.0(10)	C(45)-C(44)-C(40)	113(3)
C(35')-N(3)-Ga(2)	120(4)	C(46)-C(44)-C(40)	112(2)
C(35)-N(3)-Ga(2)	117(2)	C(36')-C(35')-C(40')	128(3)
C(32)-N(4)-C(47)	121.2(13)	C(36')-C(35')-N(3)	113(3)
C(32)-N(4)-Ga(2)	121.1(10)	C(40')-C(35')-N(3)	117(3)
C(47)-N(4)-Ga(2)	117.6(10)	C(37')-C(36')-C(35')	111(3)
N(1)-C(1)-C(2)	125.4(11)	C(37')-C(36')-C(41')	122(3)
N(1)-C(1)-C(4)	119.1(12)	C(35')-C(36')-C(41')	126(3)
C(2)-C(1)-C(4)	115.5(12)	C(36')-C(37')-C(38')	123(4)
C(1)-C(2)-C(3)	127.5(12)	C(39')-C(38')-C(37')	124(4)
N(2)-C(3)-C(2)	124.1(12)	C(38')-C(39')-C(40')	115(4)
N(2)-C(3)-C(5)	119.9(12)	C(39')-C(40')-C(35')	118(3)
C(2)-C(3)-C(5)	116.0(11)	C(39')-C(40')-C(44')	120(4)
C(11)-C(6)-C(7)	121.0(12)	C(35')-C(40')-C(44')	121(4)
C(11)-C(6)-N(1)	118.4(11)	C(42')-C(41')-C(43')	108(4)
C(7)-C(6)-N(1)	120.5(11)	C(42')-C(41')-C(36')	113(4)
C(8)-C(7)-C(6)	117.2(13)	C(43')-C(41')-C(36')	107(4)
C(8)-C(7)-C(12)	119.7(13)	C(45')-C(44')-C(46')	109(5)
C(6)-C(7)-C(12)	123.1(12)	C(45')-C(44')-C(40')	114(4)
C(9)-C(8)-C(7)	122.4(15)	C(46')-C(44')-C(40')	110(4)
C(8)-C(9)-C(10)	121.9(15)	C(48)-C(47)-C(52)	121.5(15)
C(9)-C(10)-C(11)	119.0(15)	C(48)-C(47)-N(4)	122.4(15)
C(10)-C(11)-C(6)	118.0(13)	C(52)-C(47)-N(4)	116.1(14)
C(10)-C(11)-C(15)	119.7(13)	C(47)-C(48)-C(49)	119.8(16)
C(6)-C(11)-C(15)	122.2(12)	C(47)-C(48)-C(53)	123.7(14)
C(14)-C(12)-C(7)	113.5(13)	C(49)-C(48)-C(53)	116.4(15)
C(14)-C(12)-C(13)	109.0(11)	C(48)-C(49)-C(50)	120.0(17)
C(7)-C(12)-C(13)	111.2(12)	C(51)-C(50)-C(49)	118.9(17)
C(17)-C(15)-C(16)	110.1(13)	C(50)-C(51)-C(52)	123.4(18)
C(17)-C(15)-C(11)	112.0(15)	C(51)-C(52)-C(47)	116.4(16)
C(16)-C(15)-C(11)	110.9(13)	C(51)-C(52)-C(56)	119.7(15)
C(23)-C(18)-C(19)	119.4(11)	C(47)-C(52)-C(56)	123.9(15)
C(23)-C(18)-N(2)	119.4(11)	C(54)-C(53)-C(55)	109.1(15)
C(19)-C(18)-N(2)	121.1(10)	C(54)-C(53)-C(48)	112.2(14)
C(20)-C(19)-C(18)	118.1(11)	C(55)-C(53)-C(48)	113.7(15)
C(20)-C(19)-C(24)	118.1(11)	C(57)-C(56)-C(52)	115.9(15)
C(18)-C(19)-C(24)	123.7(11)	C(57)-C(56)-C(58)	110.7(18)
C(21)-C(20)-C(19)	122.1(13)	C(52)-C(56)-C(58)	110.3(16)
C(20)-C(21)-C(22)	118.8(13)	C11#1-C11-C21	97(3)
C(23)-C(22)-C(21)	120.8(12)	C31-C21-C11	105(3)

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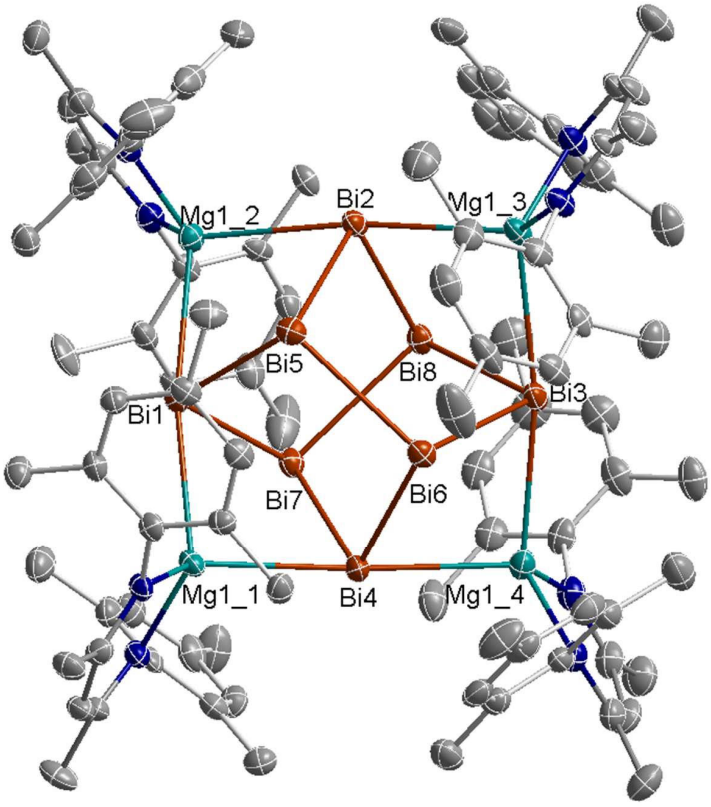

Fig. S18. Solid state structure of **4**. Hydrogen atoms and alternate positions of the disordered parts have been omitted for clarity. Displacement ellipsoids drawn at 50% probability levels.

Table S8: Bond lengths [Å] for **4** (jk_383am).

Bi(1)-Mg12	2.918(2)	C201-C231	1.508(7)	C33-C53	1.519(8)
Bi(1)-Mg11	2.929(2)	Mg12-N22	2.033(5)	C63-C113	1.392(8)
Bi(1)-Bi(5)	3.0009(10)	Mg12-N12	2.039(5)	C63-C73	1.413(8)
Bi(1)-Bi(7)	3.0010(8)	N12-C12	1.333(7)	C73-C83	1.376(9)
Bi(2)-Mg13	2.913(2)	N12-C62	1.441(7)	C73-C123	1.522(9)
Bi(2)-Mg12	2.916(2)	N22-C32	1.328(7)	C83-C93	1.389(10)
Bi(2)-Bi(5)	2.9711(6)	N22-C152	1.458(11)	C93-C103	1.389(9)
Bi(2)-Bi(8)	2.9917(10)	N22-C15'2	1.477(14)	C93-C133	1.523(9)
Bi(3)-Mg13	2.944(2)	C12-C22	1.417(8)	C103-C113	1.389(8)
Bi(3)-Mg14	2.944(2)	C12-C42	1.521(8)	C113-C143	1.509(8)
Bi(3)-Bi(8)	2.9875(10)	C22-C32	1.400(8)	C153-C203	1.402(9)
Bi(3)-Bi(6)	3.0003(6)	C32-C52	1.523(8)	C153-C163	1.426(8)
Bi(4)-Mg14	2.9045(19)	C62-C72	1.414(8)	C163-C173	1.400(9)
Bi(4)-Mg11	2.9085(18)	C62-C112	1.416(8)	C163-C213	1.513(10)
Bi(4)-Bi(7)	2.9801(8)	C72-C82	1.413(9)	C173-C183	1.387(10)
Bi(4)-Bi(6)	2.9916(8)	C72-C122	1.509(9)	C183-C193	1.392(10)

Bi(5)-Bi(6)	3.0519(10)	C82-C92	1.375(10)	C183-C223	1.525(9)
Bi(5)-Mg12	3.695(2)	C92-C102	1.401(9)	C193-C203	1.399(8)
Bi(6)-Mg14	3.684(2)	C92-C132	1.515(9)	C203-C233	1.513(9)
Bi(7)-Bi(8)	3.0421(6)	C102-C112	1.400(8)	Mg14-N24	2.036(5)
Bi(7)-Mg11	3.6816(19)	C112-C142	1.503(8)	Mg14-N14	2.037(5)
Mg11-N21	2.036(5)	C152-C162	1.393(10)	N14-C14	1.339(7)
Mg11-N11	2.037(5)	C152-C202	1.399(10)	N14-C64	1.444(7)
N11-C11	1.332(7)	C162-C172	1.407(11)	N24-C34	1.327(8)
N11-C61	1.440(7)	C162-C212	1.506(11)	N24-C154	1.431(7)
N21-C31	1.332(7)	C172-C182	1.392(11)	C14-C24	1.416(9)
N21-C151	1.437(7)	C182-C192	1.394(11)	C14-C44	1.519(8)
C11-C21	1.411(8)	C182-C222	1.515(12)	C24-C34	1.404(9)
C11-C41	1.509(8)	C192-C202	1.394(11)	C34-C54	1.527(9)
C21-C31	1.414(8)	C202-C232	1.513(12)	C64-C74	1.408(8)
C31-C51	1.522(8)	C15'2-C16'2	1.404(12)	C64-C114	1.416(8)
C61-C111	1.411(8)	C15'2-C20'2	1.415(12)	C74-C84	1.407(8)
C61-C71	1.417(8)	C16'2-C17'2	1.399(13)	C74-C124	1.511(8)
C71-C81	1.399(8)	C16'2-C21'2	1.504(14)	C84-C94	1.399(9)
C71-C121	1.517(8)	C17'2-C18'2	1.400(13)	C94-C104	1.387(9)
C81-C91	1.395(8)	C18'2-C19'2	1.397(12)	C94-C134	1.527(9)
C91-C101	1.386(8)	C18'2-C22'2	1.513(14)	C104-C114	1.395(9)
C91-C131	1.511(9)	C19'2-C20'2	1.406(13)	C114-C144	1.517(9)
C101-C111	1.392(8)	C20'2-C23'2	1.512(14)	C154-C204	1.406(8)
C111-C141	1.509(8)	Mg13-N23	2.026(5)	C154-C164	1.420(8)
C151-C161	1.408(7)	Mg13-N13	2.037(5)	C164-C174	1.403(9)
C151-C201	1.422(7)	N13-C13	1.324(7)	C164-C214	1.513(9)
C161-C171	1.399(8)	N13-C63	1.455(7)	C174-C184	1.385(9)
C161-C211	1.516(7)	N23-C33	1.345(7)	C184-C194	1.386(9)
C171-C181	1.399(8)	N23-C153	1.450(7)	C184-C224	1.506(9)
C181-C191	1.386(7)	C13-C23	1.405(8)	C194-C204	1.382(9)
C181-C221	1.513(8)	C13-C43	1.527(8)	C204-C234	1.508(8)
C191-C201	1.392(8)	C23-C33	1.406(8)		

Table S9: Bond angles [°] for **4** (jk_383am).

Mg12-Bi(1)-Mg11	169.72(5)	C112-C102-C92	122.0(6)
Mg12-Bi(1)-Bi(5)	77.25(4)	C102-C112-C62	119.2(5)
Mg11-Bi(1)-Bi(5)	98.33(4)	C102-C112-C142	120.5(6)
Mg12-Bi(1)-Bi(7)	94.59(4)	C62-C112-C142	120.3(5)
Mg11-Bi(1)-Bi(7)	76.74(4)	C162-C152-C202	122.9(10)
Bi(5)-Bi(1)-Bi(7)	98.444(14)	C162-C152-N22	117.0(11)
Mg13-Bi(2)-Mg12	172.55(5)	C202-C152-N22	119.8(11)

Mg13-Bi(2)-Bi(5)	96.91(4)	C152-C162-C172	119.3(11)
Mg12-Bi(2)-Bi(5)	77.75(4)	C152-C162-C212	121.0(13)
Mg13-Bi(2)-Bi(8)	78.57(4)	C172-C162-C212	119.5(12)
Mg12-Bi(2)-Bi(8)	97.14(4)	C182-C172-C162	119.1(12)
Bi(5)-Bi(2)-Bi(8)	100.373(14)	C172-C182-C192	119.7(10)
Mg13-Bi(3)-Mg14	169.06(5)	C172-C182-C222	117.3(12)
Mg13-Bi(3)-Bi(8)	78.16(4)	C192-C182-C222	122.9(11)
Mg14-Bi(3)-Bi(8)	98.31(4)	C202-C192-C182	123.0(11)
Mg13-Bi(3)-Bi(6)	93.58(4)	C192-C202-C152	115.9(11)
Mg14-Bi(3)-Bi(6)	76.58(4)	C192-C202-C232	122.0(12)
Bi(8)-Bi(3)-Bi(6)	98.393(11)	C152-C202-C232	122.0(13)
Mg14-Bi(4)-Mg11	176.93(5)	C16'2-C15'2-C20'2	119.1(14)
Mg14-Bi(4)-Bi(7)	100.81(4)	C16'2-C15'2-N22	122.9(16)
Mg11-Bi(4)-Bi(7)	77.39(4)	C20'2-C15'2-N22	118.0(16)
Mg14-Bi(4)-Bi(6)	77.32(4)	C17'2-C16'2-C15'2	118.6(16)
Mg11-Bi(4)-Bi(6)	100.50(4)	C17'2-C16'2-C21'2	118.6(18)
Bi(7)-Bi(4)-Bi(6)	100.78(3)	C15'2-C16'2-C21'2	122.6(18)
Bi(2)-Bi(5)-Bi(1)	91.470(15)	C16'2-C17'2-C18'2	123.9(18)
Bi(2)-Bi(5)-Bi(6)	100.022(12)	C19'2-C18'2-C17'2	116.3(15)
Bi(1)-Bi(5)-Bi(6)	103.08(2)	C19'2-C18'2-C22'2	121.9(16)
Bi(2)-Bi(5)-Mg12	50.46(3)	C17'2-C18'2-C22'2	121.6(16)
Bi(1)-Bi(5)-Mg12	50.37(4)	C18'2-C19'2-C20'2	122.0(15)
Bi(6)-Bi(5)-Mg12	130.73(3)	C19'2-C20'2-C15'2	120.0(14)
Bi(4)-Bi(6)-Bi(3)	90.039(13)	C19'2-C20'2-C23'2	119.4(16)
Bi(4)-Bi(6)-Bi(5)	99.70(3)	C15'2-C20'2-C23'2	120.6(17)
Bi(3)-Bi(6)-Bi(5)	103.590(12)	N23-Mg13-N13	93.5(2)
Bi(4)-Bi(6)-Mg14	50.28(3)	N23-Mg13-Bi(2)	106.02(15)
Bi(3)-Bi(6)-Mg14	51.02(3)	N13-Mg13-Bi(2)	125.86(16)
Bi(5)-Bi(6)-Mg14	132.76(4)	N23-Mg13-Bi(3)	124.49(17)
Bi(4)-Bi(7)-Bi(1)	90.161(19)	N13-Mg13-Bi(3)	115.83(15)
Bi(4)-Bi(7)-Bi(8)	99.70(2)	Bi(2)-Mg13-Bi(3)	93.73(5)
Bi(1)-Bi(7)-Bi(8)	103.618(18)	C13-N13-C63	118.5(5)
Bi(4)-Bi(7)-Mg11	50.44(3)	C13-N13-Mg13	124.8(4)
Bi(1)-Bi(7)-Mg11	50.75(3)	C63-N13-Mg13	116.7(3)
Bi(8)-Bi(7)-Mg11	132.54(3)	C33-N23-C153	119.2(5)
Bi(3)-Bi(8)-Bi(2)	91.27(2)	C33-N23-Mg13	123.9(4)
Bi(3)-Bi(8)-Bi(7)	103.430(18)	C153-N23-Mg13	116.7(4)
Bi(2)-Bi(8)-Bi(7)	100.158(14)	N13-C13-C23	123.8(5)
N21-Mg11-N11	93.5(2)	N13-C13-C43	119.8(5)
N21-Mg11-Bi(4)	128.03(15)	C23-C13-C43	116.5(5)
N11-Mg11-Bi(4)	108.11(14)	C13-C23-C33	129.9(5)
N21-Mg11-Bi(1)	112.73(15)	N23-C33-C23	124.2(5)

N11-Mg11-Bi(1)	124.66(15)	N23-C33-C53	119.0(5)
Bi(4)-Mg11-Bi(1)	93.02(5)	C23-C33-C53	116.8(5)
N21-Mg11-Bi(7)	162.54(15)	C113-C63-C73	120.8(5)
N11-Mg11-Bi(7)	102.84(15)	C113-C63-N13	119.9(5)
Bi(4)-Mg11-Bi(7)	52.18(3)	C73-C63-N13	119.1(5)
Bi(1)-Mg11-Bi(7)	52.51(3)	C83-C73-C63	118.2(6)
C11-N11-C61	121.4(5)	C83-C73-C123	120.9(6)
C11-N11-Mg11	123.4(4)	C63-C73-C123	120.9(6)
C61-N11-Mg11	115.0(3)	C73-C83-C93	122.6(6)
C31-N21-C151	121.9(5)	C83-C93-C103	117.7(5)
C31-N21-Mg11	124.8(4)	C83-C93-C133	120.9(7)
C151-N21-Mg11	113.3(3)	C103-C93-C133	121.4(7)
N11-C11-C21	124.5(5)	C93-C103-C113	122.3(6)
N11-C11-C41	119.5(5)	C103-C113-C63	118.4(5)
C21-C11-C41	116.0(5)	C103-C113-C143	120.4(5)
C11-C21-C31	130.2(5)	C63-C113-C143	121.1(5)
N21-C31-C21	122.7(5)	C203-C153-C163	120.2(6)
N21-C31-C51	120.0(5)	C203-C153-N23	120.2(5)
C21-C31-C51	117.2(5)	C163-C153-N23	119.2(6)
C111-C61-C71	119.3(5)	C173-C163-C153	117.5(7)
C111-C61-N11	119.6(5)	C173-C163-C213	120.7(6)
C71-C61-N11	120.8(5)	C153-C163-C213	121.8(6)
C81-C71-C61	119.3(5)	C183-C173-C163	123.3(6)
C81-C71-C121	119.0(5)	C173-C183-C193	117.8(6)
C61-C71-C121	121.7(5)	C173-C183-C223	121.4(7)
C91-C81-C71	122.1(5)	C193-C183-C223	120.8(7)
C101-C91-C81	117.2(6)	C183-C193-C203	121.9(7)
C101-C91-C131	121.1(6)	C193-C203-C153	119.3(6)
C81-C91-C131	121.7(6)	C193-C203-C233	120.7(6)
C91-C101-C111	123.5(6)	C153-C203-C233	120.0(5)
C101-C111-C61	118.6(5)	N24-Mg14-N14	93.1(2)
C101-C111-C141	121.1(5)	N24-Mg14-Bi(4)	126.85(16)
C61-C111-C141	120.3(5)	N14-Mg14-Bi(4)	107.29(15)
C161-C151-C201	120.0(5)	N24-Mg14-Bi(3)	111.93(16)
C161-C151-N21	119.6(5)	N14-Mg14-Bi(3)	128.50(16)
C201-C151-N21	119.9(5)	Bi(4)-Mg14-Bi(3)	92.88(6)
C171-C161-C151	119.0(5)	N24-Mg14-Bi(6)	161.12(16)
C171-C161-C211	120.6(5)	N14-Mg14-Bi(6)	105.13(15)
C151-C161-C211	120.4(5)	Bi(4)-Mg14-Bi(6)	52.40(3)
C161-C171-C181	121.9(5)	Bi(3)-Mg14-Bi(6)	52.40(4)
C191-C181-C171	117.6(5)	C14-N14-C64	120.6(5)
C191-C181-C221	121.2(5)	C14-N14-Mg14	123.6(4)

C171-C181-C221	121.1(5)	C64-N14-Mg14	115.5(3)
C181-C191-C201	123.2(5)	C34-N24-C154	120.5(5)
C191-C201-C151	118.1(5)	C34-N24-Mg14	124.9(4)
C191-C201-C231	121.9(5)	C154-N24-Mg14	114.6(4)
C151-C201-C231	119.9(5)	N14-C14-C24	124.0(6)
N22-Mg12-N12	94.1(2)	N14-C14-C44	119.2(6)
N22-Mg12-Bi(2)	124.37(15)	C24-C14-C44	116.8(5)
N12-Mg12-Bi(2)	109.35(15)	C34-C24-C14	129.9(6)
N22-Mg12-Bi(1)	114.72(15)	N24-C34-C24	123.3(5)
N12-Mg12-Bi(1)	122.40(16)	N24-C34-C54	119.6(6)
Bi(2)-Mg12-Bi(1)	94.28(5)	C24-C34-C54	117.1(6)
N22-Mg12-Bi(5)	161.18(16)	C74-C64-C114	118.9(5)
N12-Mg12-Bi(5)	104.49(15)	C74-C64-N14	121.3(5)
Bi(2)-Mg12-Bi(5)	51.79(3)	C114-C64-N14	119.5(5)
Bi(1)-Mg12-Bi(5)	52.38(3)	C84-C74-C64	119.0(6)
C12-N12-C62	118.0(5)	C84-C74-C124	119.3(5)
C12-N12-Mg12	123.1(4)	C64-C74-C124	121.6(5)
C62-N12-Mg12	118.8(4)	C94-C84-C74	122.2(6)
C32-N22-C152	118.5(16)	C104-C94-C84	117.9(6)
C32-N22-C15'2	121(2)	C104-C94-C134	121.1(6)
C32-N22-Mg12	124.3(4)	C84-C94-C134	121.0(6)
C152-N22-Mg12	117.2(16)	C94-C104-C114	121.8(6)
C15'2-N22-Mg12	114(2)	C104-C114-C64	120.1(6)
N12-C12-C22	124.4(5)	C104-C114-C144	120.4(6)
N12-C12-C42	119.0(5)	C64-C114-C144	119.5(6)
C22-C12-C42	116.5(5)	C204-C154-C164	119.4(6)
C32-C22-C12	130.2(5)	C204-C154-N24	120.5(5)
N22-C32-C22	123.8(5)	C164-C154-N24	119.6(5)
N22-C32-C52	119.3(5)	C174-C164-C154	118.1(6)
C22-C32-C52	116.9(5)	C174-C164-C214	121.2(6)
C72-C62-C112	119.6(5)	C154-C164-C214	120.7(6)
C72-C62-N12	121.2(5)	C184-C174-C164	122.8(6)
C112-C62-N12	119.0(5)	C174-C184-C194	117.3(6)
C82-C72-C62	118.4(6)	C174-C184-C224	120.7(6)
C82-C72-C122	120.7(6)	C194-C184-C224	121.8(7)
C62-C72-C122	120.9(6)	C204-C194-C184	122.9(6)
C92-C82-C72	122.9(6)	C194-C204-C154	119.3(6)
C82-C92-C102	117.9(6)	C194-C204-C234	120.9(6)
C82-C92-C132	121.1(7)	C154-C204-C234	119.8(6)
C102-C92-C132	121.0(7)		

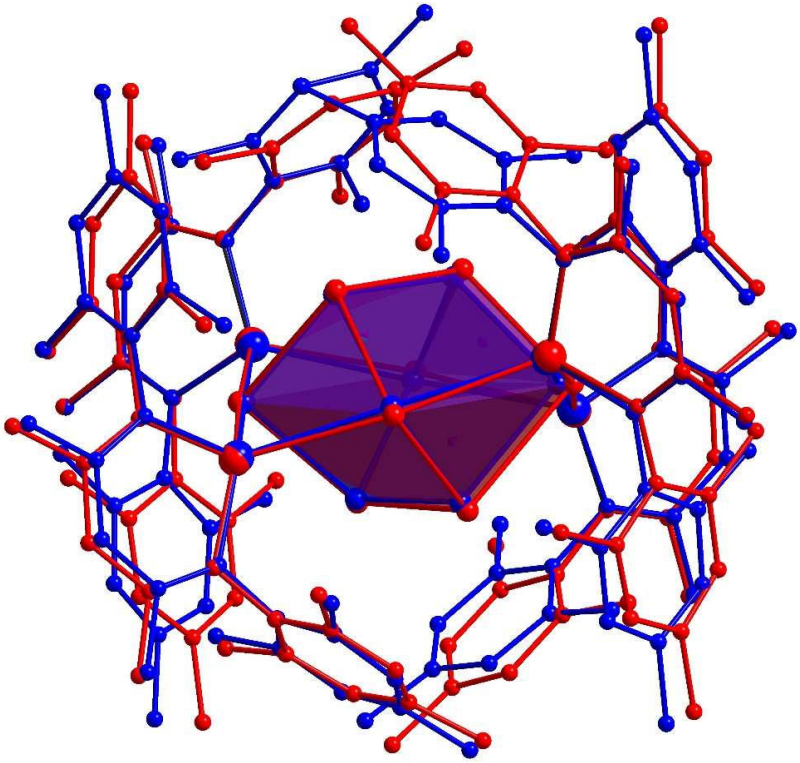

Figure S19. Overlay of the structure of $[(L^{1,2}Mg)_4(\mu_4,\eta^{2:2:2:2}\text{-}Bi_8)]$ **4** (red) and $[(L^{1,2}Mg)_4(\mu_4,\eta^{2:2:2:2}\text{-}Sb_8)]$ (blue).

Table S10. Comparison of selected bond lengths [Å] and angles [°] data of **2** with those of other dibismuthenes R_2Bi_2.

RBi=BiR				
R =	**Ga-Bi**	**Bi-Bi**	**R-Bi-Bi**	**Ref.**
L^1(Cl)Ga (**2**)	2.6793(5)	2.8031(5)	93.03(2)	***this work***
$L^1(Et_2N)Ga$	2.706	2.8132(5)	95.37	[8]
$L^1(C_6F_5O)Ga$	2.693(6)	2.8182(4)	95.52	[9]
$L^1(F_3CO_2SO)Ga$	2.655	2.8111(2)	90.56	[9]
2,6-Mes_2-C_6H_3	-	2.833	92.49	[10]
2,6-$Dipp_2$-C_6H_3	-	2.856	105.44	[11]
{(2,6-*i*-Pr_2-C_6H_3)NCH}$_2$B	-	2.796	92.19	[12]
{(2,6-[$CH(SiMe_3)_2$]$_2$-4-$Si(SiMe_3)_3$}$_2$-C_6H_3	-	2.870	104.13	[13]
2,4,6-[$CH(SiMe_3)_2$]$_3$-C_6H_2	-	2.821	100.56	[14]
{2,6-[$CH(SiMe_3)_2$]$_2$-4-*t*-Bu}$_2$-C_6H_3	-	2.854	98.84	[15]
Fc*	-	2.831	96.16	[16]
{2,6-[$CHPh_2$]$_2$-4-Me}$_2$($SiPh_3$)N	-	2.818	92.23, 98.81	[12]
2,4-*t*-Bu_2-6-CH_2NEt_2-C_6H_2	-	2.873	95.52	[17]
[Ph_2(*t*-Bu)]$_2$P	-	2.820	89.37	[18]

Fc* = 2,5-Dtp_2-1-ferrocenyl, Dtp = 3,5-di-*tert*-butylphenyl

Table S11. Comparison of selected bond lengths [Å] and angles [°] data of **1** with those of comparable stibanyl and bismuthanyl radicals of the desired type.

[L^1(X)Ga]E-X				
E =	**X =**	**Ga-E**	**Ga-E-X**	**Ref.**
Bi	L^1(Cl)Ga (**1**)	2.6485(3), 2.6619(4)	105.46(2)	***this work***
Bi	L^1(I)Ga	2.6640(9), 2.6663(9)	106.68(3)	[19]
Sb	L^1(Cl)Ga	2.5899(4), 2.5909(3)	104.89(1)	[19]
Sb	[N(Dip)CH]$_2$B	2.5959(7)	113.40(14)	[20]
Sb	2,6-$Mes_2C_6H_3$	2.635(3)	114.80(4)	[20]
Sb	N($SiMe_3$)Dip	2.6258(3)	111.45(5)	[20]
As	L^1(Cl)Ga	2.3983(11), 2.4085(14)	109.43(6)	[21]

C) Computational methods

All quantum chemical calculation were employed with the ORCA quantum chemistry package (version 4.12).[22] Ground-state geometry optimizations of **1**, **3** and **4** were calculated with a PBE0 density functional, Def2-SVP (**3'**, **4'**) and Def2-TZVP (**1'**) basis set[23] and atom-pairwise dispersion correction with Becke-Johnson damping Scheme (D3BJ).[24] The RIJCOSX approximation was employed to accelerate the calculations in conjunction with the appropriate auxiliary basis sets.[25] Additionally, effective core potentials (ECP) were utilized for Bi atoms to accelerate geometry optimizations.[26] Frequency calculations were carried out for all optimized structures. Natural bond orbital analysis was performed using the NBO version 6.0.[27]

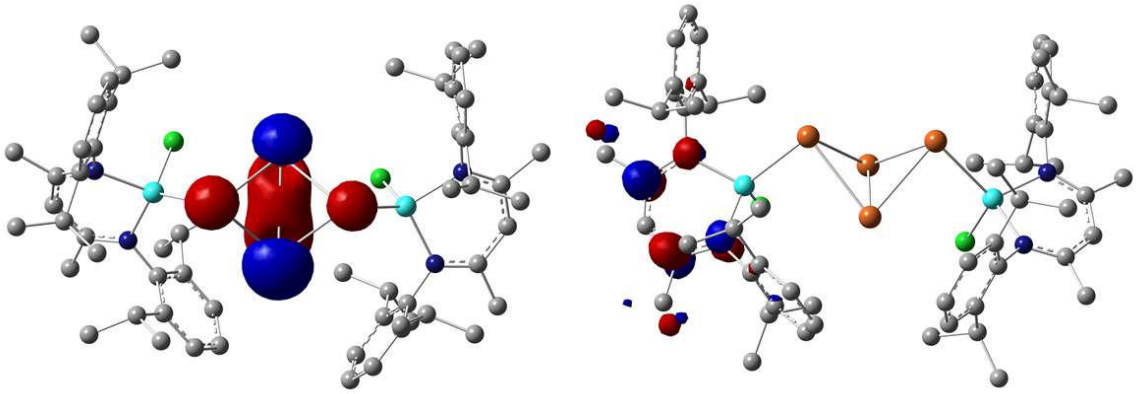

Figure S20. Calculated HOMO (left) and LUMO (right) of **3'**.

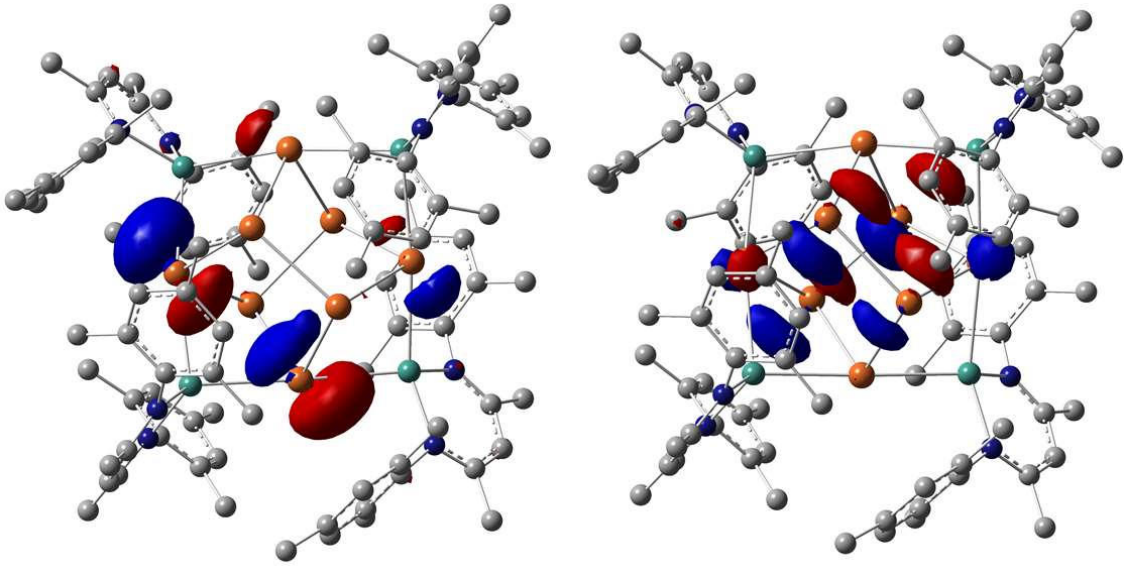

Figure S21. Calculated HOMO (left) and LUMO (right) of **4'**.

Table S12. NPA atomic charges (q, *e*), occupation numbers (ON, $|e|$) of the bonds according to NBO, Wiberg bond index (WBI), bond polarization (P) and bond orbital character (OC) for the optimized geometry of **3'**.

X-Y	q(X)	q (Y)	ON	WBI	P (X;Y)	OC (X;Y)
Bi1-Bi2	−0.18	0.18;	1.94	0.91	54%; 46%	4% s 96% p; 3% s 97% p
Bi2-Bi4	0.18	−0.21	1.94	0.91	46%; 54%	3% s 97% p; 4% s 96% p
Bi2-Bi3	0.18	0.09	1.96	0.97	50%; 50%	3% s 96% p; 3% s 97% p
Bi1-Bi3	−0.18	0.09	1.94	0.94	51%; 49%	3% s 97% p; 3% s 97% p
Bi3-Bi4	0.09	−0.21	1.93	0.92	54%; 46%	3% s 96% p; 3% s 97% p
Ga1-Bi1	1.12	−0.18	1.92	0.97	42%; 58%	40% s, 60% p; 10% s 90% p
Ga2-Bi4	1.11	−0.21	1.92	0.98	42%; 58%	40% s, 60% p; 10% s 90% p

Table S13. NPA atomic charges (q,*e*), occupation numbers (ON, $|e|$) of the bonds according to NBO, Wiberg bond index (WBI), bond polarization (P) and bond orbital character (OC) for the optimized geometry of **4'**.

X-Y	q(X)	q (Y)	ON	WBI	P (X;Y)	OC (X;Y)
Bi(1)-Mg12	−0.83	1.67	–	0.15	–	–
Bi(1)-Mg11	−0.83	1.66	–	0.16	–	–
Bi(1)-Bi(5)	−0.83	0.05	1.96	0.98	51%; 49%	5% s 95% p; 5% s 95% p
Bi(1)-Bi(7)	−0.83	0.09	1.96	0.96	53%; 47%	5% s 95% p: 5% s 95% p
Bi(2)-Mg13	−0.82	1.65	–	0.16	–	–
Bi(2)-Mg12	−0.82	1.67	–	0.16	–	–
Bi(2)-Bi(5)	−0.82	0.05	1.96	0.98	51%; 49%	4% s 95%p; 5% s 95%p
Bi(2)-Bi(8)	−0.82	0.04	1.96	0.97	52%; 48%	5% s 95% p; 5% s 95% p
Bi(3)-Mg13	−0.83	1.65	–	0.17	–	–
Bi(3)-Mg14	−0.83	1.67	–	0.16	–	–
Bi(3)-Bi(8)	−0.83	0.04	1.97	0.98	51%; 49%	5% s 95%p; 5% s 95% p
Bi(3)-Bi(6)	−0.83	0.05	1.96	0.96	53%; 47%	5% s 94% p; 5% s 95% p
Bi(4)-Mg14	−0.86	1.66	–	0.15	–	–
Bi(4)-Mg11	−0.86	1.66	–	0.17	–	–
Bi(4)-Bi(7)	−0.86	0.09	1.96	0.96	53%; 47%	5% s 95% p; 5% s 95% p
Bi(4)-Bi(6)	−0.86	0.05	1.96	0.98	53%; 47%	6% s 94% p; 5% s 95% p
Bi(5)-Bi(6)	0.05	0.05	1.95	0.89	49%; 51%	4% s 96% p; 5% s 95% p
Bi(7)-Bi(8)	0.09	0.04	1.95	0.91	49%; 51%	5% s 95% p; 5% s 95% p

Table S14. Cartesian coordinates (x,y,z) for the optimized geometry of **1'**.

Bi	2,91296	20,16517	3,44633	C	3,09856	23,47814	6,18321
Ga	1,58583	21,84893	1,81867	H	3,40151	22,429	6,21638
Ga	3,31595	18,08329	1,78259	H	2,77677	23,77738	7,18424
Cl	0,15896	21,17772	0,25395	H	3,97841	24,0765	5,9365
Cl	3,98277	18,57511	-0,28015	C	5,00934	15,78915	2,09951
N	2,55465	23,35594	0,95906	C	4,01682	15,02102	1,50096
N	0,42509	23,00212	2,92279	H	4,30351	14,02168	1,20599
N	4,80071	17,0227	2,54792	C	2,64627	15,30592	1,41451
N	2,11898	16,51338	1,55395	C	6,36579	15,175	2,26639
C	1,91354	24,50437	0,80783	H	6,36184	14,12667	1,9732
C	0,66317	24,80015	1,37117	H	6,72655	15,26704	3,29145
H	0,23072	25,739	1,05349	H	7,07592	15,71141	1,63238
C	8,30E-04	24,14616	2,40668	C	1,74438	14,13001	1,17419
C	2,51485	25,6133	-0,00714	H	1,36222	14,12957	0,15212
H	1,97507	25,69424	-0,95413	H	0,87097	14,17141	1,82353
H	3,56661	25,4481	-0,22779	H	2,28328	13,20169	1,35218
H	2,3964	26,56032	0,52011	C	5,64859	17,57294	3,55418
C	-1,24066	24,78824	2,94931	C	6,75816	18,35825	3,2203
H	-1,27476	25,84858	2,7044	C	7,48534	18,94905	4,25003
H	-1,32687	24,65344	4,02786	H	8,33868	19,57039	4,00293
H	-2,10794	24,30537	2,49024	C	7,14321	18,75537	5,57354
C	3,83663	23,16417	0,34802	H	7,71824	19,2302	6,36017
C	3,92212	22,85727	-1,0188	C	6,06789	17,94399	5,89241
C	5,18565	22,69481	-1,57899	H	5,80875	17,78592	6,93211
H	5,26387	22,44358	-2,63055	C	5,30339	17,3429	4,90113
C	6,33289	22,85163	-0,82891	C	7,197	18,5701	1,79136
H	7,30626	22,72809	-1,28995	H	6,5651	17,95344	1,14783
C	6,233	23,15435	0,51684	C	8,65207	18,15639	1,5867
H	7,13512	23,27226	1,10321	H	8,92837	18,2661	0,53488
C	4,99588	23,30121	1,13094	H	8,83122	17,12208	1,88957
C	2,71158	22,71194	-1,91233	H	9,32812	18,7875	2,16856
H	1,82243	22,94475	-1,32545	C	7,00125	20,01598	1,36224
C	2,77049	23,67361	-3,10044	H	7,27352	20,1453	0,31256
H	3,57569	23,40331	-3,78811	H	7,62537	20,68672	1,95873
H	2,94453	24,70453	-2,78521	H	5,96213	20,32901	1,47164
H	1,83516	23,63768	-3,66376	C	4,13976	16,44997	5,27537
C	2,56543	21,2738	-2,39859	H	3,42693	16,50283	4,44991
H	1,63438	21,15429	-2,95727	C	4,55949	14,98647	5,41516
H	2,55575	20,57449	-1,56482	H	4,9234	14,57115	4,47579
H	3,39342	20,99576	-3,0574	H	3,70801	14,38148	5,7381
C	4,92012	23,67279	2,59458	H	5,34975	14,88106	6,16351
H	3,99203	23,24802	2,98616	C	3,42317	16,88463	6,54658
C	6,06268	23,11004	3,42881	H	3,16299	17,94501	6,52817
H	6,18356	22,03569	3,28111	H	4,03104	16,69222	7,43418
H	5,86456	23,28422	4,48861	H	2,50256	16,30896	6,66353
H	7,01289	23,59713	3,19472	C	0,69458	16,63033	1,44213

C	4,84809	25,18819	2,7618	C	0,10516	16,72453	0,1713
H	5,7085	25,66228	2,28152	C	-1,28405	16,75154	0,09427
H	4,85769	25,46186	3,82019	H	-1,7548	16,84128	-0,87859
H	3,94334	25,60371	2,31727	C	-2,07135	16,66874	1,22788
C	-0,00521	22,52082	4,19001	H	-3,15216	16,67445	1,14422
C	-1,14129	21,71501	4,32042	C	-1,47231	16,58964	2,47057
C	-1,4259	21,17684	5,57259	H	-2,09022	16,52925	3,35916
H	-2,29554	20,54026	5,68623	C	-0,08899	16,58888	2,60442
C	-0,62231	21,4328	6,66459	C	0,91422	16,8273	-1,10309
H	-0,86504	20,99798	7,6277	H	1,97155	16,7928	-0,83832
C	0,48725	22,25166	6,52671	C	0,64546	15,69006	-2,08446
H	1,10958	22,45943	7,38799	H	-0,40762	15,64653	-2,37602
C	0,81508	22,80731	5,29807	H	0,91978	14,7143	-1,67863
C	-2,0618	21,41657	3,16336	H	1,23277	15,84363	-2,99262
H	-1,72706	22,00529	2,30786	C	0,66738	18,17218	-1,77779
C	-3,50569	21,79959	3,48585	H	1,33618	18,28863	-2,63339
H	-4,13055	21,6913	2,59607	H	0,84475	18,9964	-1,0898
H	-3,58679	22,82862	3,84534	H	-0,36208	18,25623	-2,13796
H	-3,92323	21,1493	4,25819	C	0,519	16,47952	3,98426
C	-1,98367	19,95068	2,75663	H	1,5929	16,64026	3,88121
H	-2,60202	19,76546	1,87604	C	0,31243	15,08154	4,56512
H	-2,33691	19,30215	3,5621	H	-0,75206	14,8365	4,61322
H	-0,96564	19,65504	2,50437	H	0,71886	15,02003	5,57799
C	2,01003	23,72052	5,14914	H	0,80573	14,31689	3,96318
H	2,43638	23,52155	4,16202	C	-0,00867	17,54698	4,93513
C	1,59805	25,19272	5,16851	H	0,16017	18,55076	4,54009
H	0,90354	25,43442	4,36588	H	0,49813	17,47461	5,89958
H	2,47702	25,8302	5,04268	H	-1,08133	17,4384	5,11568
H	1,1213	25,44656	6,1196				

Table S15. Cartesian coordinates (x,y,z) for the optimized geometry of **3'**.

Bi	4,23239	2,36226	3,46455	H	3,27961	-4,43684	6,50446
Bi	3,55602	-0,53021	2,93496	H	3,13866	-4,64723	4,75652
Bi	1,3584	2,2617	4,31621	C	5,79576	-4,92526	5,44093
Bi	3,4659	0,62739	5,73831	H	5,42857	-5,68032	4,7281
Ga	6,189	-0,9965	3,09699	H	5,73714	-5,3568	6,45279
Ga	1,85172	4,31497	5,97185	H	6,85476	-4,74449	5,21144
Cl	7,46055	0,86402	3,03014	C	0,57314	6,84183	6,54762
Cl	3,99503	4,93395	6,18539	C	0,61002	6,51379	7,91115
N	6,88944	-2,14686	1,66187	H	0,2914	7,30385	8,58993
N	7,09992	-1,93548	4,57539	C	0,8744	5,27252	8,52264
N	0,91836	5,99939	5,57555	C	0,11277	8,22622	6,1805
N	1,30791	4,19763	7,87634	H	0,98216	8,83111	5,88016
C	8,03414	-2,80763	1,82195	H	-0,38037	8,7198	7,02631
C	8,68576	-2,9465	3,05651	H	-0,56726	8,21133	5,31789
H	9,63417	-3,48036	3,03047	C	0,64236	5,20957	10,00683
C	8,21196	-2,62323	4,34345	H	0,53982	4,17922	10,36754

C	8,65113	-3,47654	0,62695	H	-0,25034	5,78562	10,28251
H	7,97413	-4,24019	0,22012	H	1,49917	5,66417	10,52738
H	9,60424	-3,95299	0,88486	C	0,6743	6,33689	4,21001
H	8,81406	-2,74711	-0,17965	C	-0,50554	5,84484	3,60515
C	9,04171	-3,10069	5,50114	C	-0,77661	6,21341	2,28534
H	8,42747	-3,30055	6,38858	H	-1,68151	5,84503	1,79877
H	9,76446	-2,31616	5,77381	C	0,09111	7,03926	1,57685
H	9,60859	-4,00053	5,23281	H	-0,15071	7,33701	0,55358
C	6,15313	-2,22997	0,44122	C	1,26953	7,47309	2,16961
C	6,22793	-1,17141	-0,49006	H	1,96459	8,09552	1,6001
C	5,43485	-1,23664	-1,64053	C	1,59325	7,12207	3,4842
H	5,47746	-0,41783	-2,36363	C	-1,46485	4,95715	4,37932
C	4,5941	-2,31698	-1,87629	H	-0,85045	4,3665	5,0801
H	3,98502	-2,35305	-2,78234	C	-2,44705	5,76542	5,22788
C	4,53802	-3,3575	-0,95564	H	-3,07036	6,41573	4,59245
H	3,87902	-4,20775	-1,14887	H	-1,9304	6,39625	5,96323
C	5,30539	-3,3396	0,2129	H	-3,1174	5,0908	5,78479
C	7,14234	0,01826	-0,27924	C	-2,21671	3,96939	3,49527
H	7,63894	-0,10717	0,69136	H	-2,93964	4,4791	2,83827
C	6,35319	1,32387	-0,20491	H	-2,78609	3,26479	4,12185
H	5,86468	1,56162	-1,16437	H	-1,53269	3,38415	2,86139
H	7,02054	2,15816	0,05795	C	2,92307	7,55467	4,06668
H	5,57025	1,26903	0,56593	H	2,94225	7,24402	5,12176
C	8,24203	0,09728	-1,33716	C	3,1354	9,06653	4,00985
H	7,82971	0,30144	-2,33899	H	4,03865	9,34435	4,5744
H	8,82194	-0,83667	-1,39586	H	2,28907	9,62408	4,4376
H	8,94322	0,91039	-1,0921	H	3,27298	9,42159	2,97606
C	5,19687	-4,50299	1,18529	C	4,07681	6,82797	3,37282
H	5,91671	-4,3267	1,9989	H	3,93587	5,73873	3,40171
C	5,5427	-5,84183	0,52906	H	5,02696	7,04887	3,88307
H	4,83257	-6,08798	-0,27513	H	4,16604	7,13875	2,31906
H	5,49019	-6,65367	1,27135	C	1,48208	2,93574	8,5231
H	6,55045	-5,84648	0,08645	C	0,46643	1,96513	8,35765
C	3,80666	-4,58627	1,81665	C	0,63918	0,70686	8,93836
H	3,51651	-3,63576	2,28905	H	-0,13738	-0,05099	8,82374
H	3,77636	-5,37266	2,58706	C	1,7919	0,40226	9,65592
H	3,0438	-4,83488	1,06219	H	1,91902	-0,58769	10,10105
C	6,57221	-1,75165	5,88866	C	2,78276	1,3617	9,80443
C	7,05735	-0,73247	6,73571	H	3,68391	1,11524	10,37089
C	6,44402	-0,56647	7,98395	C	2,65763	2,64022	9,24672
H	6,79963	0,22517	8,64697	C	-0,79411	2,29966	7,58587
C	5,37965	-1,36311	8,38136	H	-0,50289	3,02744	6,81092
H	4,90454	-1,19661	9,35063	C	-1,40692	1,09866	6,87717
C	4,90317	-2,3566	7,52934	H	-2,18525	1,43389	6,17473
H	4,05363	-2,96655	7,84026	H	-1,88453	0,4035	7,58599
C	5,48037	-2,56683	6,27471	H	-0,65165	0,53954	6,30438
C	8,17713	0,2121	6,34422	C	-1,82809	2,99068	8,47337
H	8,49914	-0,04621	5,3253	H	-1,42656	3,90001	8,94121

C	7,67892	1,65703	6,30485	H	-2,16314	2,31829	9,27904
H	8,45368	2,31655	5,88628	H	-2,70959	3,28041	7,87951
H	7,43111	2,02404	7,31361	C	3,78099	3,63873	9,45239
H	6,78292	1,75878	5,67727	H	3,51569	4,55791	8,90974
C	9,3806	0,09736	7,2791	C	5,093	3,13197	8,85346
H	9,76645	-0,93065	7,34489	H	5,4492	2,22665	9,37094
H	9,12316	0,41953	8,30129	H	5,87617	3,89962	8,94777
H	10,19906	0,74448	6,92752	H	4,98329	2,90071	7,78527
C	4,96072	-3,64727	5,34464	C	3,96728	3,97933	10,93426
H	5,07912	-3,2605	4,31829	H	4,72948	4,76394	11,05862
C	3,48172	-3,95277	5,53619	H	4,30799	3,10088	11,50617
H	2,87368	-3,03807	5,47	H	3,03784	4,33585	11,40154

Table S16. Cartesian coordinates (x,y,z) for the optimized geometry of **4'**.

Bi	7,22024	9,61371	4,39626	Mg	4,64686	10,59647	3,4345
Bi	7,95033	12,236	3,18803	N	2,76021	10,08018	4,01225
Bi	9,94981	13,17594	5,25273	N	4,24336	10,0963	1,48063
Bi	6,99577	10,39209	7,27958	C	1,85527	9,47109	3,25832
Bi	5,7567	13,12275	7,0968	C	2,03887	9,1867	1,89075
Bi	8,19835	14,86191	6,99066	H	1,2064	8,68597	1,39695
Bi	9,92119	10,97313	7,28309	C	3,12514	9,5238	1,0554
Bi	5,34105	13,36631	4,14986	C	0,5534	9,0493	3,89206
Mg	9,95205	13,45221	8,88311	H	-0,1292	8,59725	3,16235
N	11,73296	14,35437	9,43566	H	0,05194	9,90052	4,37616
N	9,22704	13,31605	10,79858	H	0,7507	8,31864	4,69225
C	11,90379	14,82633	10,67347	C	2,96218	9,24264	-0,41658
C	11,001	14,66858	11,73968	H	2,75457	10,18512	-0,94962
H	11,31136	15,13825	12,67188	H	2,12929	8,55525	-0,60796
C	9,81543	13,91145	11,82742	H	3,87962	8,8303	-0,85845
C	13,18198	15,56029	11,00749	C	2,45421	10,59113	5,29568
H	14,03652	14,86605	11,00102	C	2,90007	9,92545	6,45083
H	13,12373	16,02887	11,99737	C	2,73865	10,55327	7,68982
H	13,41008	16,33092	10,25838	H	3,09145	10,03843	8,58738
C	9,2378	13,74584	13,2089	C	2,14899	11,81299	7,81328
H	8,16292	13,97601	13,23327	C	1,69701	12,44216	6,64978
H	9,75641	14,3805	13,93662	H	1,24262	13,43367	6,71828
H	9,34221	12,69611	13,52666	C	1,83767	11,85635	5,3913
C	12,84783	14,46858	8,56037	C	3,52627	8,56757	6,34591
C	12,98348	15,58308	7,7138	H	2,88999	7,87389	5,77648
C	14,15012	15,71733	6,954	H	3,70529	8,13789	7,34096
H	14,25966	16,60248	6,32	H	4,49554	8,59335	5,81986
C	15,18919	14,7868	7,01754	C	2,04081	12,49476	9,14578
C	15,0091	13,66486	7,83165	H	1,10731	13,06985	9,23424
H	15,80228	12,91219	7,89223	H	2,87466	13,20399	9,28702
C	13,85264	13,48235	8,59349	H	2,08219	11,77088	9,97235
C	11,92887	16,64569	7,6891	C	1,37107	12,55971	4,15105

H	12,18496	17,44247	6,97844	H	0,57295	12,00355	3,63372
H	11,79763	17,10306	8,68296	H	2,19446	12,66325	3,42584
H	10,94596	16,23237	7,409	H	0,99785	13,56517	4,38387
C	16,48185	15,00775	6,28454	C	5,36186	10,29919	0,63679
H	16,3576	15,69563	5,43578	C	6,28444	9,24629	0,46584
H	16,90145	14,06505	5,90069	C	7,48587	9,49943	-0,19558
H	17,23805	15,45021	6,95478	H	8,20401	8,68189	-0,313
C	13,68357	12,27464	9,46403	C	7,79863	10,7636	-0,70403
H	12,76841	11,72258	9,19122	C	6,84832	11,77551	-0,56257
H	13,57669	12,54849	10,52615	H	7,05917	12,76589	-0,97572
H	14,53905	11,5921	9,37017	C	5,62931	11,56856	0,09438
C	8,05847	12,53529	11,00163	C	5,9664	7,88233	0,99458
C	6,78813	13,14354	10,97645	H	5,02578	7,48738	0,57985
C	5,65287	12,33892	11,11544	H	5,84411	7,89621	2,08966
H	4,66844	12,81575	11,10497	H	6,76793	7,17586	0,74874
C	5,73979	10,95619	11,28477	C	9,12141	11,00637	-1,3737
C	7,01195	10,38188	11,32102	H	9,31151	10,27717	-2,17607
H	7,10667	9,30257	11,47353	H	9,94994	10,90804	-0,65393
C	8,17488	11,14402	11,1893	H	9,17985	12,01126	-1,81548
C	6,65046	14,62913	10,82853	C	4,61027	12,66244	0,20674
H	6,96229	14,96439	9,82525	H	4,92512	13,55683	-0,34635
H	7,2844	15,17818	11,54047	H	4,43832	12,9591	1,25572
H	5,60839	14,94264	10,98324	H	3,63453	12,3377	-0,18601
C	4,51088	10,10648	11,42253	Mg	6,70735	15,85144	4,69096
H	3,65041	10,69455	11,77266	N	5,24345	17,27881	4,82566
H	4,67271	9,27997	12,12951	N	7,84322	16,93375	3,36752
H	4,23203	9,65189	10,45701	C	5,4609	18,5327	4,43658
C	9,52345	10,49372	11,2638	C	6,6295	18,98196	3,79522
H	9,98295	10,41932	10,26294	H	6,65848	20,05181	3,58677
H	9,4509	9,47866	11,67764	C	7,67087	18,2376	3,20281
H	10,22446	11,07346	11,88155	C	4,37701	19,56206	4,63235
Mg	9,84053	8,72051	5,34382	H	3,5144	19,33912	3,98639
N	9,57817	6,68024	5,22395	H	4,74232	20,56721	4,38844
N	11,79109	8,57338	4,70636	H	3,99586	19,5486	5,66461
C	10,57303	5,80757	5,06276	C	8,60238	19,02646	2,31365
C	11,91191	6,16321	4,8415	H	9,22422	18,37863	1,68318
H	12,61026	5,33177	4,73959	H	9,27095	19,64172	2,93756
C	12,46642	7,44046	4,60097	H	8,02926	19,71125	1,67314
C	10,2537	4,33345	5,10373	C	3,92651	16,89238	5,17783
H	9,48783	4,06824	4,36271	C	3,54668	16,7314	6,52058
H	9,82636	4,06923	6,08428	C	2,21921	16,39123	6,81067
H	11,1451	3,722	4,91888	H	1,92451	16,2838	7,85963
C	13,91338	7,44887	4,17096	C	1,26203	16,21773	5,81362
H	14,55713	7,12977	5,00512	C	1,68417	16,31206	4,4822
H	14,24193	8,44076	3,83657	H	0,96155	16,14646	3,67698
H	14,06943	6,72835	3,35586	C	2,99997	16,61893	4,14532
C	8,24024	6,24066	5,08011	C	4,52049	16,96081	7,63784
C	7,74731	5,96868	3,78468	H	5,5571	16,78266	7,31643

C	6,40082	5,63954	3,63121	H	4,30327	16,29977	8,4894
H	6,02285	5,41882	2,62877	H	4,47462	18,00054	8,00519
C	5,51644	5,60867	4,71358	C	-0,17589	15,93732	6,1412
C	6,03168	5,87198	5,98382	H	-0,84356	16,64645	5,62823
H	5,36521	5,83233	6,85054	H	-0,36692	16,01948	7,22061
C	7,38054	6,18151	6,19004	H	-0,48151	14,92758	5,81805
C	8,64308	6,10192	2,58852	C	3,44219	16,64027	2,71257
H	8,91503	7,16029	2,42589	H	3,791	17,6325	2,38374
H	8,14386	5,73177	1,68333	H	2,63428	16,31324	2,04388
H	9,59203	5,55894	2,69956	H	4,29399	15,95633	2,57284
C	4,05603	5,33735	4,49635	C	8,76701	16,21281	2,57161
H	3,54925	6,22466	4,08094	C	10,11185	16,06553	2,95329
H	3,54811	5,07559	5,43517	C	10,95764	15,29093	2,14786
H	3,89547	4,51626	3,78161	H	11,99903	15,17427	2,45249
C	7,90456	6,46421	7,56598	C	10,51517	14,67577	0,97846
H	8,78848	5,85149	7,79851	C	9,17056	14,82729	0,62949
H	7,13786	6,27645	8,32994	H	8,79502	14,33974	-0,27438
H	8,2181	7,5183	7,67272	C	8,28924	15,58124	1,40134
C	12,38818	9,83026	4,4526	C	10,65913	16,76579	4,16264
C	12,02955	10,52086	3,27919	H	11,4884	16,19786	4,60866
C	12,53624	11,80662	3,06951	H	9,88589	16,91022	4,93077
H	12,23631	12,34131	2,16633	H	11,04773	17,76402	3,89504
C	13,40248	12,41688	3,98018	C	11,43788	13,89892	0,08576
C	13,73136	11,71325	5,14001	H	11,6272	14,44618	-0,85216
H	14,37522	12,18779	5,88314	H	11,00134	12,92783	-0,19164
C	13,23411	10,43539	5,40327	H	12,41272	13,71273	0,5573
C	11,14206	9,87214	2,25758	C	6,85476	15,72604	0,99563
H	11,59212	8,94796	1,86056	H	6,54811	16,7809	0,92462
H	10,94919	10,55421	1,41903	H	6,18852	15,2548	1,7379
H	10,16037	9,58356	2,67291	H	6,66729	15,24248	0,02831
C	13,92618	13,80589	3,76033	C	13,59656	9,73125	6,67763
H	13,31277	14,54257	4,30415	H	14,32271	8,91983	6,51159
H	13,92251	14,08113	2,69615	H	12,71213	9,27687	7,15042
H	14,95263	13,91408	4,13699	H	14,04389	10,43544	7,38927

D) References

[1] N. J. Hardman, B. E. Eichler, P. P. Power, *Chem. Commun*. **2000**, 1991-1992.

[2] a) S. P. Green, C. Jones, A. Stasch, *Science* **2007**, *318*, 1754-1757; b) S. J. Bonyhady, C. Jones, S. Nembenna, A. Stasch, A. J. Edwards, G. J. McIntyre, *Chem. Eur. J*., **2010**, *16*, 938-955.

[3] R. J. Wiacek, J. N. Jones, C. L. Macdonald, A. H. Cowley, *Can. J. Chem*., **2002**, *80*, 1518-1523.

[4] F. Calderazzo, R. Poli, G. Pelizzi, *Dalton Trans.* **1984**, *11*, 2365-2369.

[5] SHELXS-97; G. M. Sheldrick, *Acta Crystallogr.* **1990**, *A46*, 467-473.

[6] a) SHELXL-2014; Sheldrick, G. M. *Acta Crystallogr*. **2008**, *A64*, 112-122; b) shelXle, C. B. Hübschle, G. M. Sheldrick, B. Dittrich, *J. Appl. Cryst.* **2011**, *44*, 1281-1284.

[7] A. L. Spek, *Acta Cryst.* **1990**, *A46*, 194-201.

[8] L. Tuscher, C. Helling, C. Wölper, W. Frank, A., S. Nizovtsev, S. Schulz, *Chem. Eur. J.* **2018**, *24*, 3241-3250.

[9] G. Prabusankar, C. Gemel, P. Parameswaran, C. Flener, G. Frenking. R. A. Fischer, *Angew. Chem.* **2009**, *121*, 5634-5637; *Angew. Chem. Int. Ed*. **2009**, *48*, 5526-5529.

[10] B. Twamley, C. D. Sofield, M. M. Olmstead, P. P. Power, *J. Am. Chem. Soc*. **1999**, *121*, 3357-3367.

[11] R. Wolf, J. Fischer, R. C. Fischer, J. C. Fettinger, P. P. Power, *Eur. J. Inorg. Chem*. **2008**, 2515-2521.

[12] D. Dange, A. Davey, J. A. B. Abdalla, S. Aldridge, C. Jones, *Chem. Commun*. **2015**, *51*, 7128-7131.

[13] T. Sasamori, Y. Arai, N. Takeda, R. Okazaki, Y. Furukawa, M. Kimura, S. Nagase, N. Tokitoh *Bull. Chem. Soc. Jpn*. **2002**, *75*, 661-675.

[14] N. Tokitoh, Y. Arai, R. Okazaki, S. Nagase, *Science* **1997**, *277*, 78.

[15] P. K. Majhi, H. Ikeda, T. Sasamori, H. Tsurugi, K. Mashima, N. Tokitoh, *Organometallics* **2017**, *36*, 1224-1226.

[16] M. Sakagami, T. Sasamori, H. Sakai, Y. Furukawa, N. Tokitoh, *Chem. Asian J*. **2013**, *8*, 690-693.

[17] I. Vranova, M. Alonso, R. Lo, R. Sedlak, R. Jambor, A. Ruzicka, F. De Proft, P. Hobza, L. Dostal, *Chem. Eur. J*. **2015**, *21*, 16917-16928.

[18] C. von Hänisch, D. Nikolova, *Eur. J. Inorg. Chem*. **2006**, 4770-4773.

[19] C. Ganesamoorthy, C. Helling, C. Wölper, W. Frank, E. Bill, G. E. Cutsail III, S. Schulz, *Nat. Commun.* **2018**, *9*, 87.

[20] C. Helling, G. E. Cutsail III, H. Weinert, C. Wölper, S. Schulz, *Angew. Chem. Int. Ed*., DOI:10.1002/anie.202000586; *Angew. Chem*., DOI:10.1002/ange.202000586

[21] C. Helling, C. Wölper, Y. Schulte, G. E. Cutsail III, S. Schulz, *Inorg. Chem.* **2019**, *58*, 10323-10332

[22] F. Neese, The ORCA program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science* **2012**, *2*, 73.

[23] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

[24] a) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456-1465; b) S. Grimme, J. Antony, S. Ehrlich; H. Krieg, *J. Chem. Phys*. **2010**, *132*, 154104.

[25] S. Kossmann, F. Neese, *Chem. Phys. Lett*. **2009**, *481*, 240-243.

[26] a) M. Dolg, H. Stoll, H. Preuss, *J. Chem. Phys*. **1989**, *90*, 1730-1734; b) D. Andrae, U. Häußermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta* **1990**, *77*, 123-141; c) B. Metz, H. Stoll, M. Dolg, *J. Chem. Phys.* **2000**, *113*, 2563-2569; d) K. A. Peterson, D. Figgen, E. Goll, H. Stoll, M. Dolg, *J. Chem. Phys.* **2003**, *119*, 11113-11123; e) T. Leininger, A. Nicklass, W. Kuechle, H. Stoll, M. Dolg, A. Bergner, *Chem. Phys. Lett.* **1996**, *255*, 274-280; f) M. Kaupp, P. V. Schleyer, H. Stoll and H. Preuss, *J. Chem. Phys.* **1991**, *94*, 1360-1366; g) M. Dolg, H. Stoll, A. Savin, H. Preuss, *Theor. Chim. Acta* **1989**, *75*, 173-194; h) X. Cao, M. Dolg, *J. Chem. Phys*. **2001**, *115*, 7348-7355.

[27] NBO 6.0: E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, F. Weinhold (Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, 2013); http://nbo6.chem.wisc.edu/.