Supporting Information

"Reactivity of Group 13 Metal-Substituted Dipnictenes in Cycloaddition and Single Electron Transfer Reactions"

Hanns Micha Weinert

Universität Duisburg-Essen

Essen 2022

Table of Content

List of Figures

List of Tables

List of Compounds

		Identification code (crystallographic Appendix)
1	$L(^{i}PrO)GaAs(O^{i}Pr)_2$	mw_129_3m
2	$L(EtO)GaAs(OEt)_2$	mw_024_llm
3	$L(MeO)GaAs(OMe)_2$	mw_138m
4	$[L(MeO)GaAs]_2$	mw_141_4m
5	$L(Me_2N)GaSbGaL$	mw_017m
6	$[L(Me_2N)AlSb]_2$	mw_031_1m
	$LAl(NMe_2)_2$	
7	$[L(Et_2N)Al]_2SbH$	mw_096m
8	$[L(Me_2N)GaBi]_2$	mw_060m
9	$[L(TfO)Ga]_2Bi$•	mw_117_10m
	LGa(H)OTf	mw_117_1lm
10	$[L(EtO)GaBi]_2$	mw_085_1m
11	$[\{L(EtO)Ga\}_2\text{-}\mu,\eta^{1:1}\text{-}Bi_4]$	mw_084lfsm
12	$[L(Et_2N)AlBi]_2$	mw_036_1m
	$LAl(NEt_2)_2$	mw_036_5m
13	$L(Et_2N)GaTEMPO$	mw_053m
14	$[L(TfO)GaSb]_2$	mw_073_0m
15	$[L(DMAP)GaSb]_2[OTf]_2$	mw_076_2m
16	$[L(DMAP)GaBi]_2[OTf]_2$	mw_132_2m
17	$[LGaSb]_2[BArF_{24}]_2$	mw_155_3m
18	$[LGaBi]_2[BArF_{24}]_2$	mw_154_3bm and mw_154bm
19	$[L(Me_2N)Ga]SbSb[N(SiMe_3)Ga(NMe_2)L]$	mw_071_7m
20	$[L(Me_2N)Ga]SbSb[N(SiMe_3)Ga(N(H)SiMe_3)L]$	mw_071_7m
21	$[L(Me_2N)GaSb][L(Me_2N)GaN(SiMe_3)Sb]N\text{-}SiMe_3$	mw_071m
22	$[L(Me_2N)GaSb]_2NPh$	mw_124_1m_sq
23	$[L(Me_2N)GaSb]_2N(p\text{-}CF_3Ph)$	mw_125_5m
24	$[L(Me_2N)GaSb]_2N(ada)$	mw_097_3m
25	$[L(Me_2N)Ga]SbSb[N(Ph)Ga(NMe_2)L]$	mw_130_4m_sq
26	$[L(Me_2N)Ga]SbSb[N(p\text{-}CF_3Ph)Ga(NMe_2)L]$	mw_143_4m
27	$[(L(NPh)Ga\text{-}\kappa Ga,\kappa N)_2\text{-}(\mu,\eta^{1:1:1:1}\text{-}Sb_4)]$	mw_130_1m
28	$[L(Me_2N)GaSb][L(Me_2N)GaN(Ph)Sb]NPh$	mw_145_1m
29	$[L(Me_2N)GaN(Ph)Sb]_2$	mw_150_2m
30	$[L(Me_2N)GaSb]_2C(H)SiMe_3$	mw_089_1fsm
31	$[L(EtO)GaSb]_2C(H)SiMe_3$	mw_099_tw5
32	$[L(Cl)GaSb]_2C(H)SiMe_3$	mw_112_3frm
33	$(DME)[K(B\text{-}18\text{-}C\text{-}6)][L(Me_2N)GaSb]_2$	mw_022_4m_sq
34	$(DME)[K(B\text{-}18\text{-}C\text{-}6)][L(Et_2N)GaBi]_2$	mw_022_16m_sq

NMR and ATR-IR spectra:

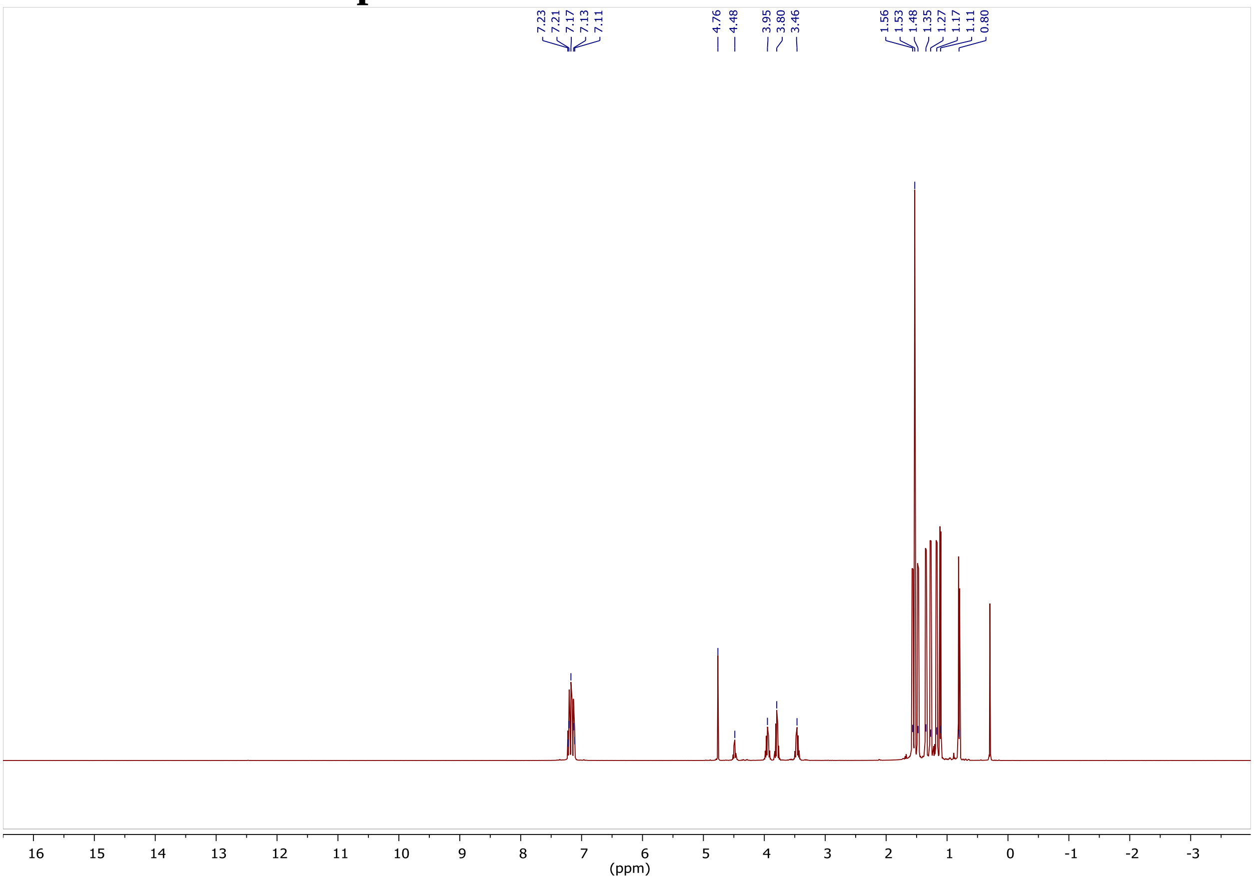

Figure 1: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of L(^{i}PrO)GaAs(O^{i}Pr)$_2$ (**1**).

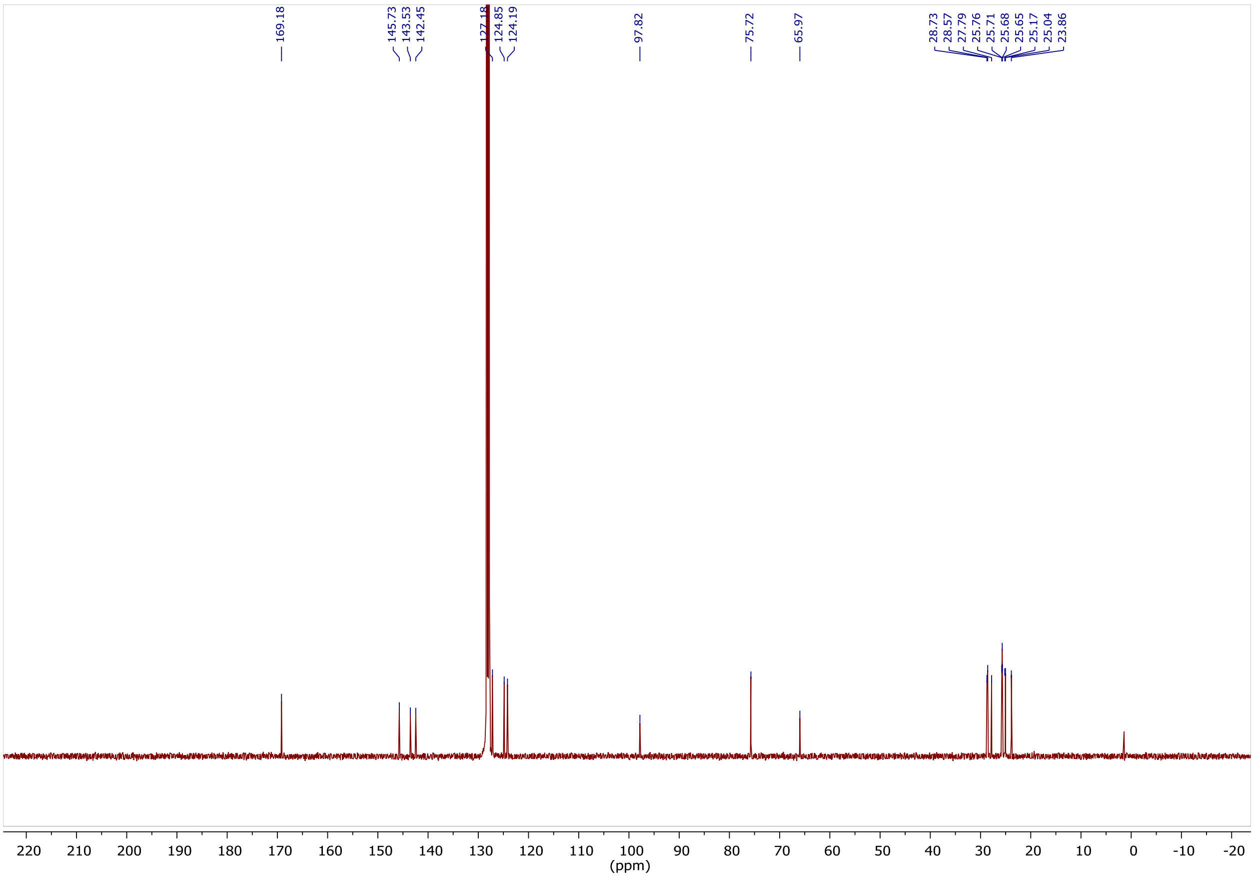

Figure 2: ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) of L(^{i}PrO)GaAs(O^{i}Pr)$_2$ (**1**).

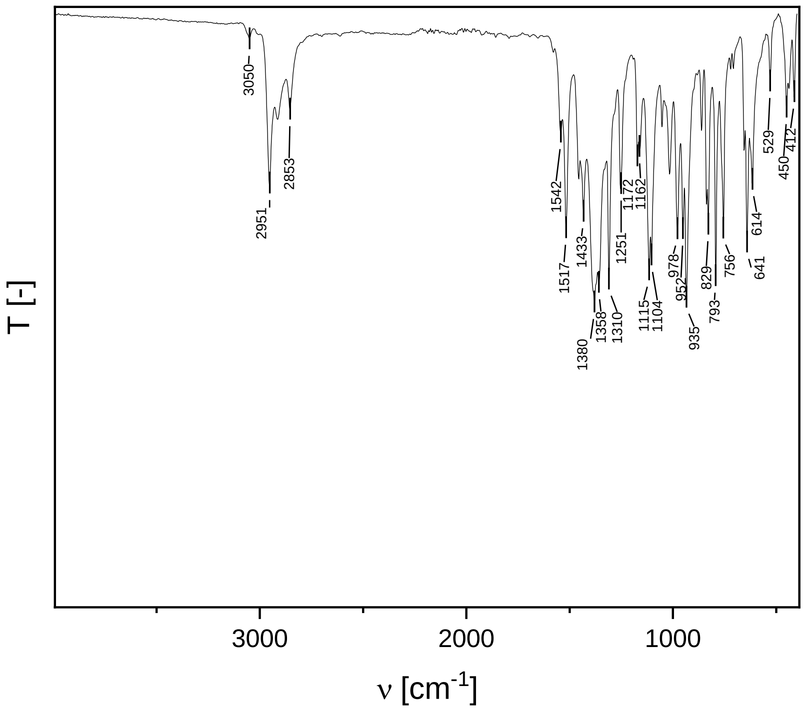

Figure 3: ATR-IR spectrum of L(^{i}PrO)GaAs(O^{i}Pr)$_2$ (**1**).

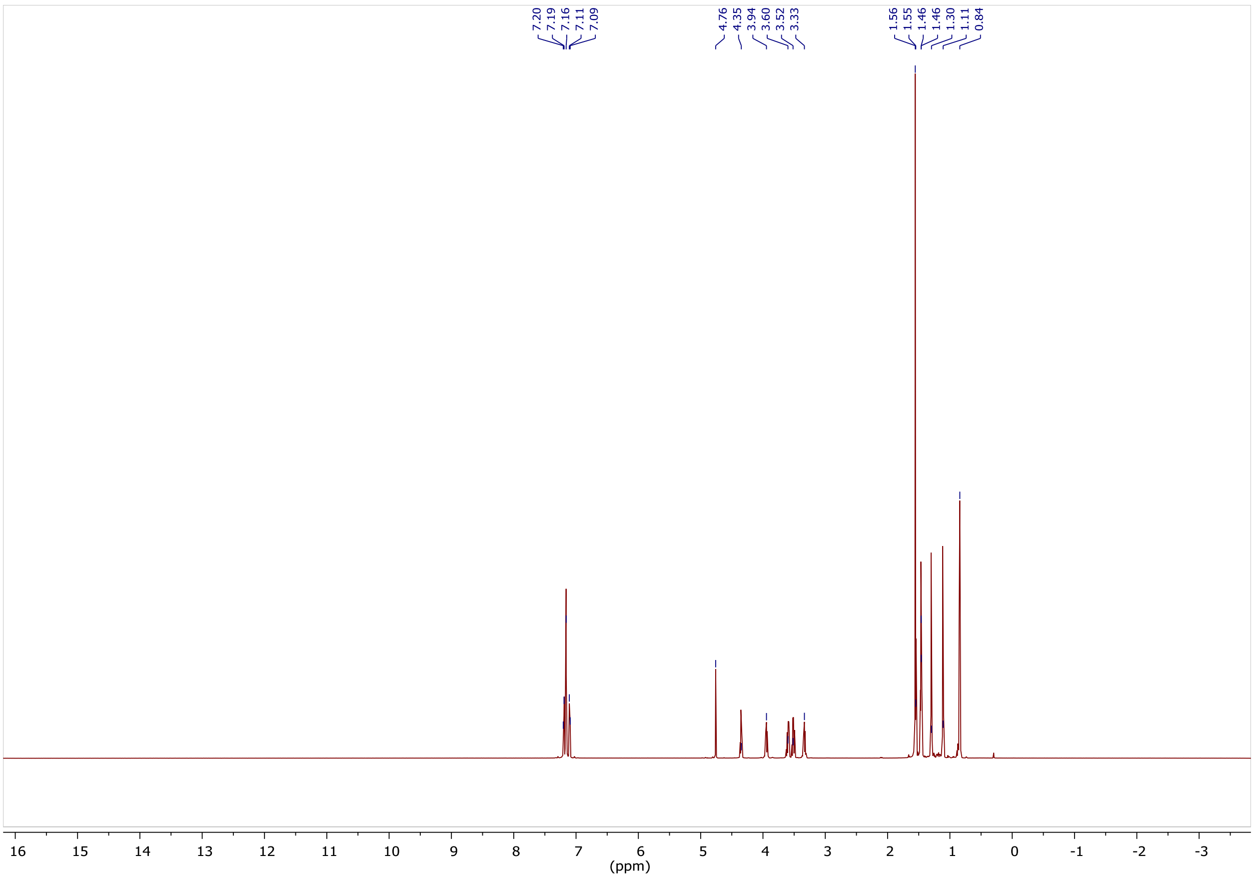

Figure 4: ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of L(EtO)GaAs(OEt)$_2$ (**2**).

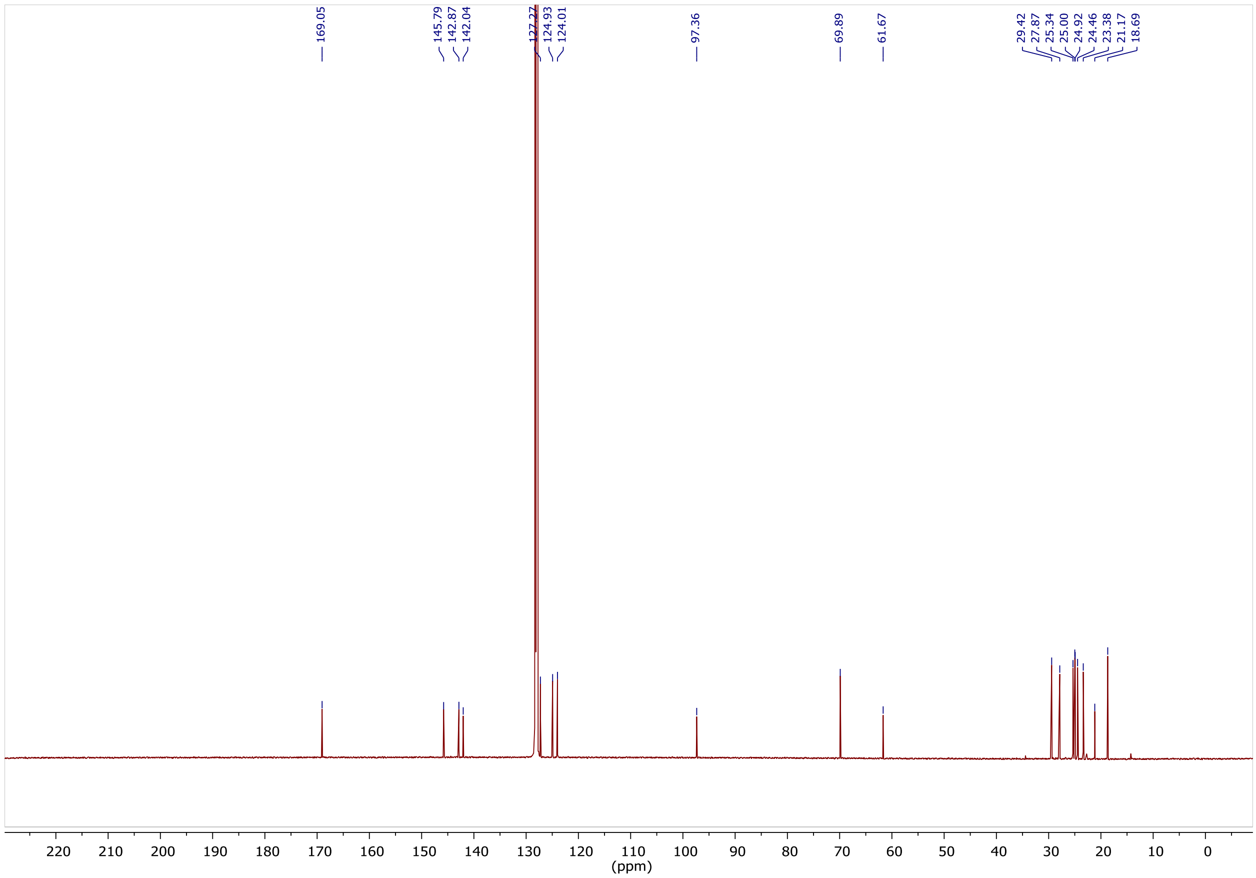

Figure 5: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of L(EtO)GaAs(OEt)$_2$ (**2**).

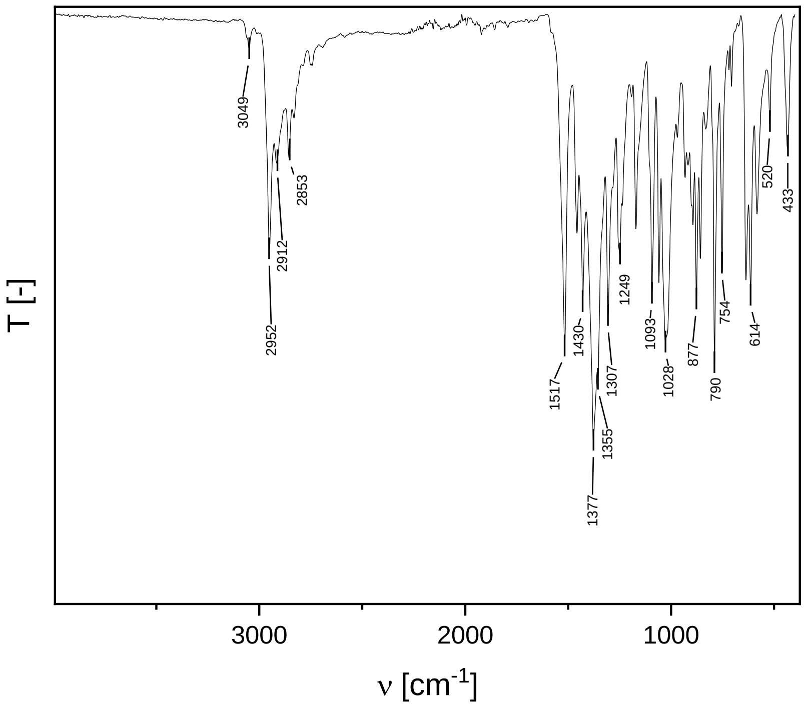

Figure 6: ATR-IR spectrum of L(EtO)GaAs(OEt)$_2$ (**2**).

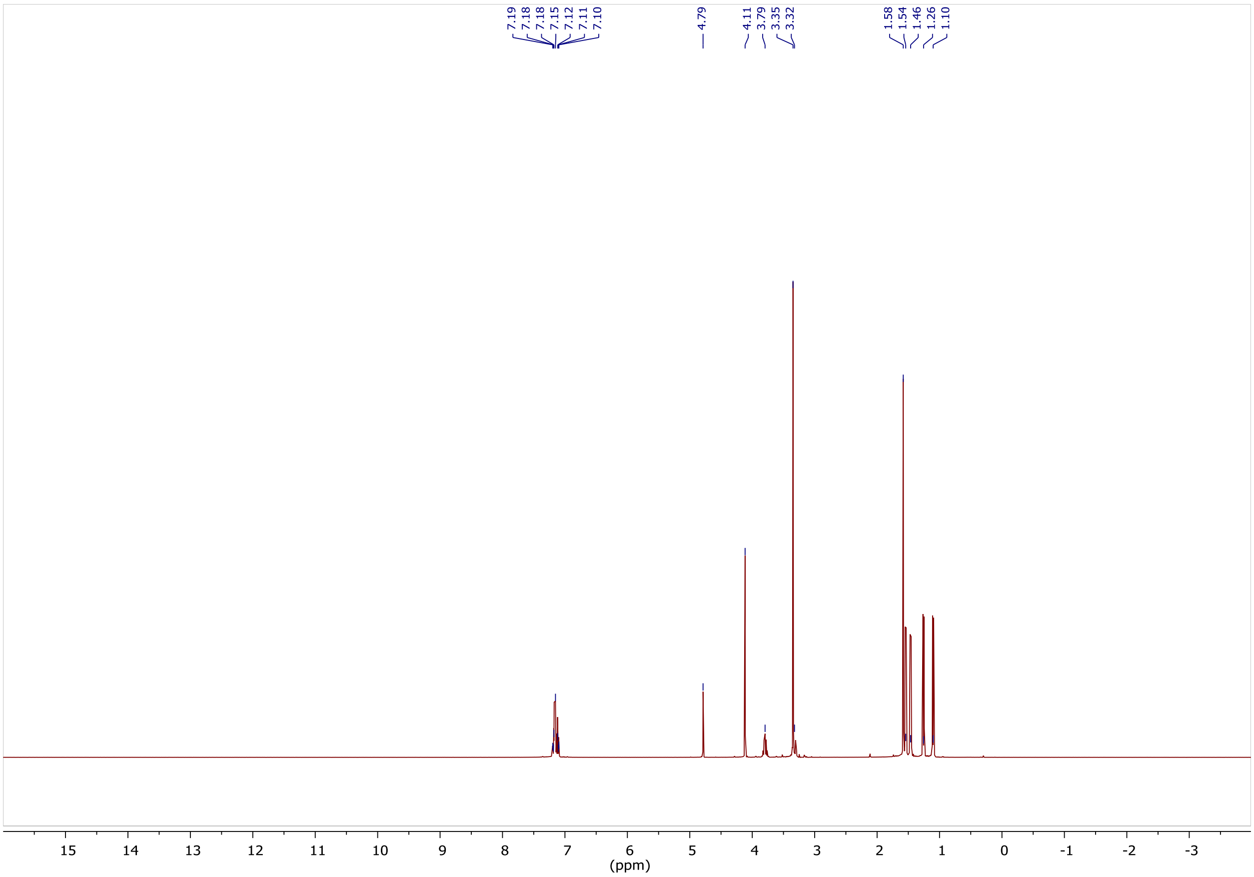

Figure 7: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $L(EtO)GaAs(OEt)_2$ (**3**).

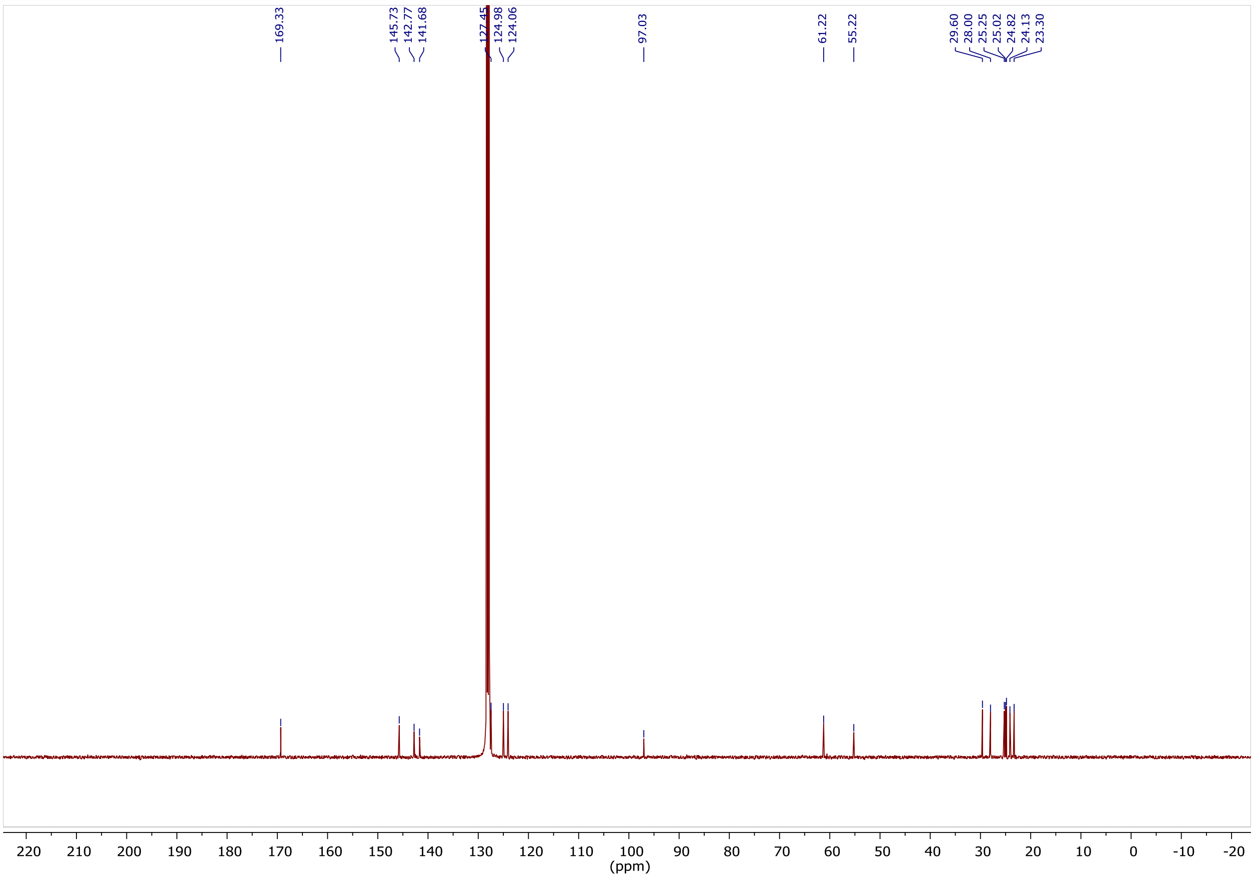

Figure 8: ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) of $L(EtO)GaAs(OEt)_2$ (**3**).

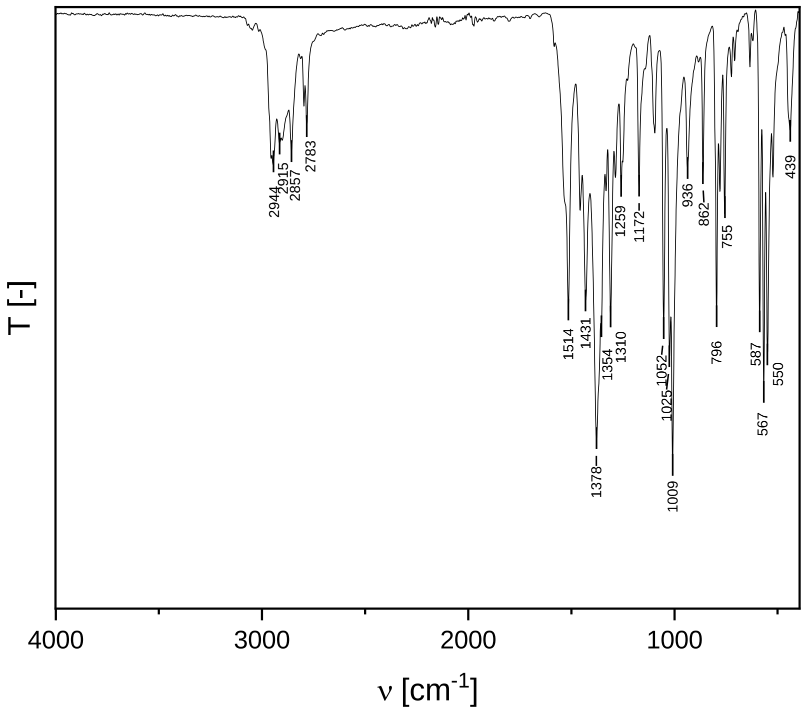

Figure 9: ATR-IR spectrum of L(EtO)GaAs(OEt)$_2$ (**3**).

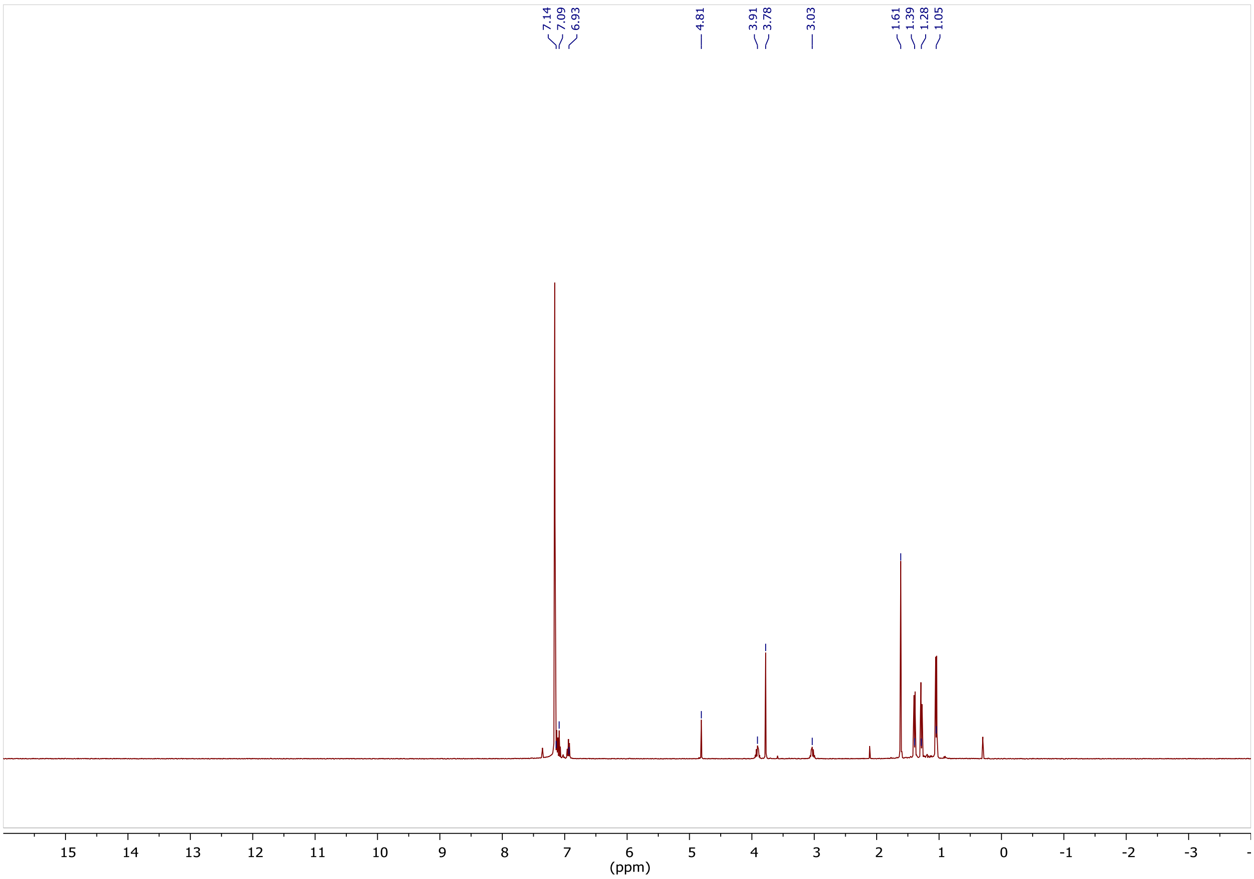

Figure 10: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of [L(MeO)GaAs]$_2$ (**4**).

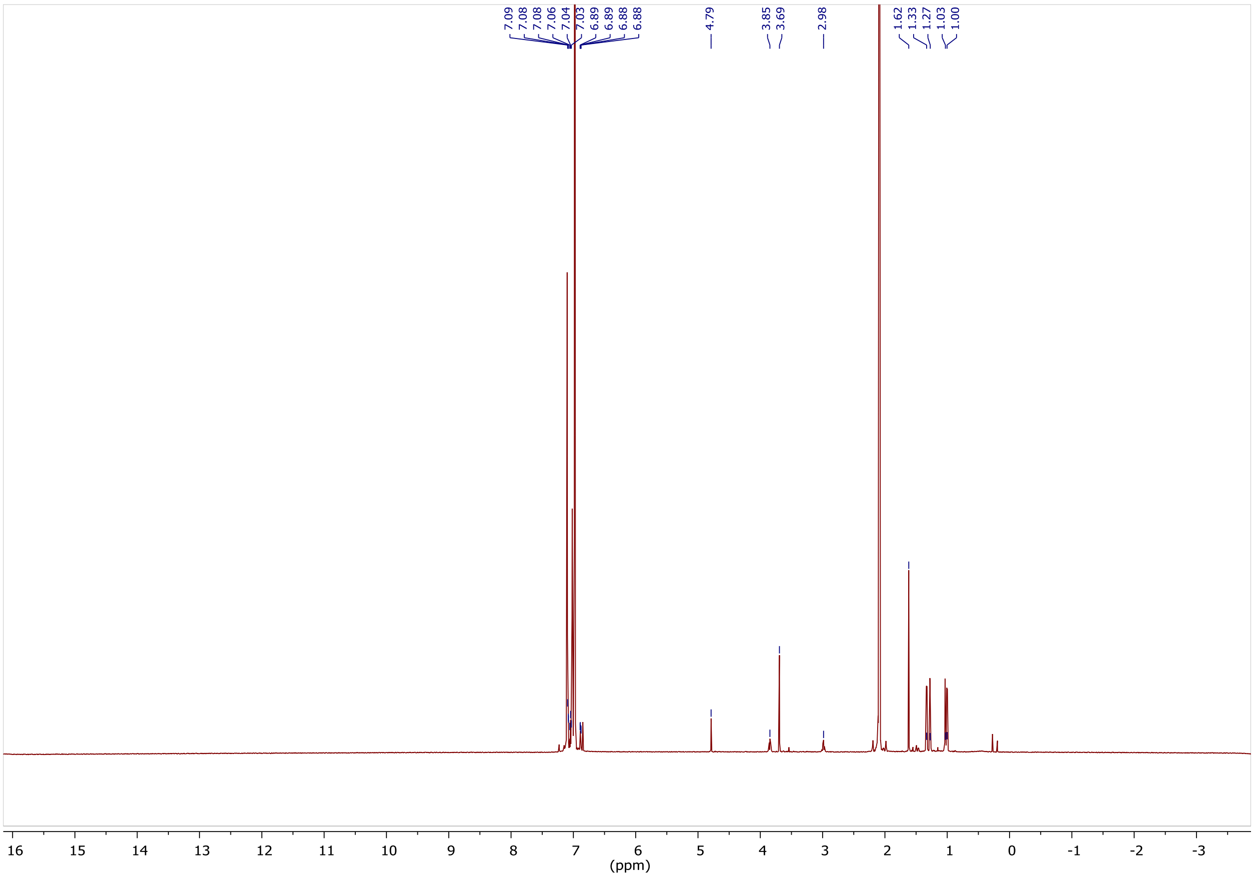

Figure 11: ^{1}H NMR spectrum (600 MHz, C_7D_8, 25 °C) of $[L(MeO)GaAs]_2$ (**4**).

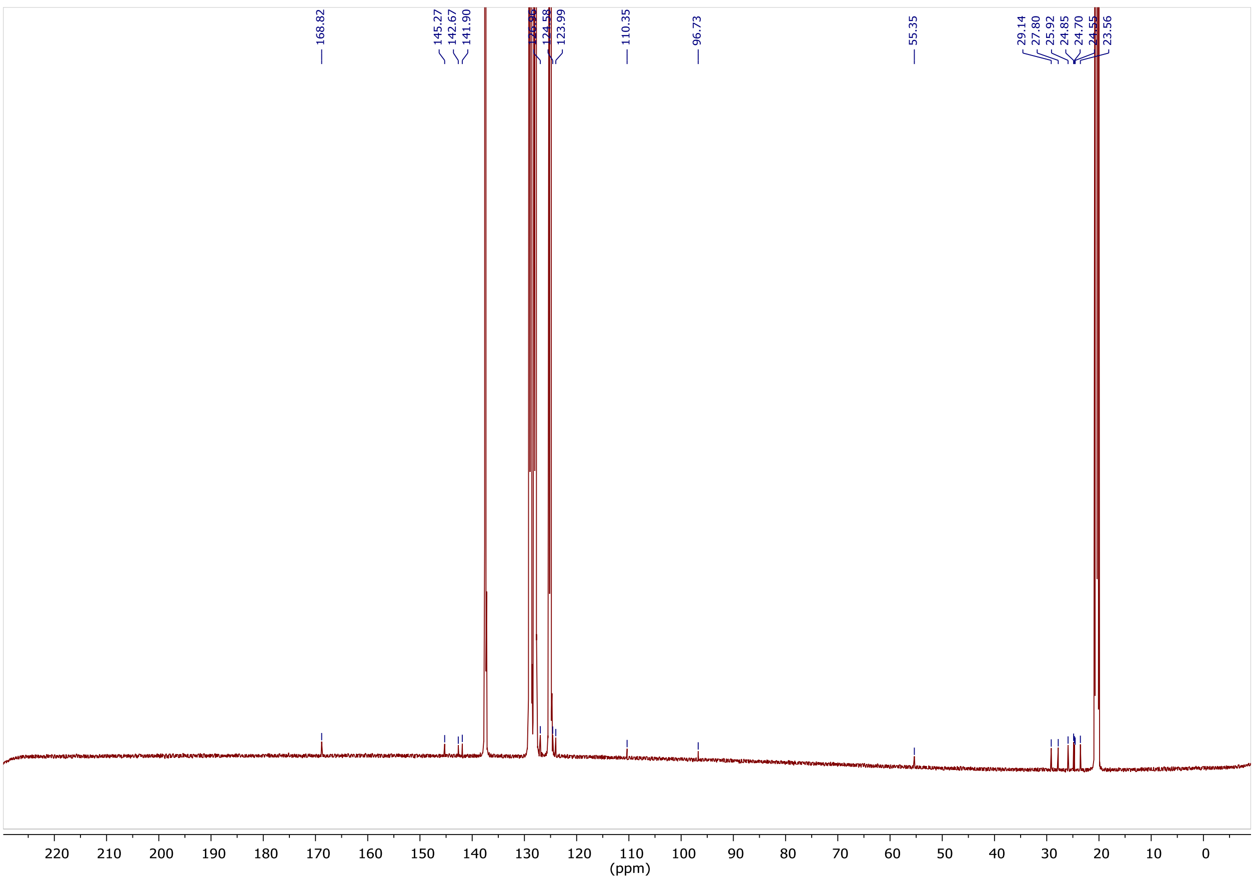

Figure 12: ^{13}C NMR spectrum (150.9 MHz, C_7D_8, 25 °C) of $[L(MeO)GaAs]_2$ (**4**).

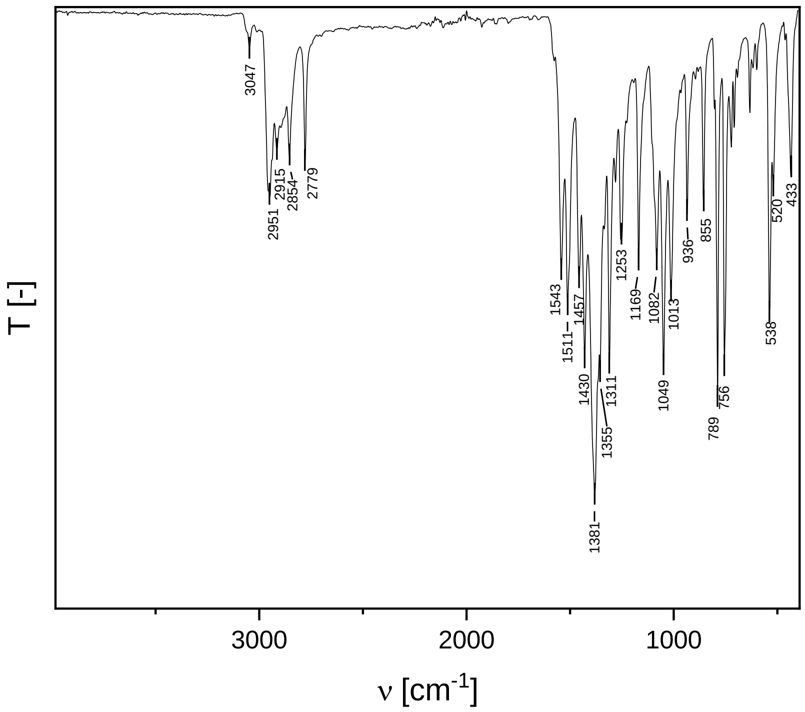

Figure 13: ATR-IR spectrum of $[L(MeO)GaAs]_2$ (**4**).

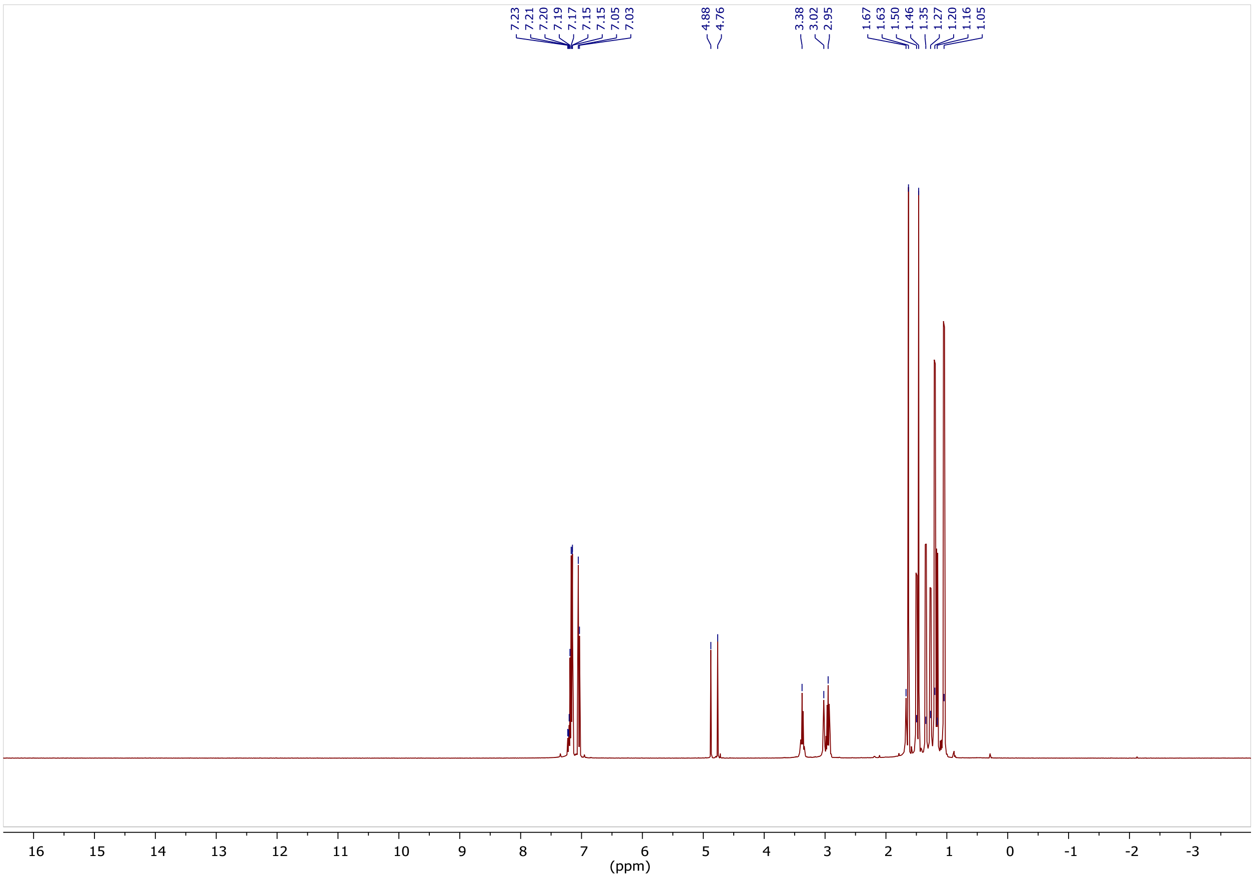

Figure 14: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $L(Me_2N)GaSbGaL$ (**5**).

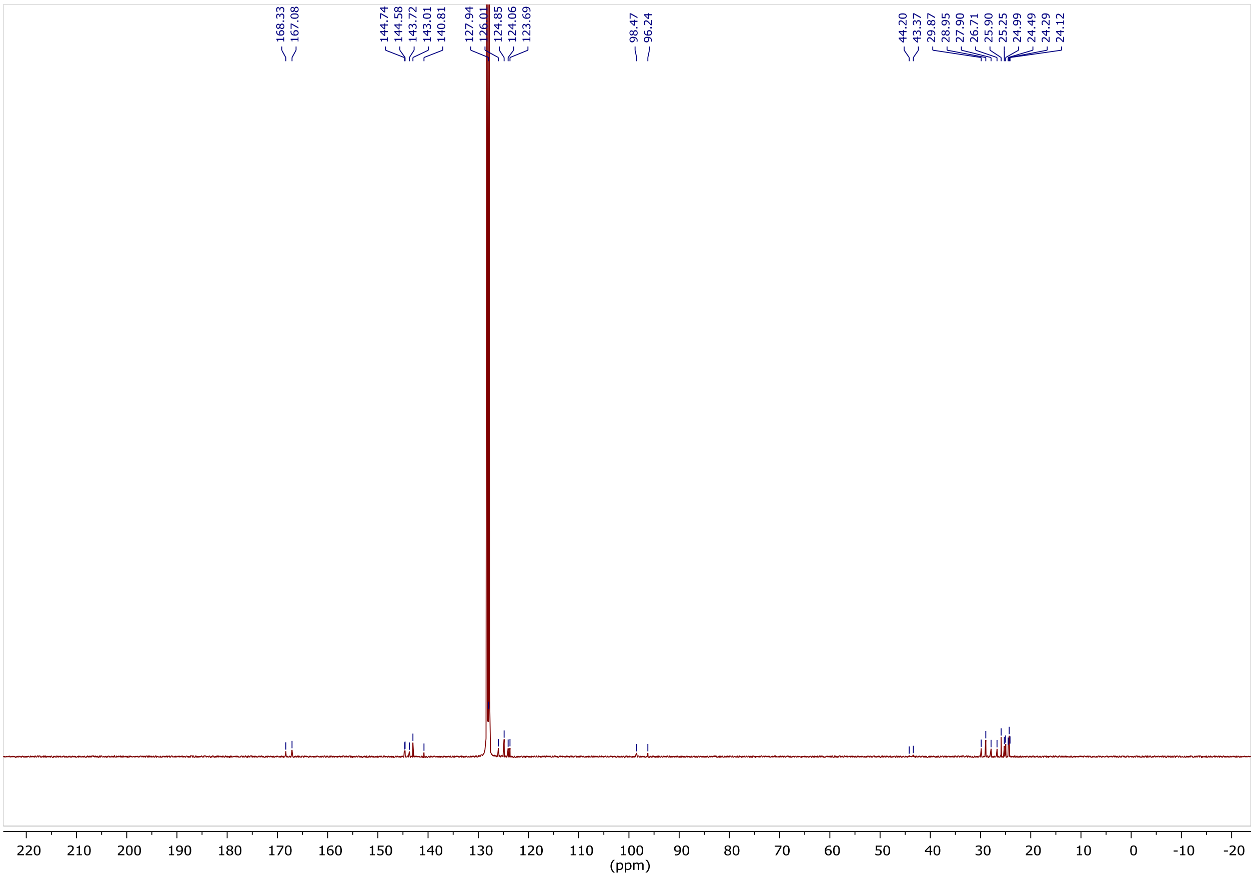

Figure 15: ^{13}C NMR spectrum (100.7 MHz, C_6D_6, 25 °C) of L(Me_2N)GaSbGaL (**5**).

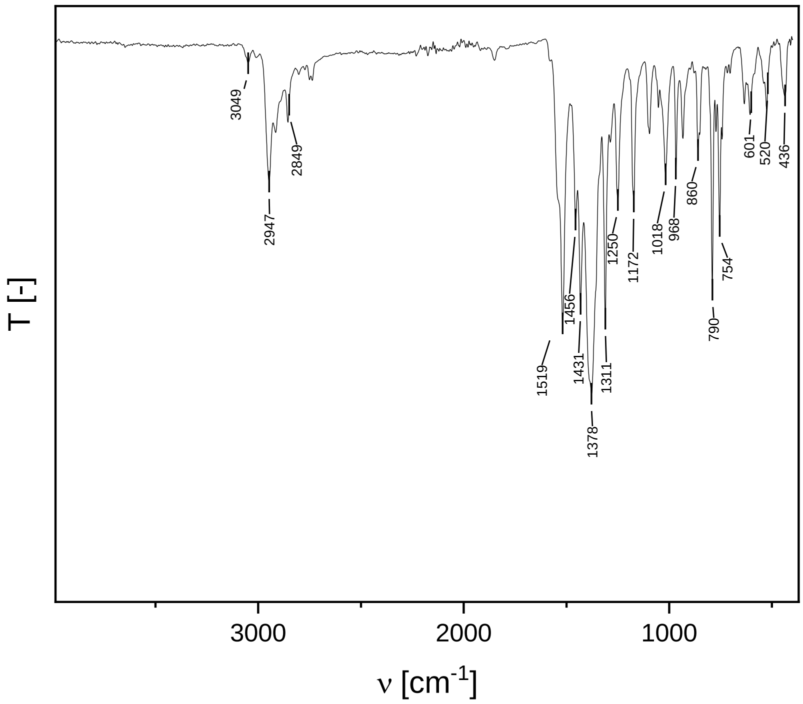

Figure 16: ATR-IR spectrum of L(Me_2N)GaSbGaL (**5**).

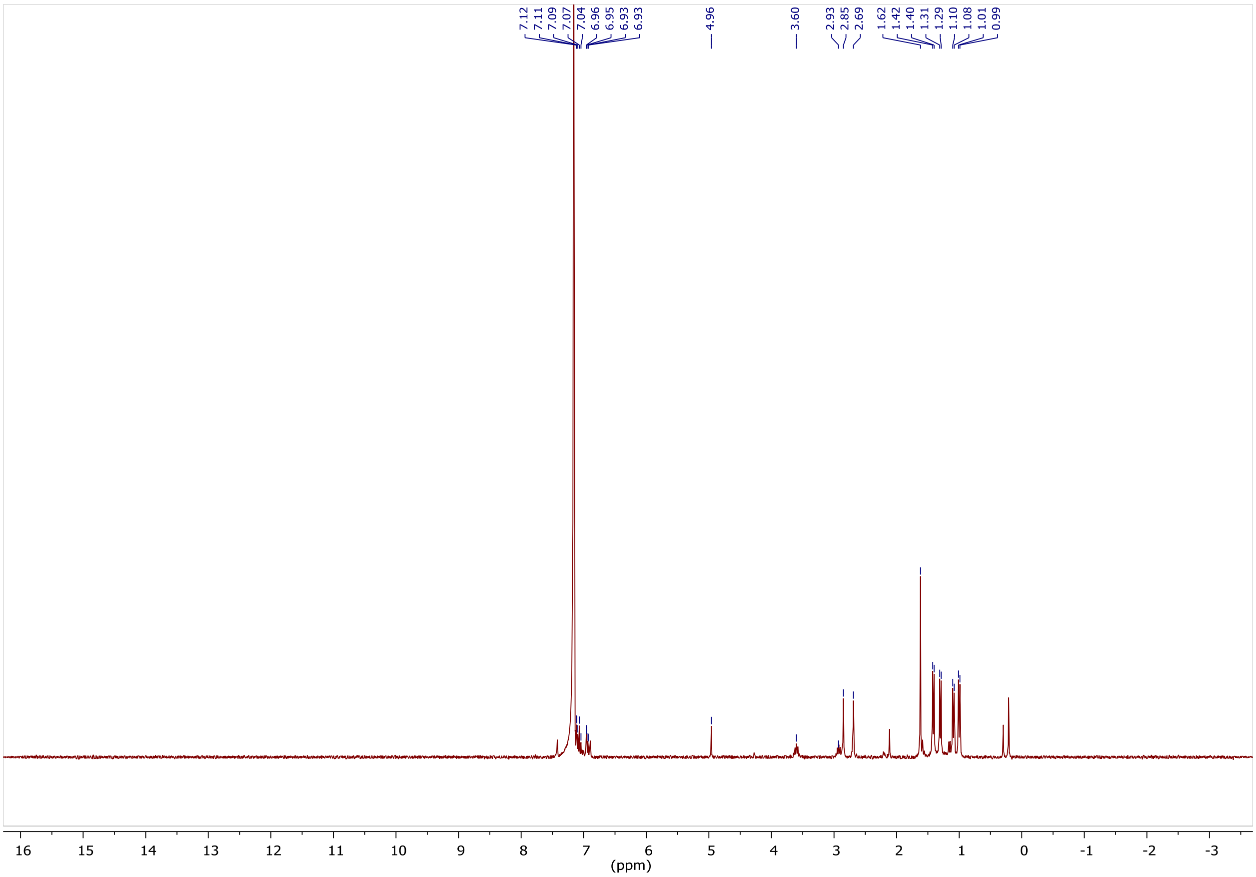

Figure 17: ^{1}H NMR spectrum (300 MHz, C_6D_6, 25 °C) of $[L(Me_2N)AlSb]_2$ (**6**).

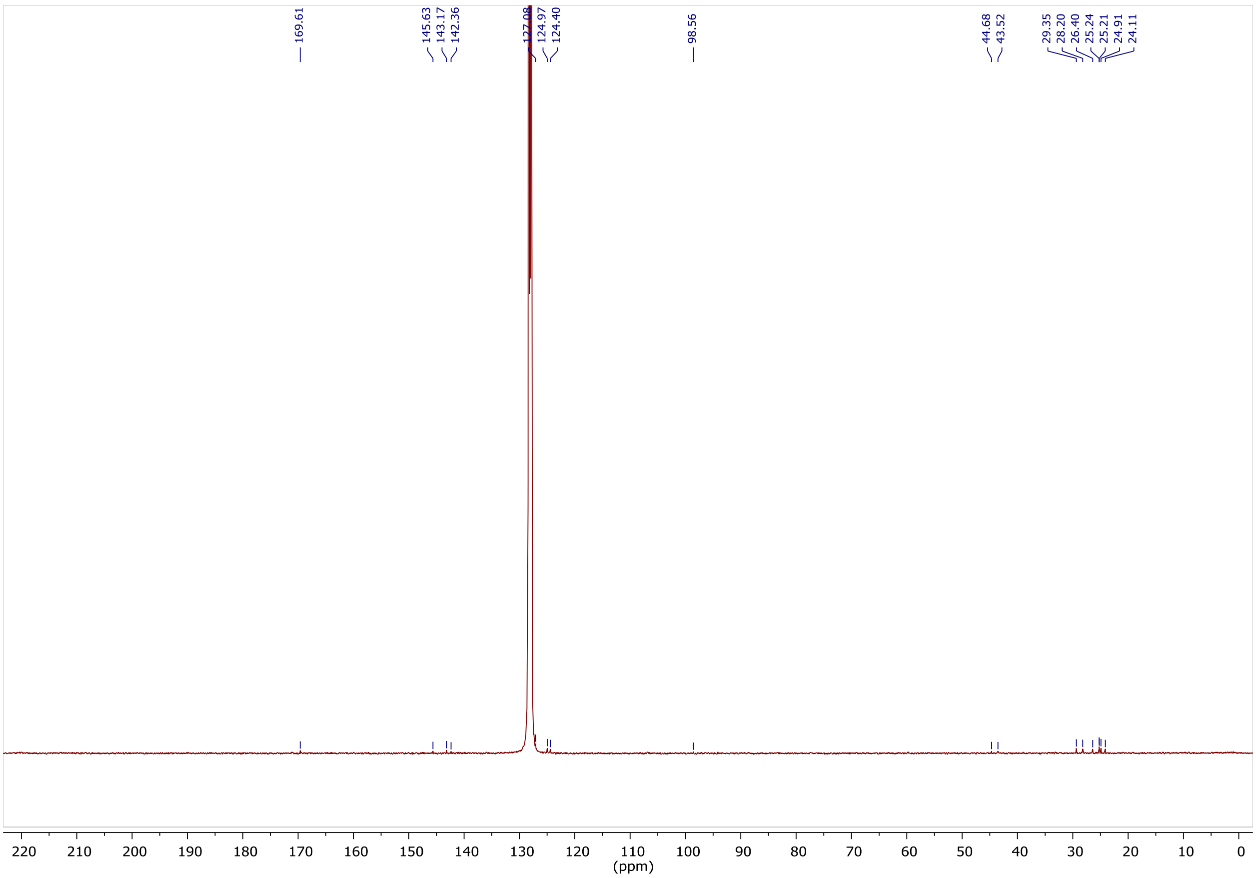

Figure 18: ^{13}C NMR spectrum (100.7 MHz, C_6D_6, 25 °C) of $[L(Me_2N)AlSb]_2$ (**6**).

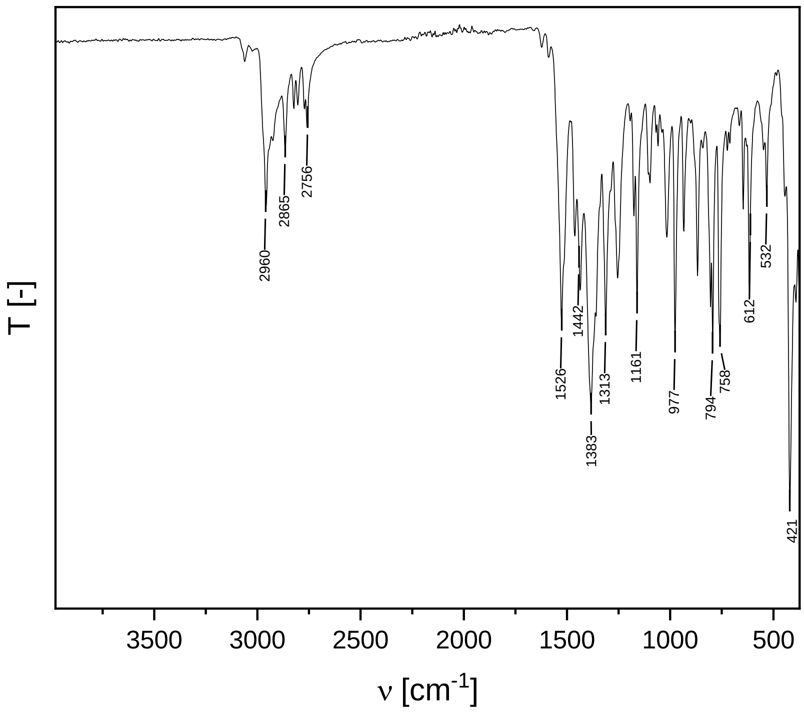

Figure 19: ATR-IR spectrum of $[L(Me_2N)AlSb]_2$ (**6**).

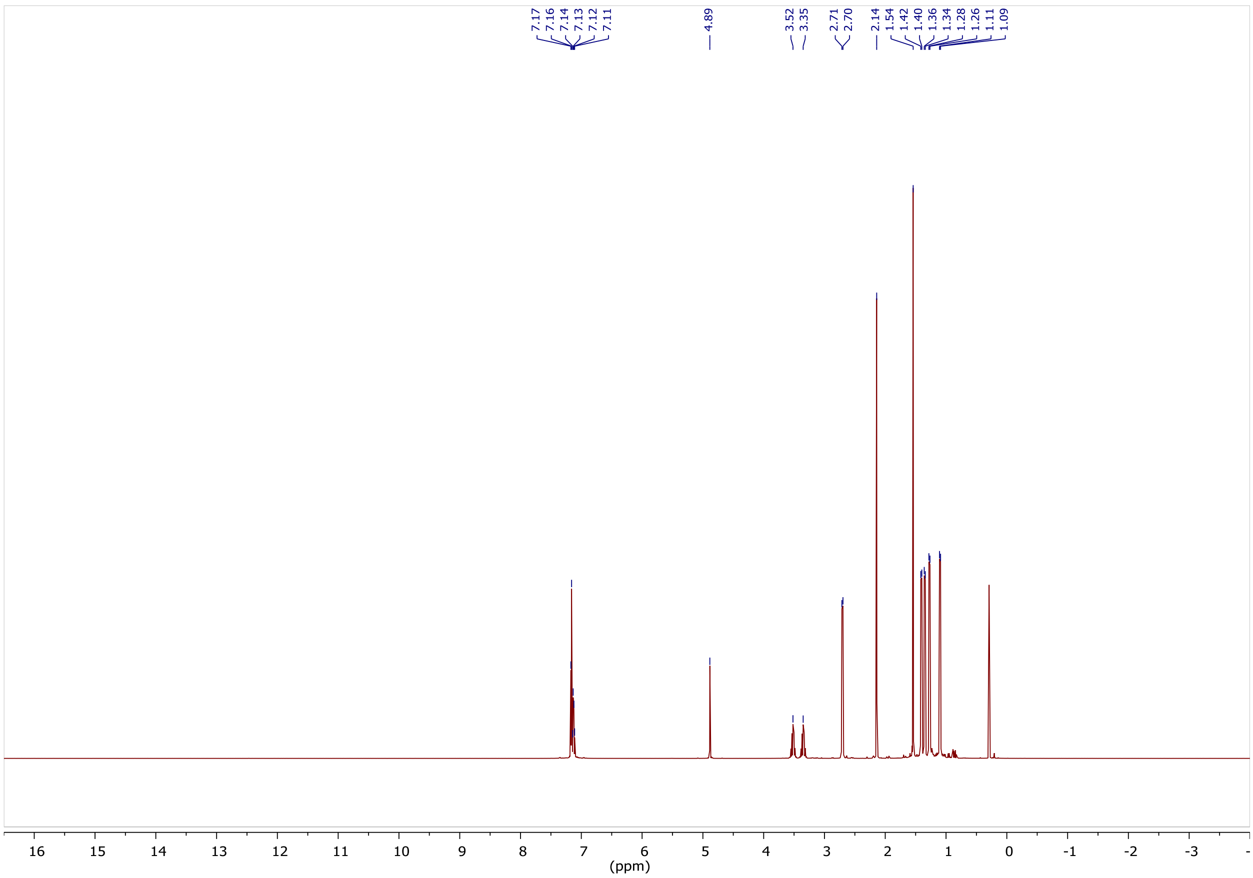

Figure 20: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $LAl(NMe_2)_2$.

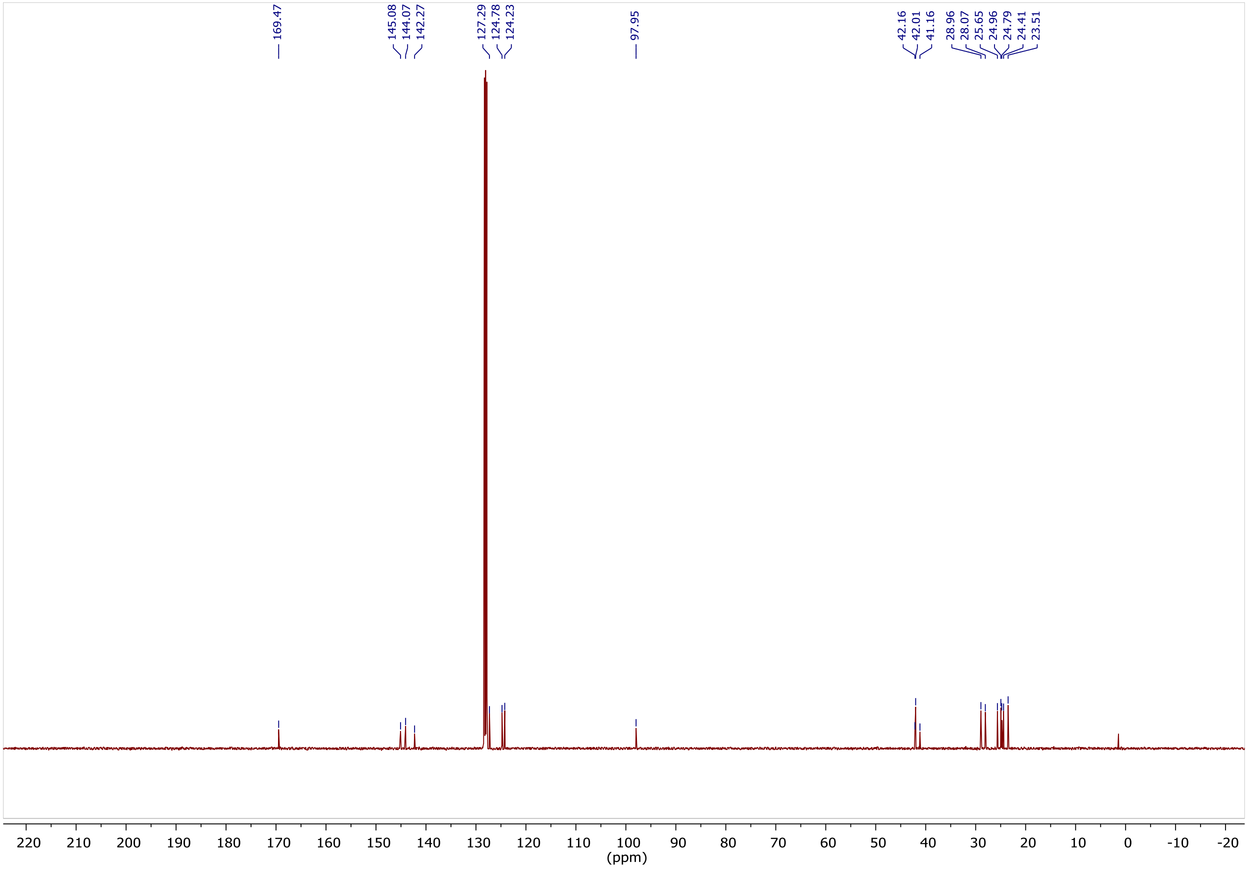

Figure 21: ^{13}C NMR spectrum (100.7 MHz, C_6D_6, 25 °C) of $LAl(NMe_2)_2$.

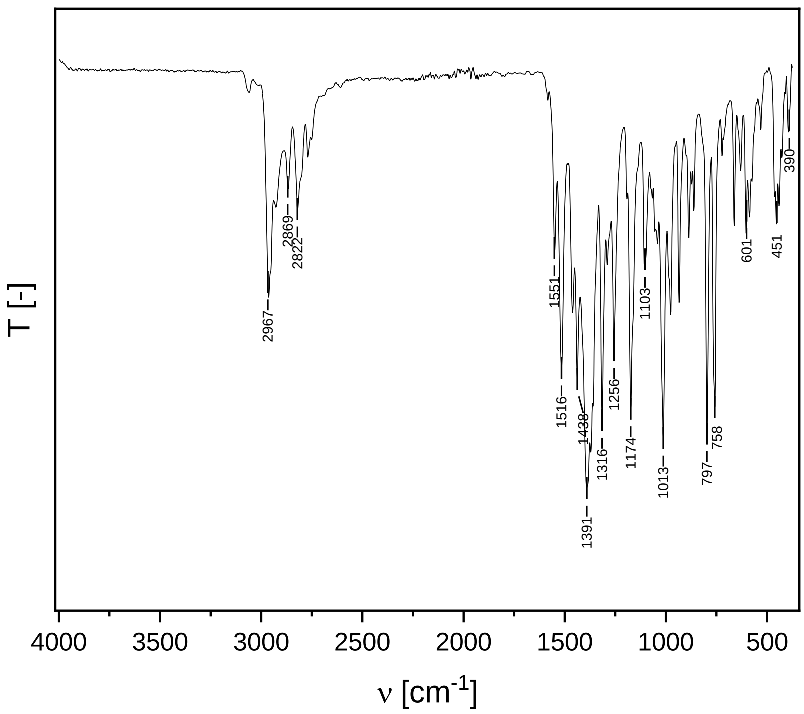

Figure 22: ATR-IR spectrum of $LAl(NMe_2)_2$.

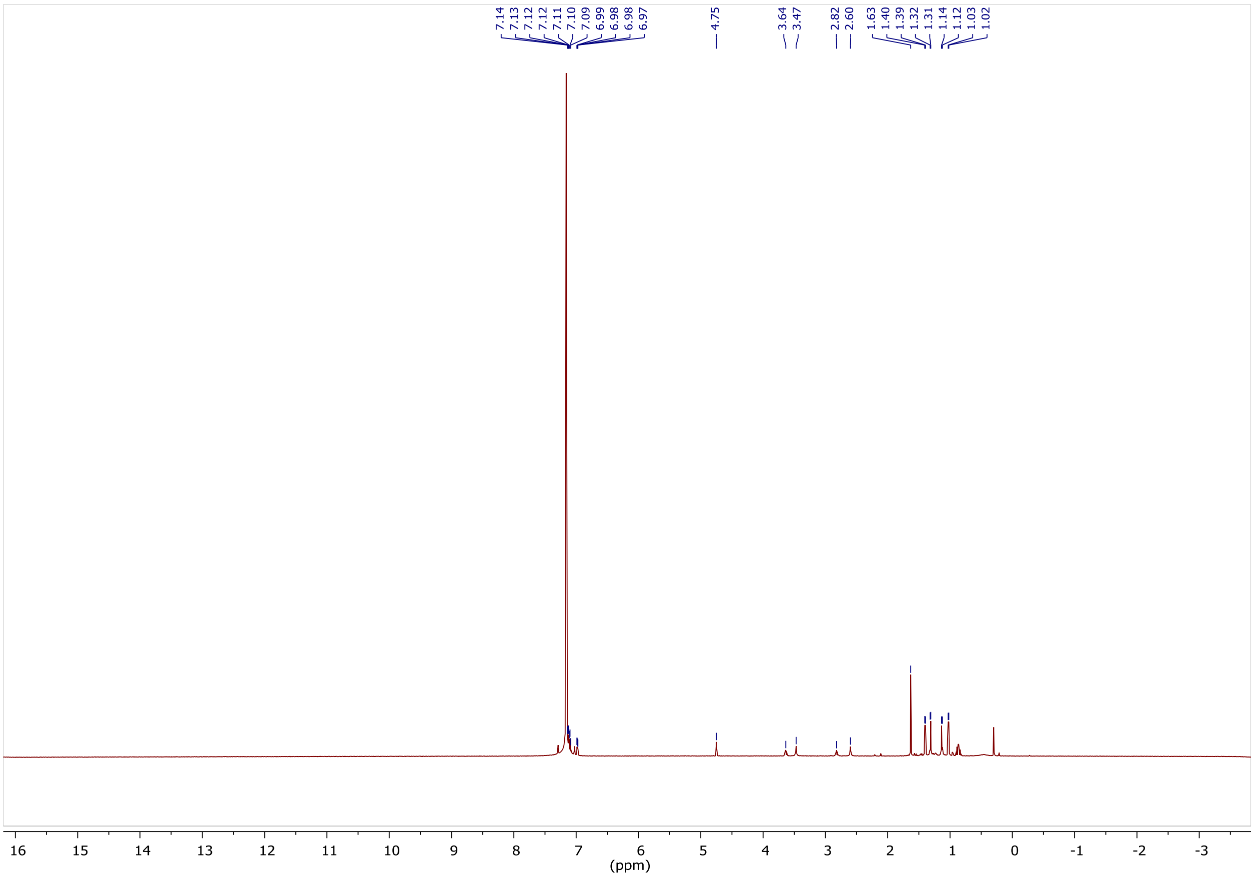

Figure 23: ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaBi]_2$ (**8**).

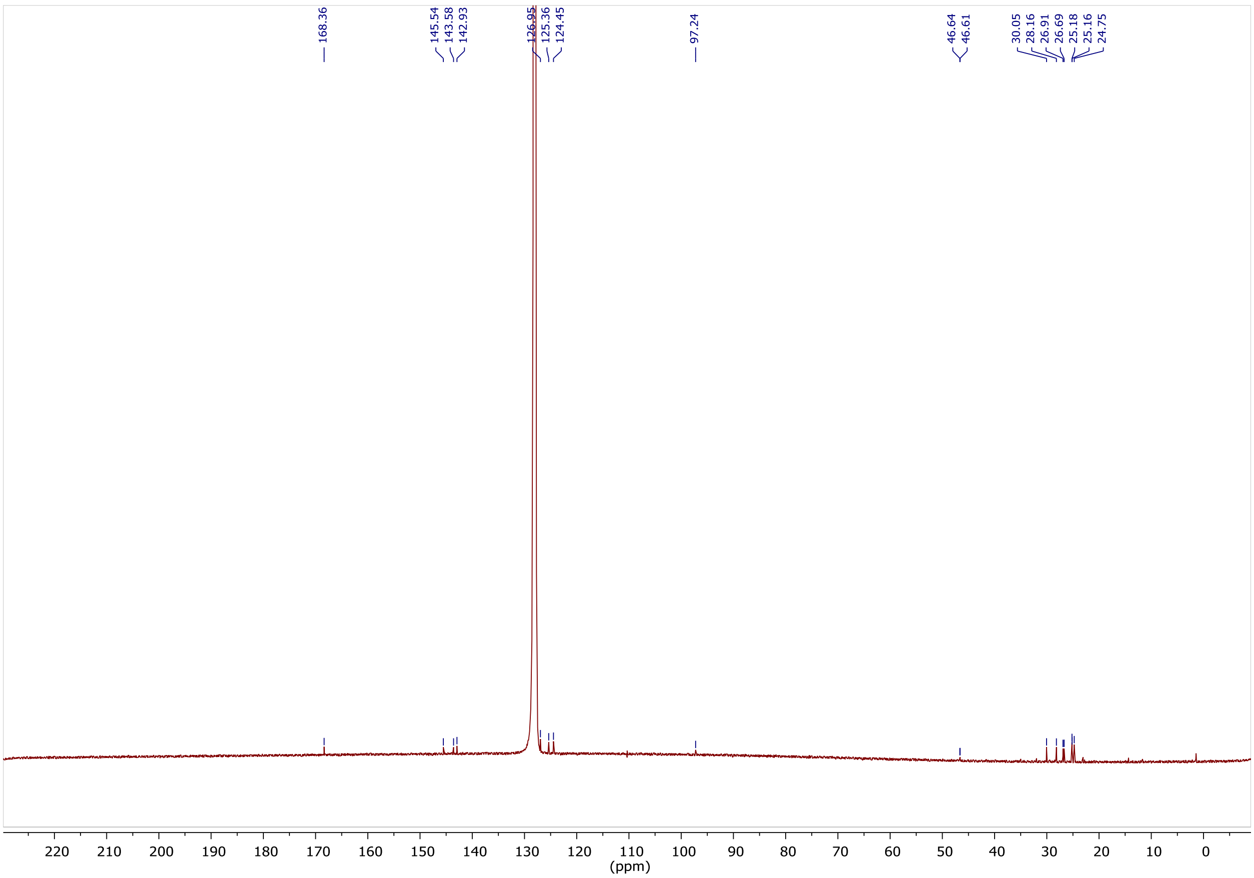

Figure 24: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaBi]_2$ (**8**).

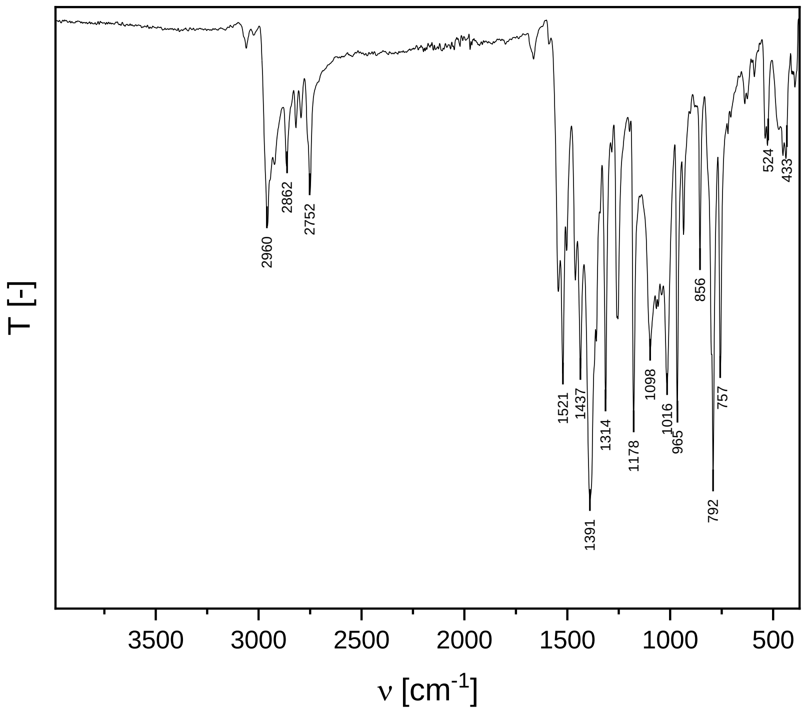

Figure 25: ATR-IR spectrum of [L(Me$_2$N)GaBi]$_2$ (**8**).

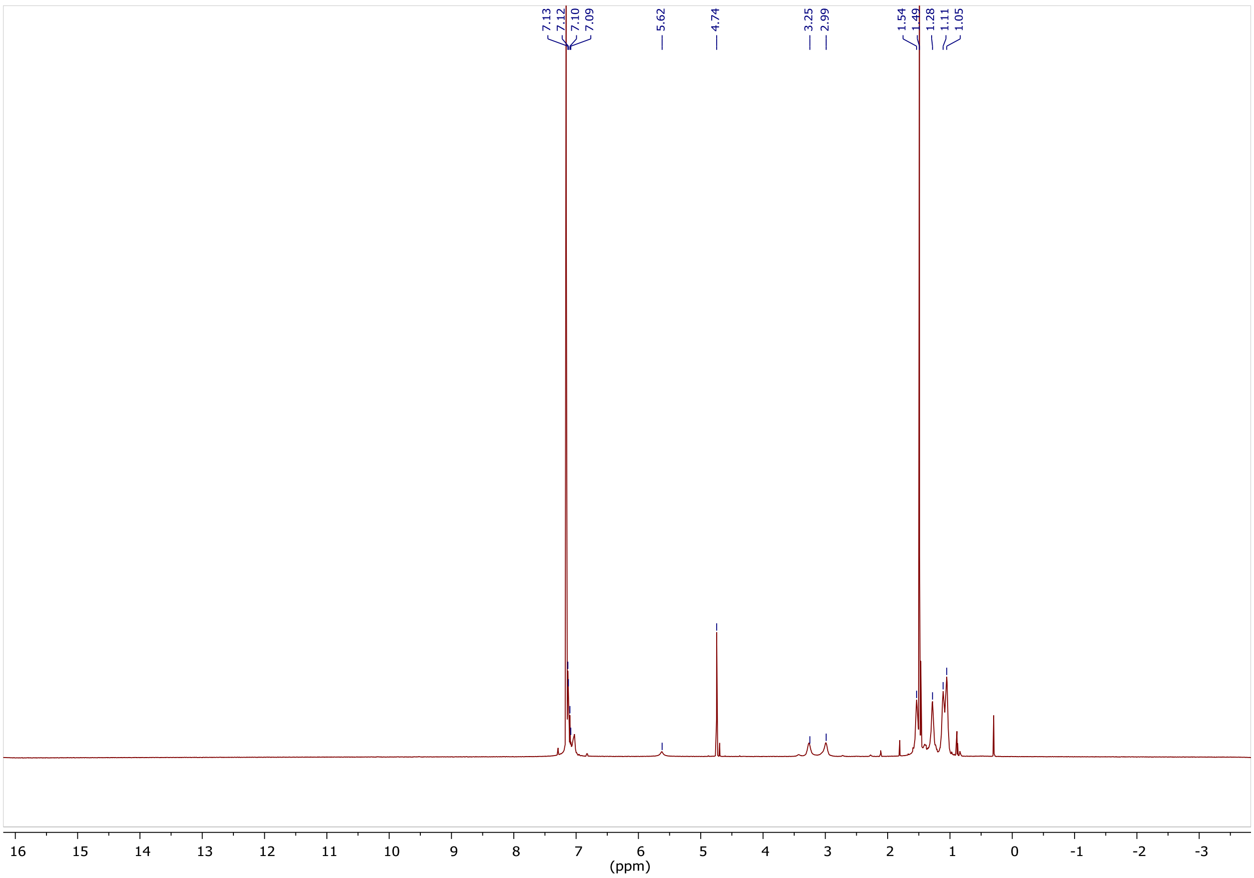

Figure 26: ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of LGa(H)OTf.

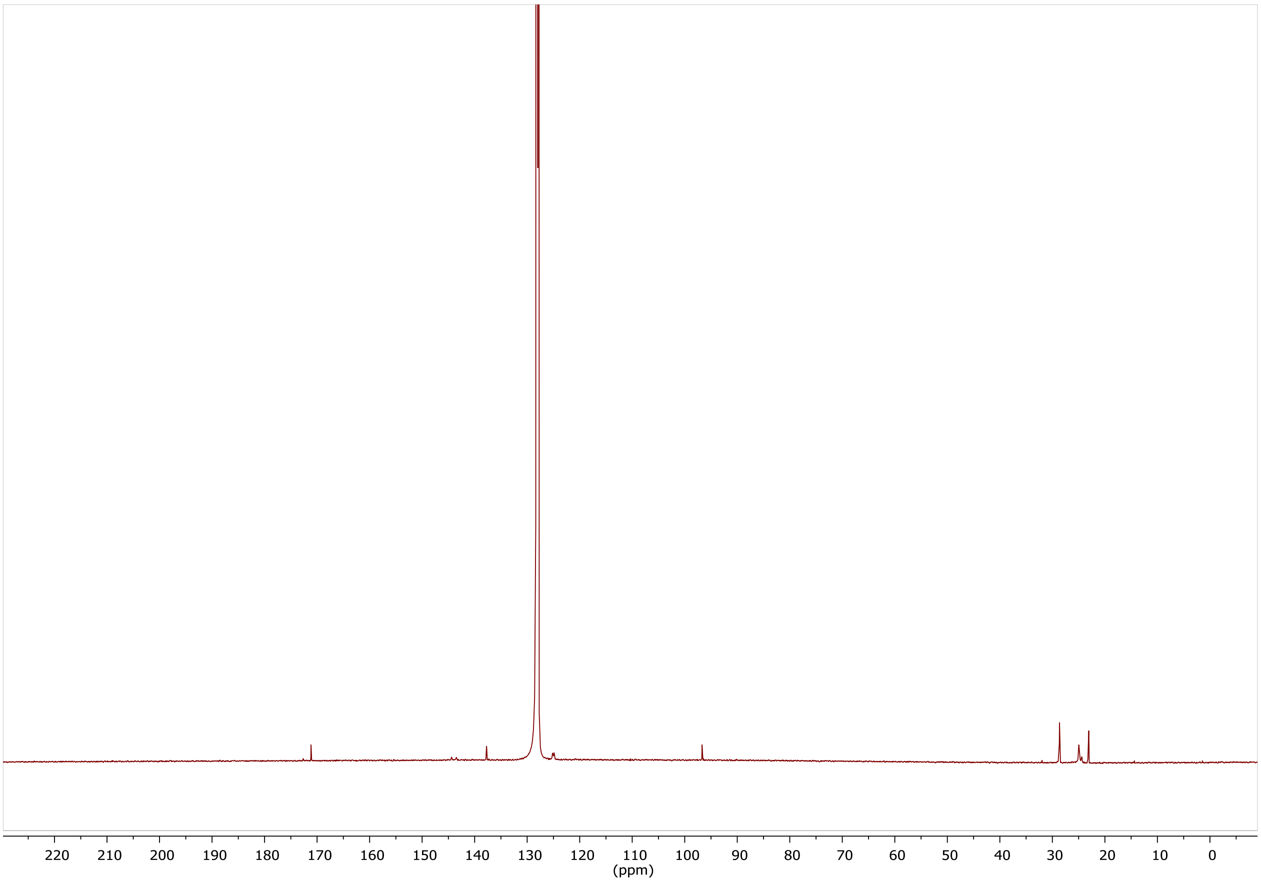

Figure 27: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of LGa(H)OTf.

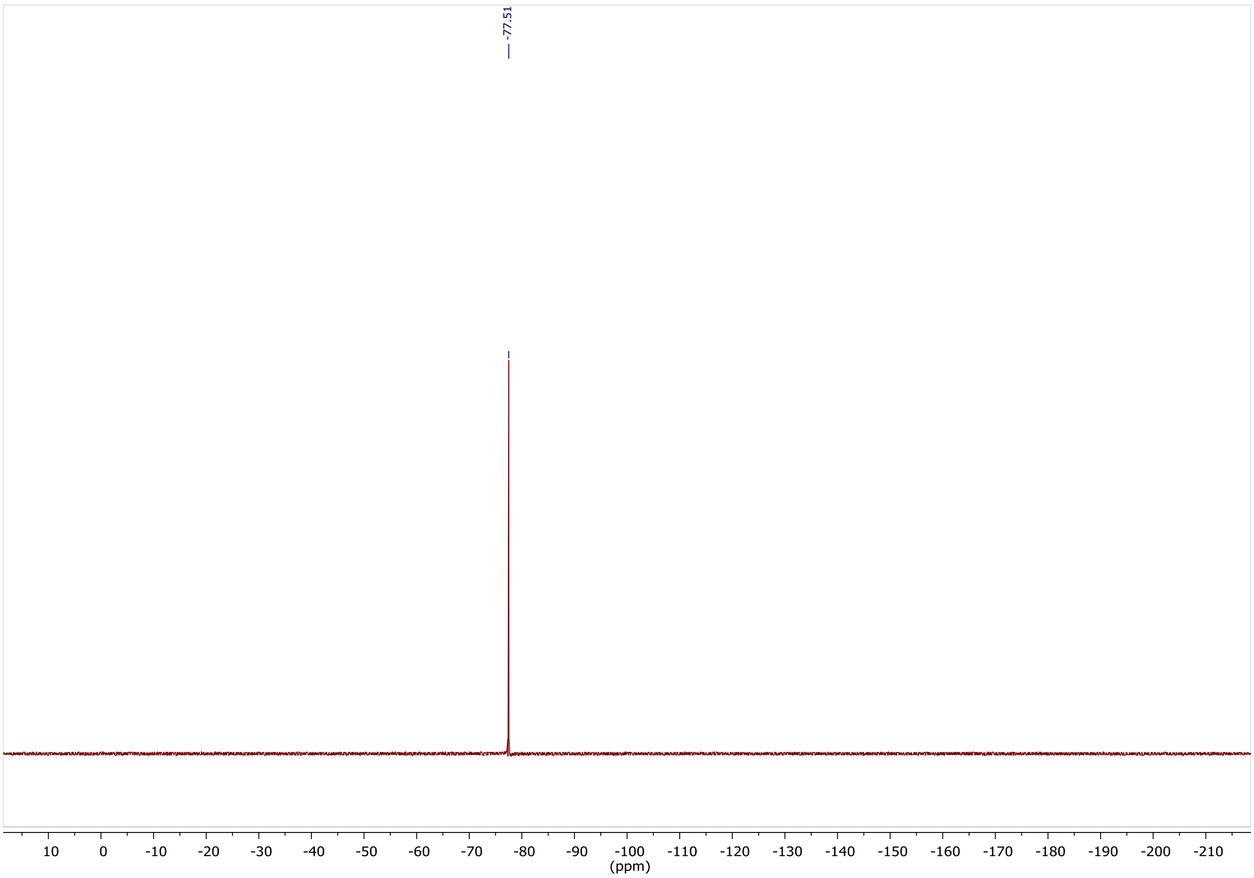

Figure 28: ^{19}F NMR spectrum (564.6 MHz, C_6D_6, 25 °C) of LGa(H)OTf.

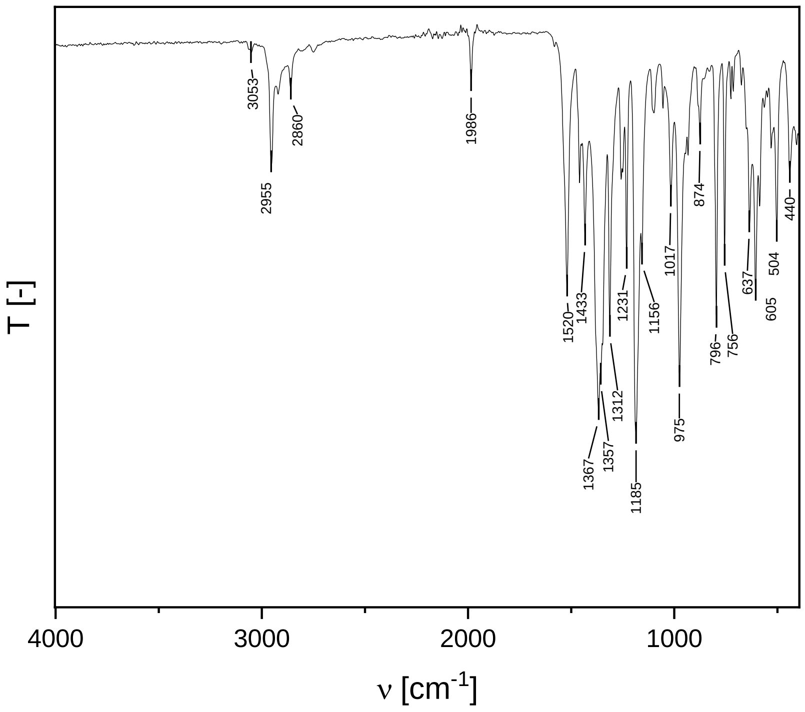

Figure 29: ATR-IR spectrum of LGa(H)OTf.

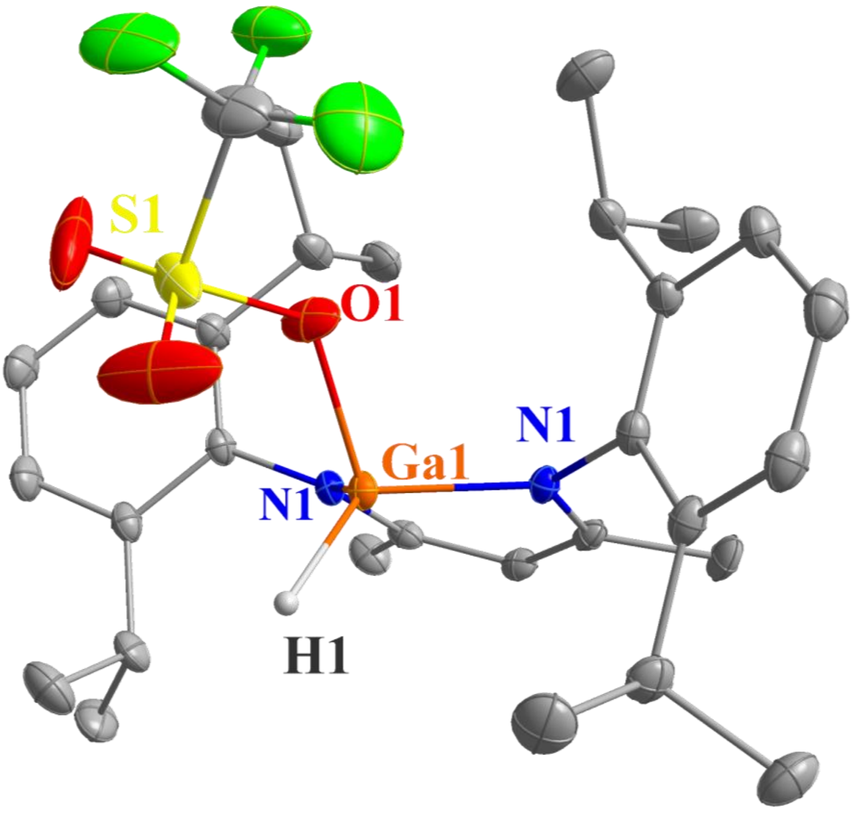

Figure 30: Molecular structure of LGa(H)OTf in the crystal. H atoms are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level. Only one component for the disorder of the OTf unit is displayed.

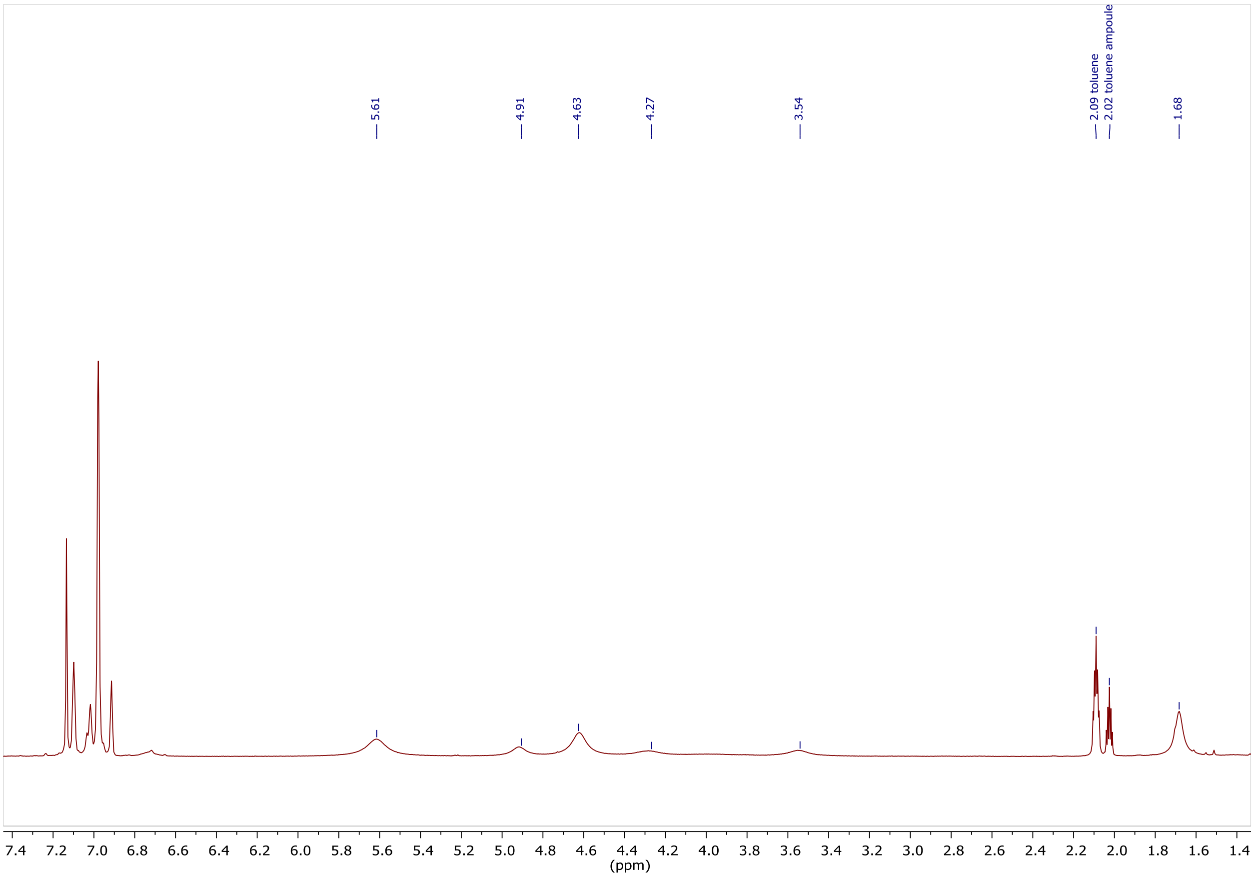

Figure 31: ^{1}H NMR (300 MHz toluene-d_8, 25 °C) of $[L(TfO)Ga]_2Bi\bullet$ (**9**) for Evans' method.

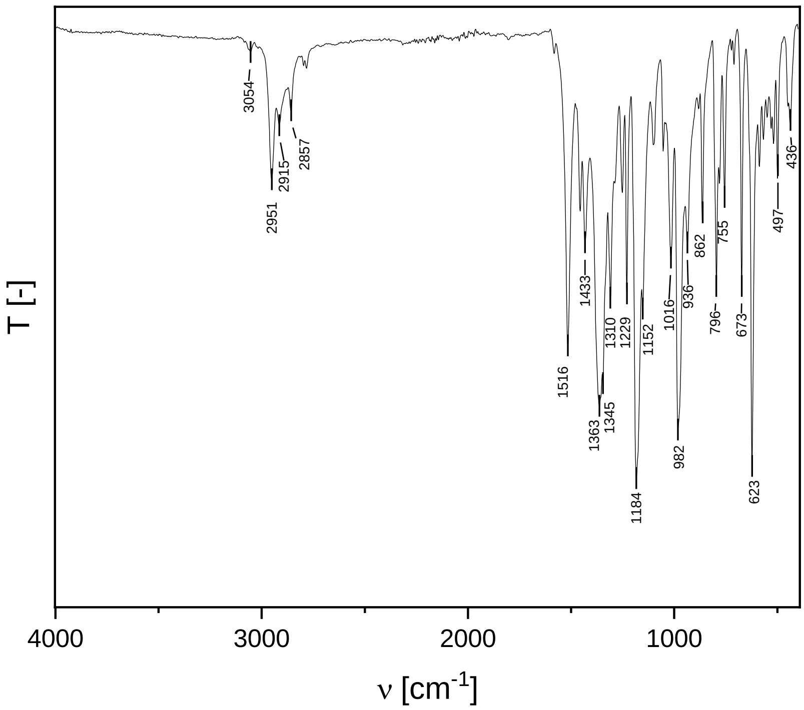

Figure 32: ATR-IR spectrum of $[L(TfO)Ga]_2Bi\bullet$ (**9**).

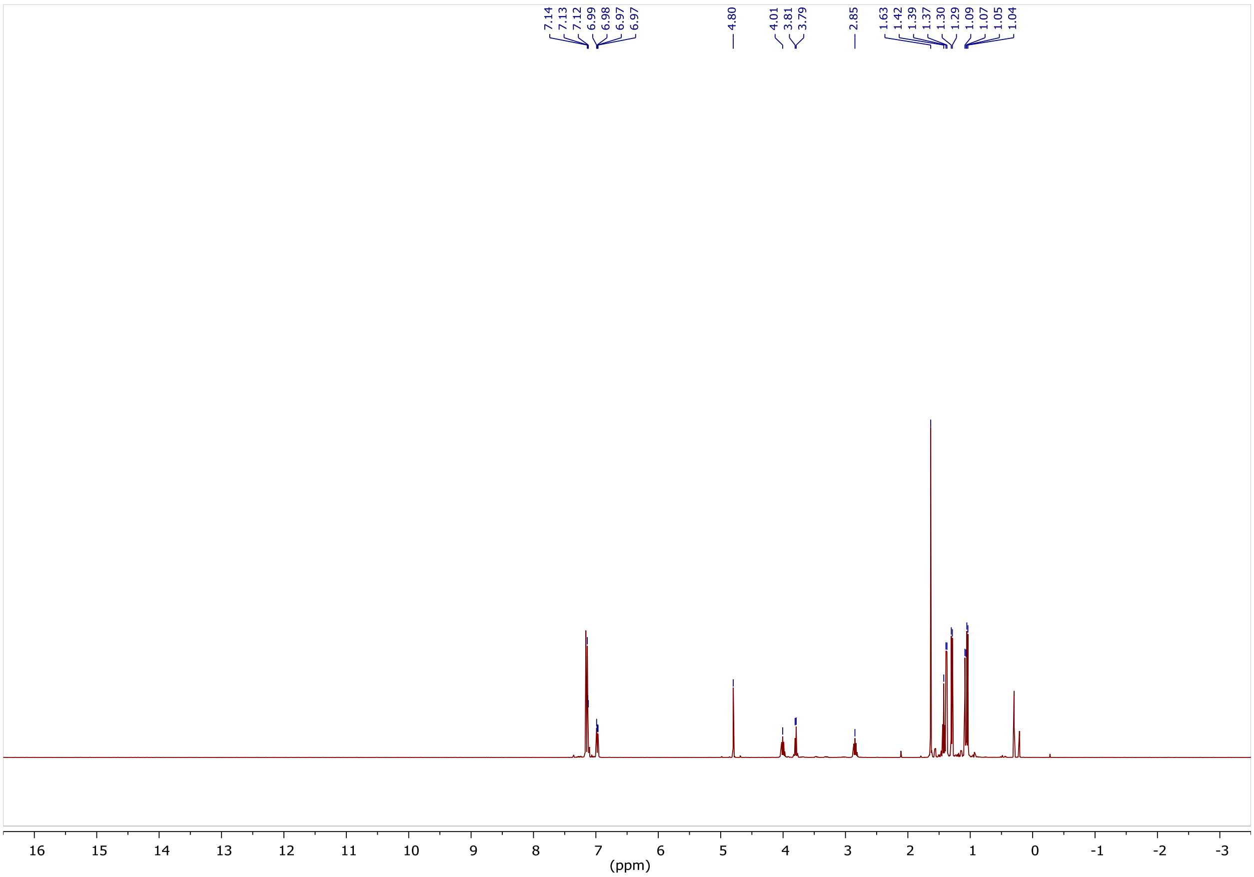

Figure 33: ^{1}H NMR spectrum (300 MHz, C_6D_6, 25 °C) of $[L(EtO)GaBi]_2$ (**10**).

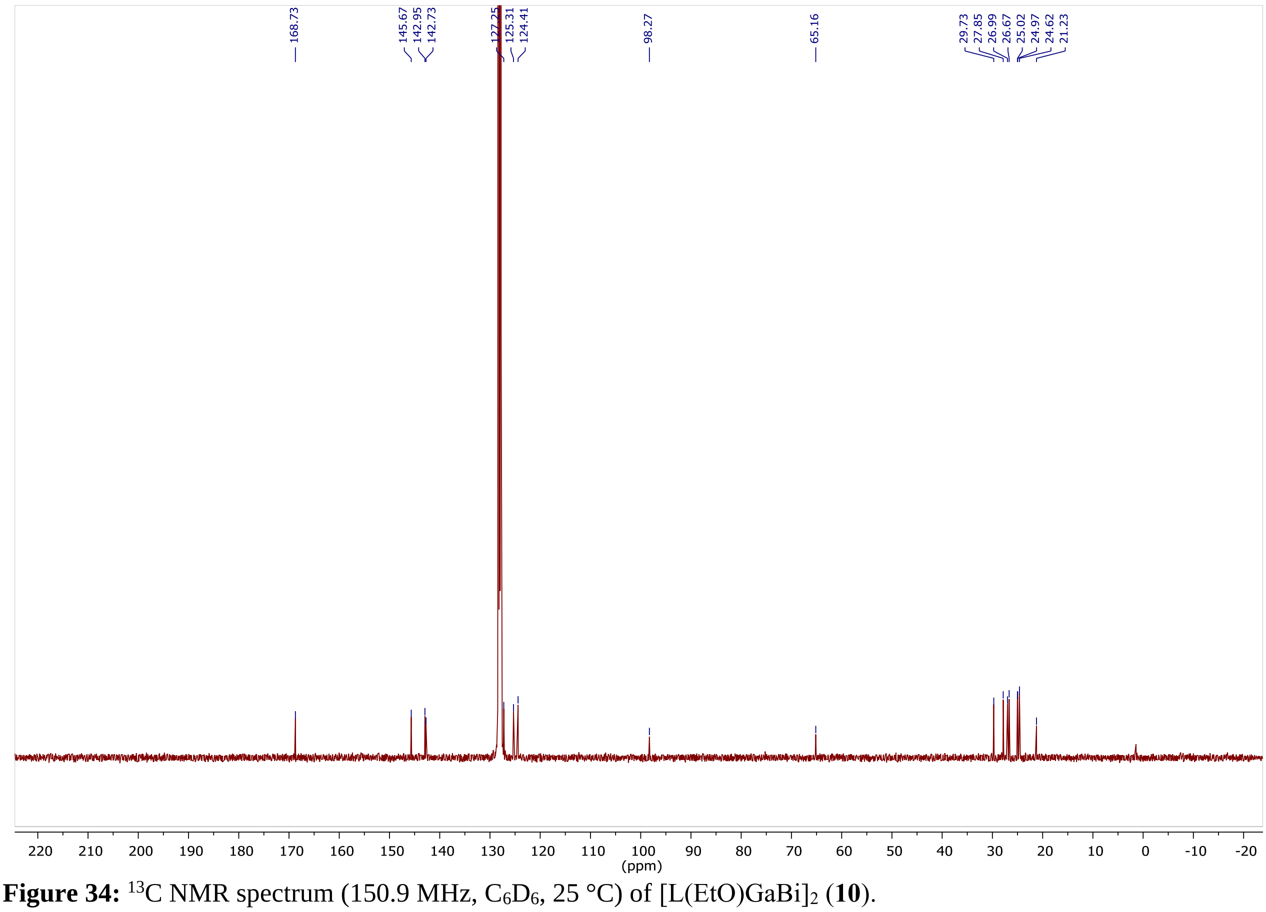

Figure 34: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(EtO)GaBi]_2$ (**10**).

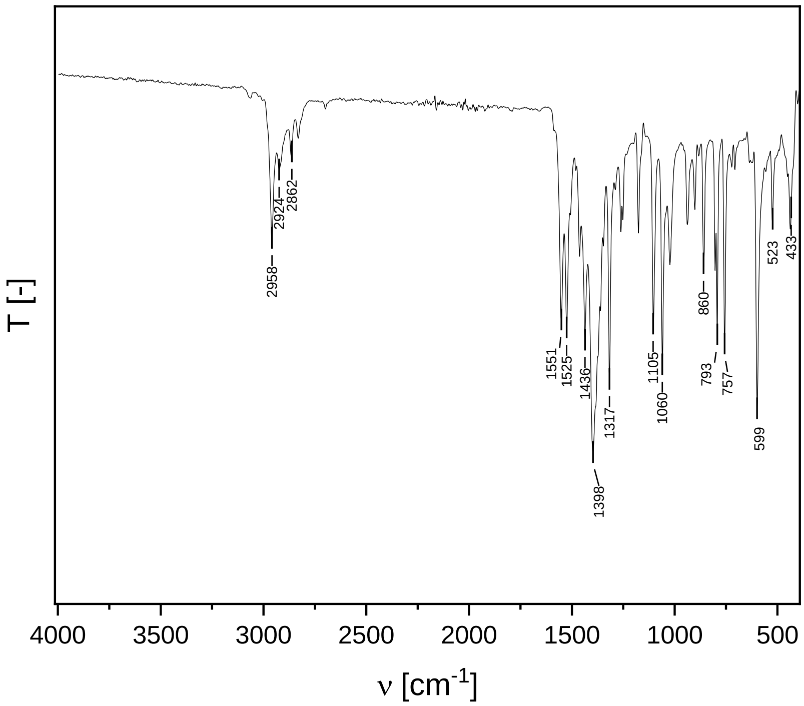

Figure 35: ATR-IR spectrum of $[L(EtO)GaBi]_2$ (**10**).

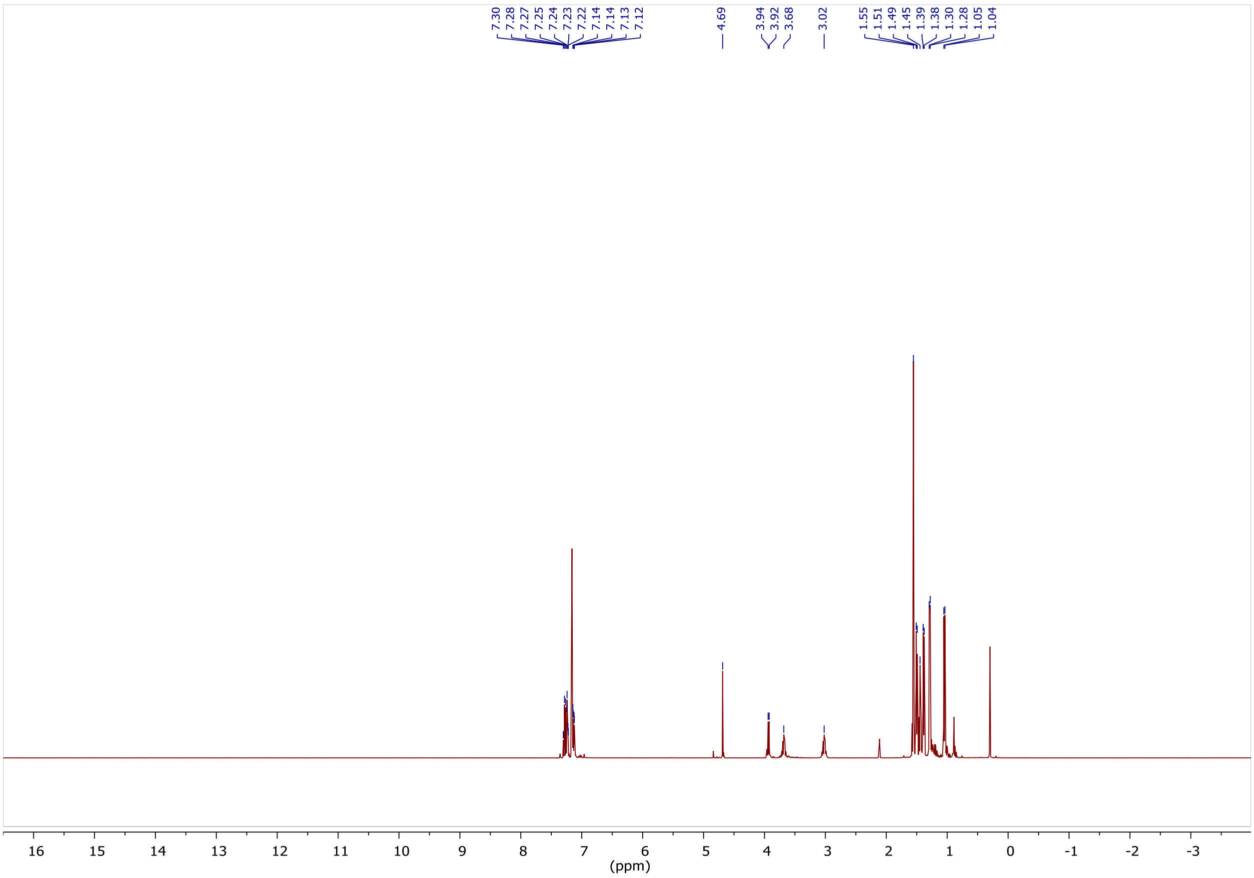

Figure 36: ^{1}H NMR spectrum (300 MHz, C_6D_6, 25 °C) of $[\{L(EtO)Ga\}_2\text{-}\mu,\eta^{1:1}\text{-}Bi_4]$ (**11**).

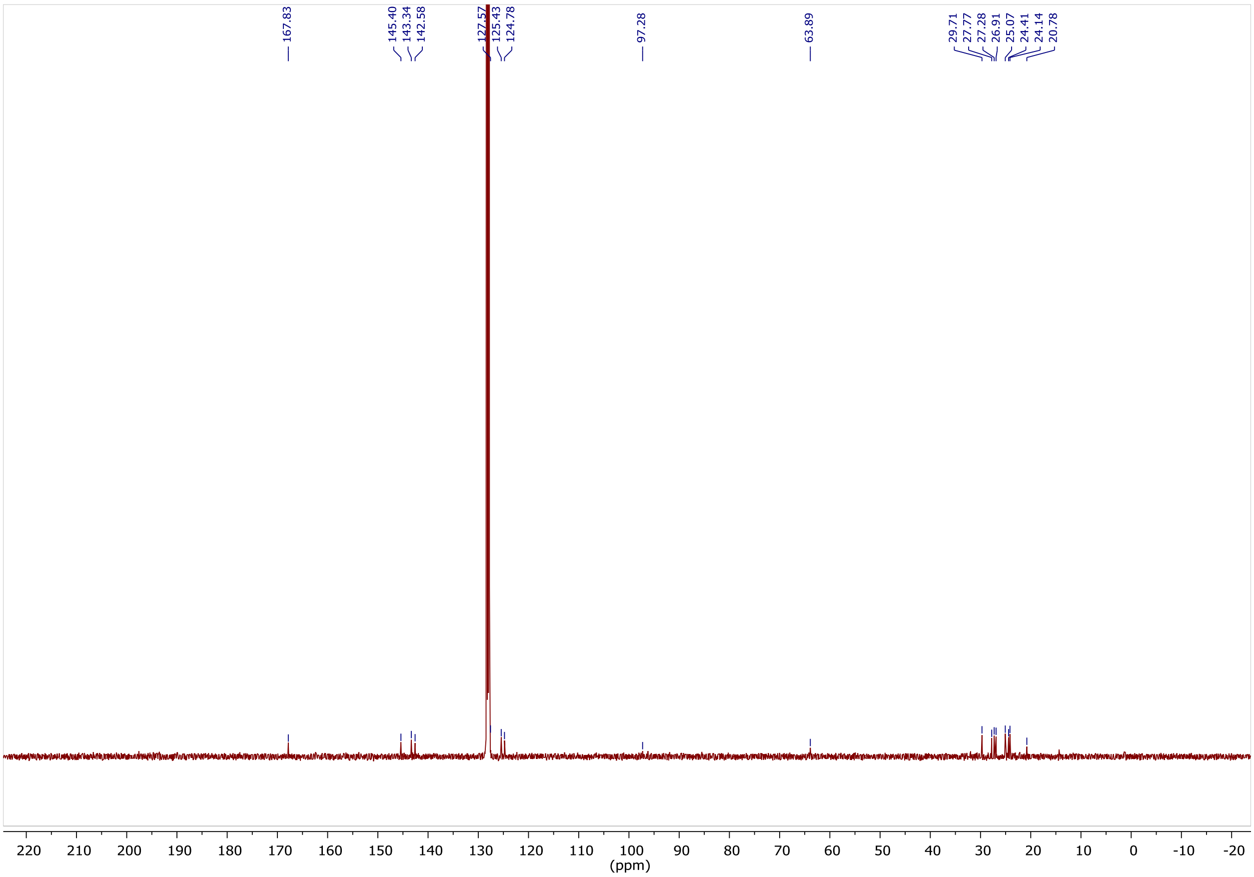

Figure 37: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of [{L(EtO)Ga}$_2$-μ,η$^{1:1}$-Bi_4] (**11**).

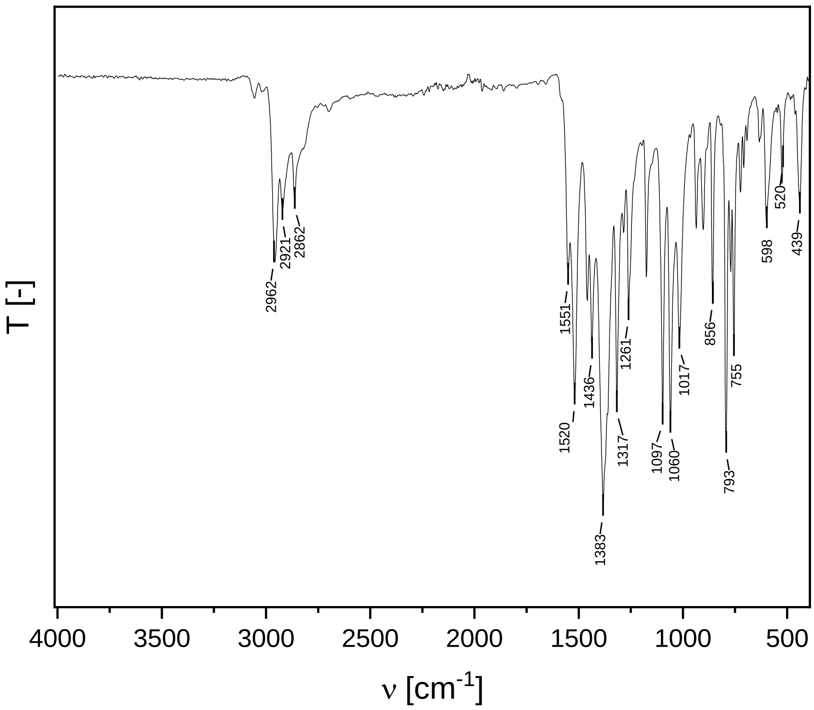

Figure 38: ATR-IR spectrum of [{L(EtO)Ga}$_2$-μ,η$^{1:1}$-Bi_4] (**11**).

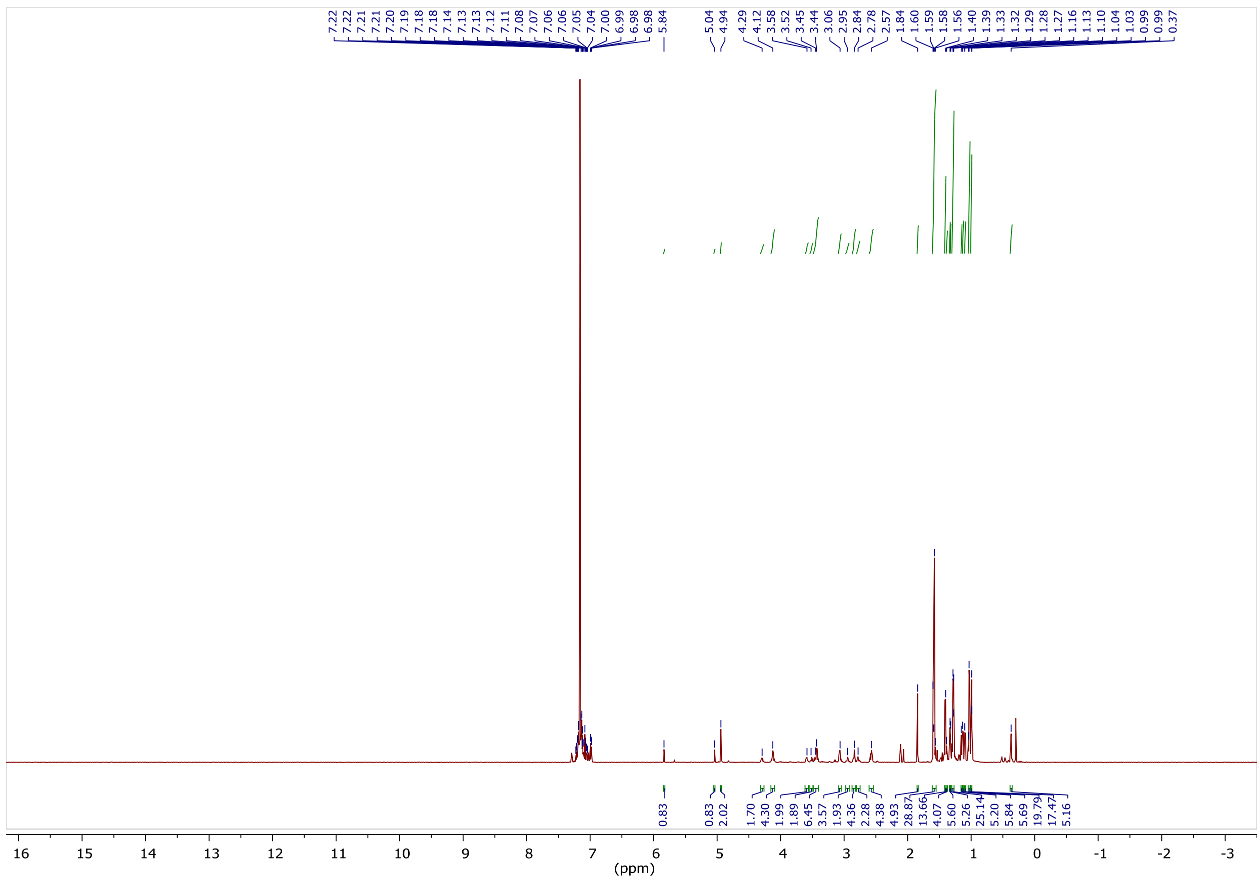

Figure 39: ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of $[L(Et_2N)AlBi]_2$ (**12**).

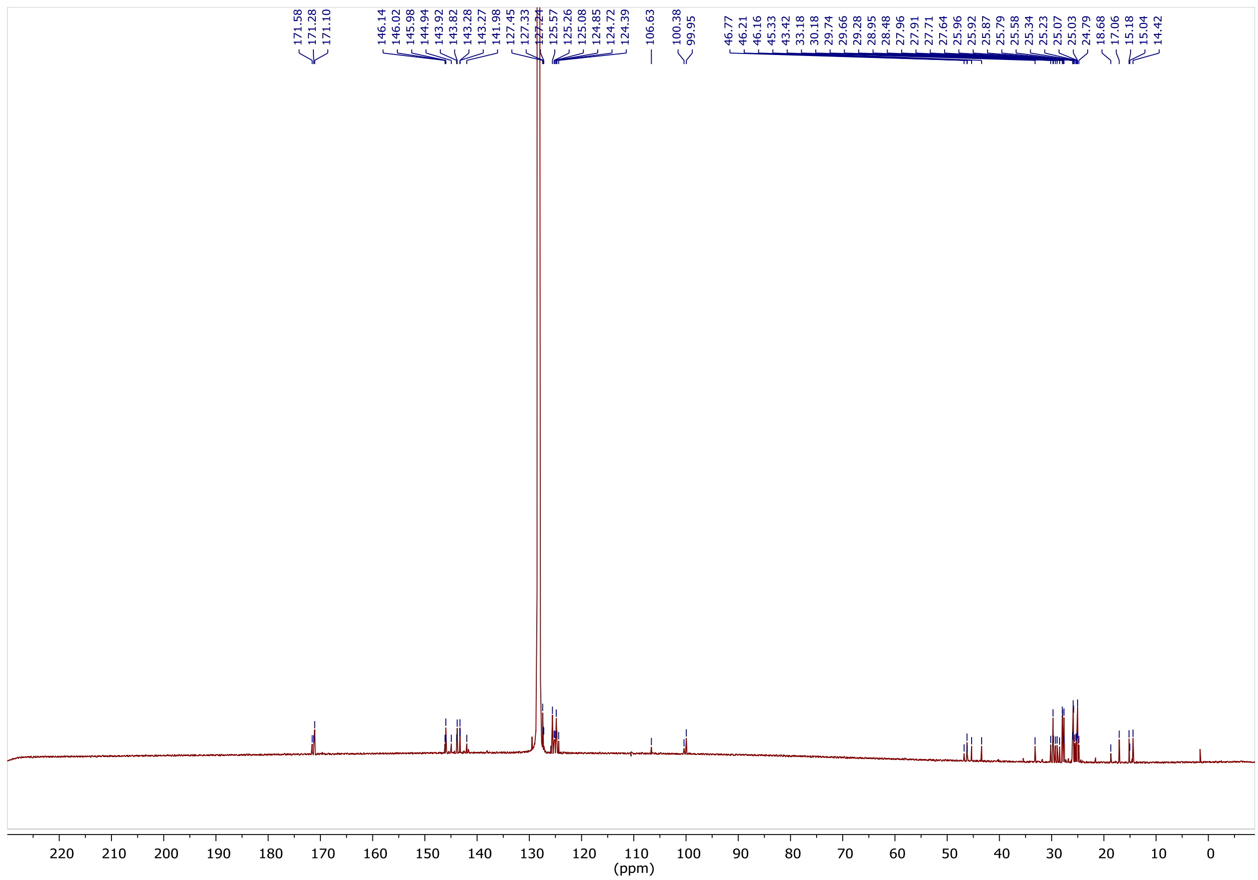

Figure 40: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Et_2N)AlBi]_2$ (**12**).

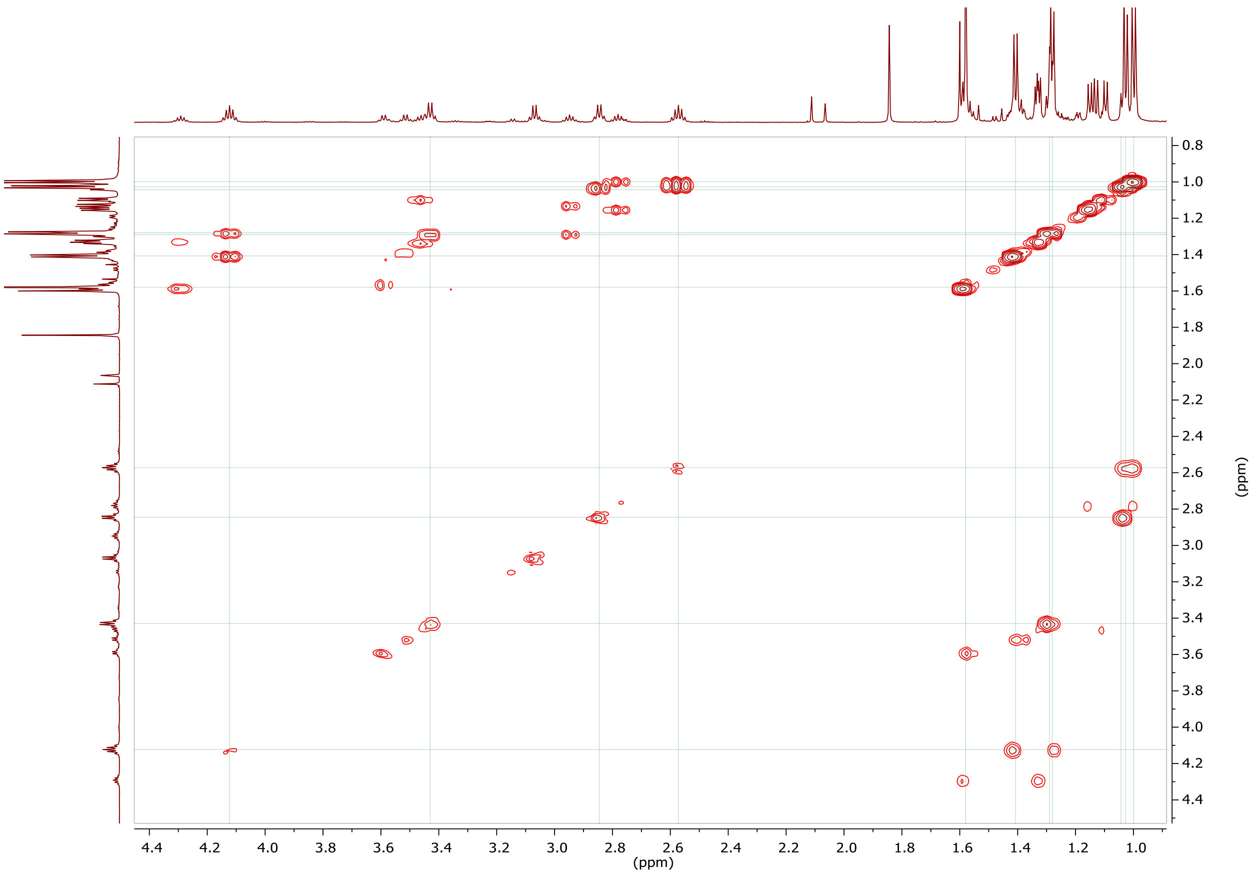

Figure 41: COSY 2D-NMR spectrum (600 MHz, C_6D_6, 25 °C) of $[L(Et_2N)AlBi]_2$ (**12**). The correlations of symmetric conformer are marked.

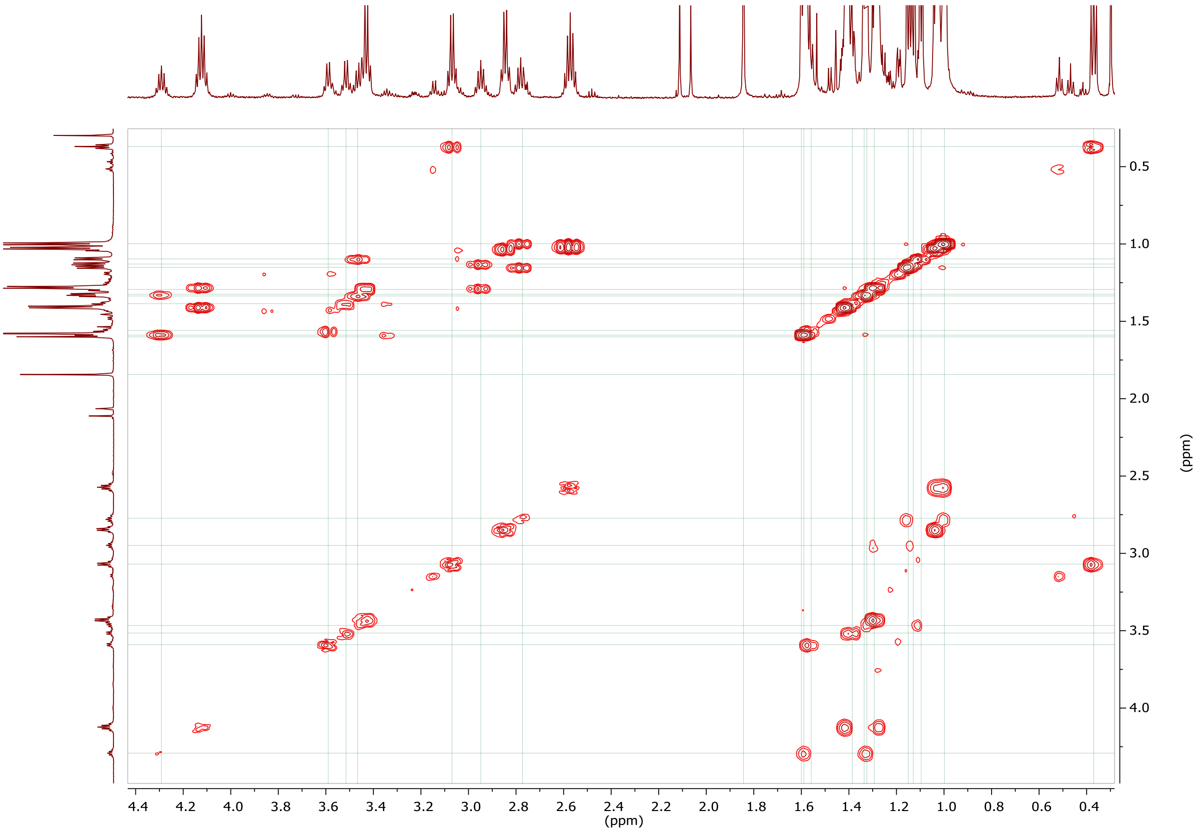

Figure 42: COSY 2D-NMR spectrum (600 MHz, C_6D_6, 25 °C) of $[L(Et_2N)AlBi]_2$ (**12**). The correlations of unsymmetric conformer are marked.

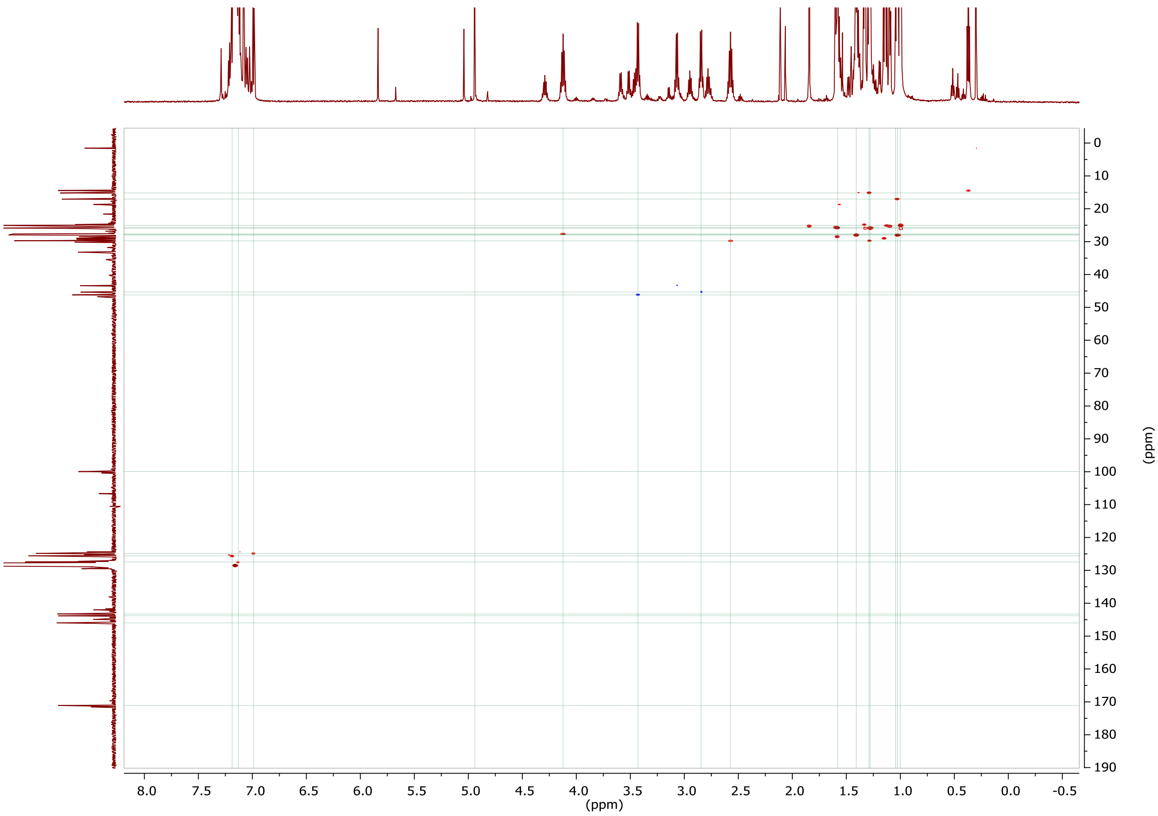

Figure 43: HSQC 2D-NMR spectrum (600/150.9 MHz, C_6D_6, 25 °C) of $[L(Et_2N)AlBi]_2$ (**12**). The correlations of symmetric conformer are marked.

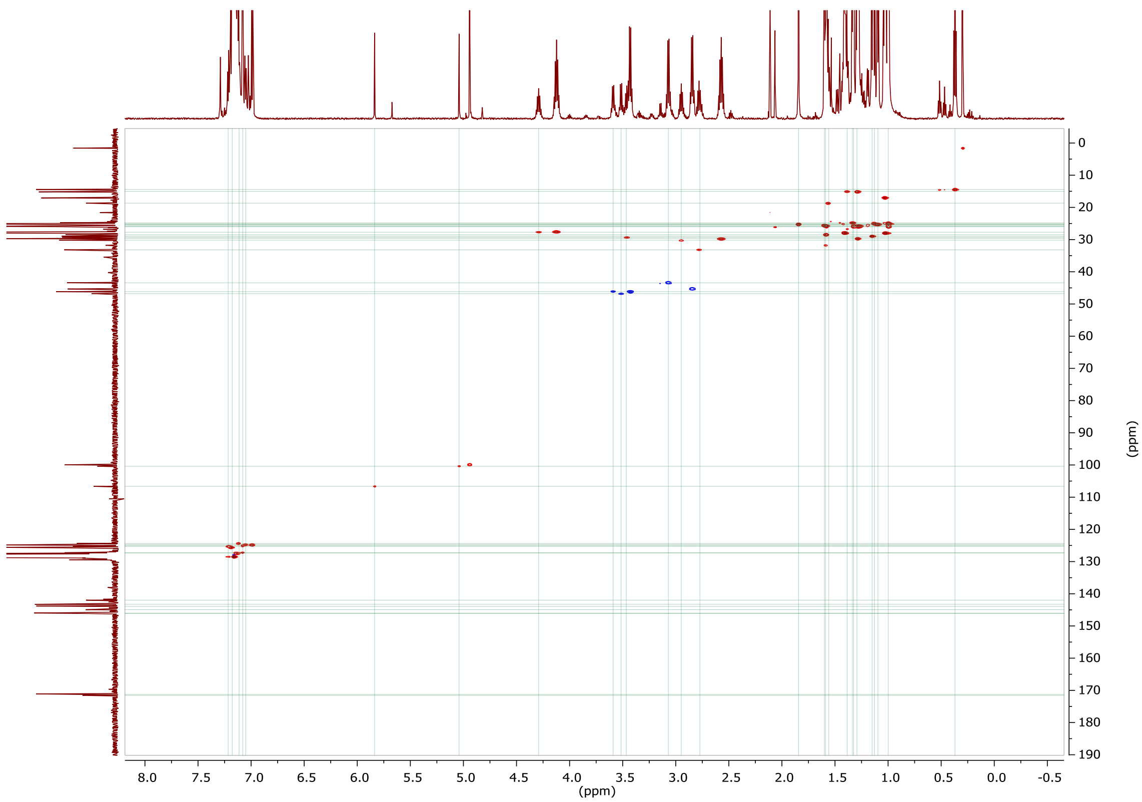

Figure 44: HSQC 2D-NMR spectrum (600/150.9 MHz, C_6D_6, 25 °C) of $[L(Et_2N)AlBi]_2$ (**12**). The correlations of unsymmetric conformer are marked.

Table 1: DOSY NMR Results of chosen peaks of $[L(Et_2N)AlBi]_2$ (**12**).

Peak number	F2 [ppm]	Io	Error	D [m2/s]	Error
1	7.081	3.50e+09	2.321e+06	5.72e-10	1.194e-12
2	5.834	2.96e+08	2.278e+06	5.90e-10	1.153e-11
3	5.079	3.03e+08	3.295e+06	5.33e-10	1.368e-11
4	4.967	1.24e+09	4.087e+06	6.67e-10	4.214e-12
5	4.266	4.46e+08	3.015e+06	5.48e-10	1.047e-11
6	4.103	1.25e+09	2.774e+06	5.44e-10	3.238e-12
7	3.469	0.00	0.000	0.00	0.000
8	2.533	1.22e+09	2.339e+06	5.62e-10	3.315e-12
9	2.098	2.04e+10	3.019e+06	2.12e-09	7.980e-13
10	1.587	7.36e+09	3.240e+06	6.95e-10	7.008e-13
11	1.341	3.21e+10	7.596e+06	2.68e-09	9.447e-13
12	0.939	0.00	0.000	0.00	0.000
13	0.308	2.42e+09	2.366e+06	2.05e-10	6.393e-13

B values variable. Little delta = 0.001 s. Big delta = 0.03 s. Random error estimation of data: RMS per Spectrum (or trace/plane). Systematic error estimation: worst case per peak scenario. Fit parameter Error estimation method: from fit using calculated y uncertainties. Confidence level: 95 %. Used integrals: area integral.

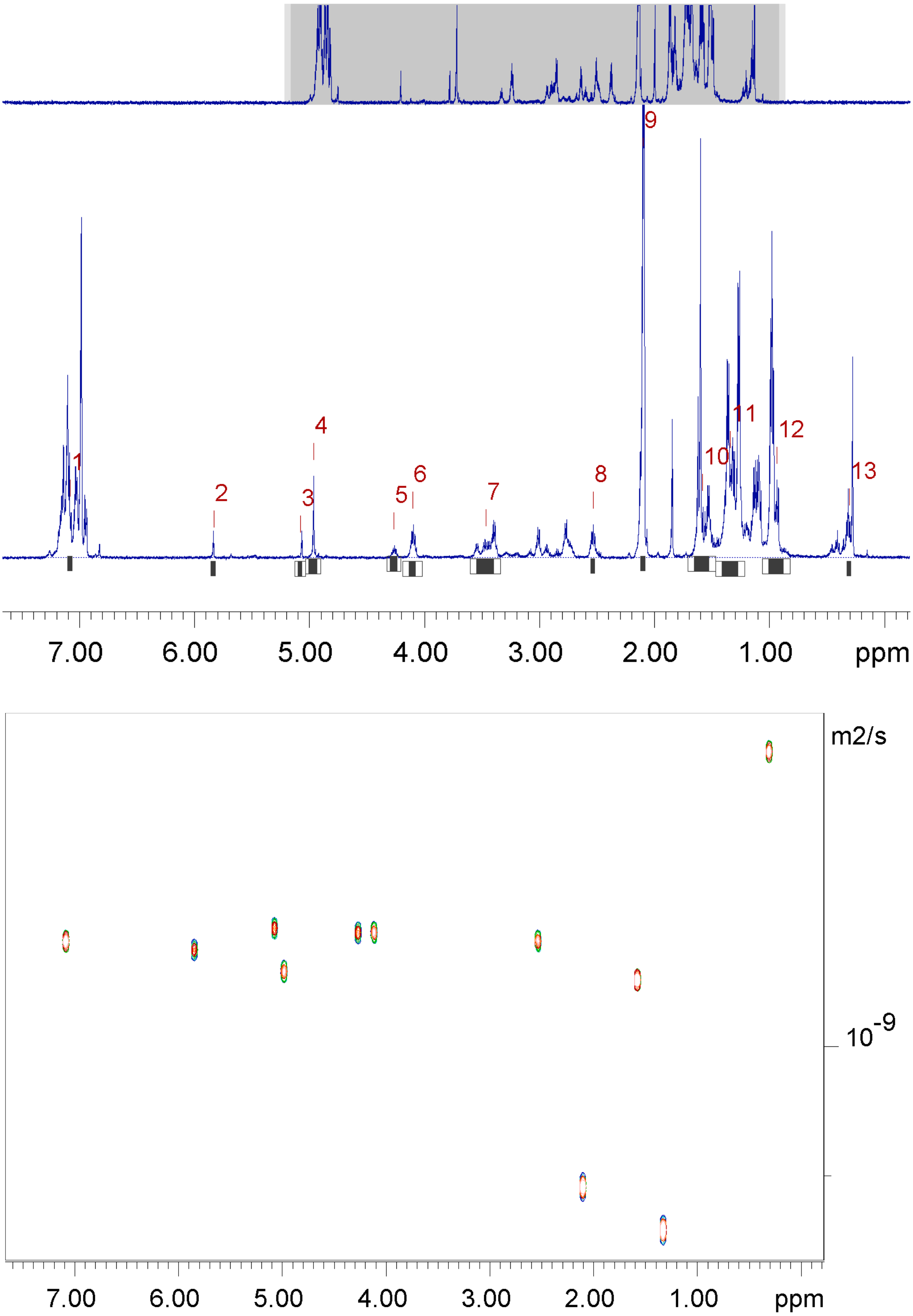

Figure 45: DOSY NMR of $[L(Et_2N)AlBi]_2$ (**12**). The three deviating signals are from left to right toluene, *n*-hexane, and silicon grease.

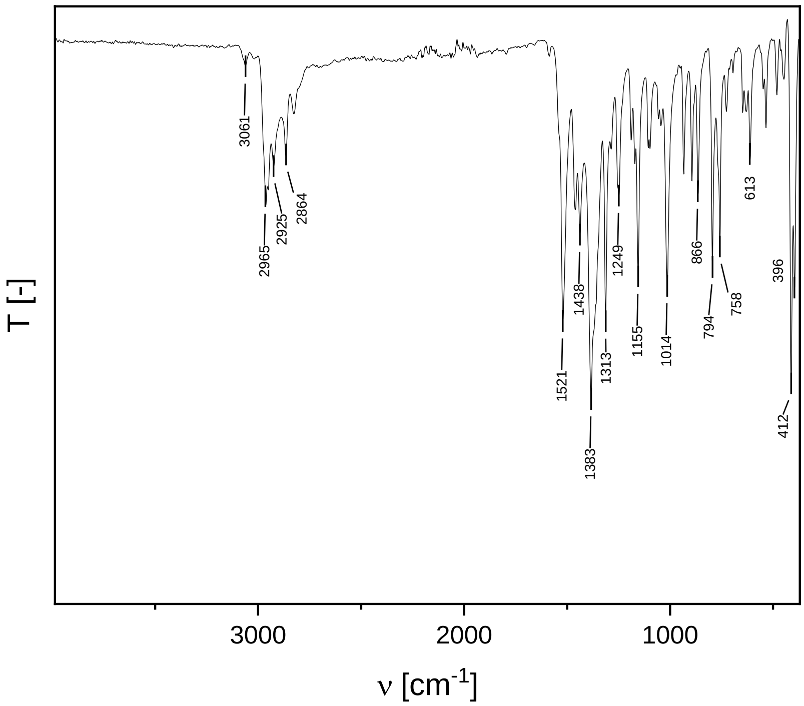

Figure 46: ATR-IR spectrum of $[L(Et_2N)AlBi]_2$ (**12**).

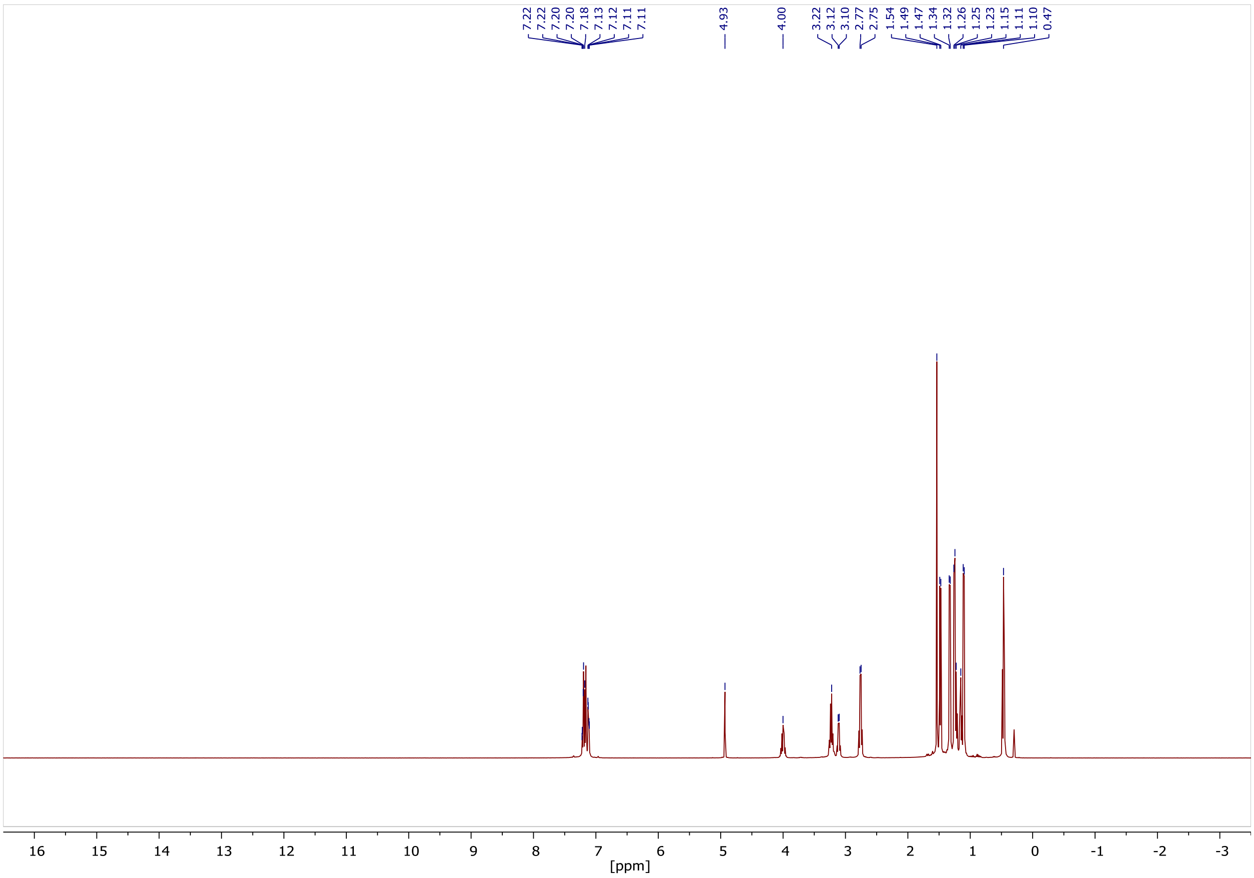

Figure 47: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $LAl(NEt_2)_2$.

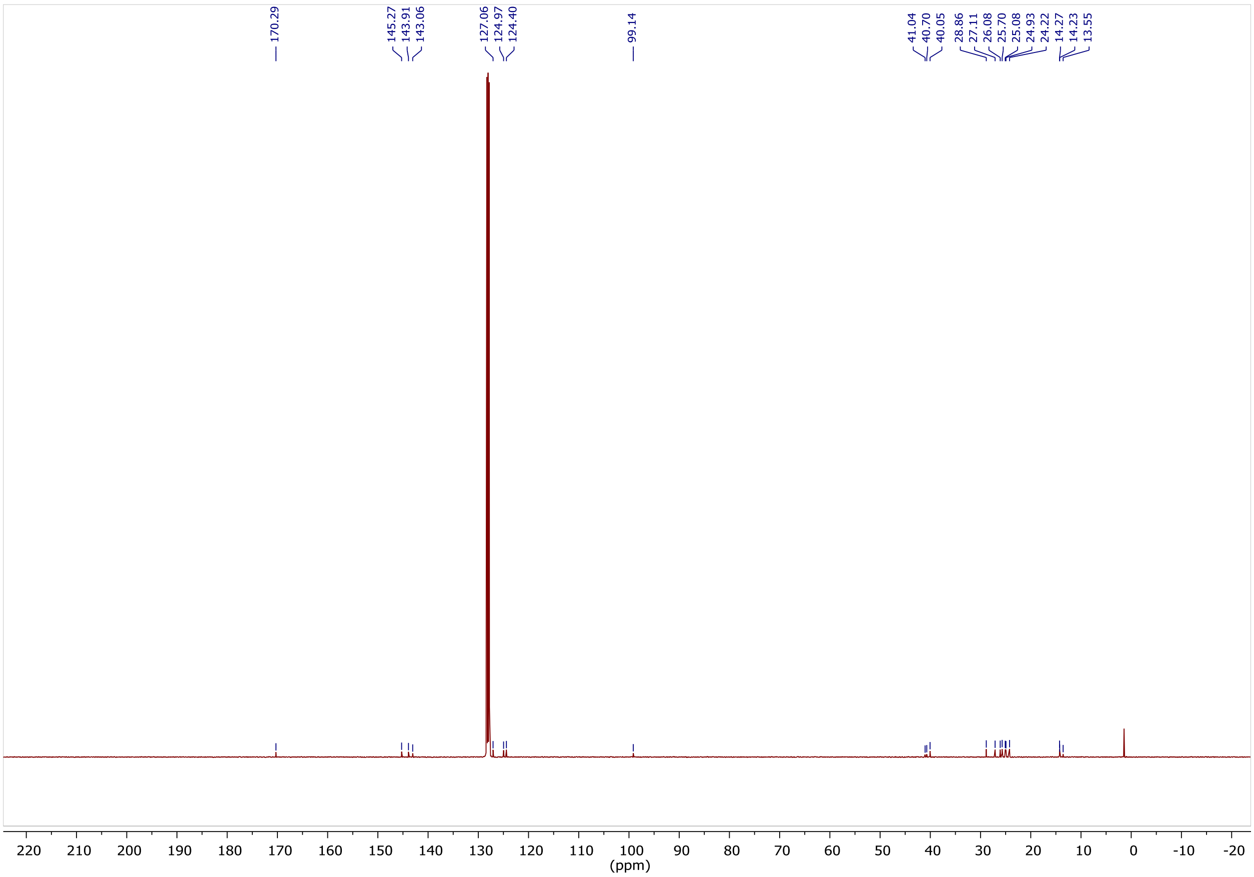

Figure 48: ^{13}C NMR spectrum (100.7 MHz, C_6D_6, 25 °C) of $LAl(NEt_2)_2$.

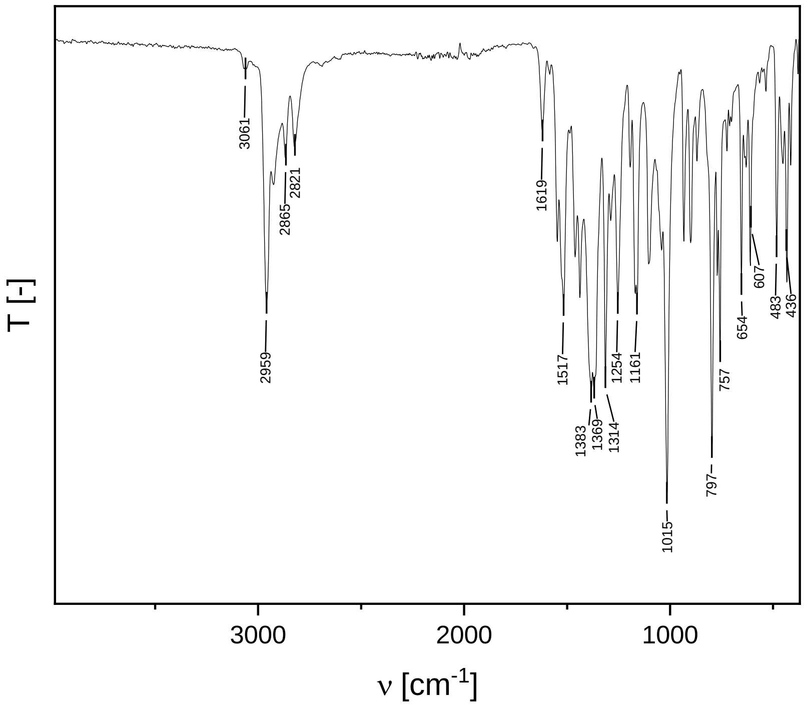

Figure 49: ATR-IR spectrum of $LAl(NEt_2)_2$.

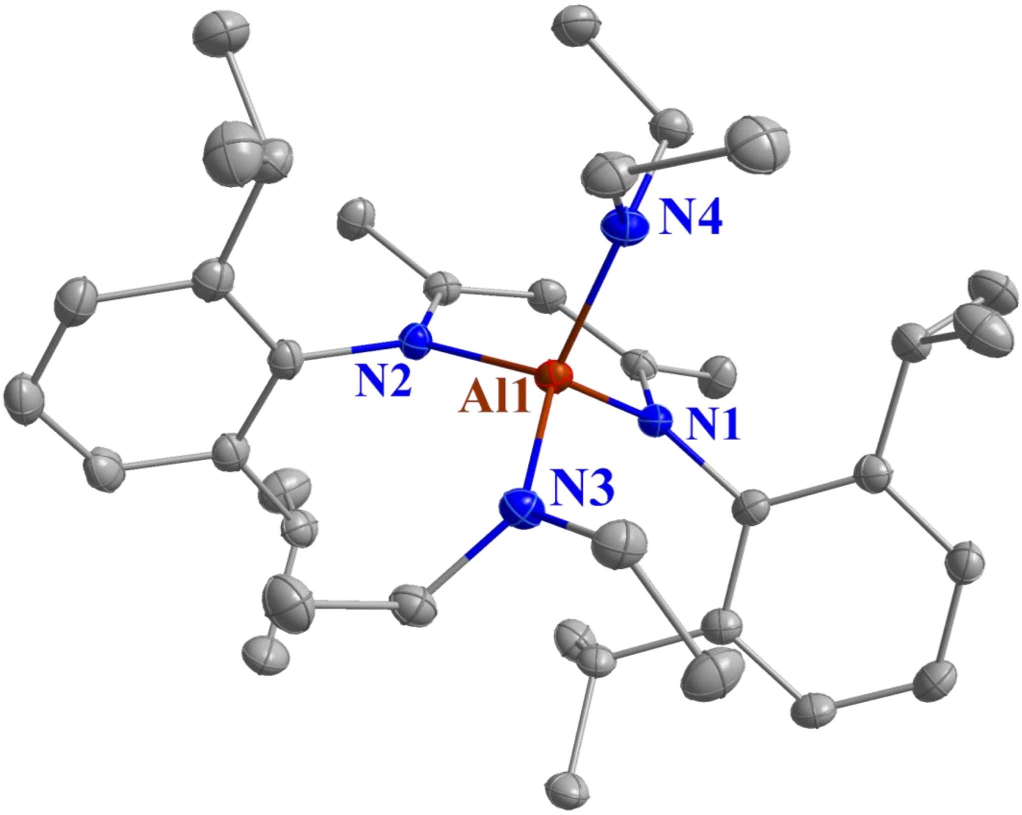

Figure 50: Molecular structure of $LAl(NEt_2)_2$ in the crystal. H atoms have been omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

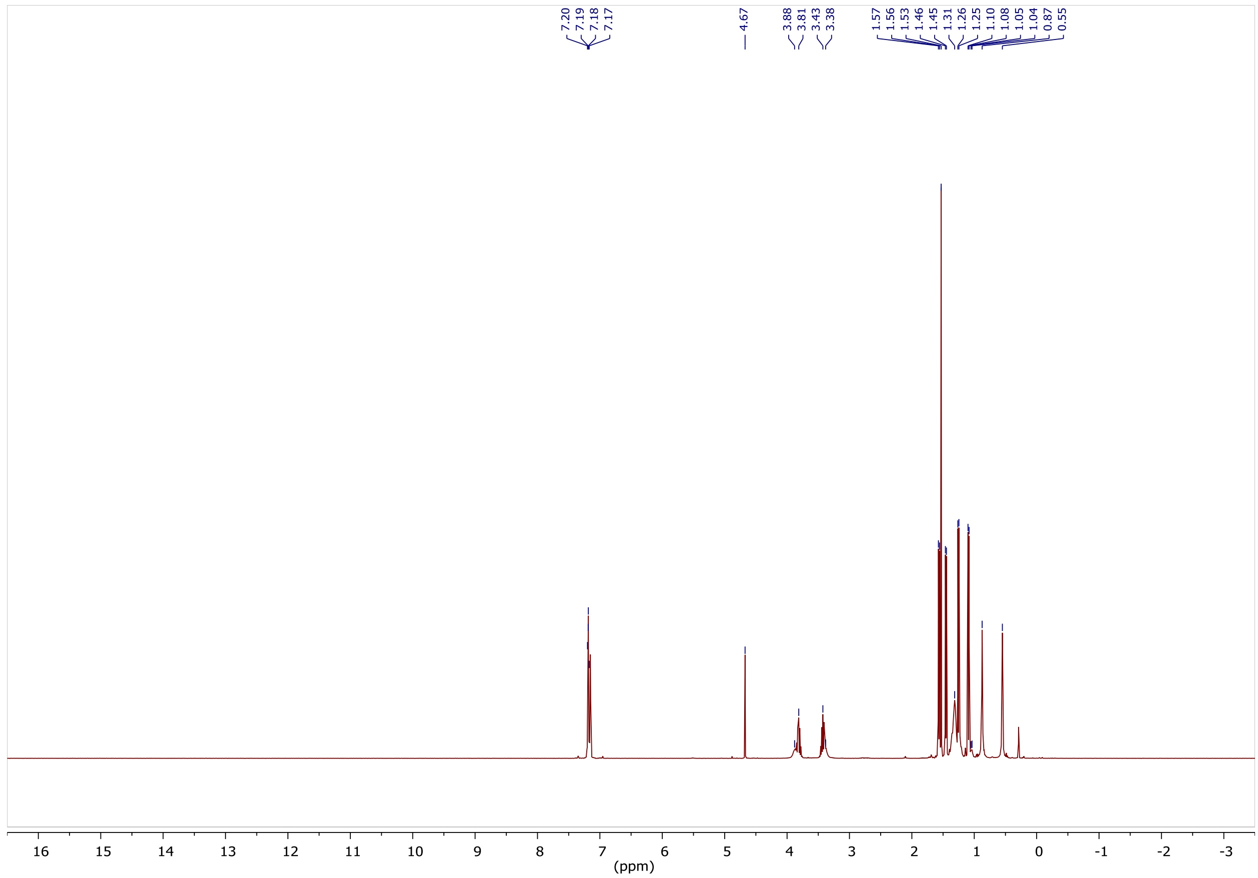

Figure 51: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $L(Et_2N)GaTEMPO$ (**13**).

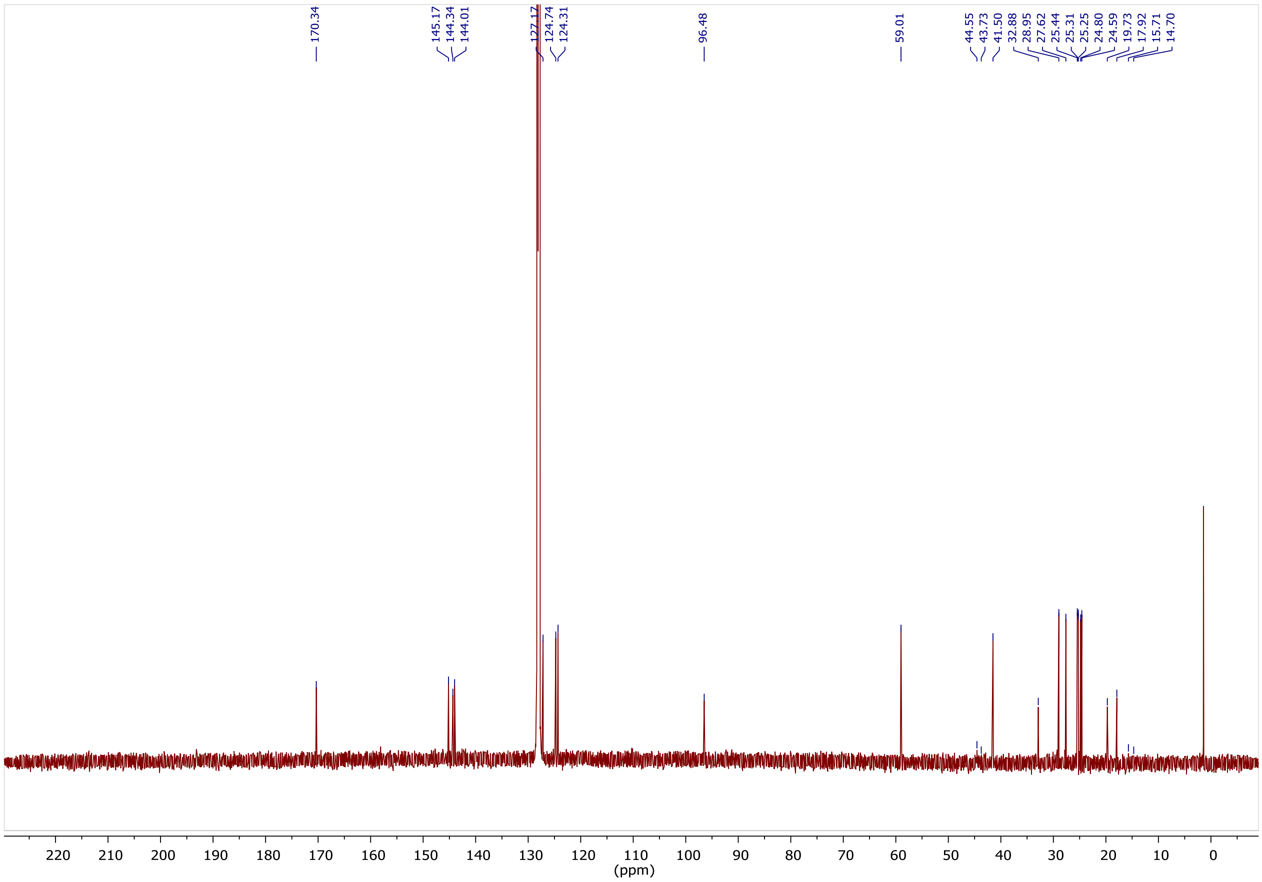

Figure 52: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of L(Et_2N)GaTEMPO (**13**).

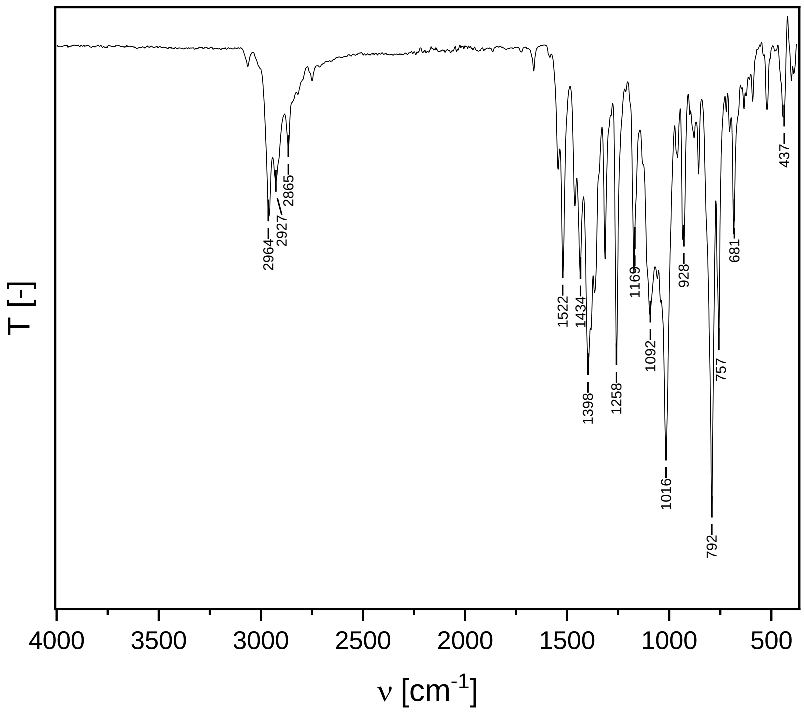

Figure 53: ATR-IR spectrum of L(Et_2N)GaTEMPO (**13**).

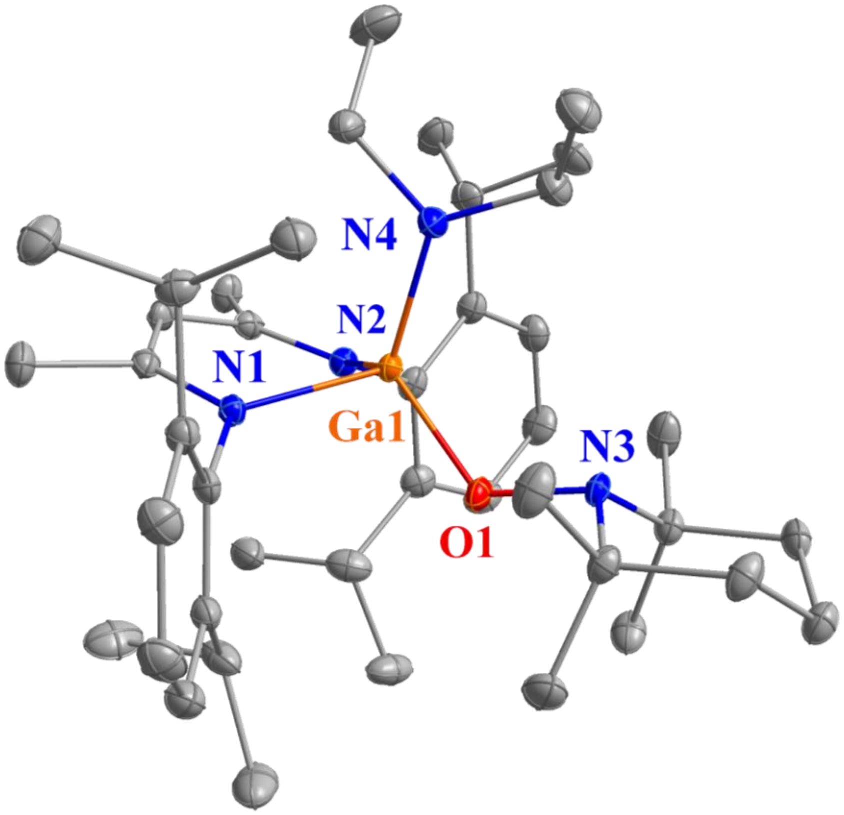

Figure 54: Molecular structure of L(Et$_2$N)GaTEMPO (**13**) in the crystal. H atoms have been omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

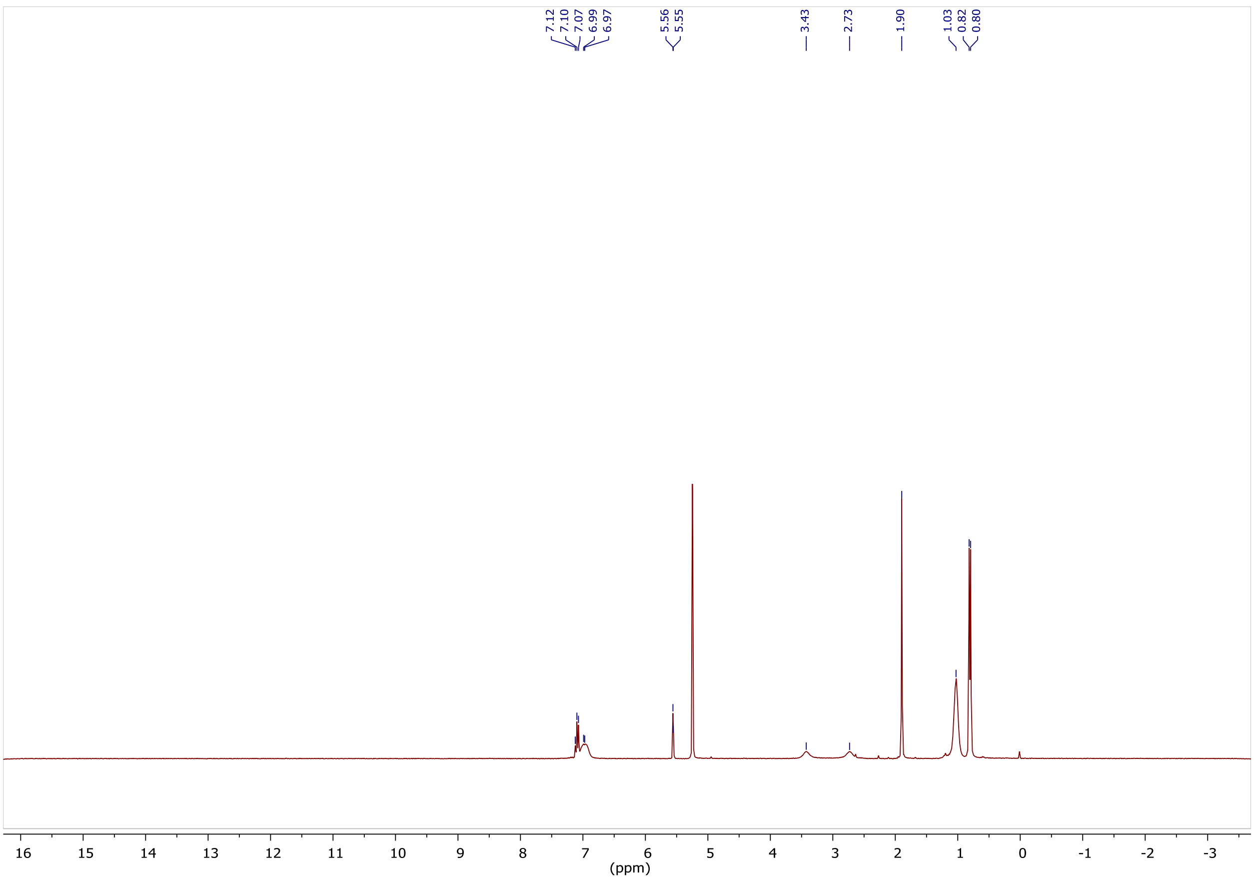

Figure 55: ^{1}H NMR spectrum (300 MHz, DCM-d$_2$, 25 °C) of [L(TfO)GaSb]$_2$ (**14**).

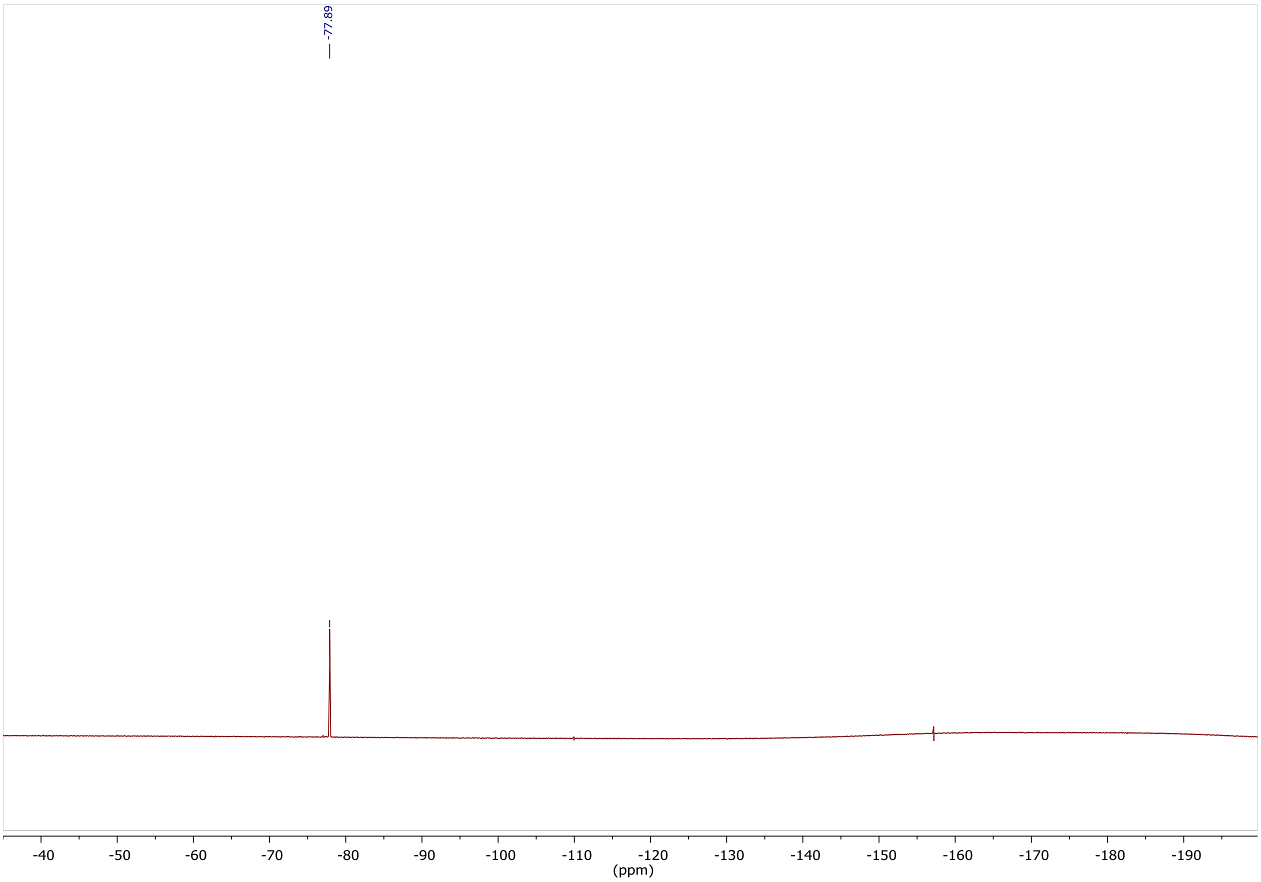

Figure 56: ^{19}F NMR spectrum (282.3 MHz, DCM-d_2, 25 °C) of $[L(TfO)GaSb]_2$ (**14**).

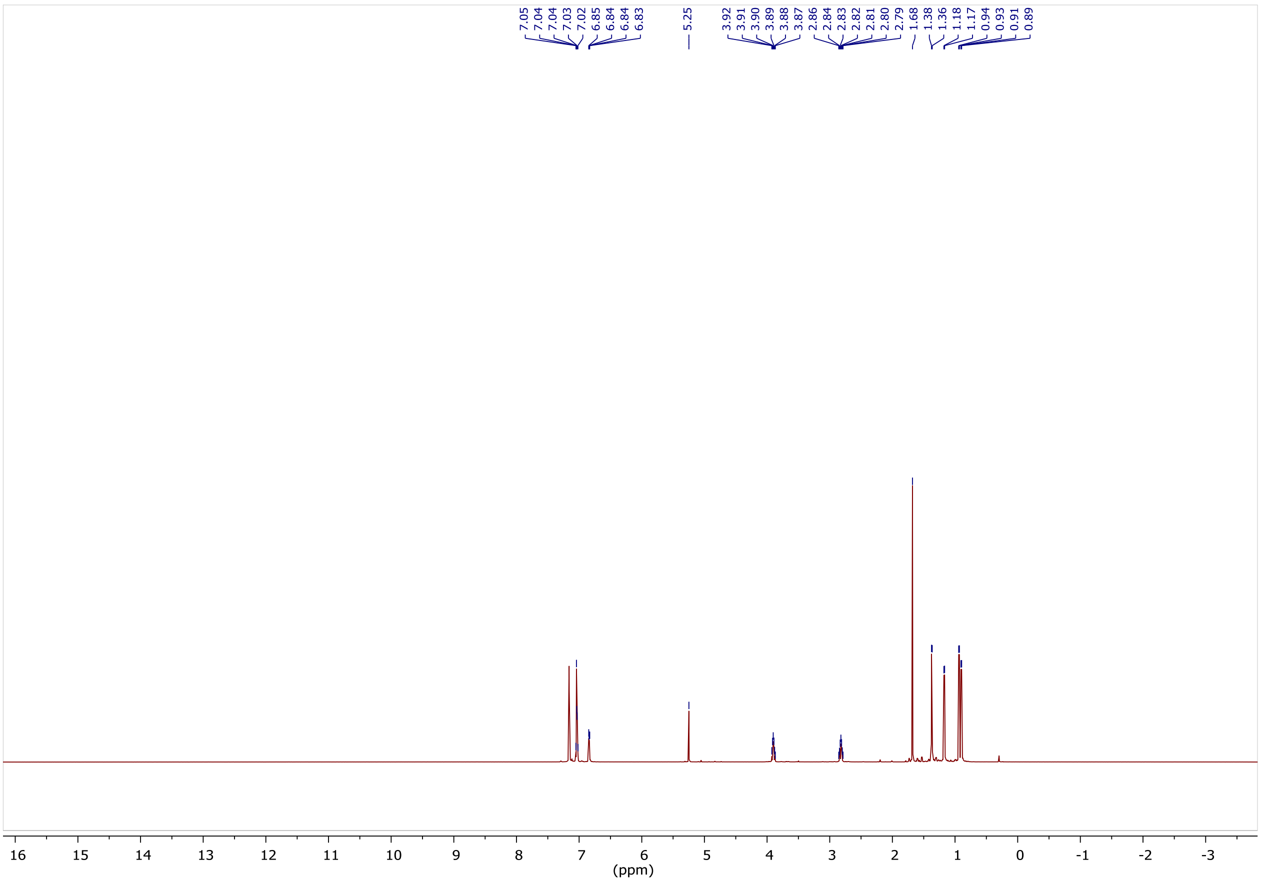

Figure 57: ^{1}H NMR spectrum (300 MHz, C_6D_6, 25 °C) of $[L(TfO)GaSb]_2$ (**14**).

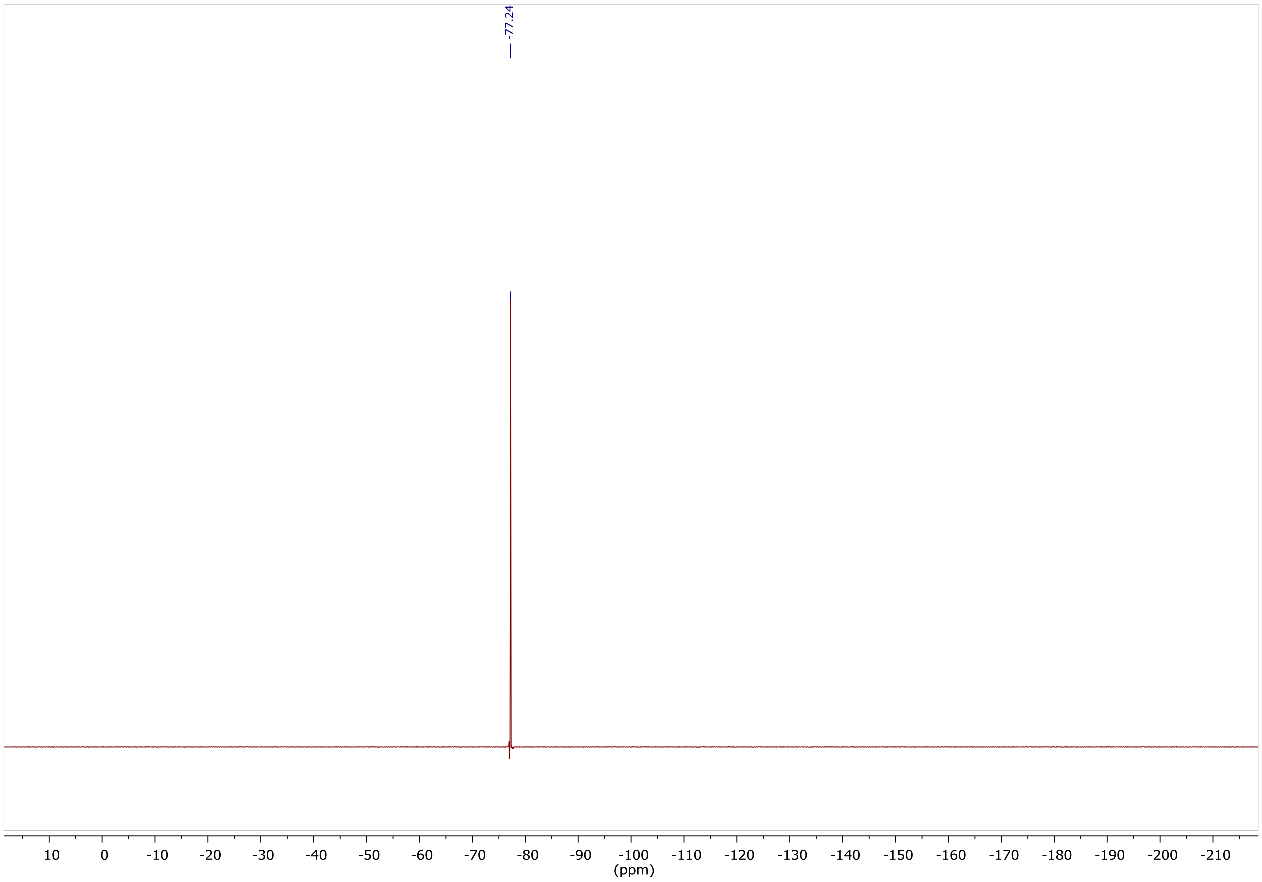

Figure 58: ^{19}F NMR spectrum (282.3 MHz, C_6D_6, 25 °C) of $[L(TfO)GaSb]_2$ (**14**).

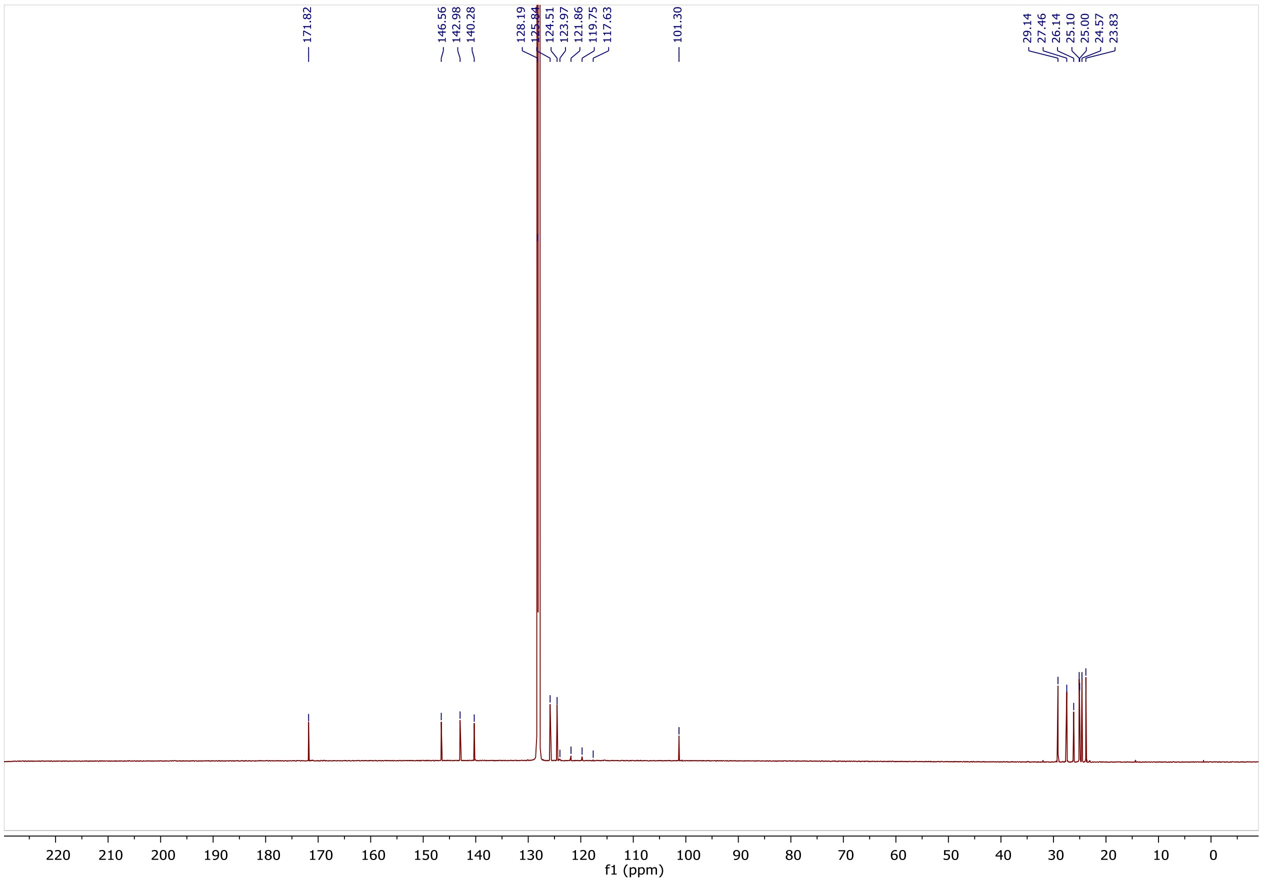

Figure 59: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(TfO)GaSb]_2$ (**14**).

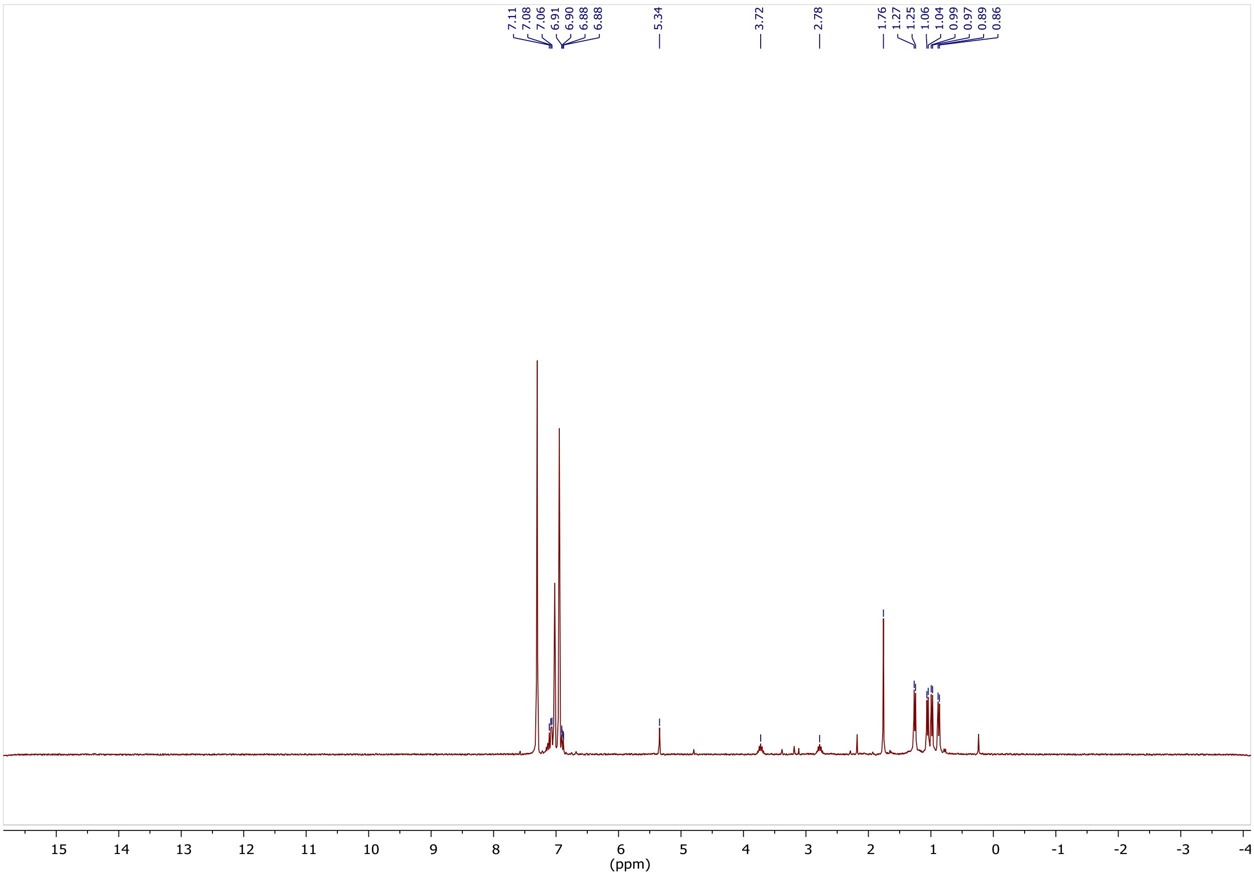

Figure 60: ^{1}H NMR spectrum (300 MHz, C_6D_5Br,25 °C) of $[L(TfO)GaSb]_2$ (**14**).

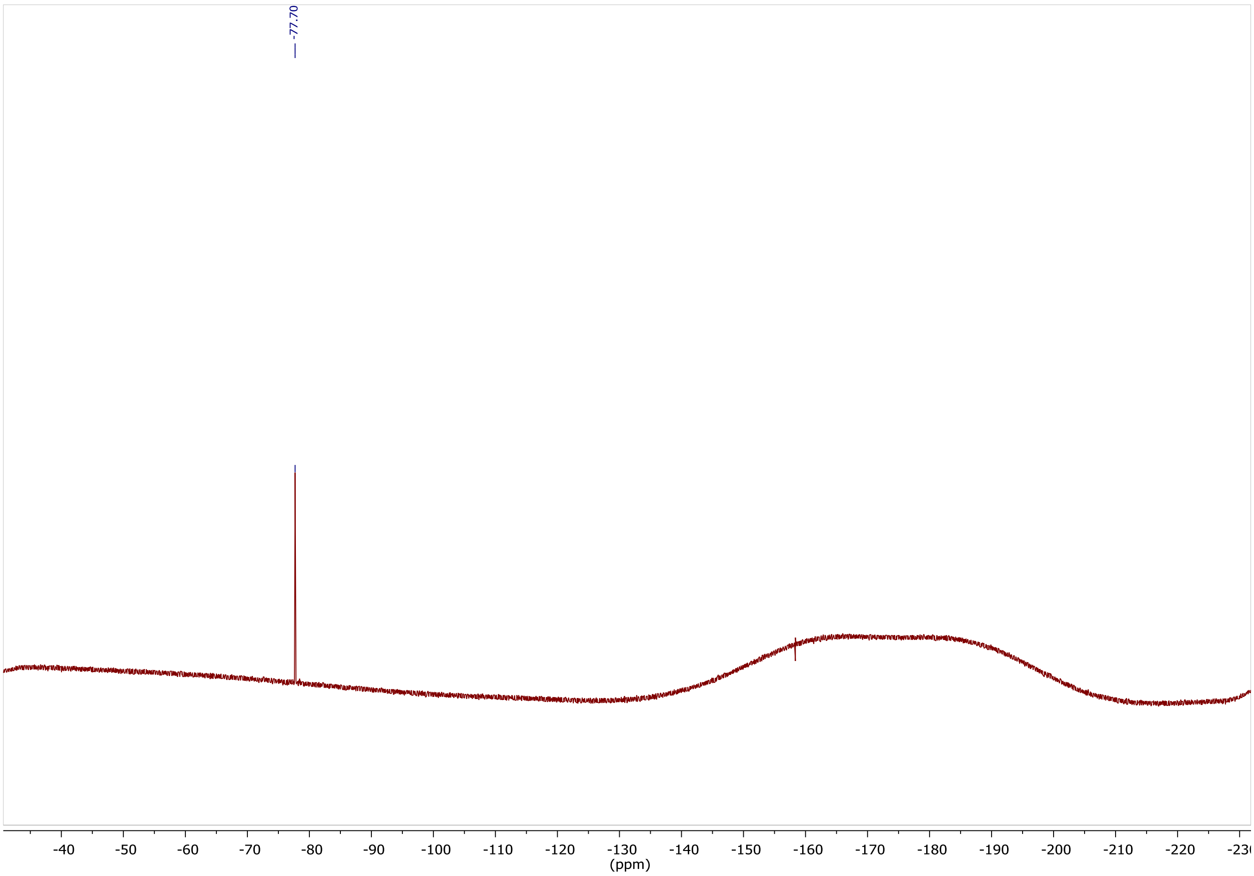

Figure 61: ^{19}F NMR spectrum (282.4 MHz, C_6D_5Br,25 °C) of $[L(TfO)GaSb]_2$ (**14**).

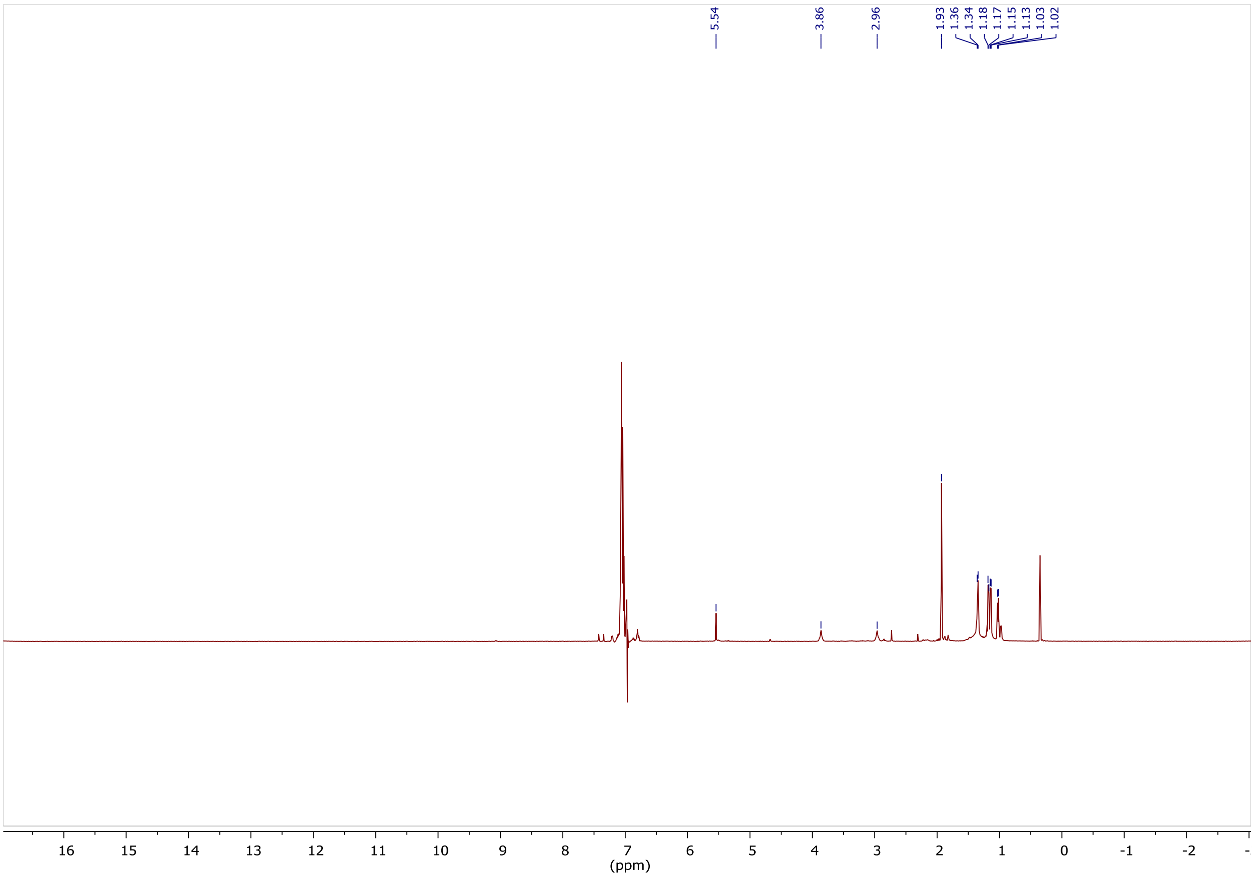

Figure 62: [1]H NMR spectrum (600 MHz, $C_6H_4F_2$/C_6D_5Br, suppressing the 2 strongest signals 25°C) [L(TfO)GaSb]$_2$ (**14**).

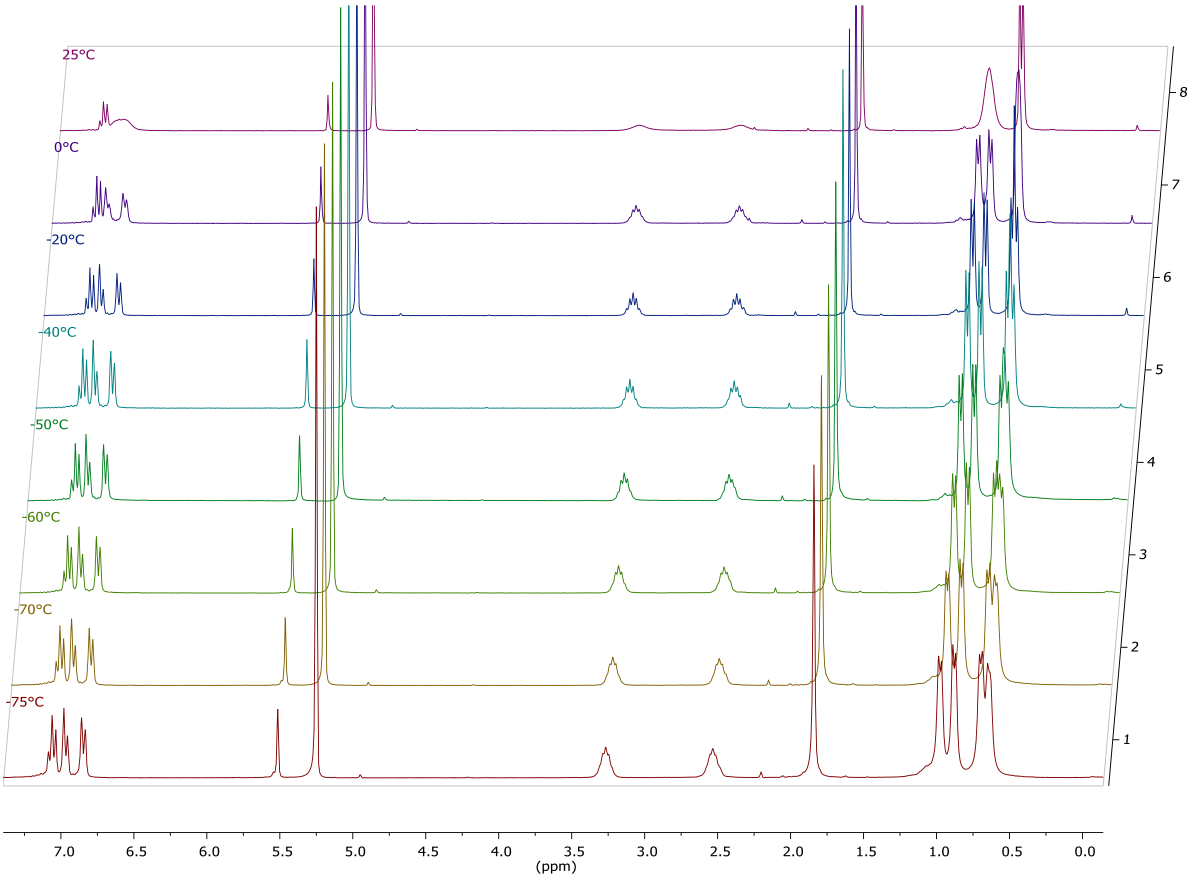

Figure 63: Variable-temperature [1]H NMR spectra (300 MHz, C_6D_6, −75–25 °C) of [L(TfO)GaSb]$_2$ (**14**).

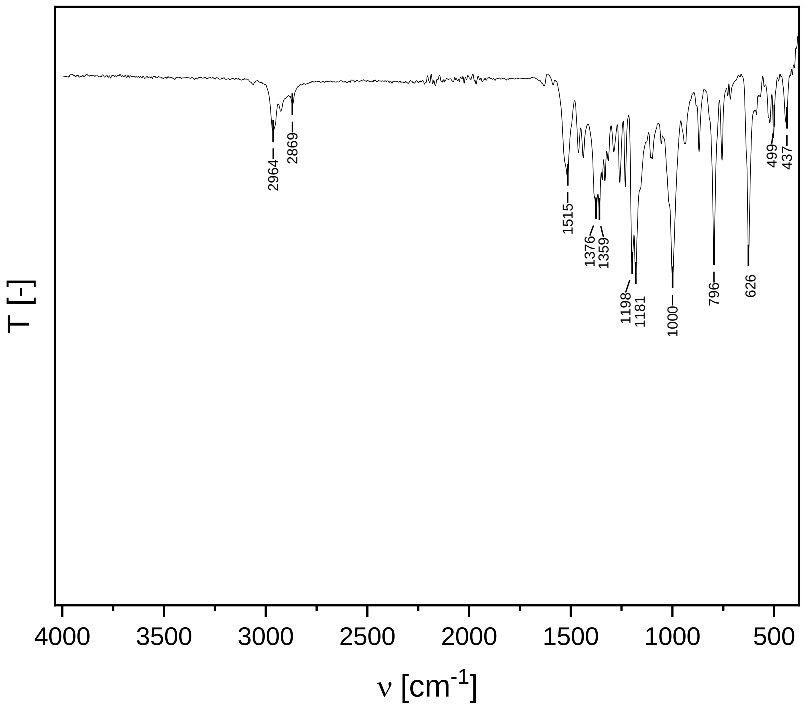

Figure 64: ATR-IR spectrum of $[L(TfO)GaSb]_2$ (**14**).

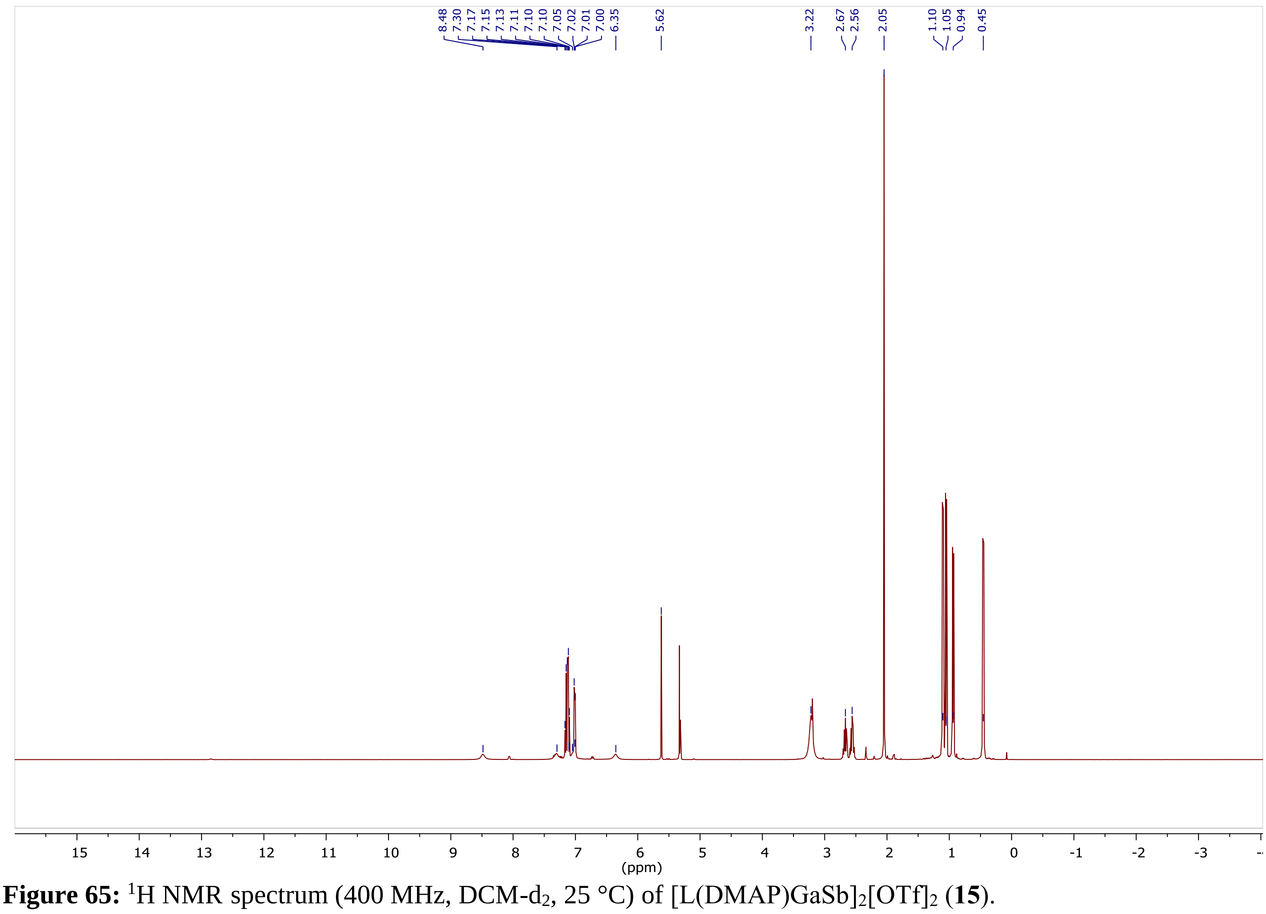

Figure 65: ^{1}H NMR spectrum (400 MHz, DCM-d_2, 25 °C) of $[L(DMAP)GaSb]_2[OTf]_2$ (**15**).

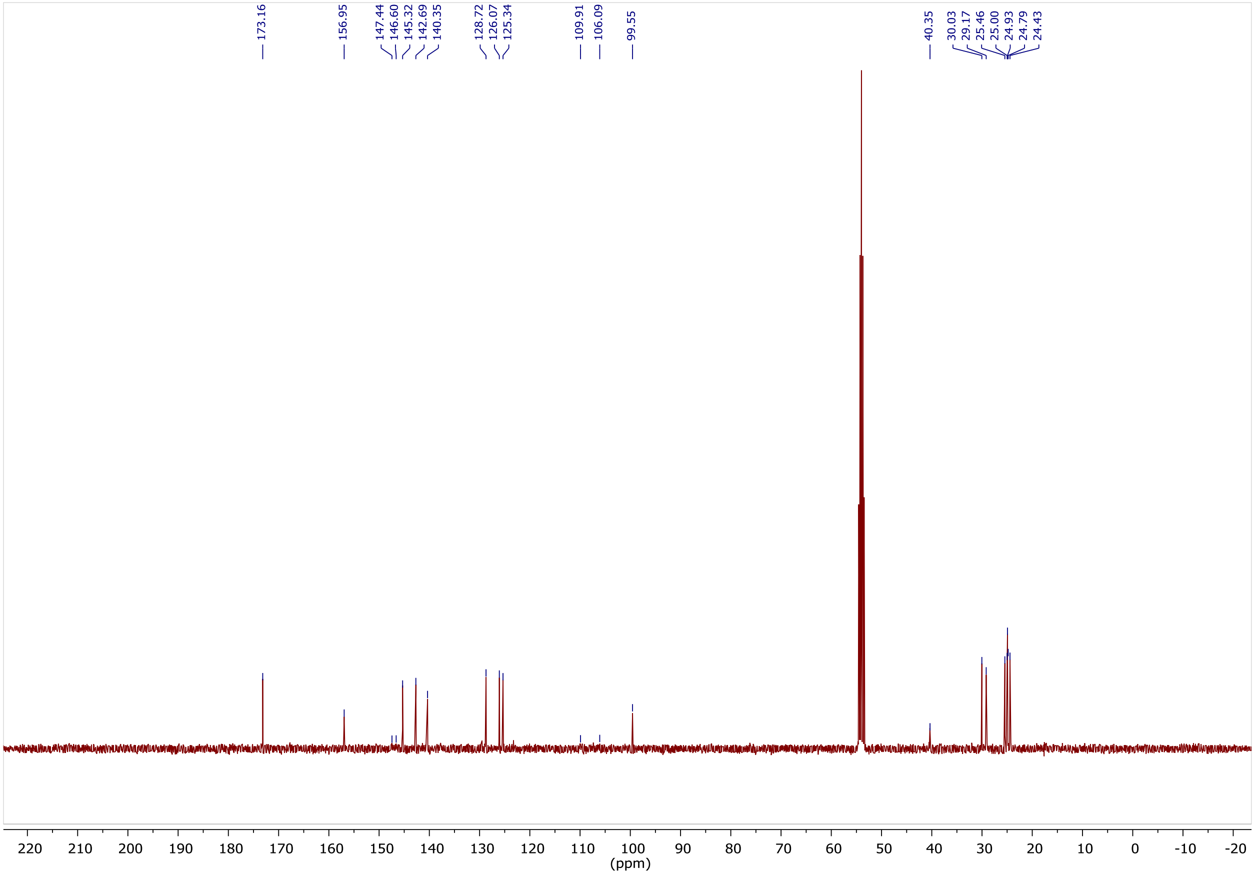

Figure 66: ^{13}C NMR spectrum (100.6 MHz, DCM-d_2, 25 °C) of $[L(DMAP)GaSb]_2[OTf]_2$ (**15**).

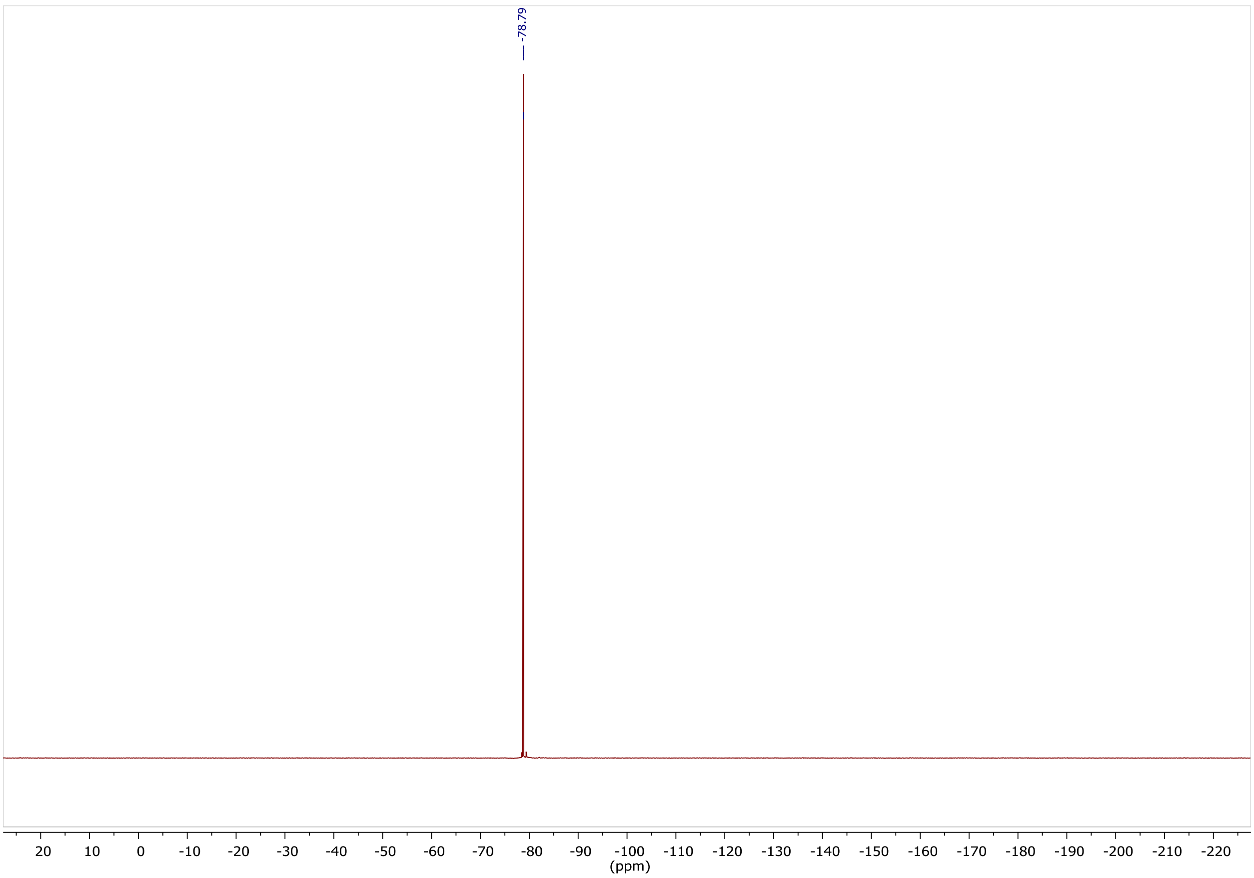

Figure 67: ^{19}F NMR spectrum (376.5 MHz, DCM-d_2, 25 °C) of $[L(DMAP)GaSb]_2[OTf]_2$ (**15**).

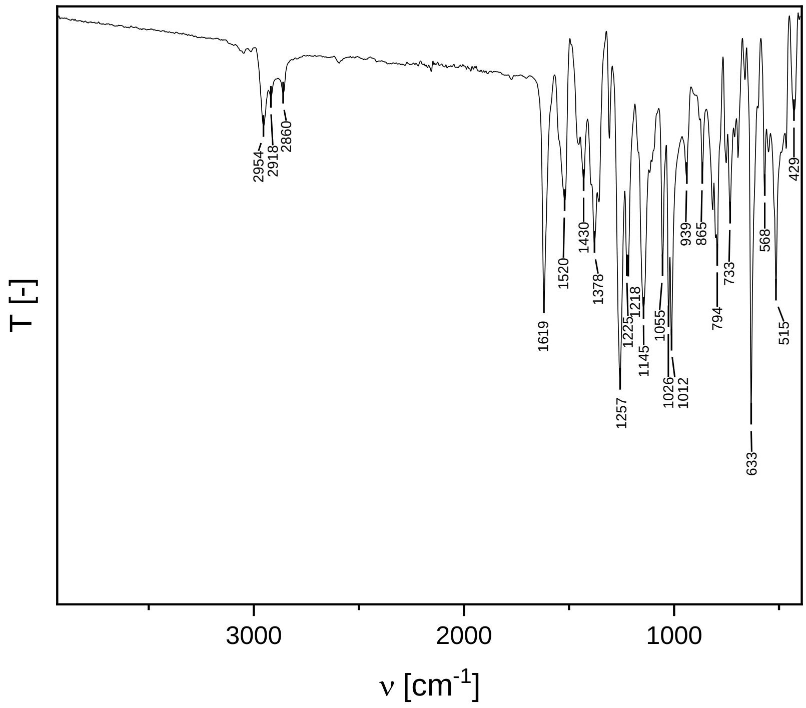

Figure 68: ATR-IR spectrum of $[L(DMAP)GaSb]_2[OTf]_2$ (**15**).

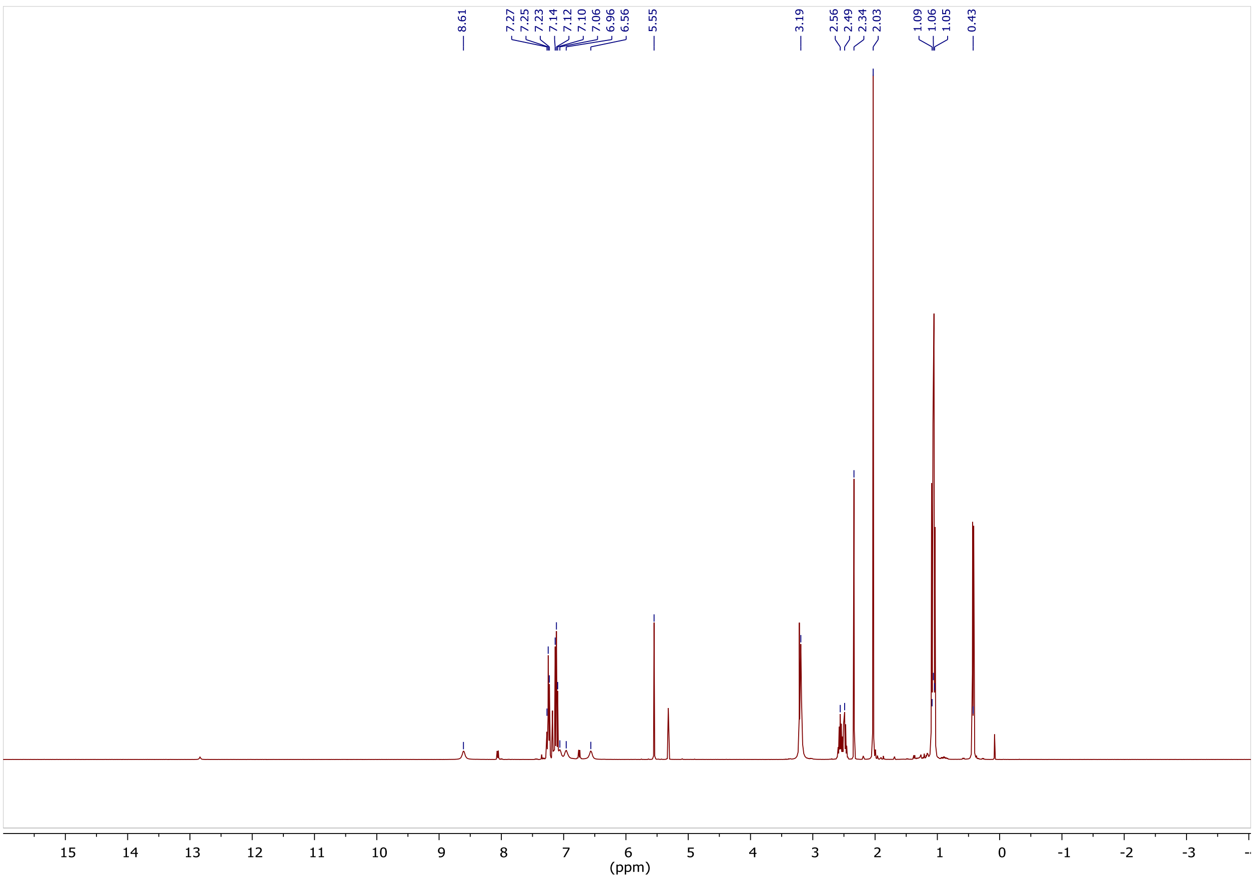

Figure 69: ^{1}H NMR spectrum (400 MHz, DCM-d_2, 25 °C) of $[L(DMAP)GaBi]_2[OTf]_2$ (**16**).

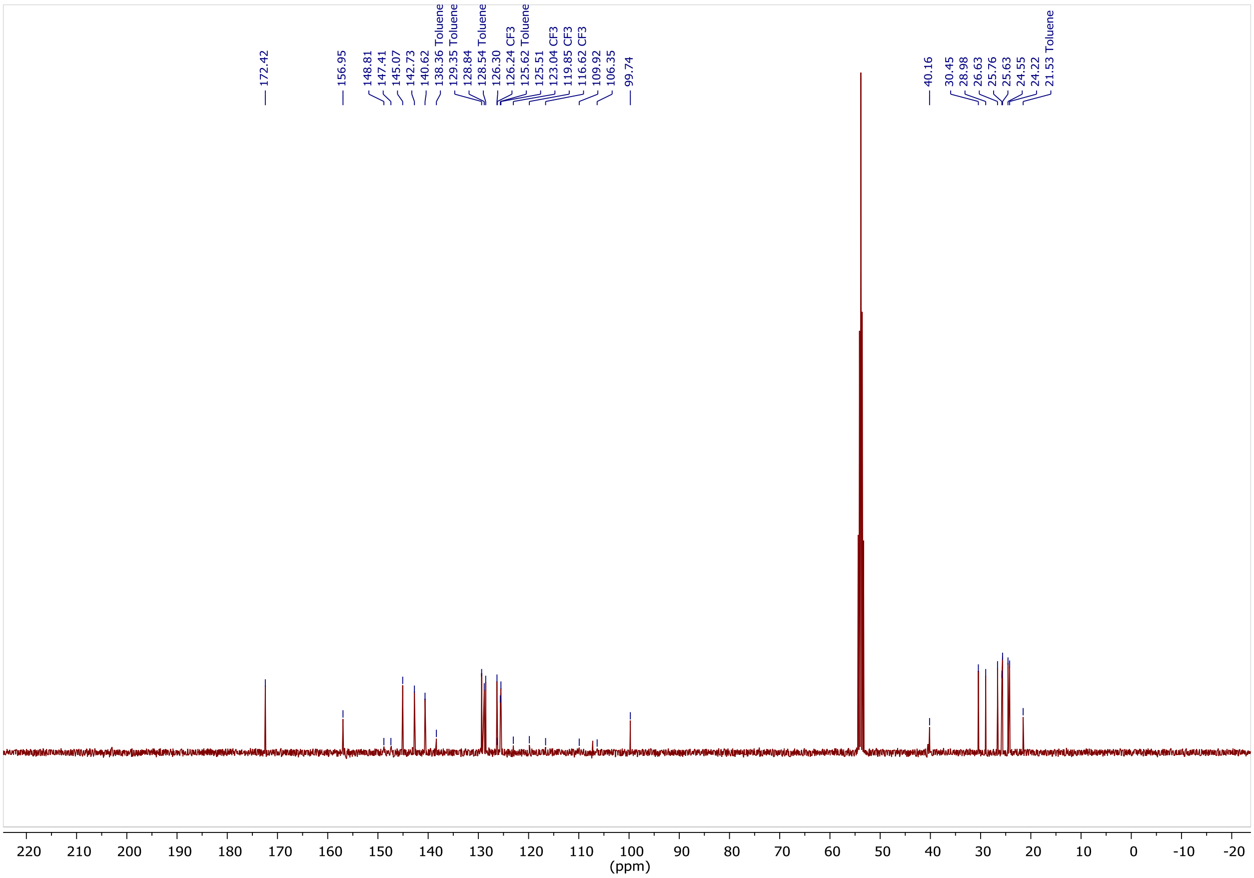

Figure 70: ^{13}C NMR spectrum (100.6 MHz, DCM-d$_2$, 25 °C) of [L(DMAP)GaBi]$_2$[OTf]$_2$ (**16**).

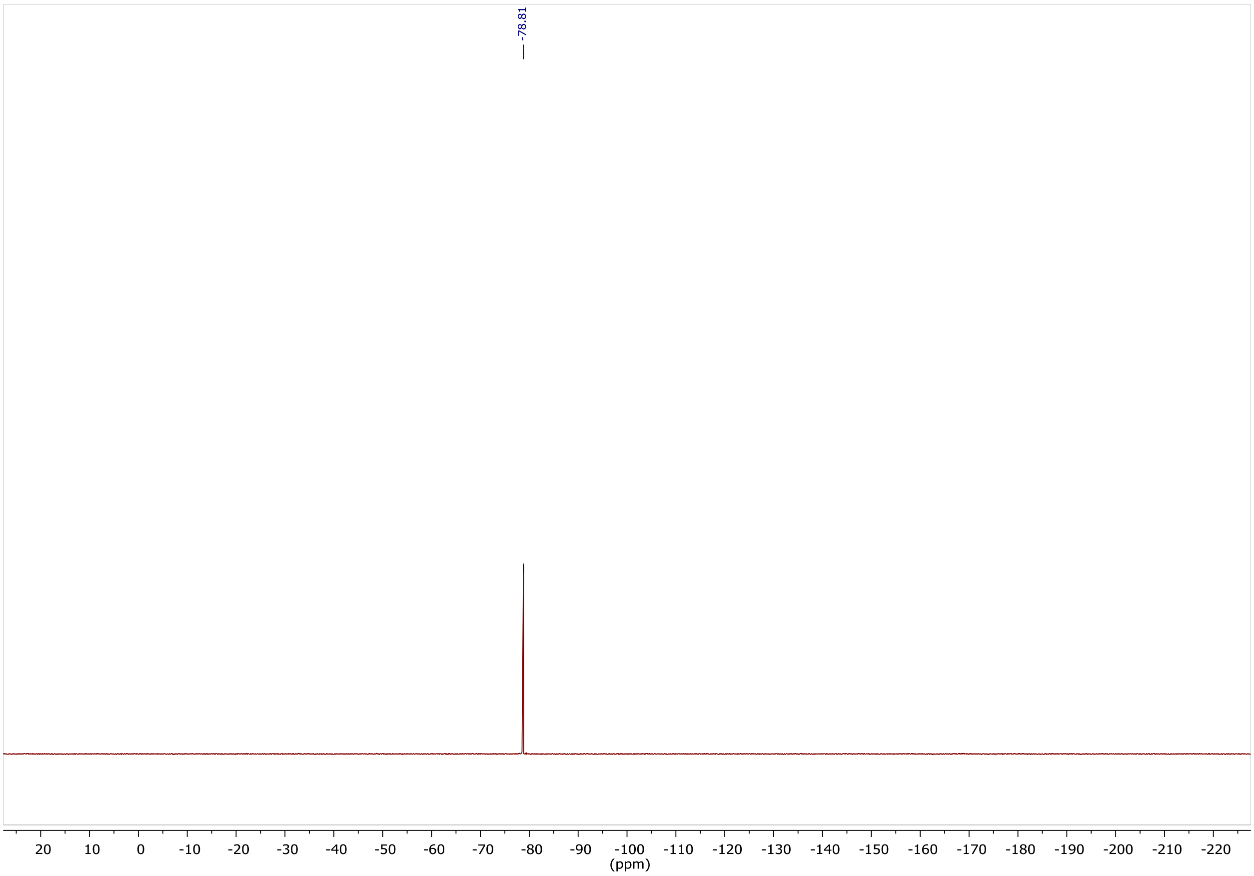

Figure 71: ^{19}F NMR spectrum (376.5 MHz, DCM-d$_2$, 25 °C) of [L(DMAP)GaBi]$_2$[OTf]$_2$ (**16**).

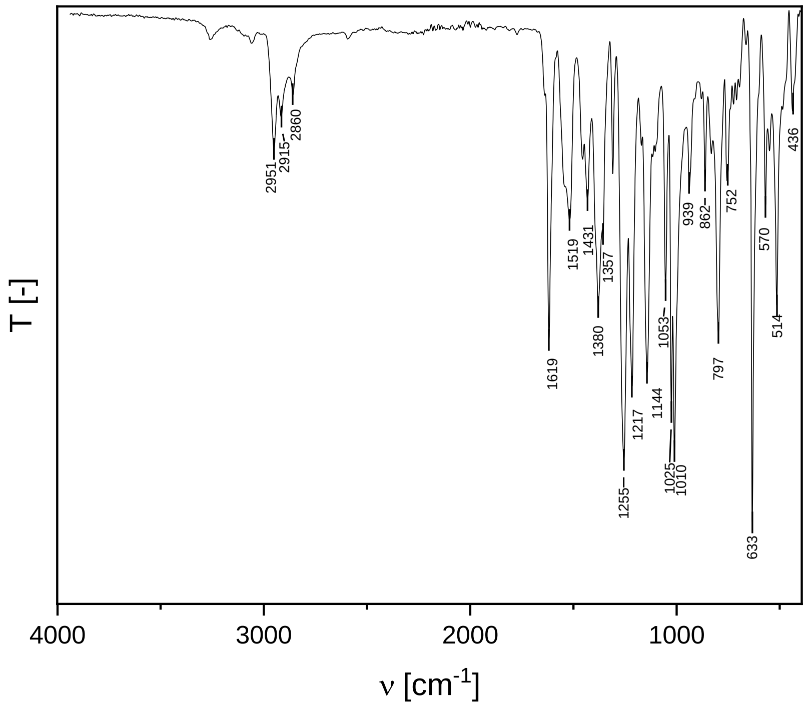

Figure 72: ATR-IR spectrum of $[L(DMAP)GaBi]_2[OTf]_2$ (**16**).

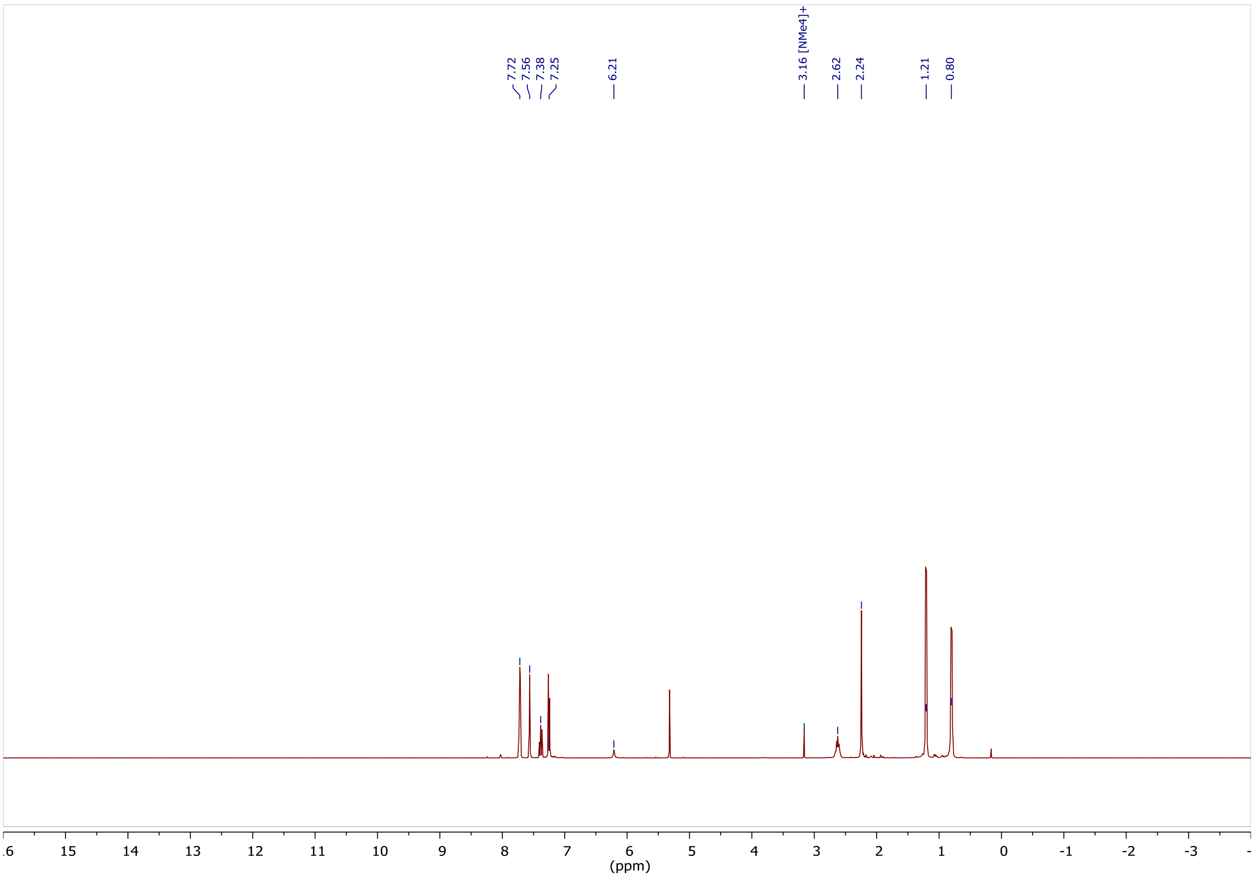

Figure 73: ^{1}H NMR spectrum (400 MHz, DCM-d$_2$, 25 °C) of $[LGaSb]_2[BarF_{24}]_2$ (**17**).

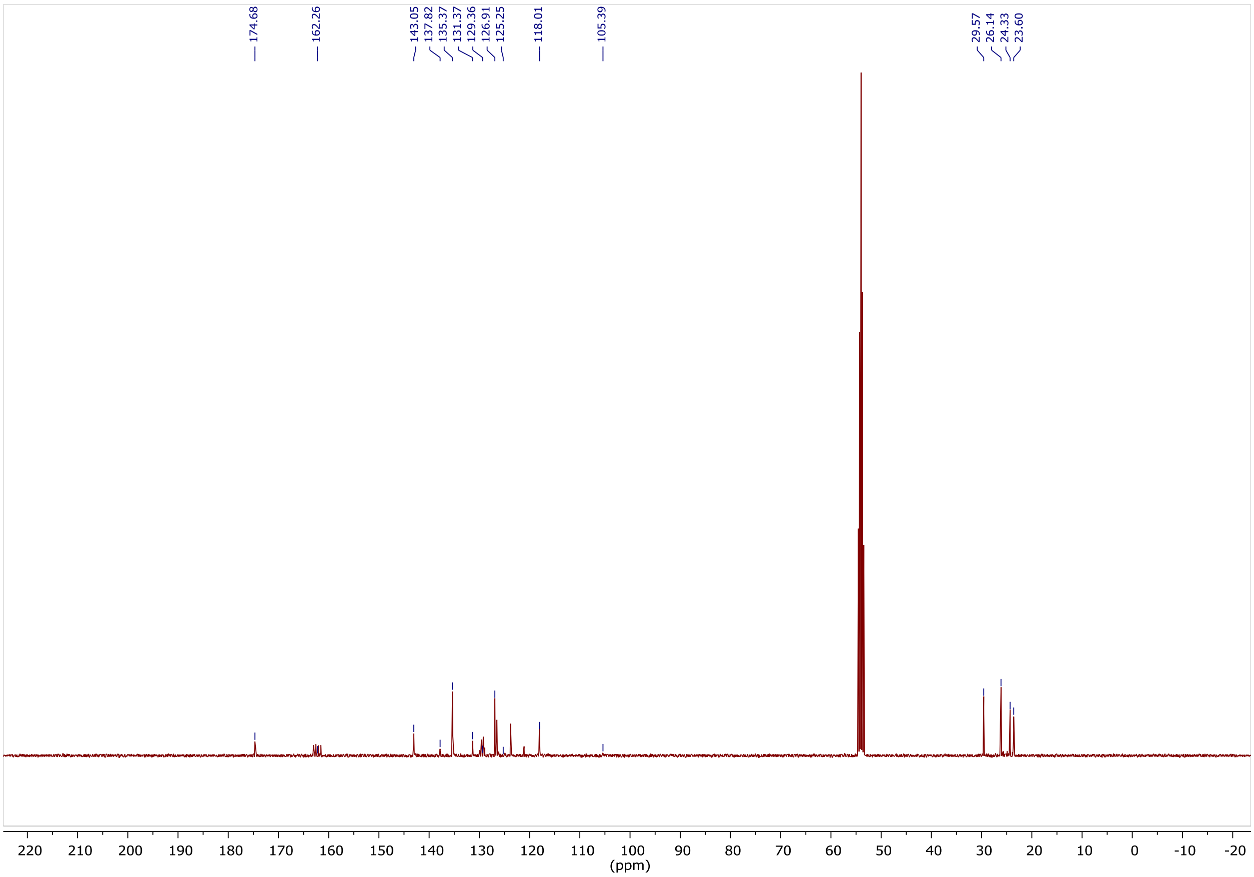

Figure 74: ^{13}C NMR spectrum (150.9 MHz, DCM-d$_2$, 25 °C) of [LGaSb]$_2$[BarF$_{24}$]$_2$ (**17**).

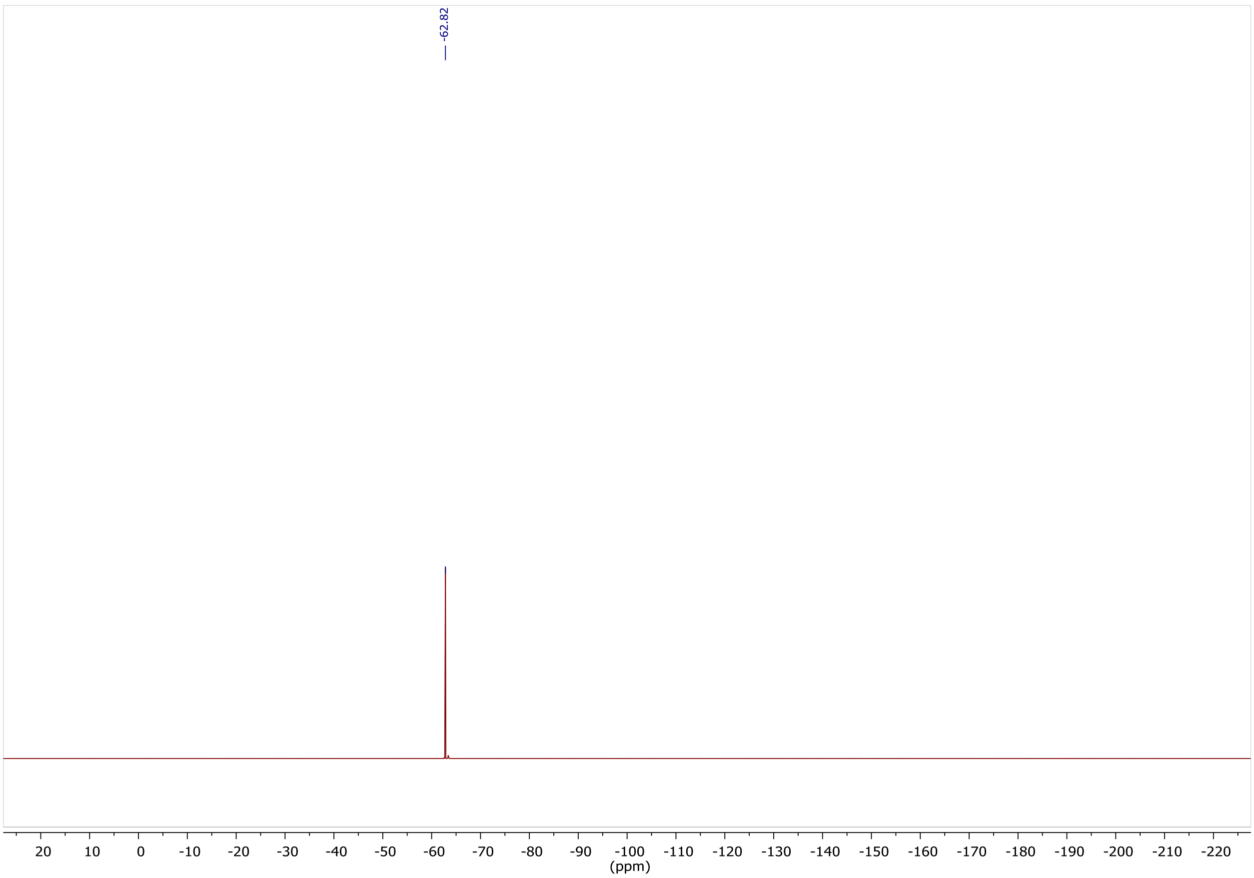

Figure 75: ^{19}F NMR spectrum (376.5 MHz, DCM-d$_2$, 25 °C) of [LGaSb]$_2$[BarF$_{24}$]$_2$ (**17**).

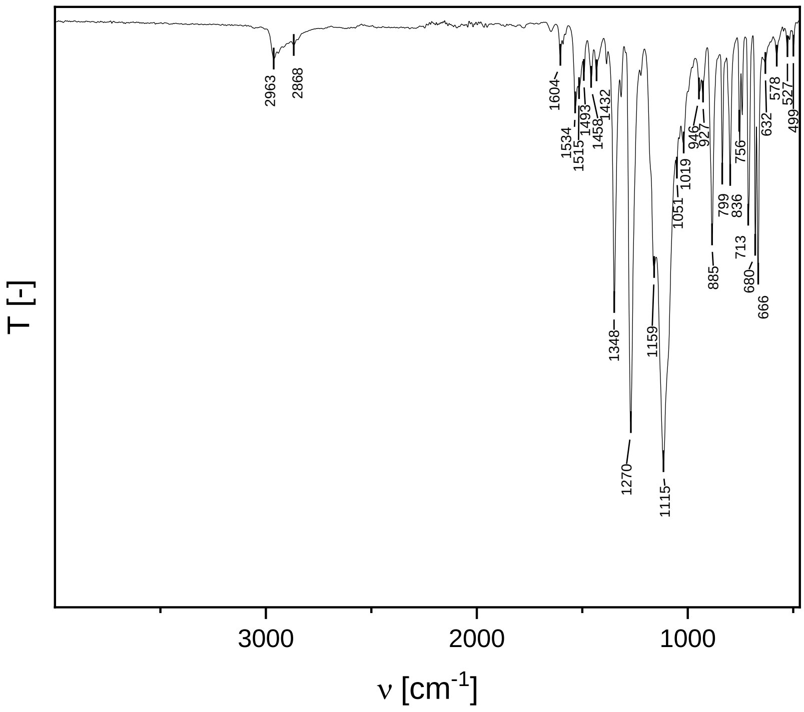

Figure 76: ATR-IR spectrum of $[LGaSb]_2[BarF_{24}]_2$ (**17**).

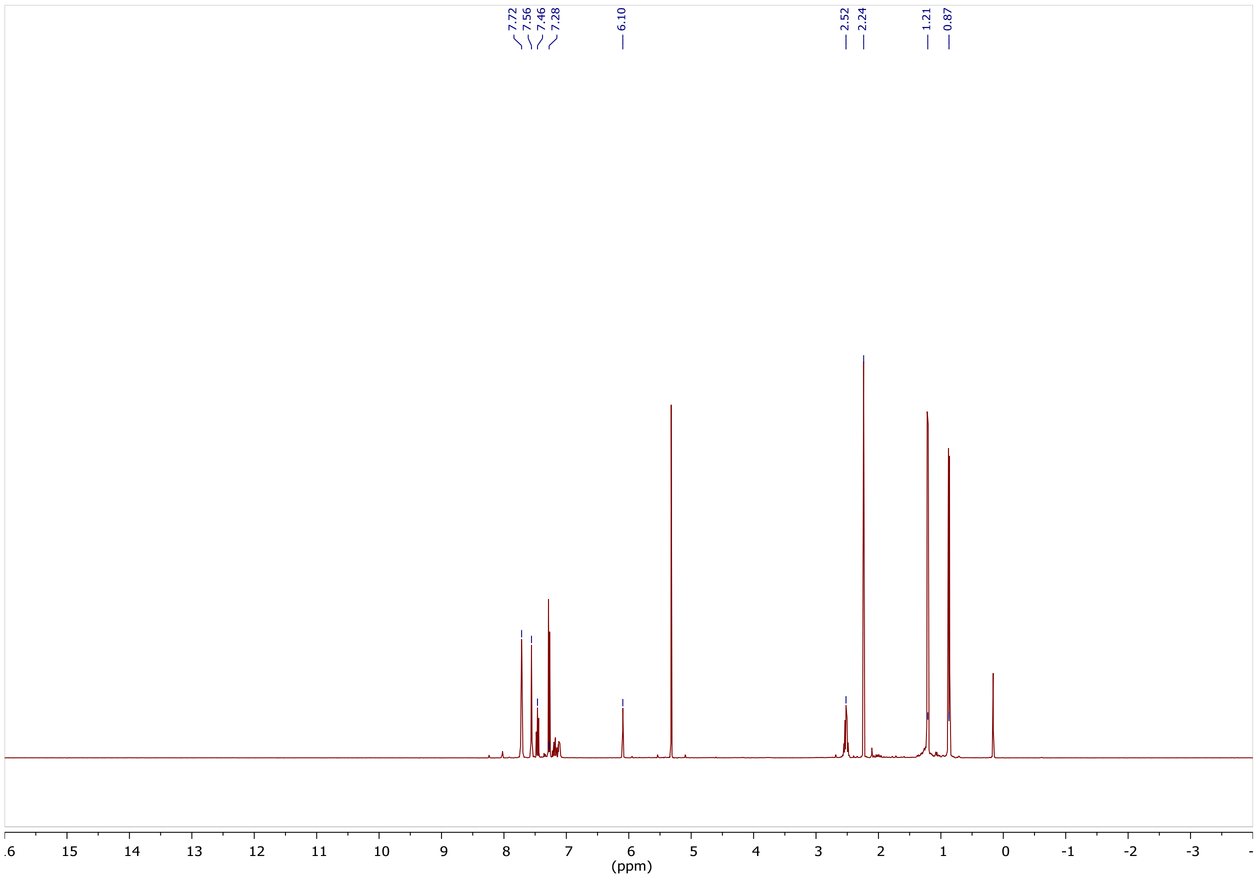

Figure 77: ^{1}H NMR spectrum (400 MHz, DCM-d$_2$, 25 °C) of $[LGaBi]_2[BarF_{24}]_2$ (**18**).

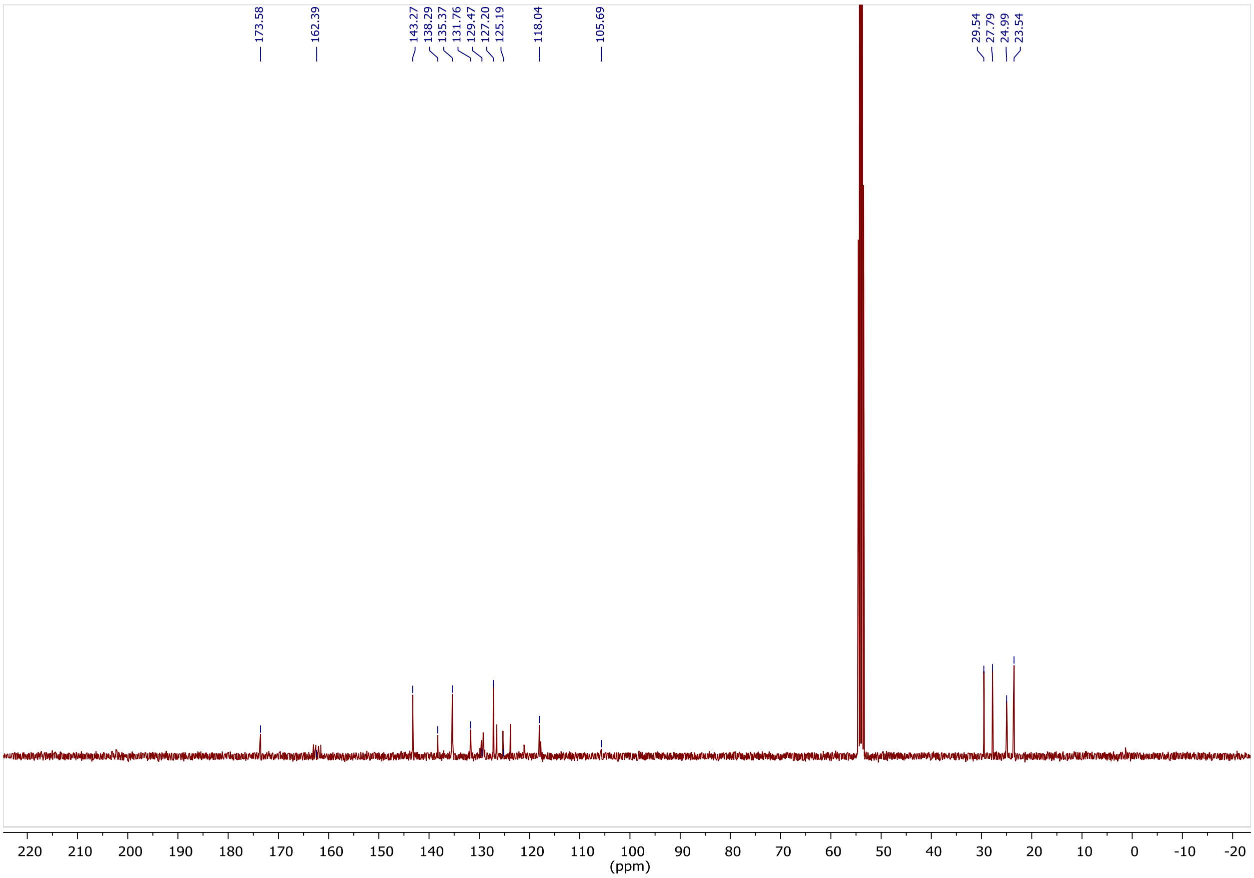

Figure 78: ^{13}C NMR spectrum (150.9 MHz, DCM-d$_2$, 25 °C) of $[LGaBi]_2[BarF_{24}]_2$ (**18**).

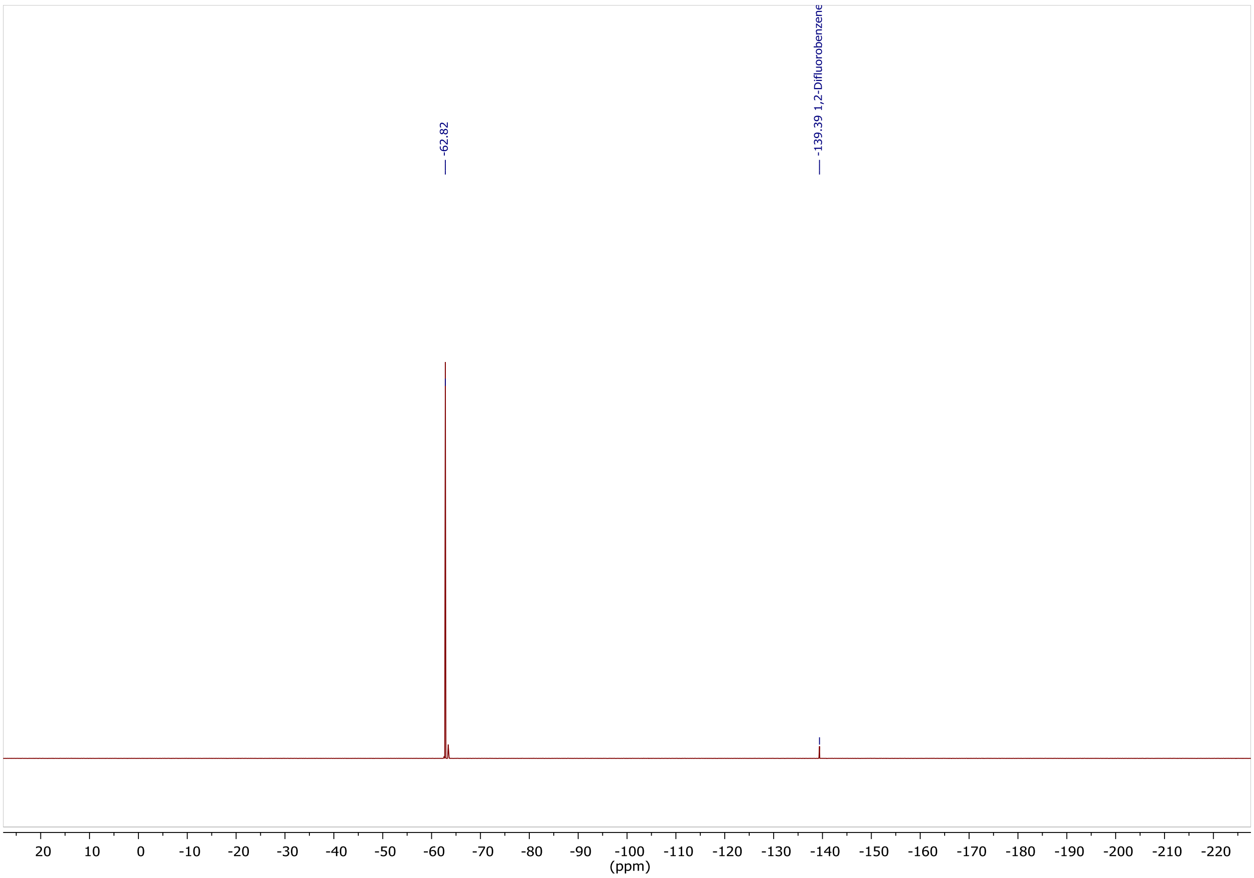

Figure 79: ^{19}F NMR spectrum (376.5 MHz, DCM-d2, 25 °C) of $[LGaBi]_2[BarF_{24}]_2$ (**18**).

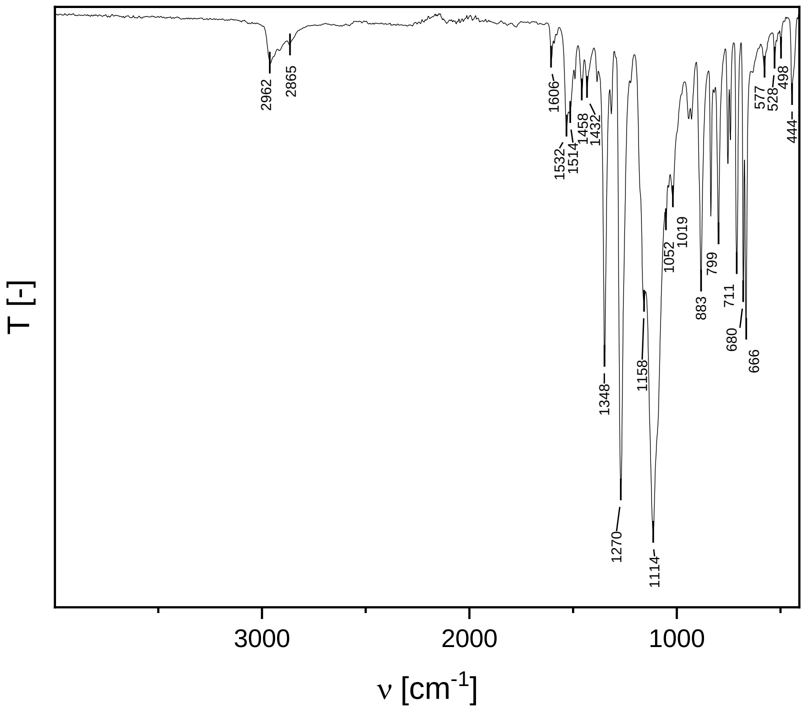

Figure 80: ATR-IR spectrum of $[LGaBi]_2[BarF_{24}]_2$ (**18**).

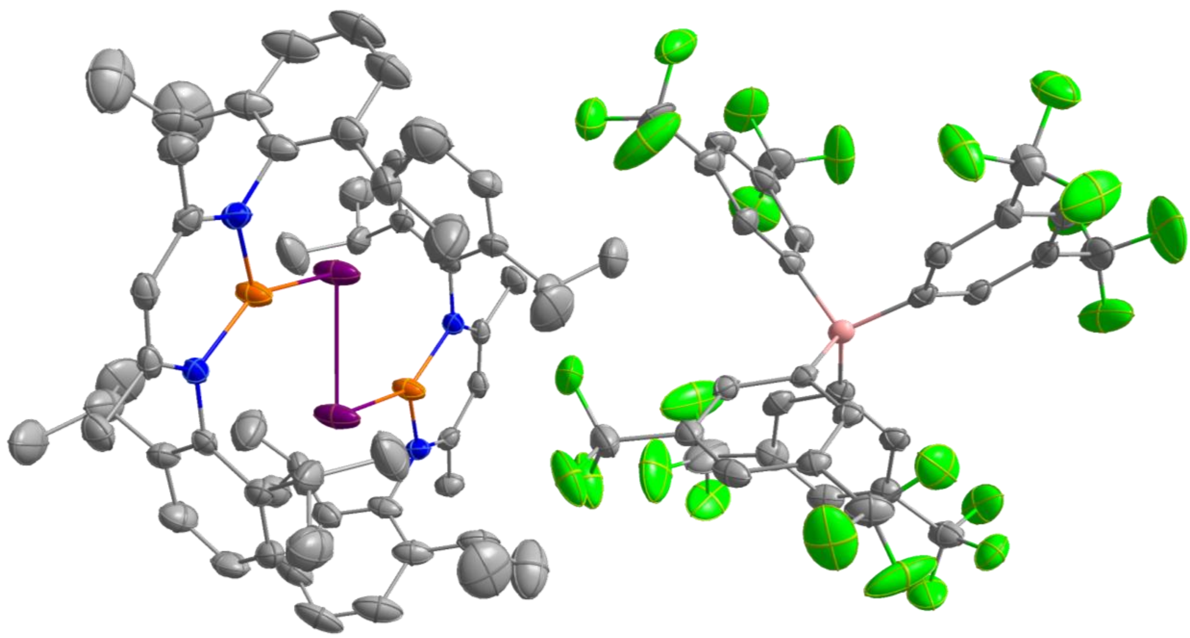

Figure 81: Molecular structure of $[LGaBi]_2[BarF_{24}]_2$ (**18**) in the crystal. H atoms have been omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

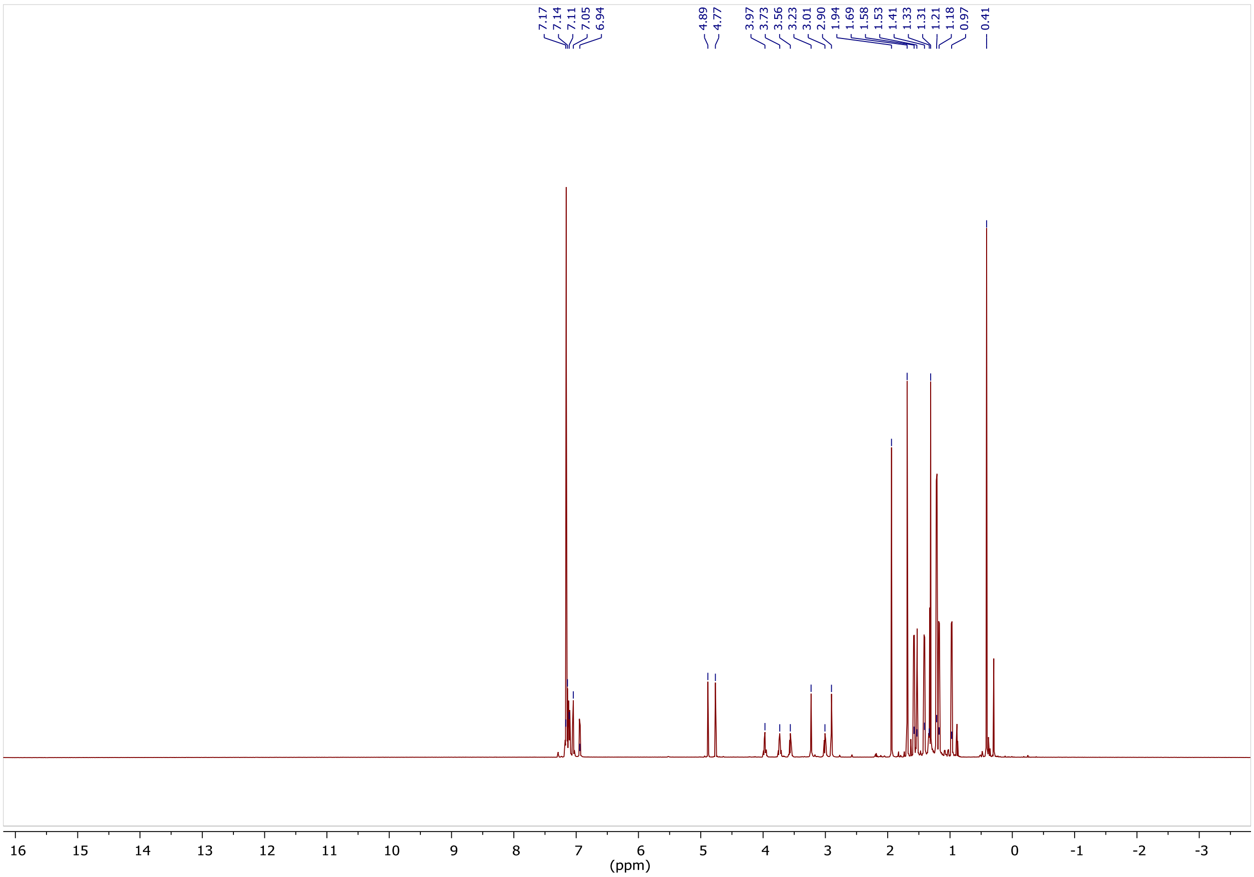

Figure 82: [1]H NMR spectrum (600 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**19**).

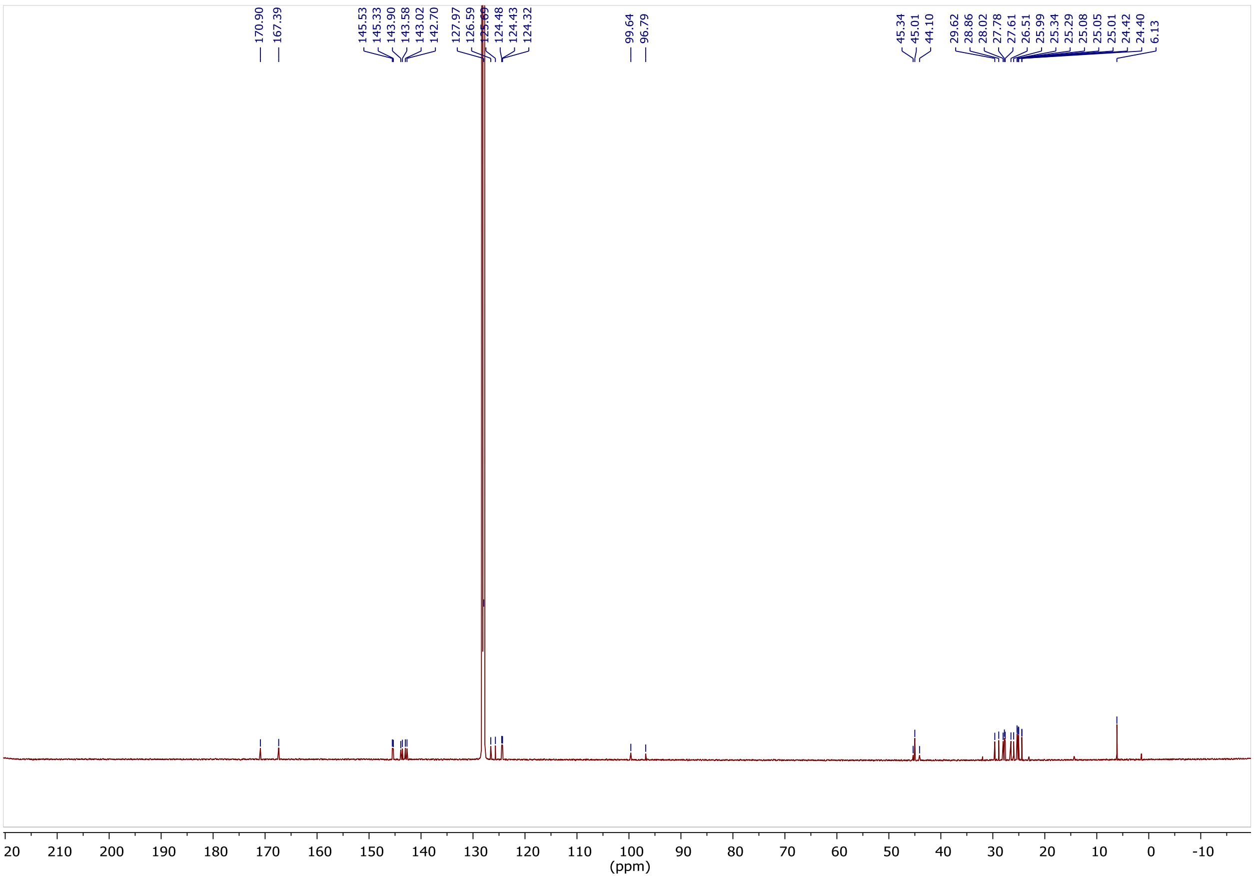

Figure 83: [13]C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**19**).

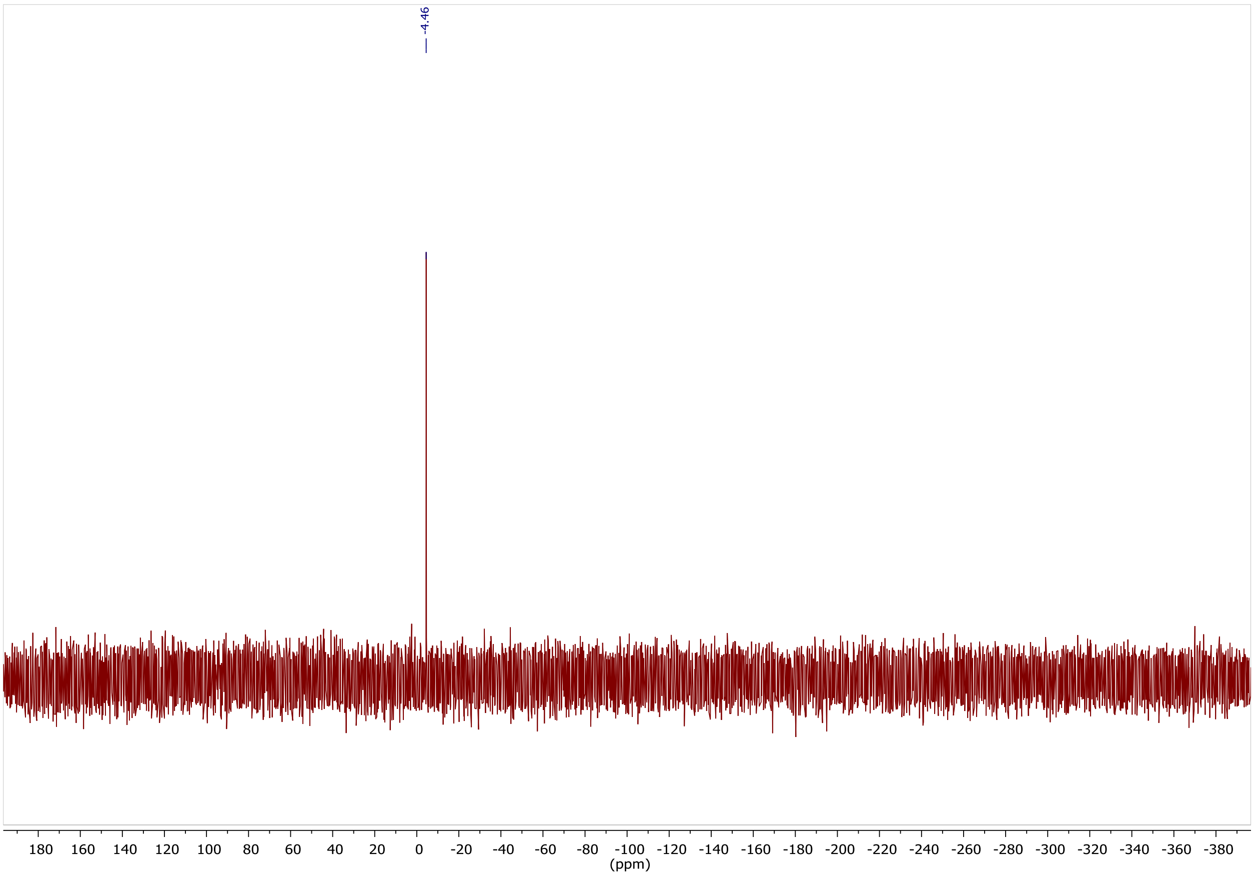

Figure 84: DEPT ^{29}Si NMR spectrum (79.5 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**19**).

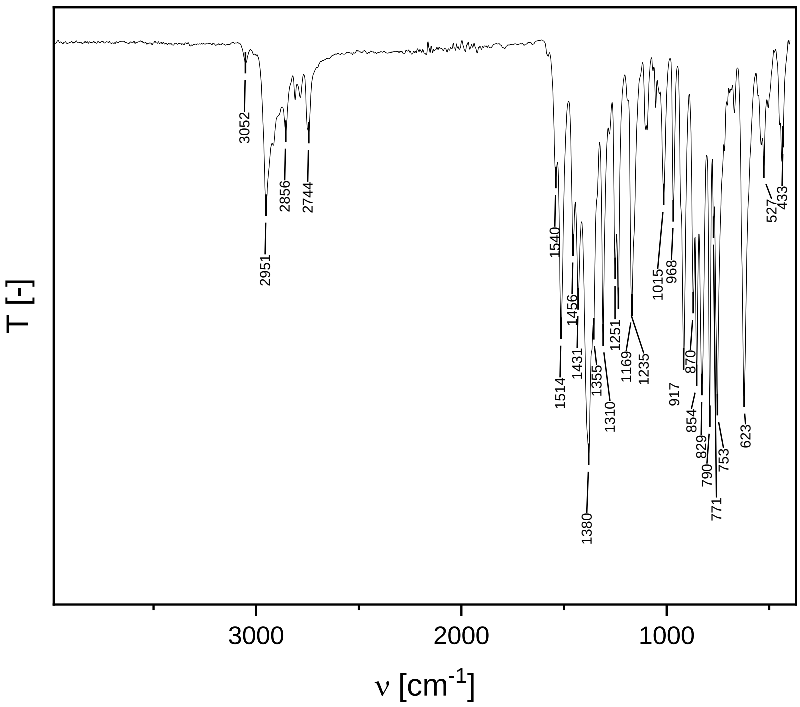

Figure 85: ATR-IR spectrum of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**19**).

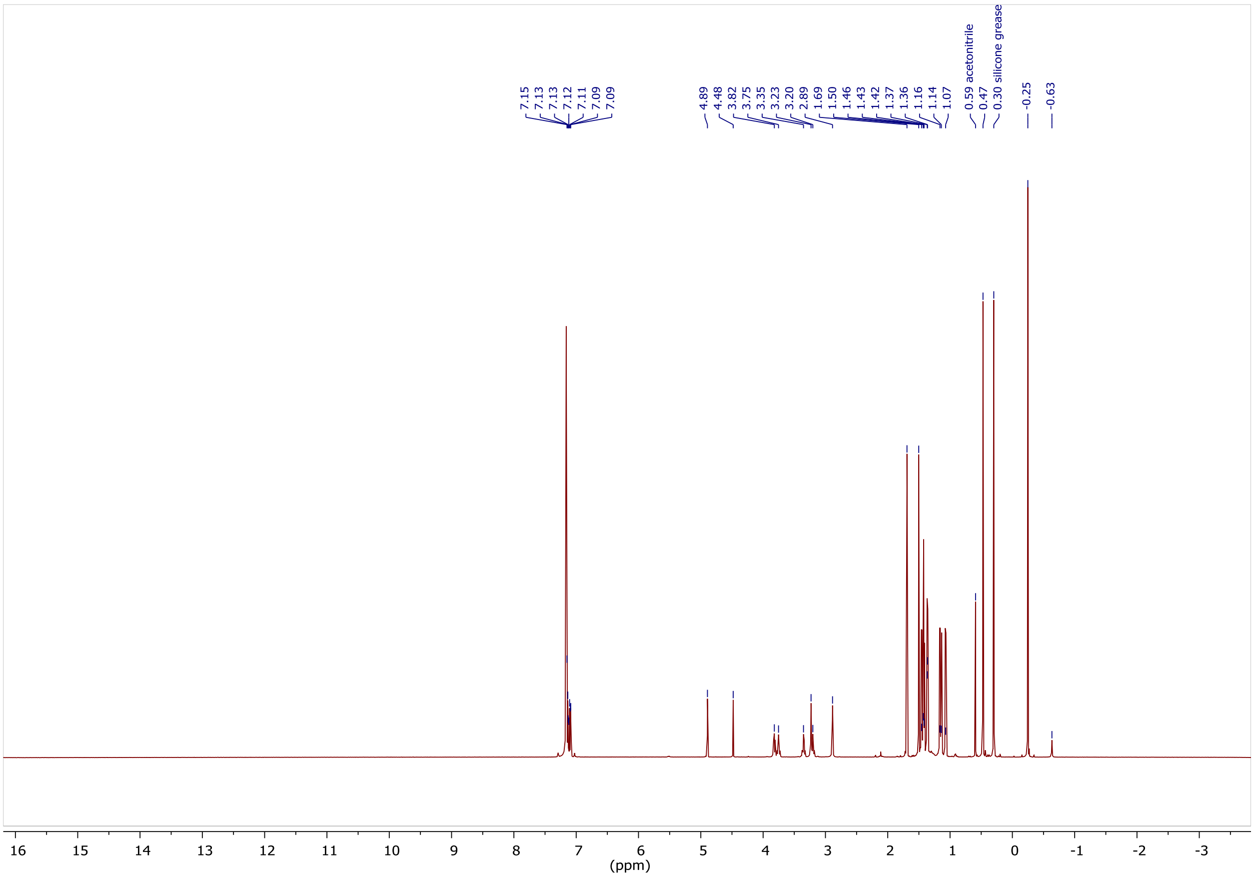

Figure 86: ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(N(H)$SiMe_3$)L] (**20**).

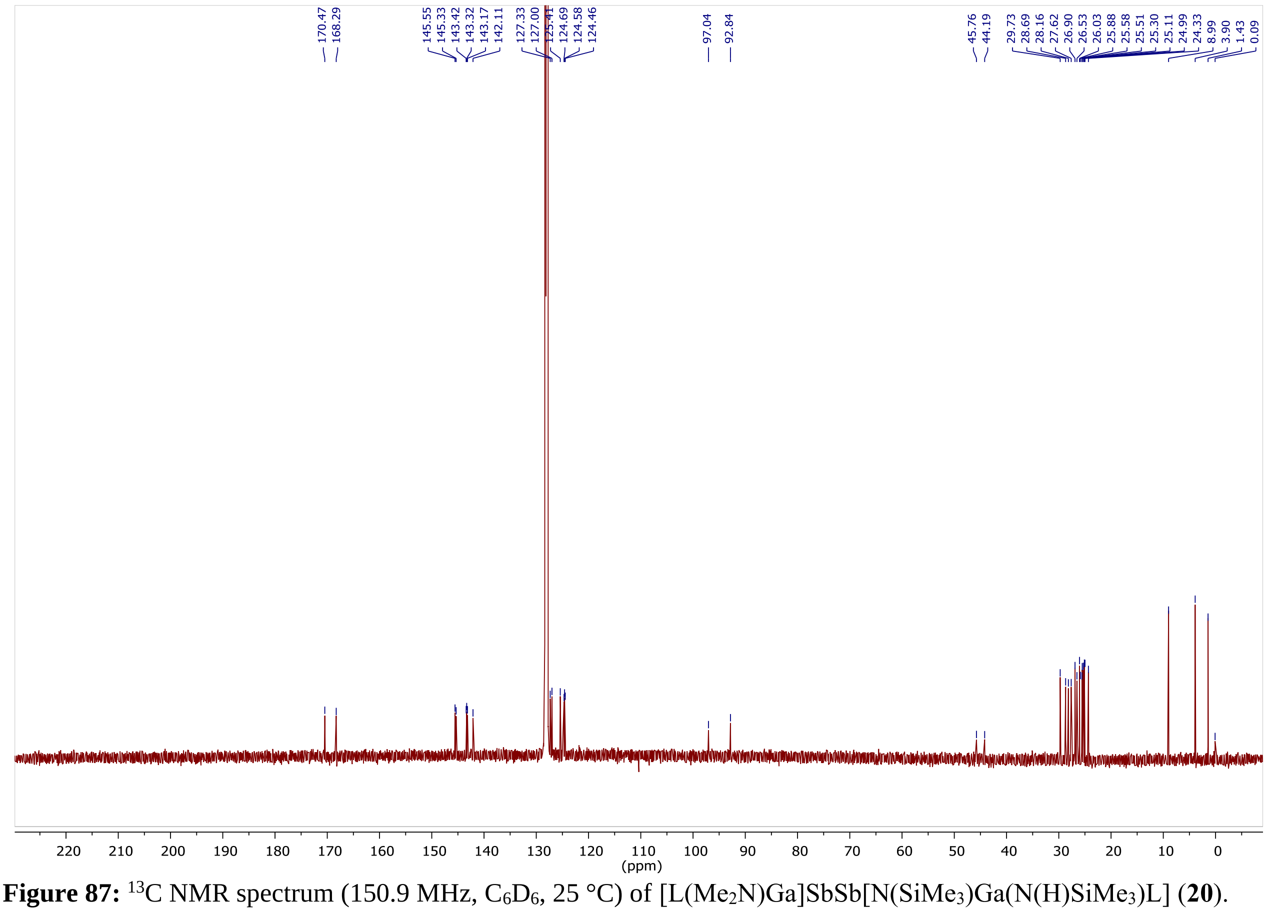

Figure 87: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(N(H)$SiMe_3$)L] (**20**).

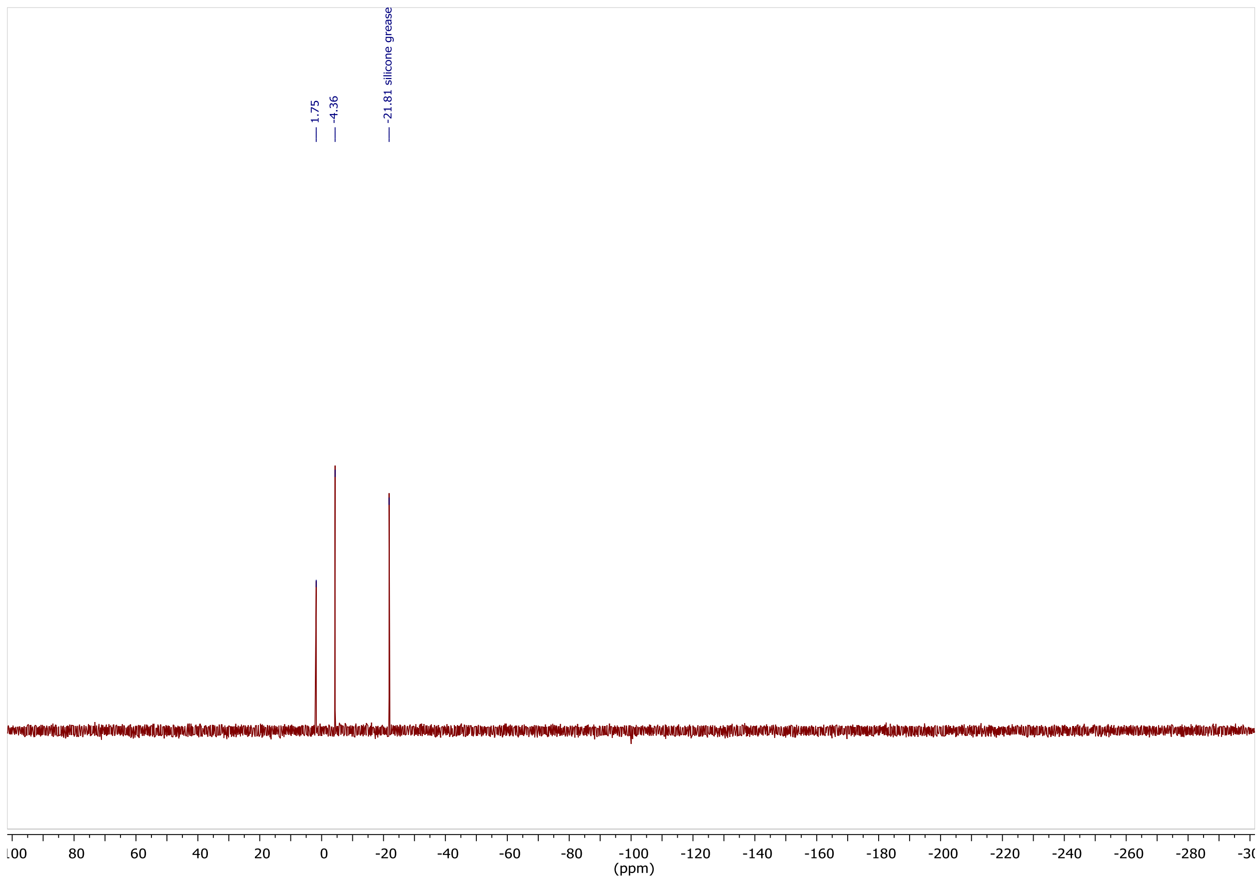

Figure 88: DEPT ^{29}Si NMR spectrum (119.2 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(N(H)$SiMe_3$)L] (**20**).

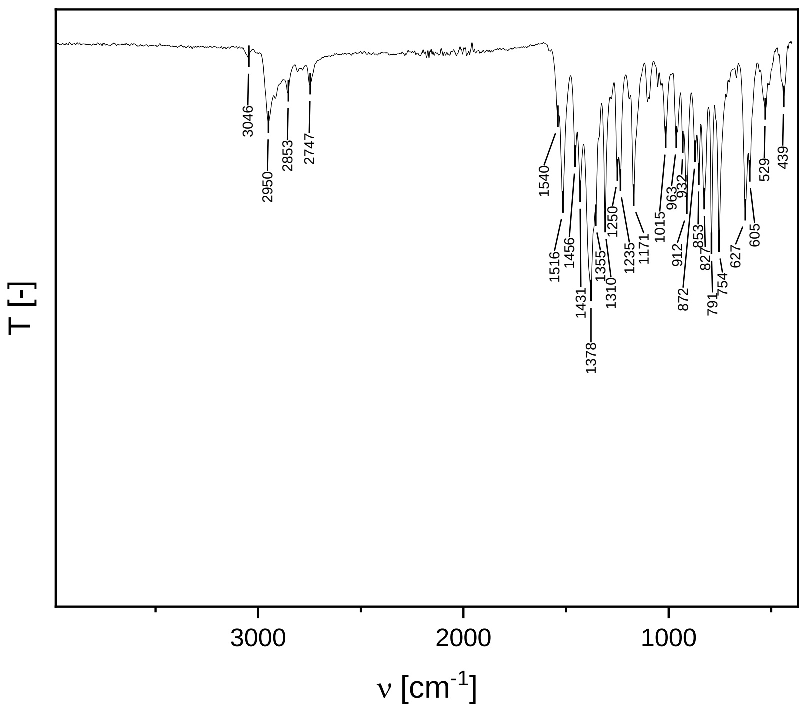

Figure 89: ATR-IR spectrum of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(N(H)$SiMe_3$)L] (**20**).

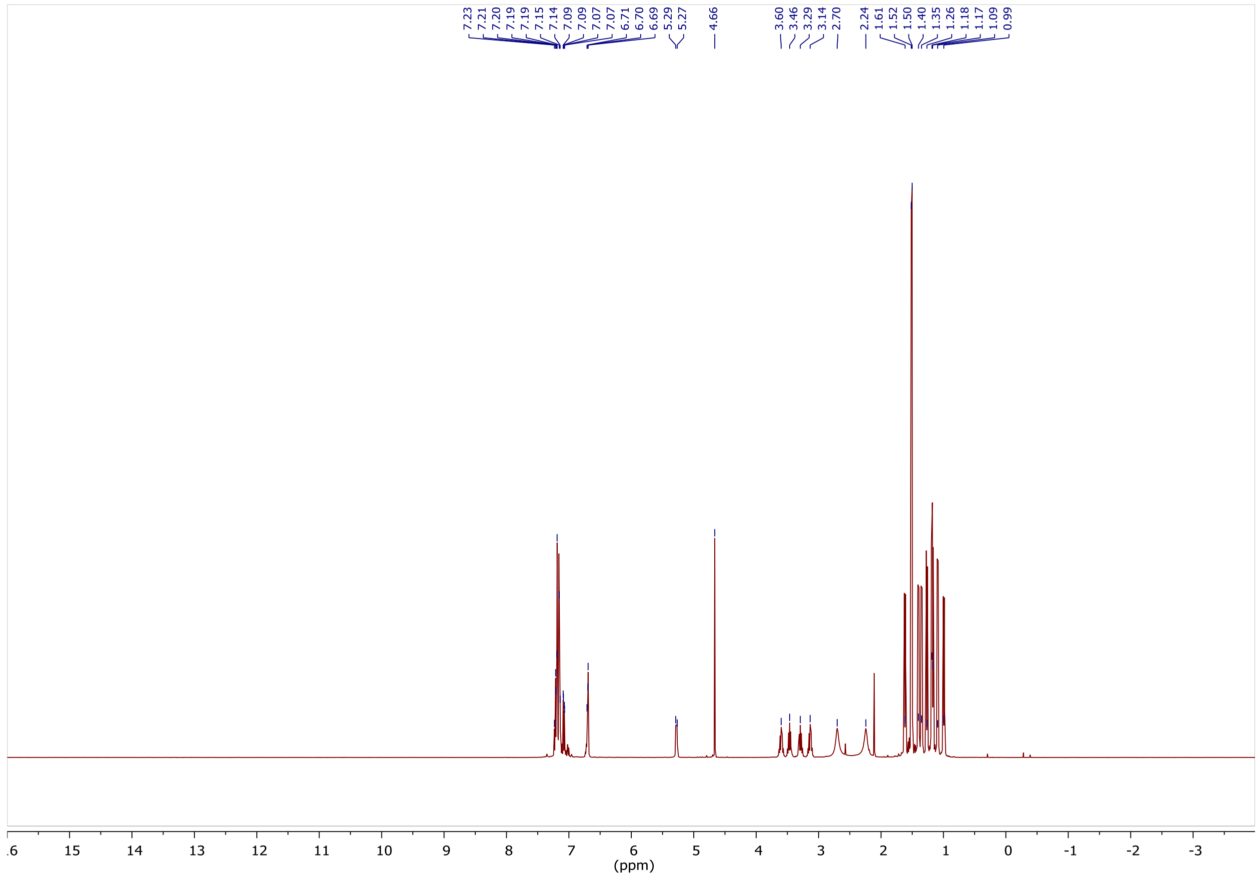

Figure 90: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2NPh$ (**22**).

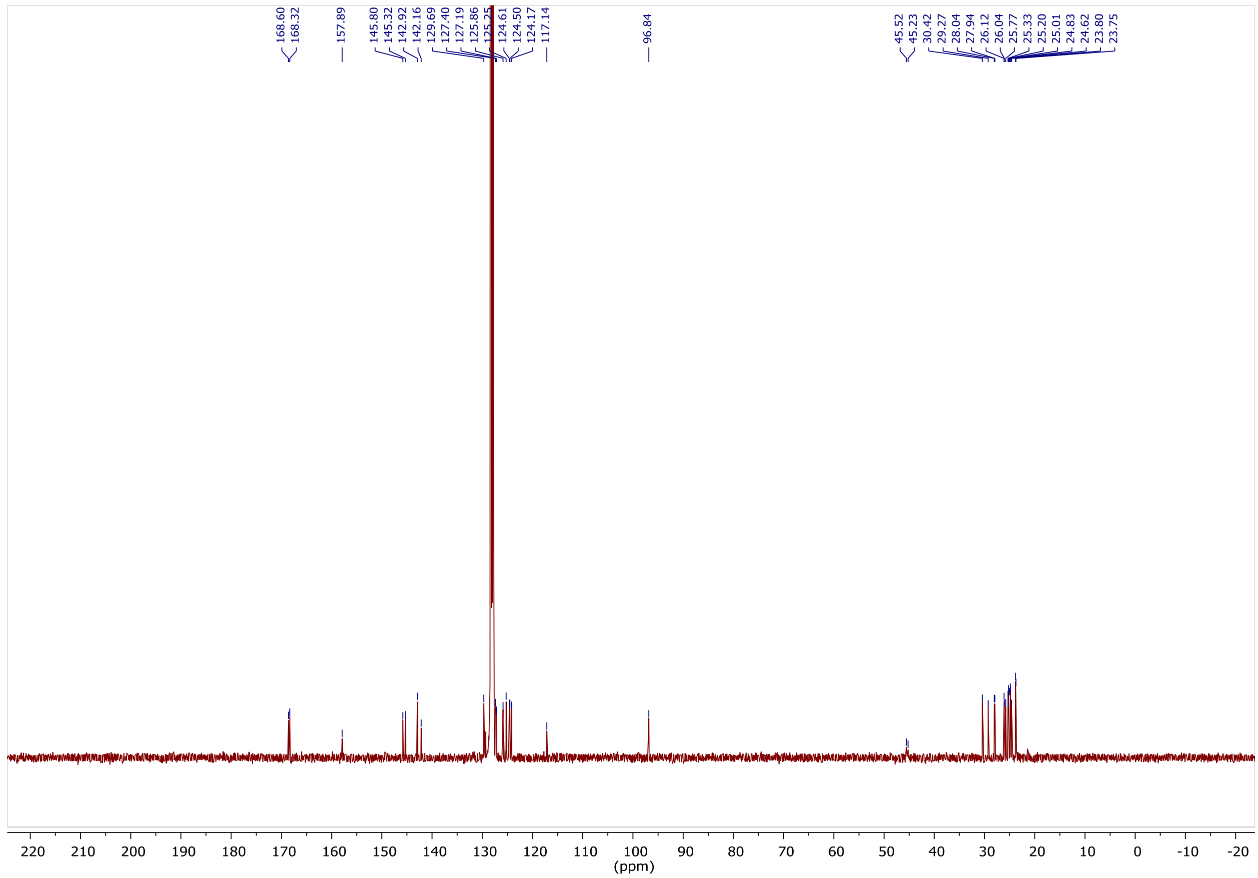

Figure 91: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2NPh$ (**22**).

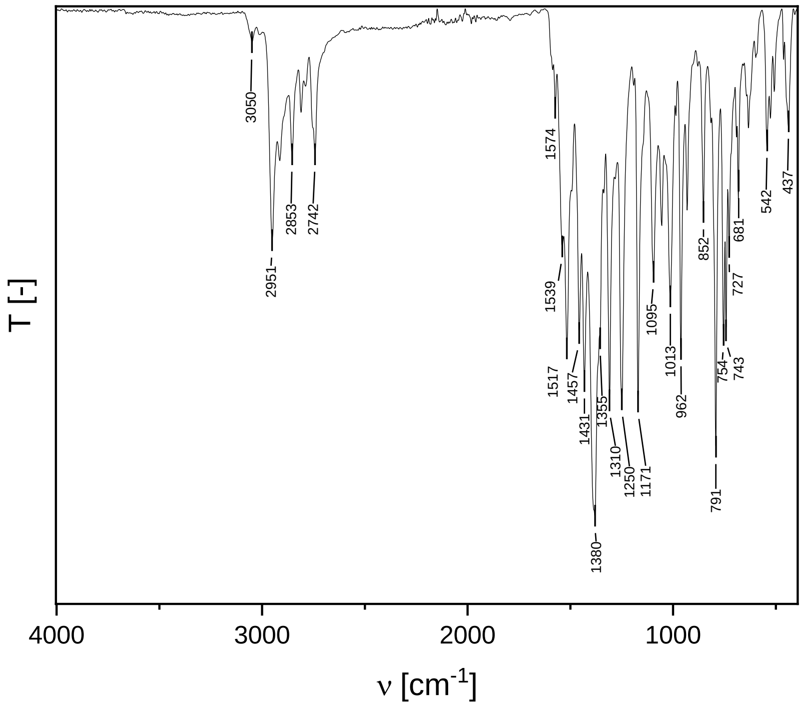

Figure 92: ATR-IR spectrum of [L(Me$_2$N)GaSb]$_2$NPh (**22**).

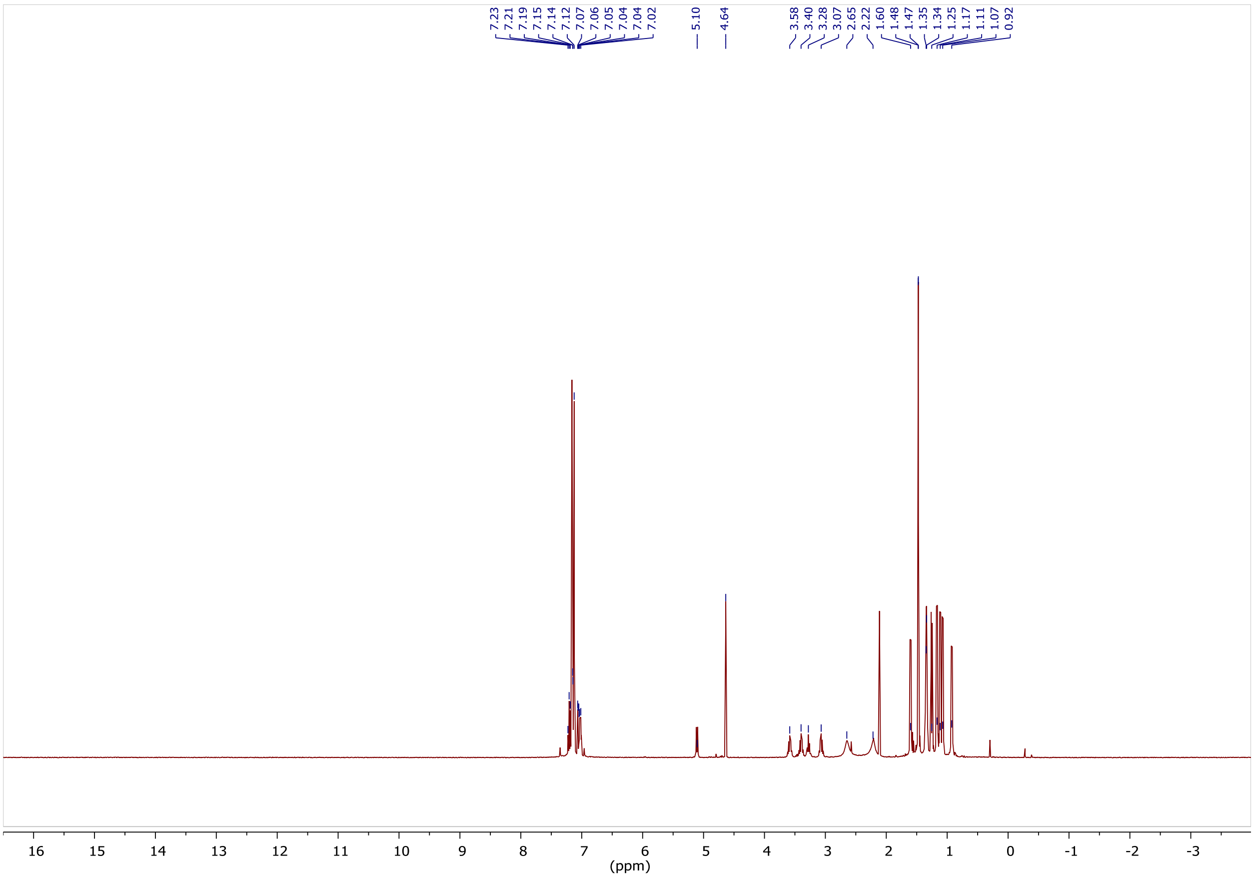

Figure 93: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of [L(Me$_2$N)GaSb]$_2$N(*p*-CF$_3$Ph) (**23**).

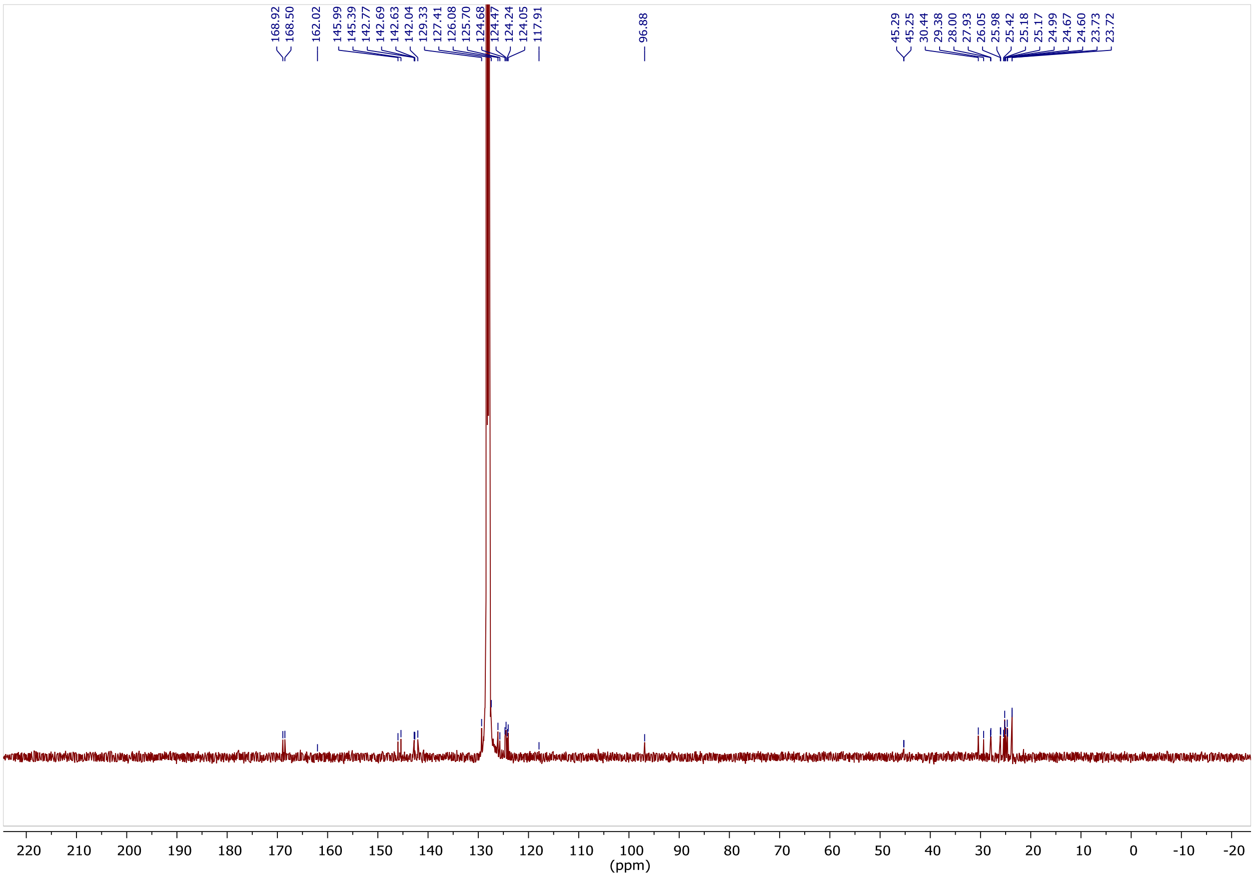

Figure 94: ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2N(p\text{-}CF_3Ph)$ (**23**).

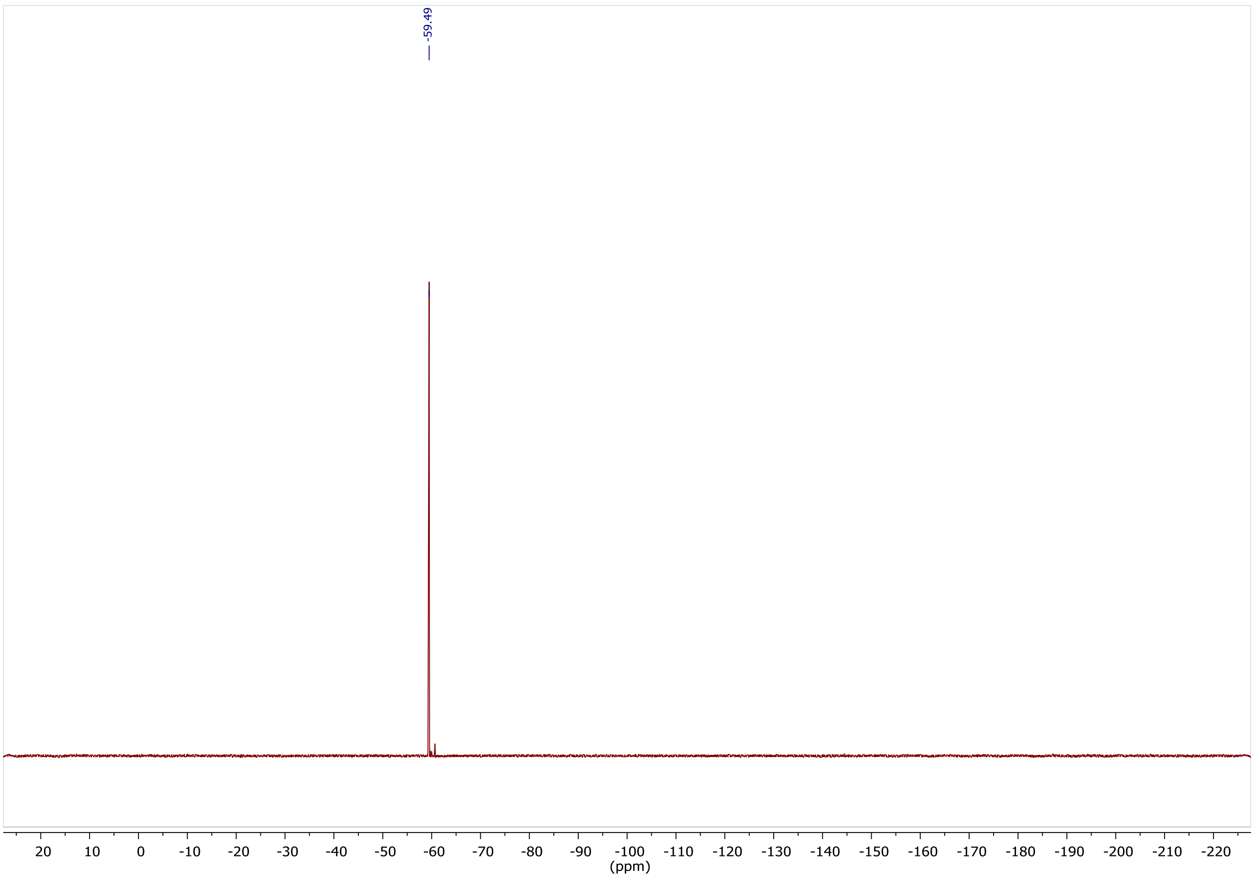

Figure 95: ^{19}F NMR spectrum (376.5 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2N(p\text{-}CF_3Ph)$ (**23**).

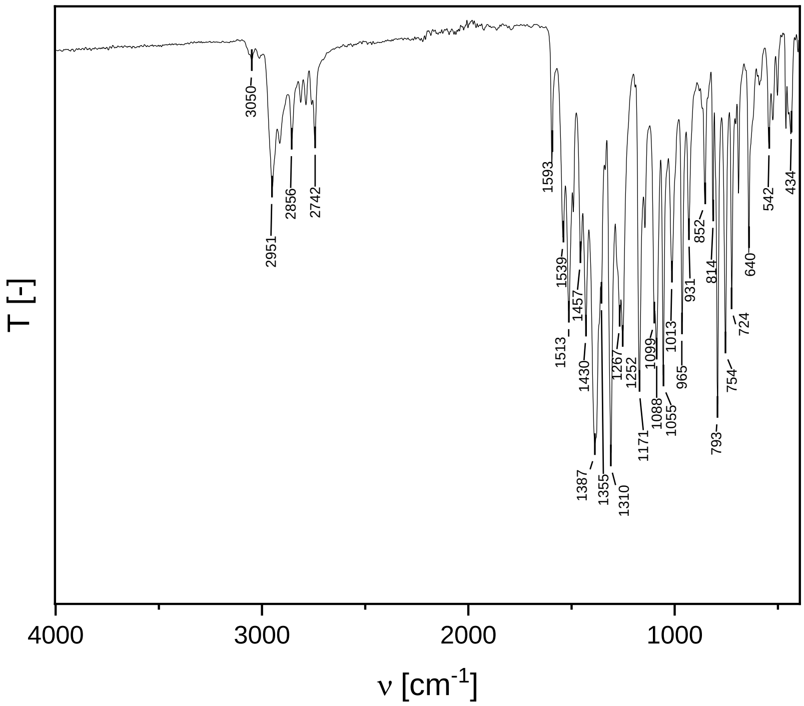

Figure 96: ATR-IR spectrum of [L(Me$_2$N)GaSb]$_2$N(*p*-CF$_3$Ph) (**23**).

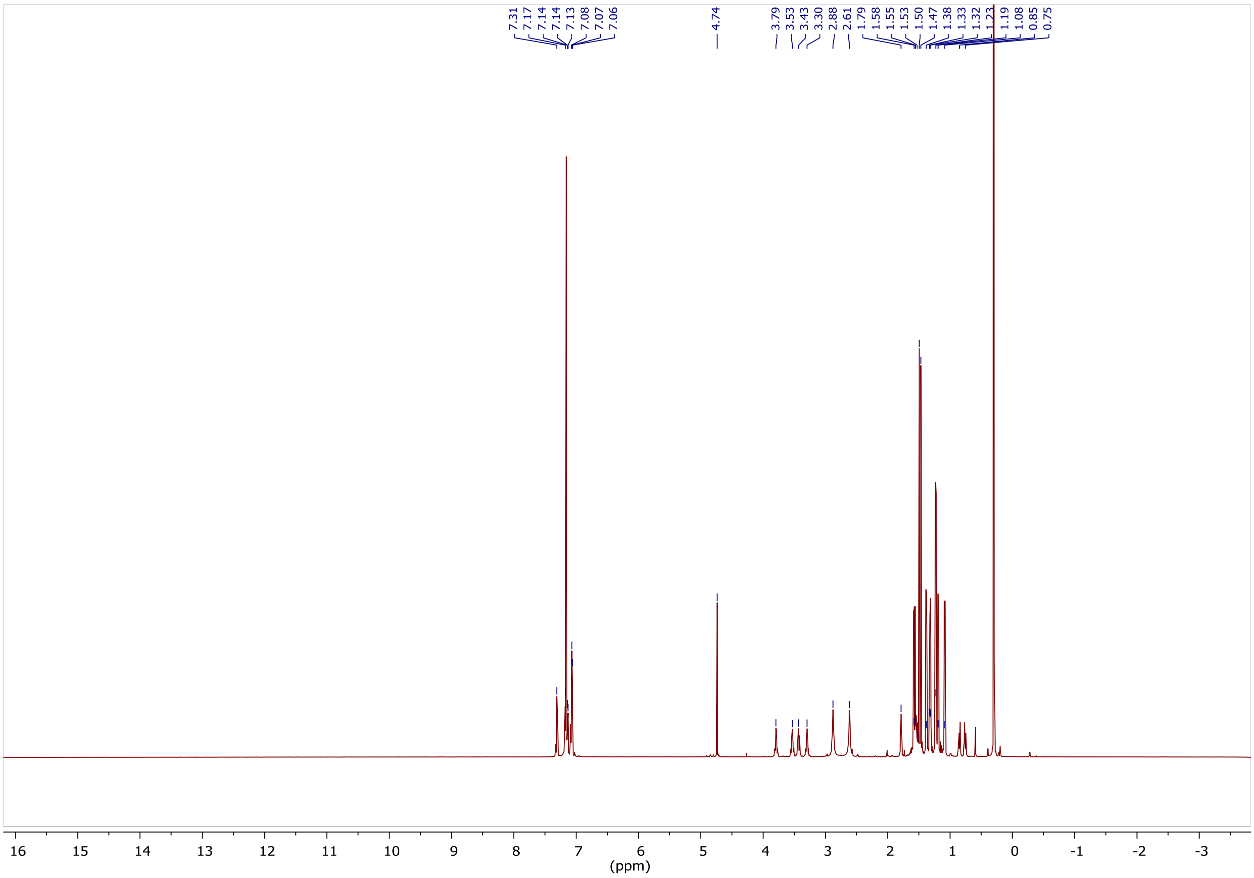

Figure 97: ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of [L(Me$_2$N)GaSb]$_2$N(ada) (**24**).

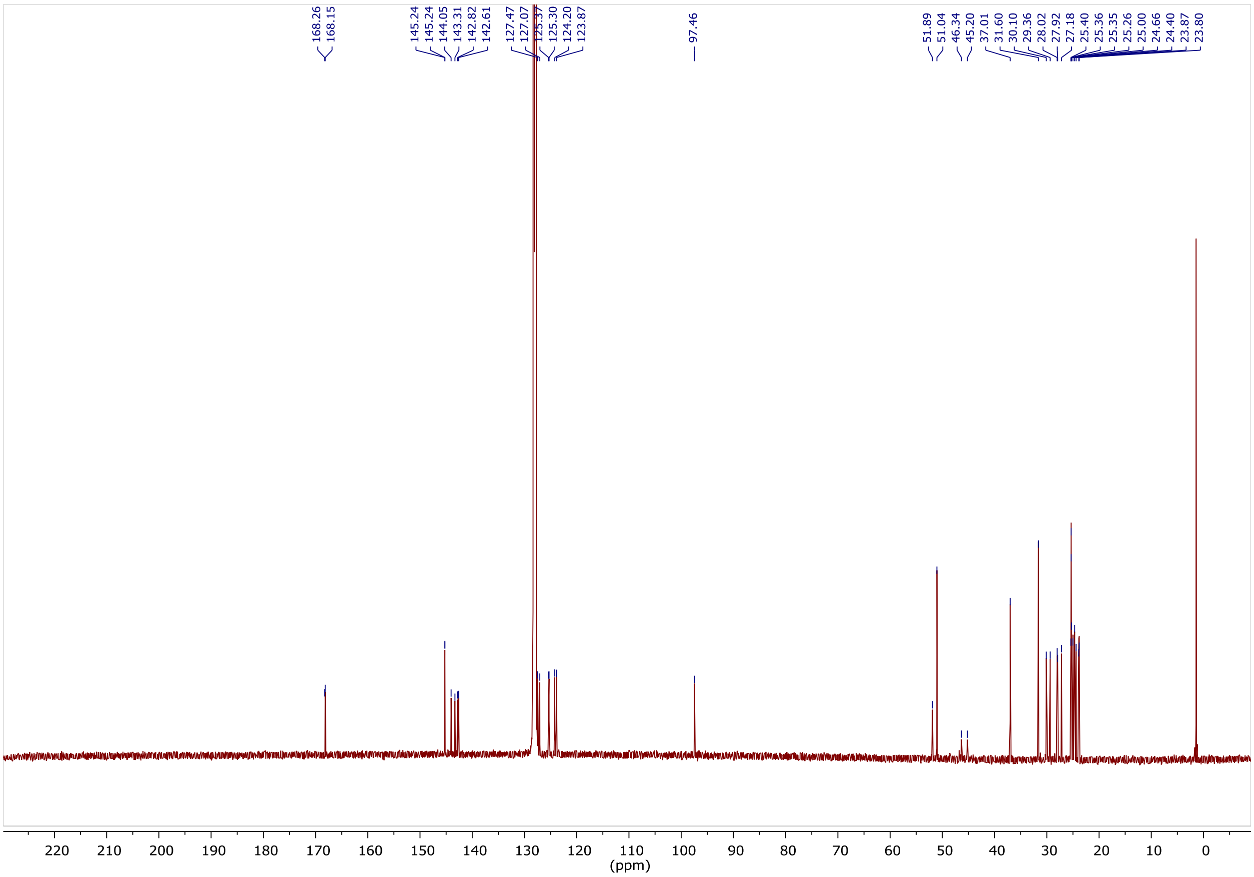

Figure 98: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2N(ada)$ (**24**).

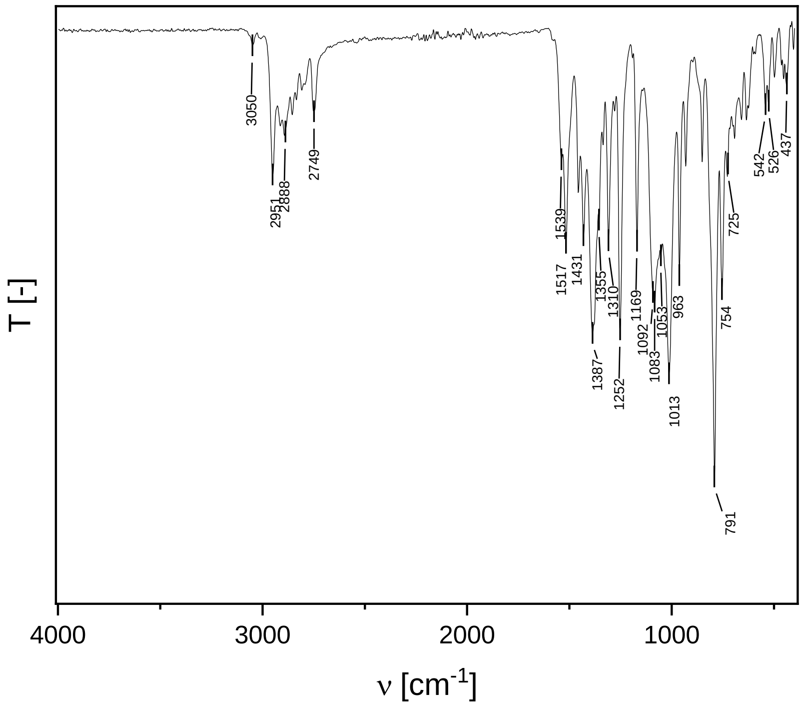

Figure 99: ATR-IR spectrum of $[L(Me_2N)GaSb]_2N(ada)$ (**24**).

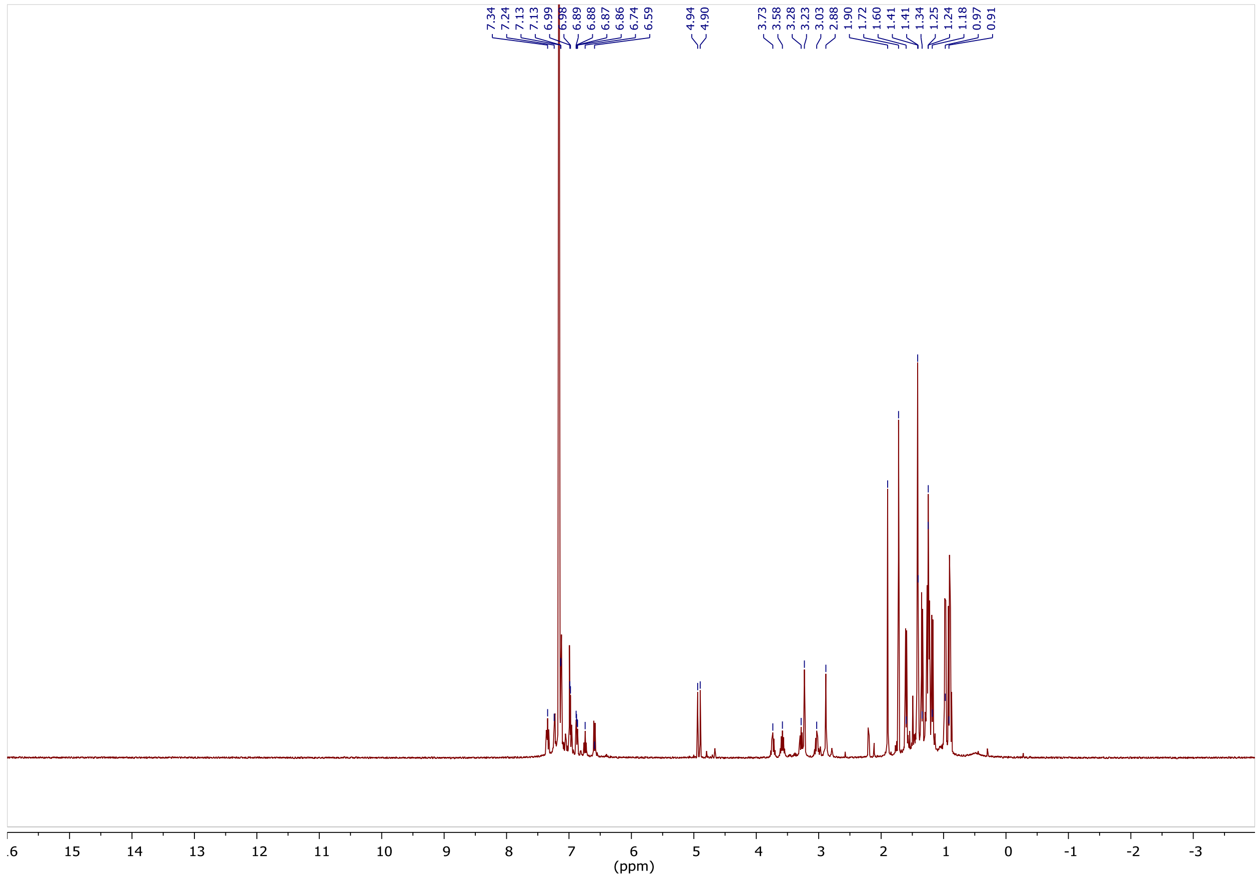

Figure 100: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of [L(Me$_2$N)Ga]SbSb[N(Ph)Ga(NMe$_2$)L] (**25**).

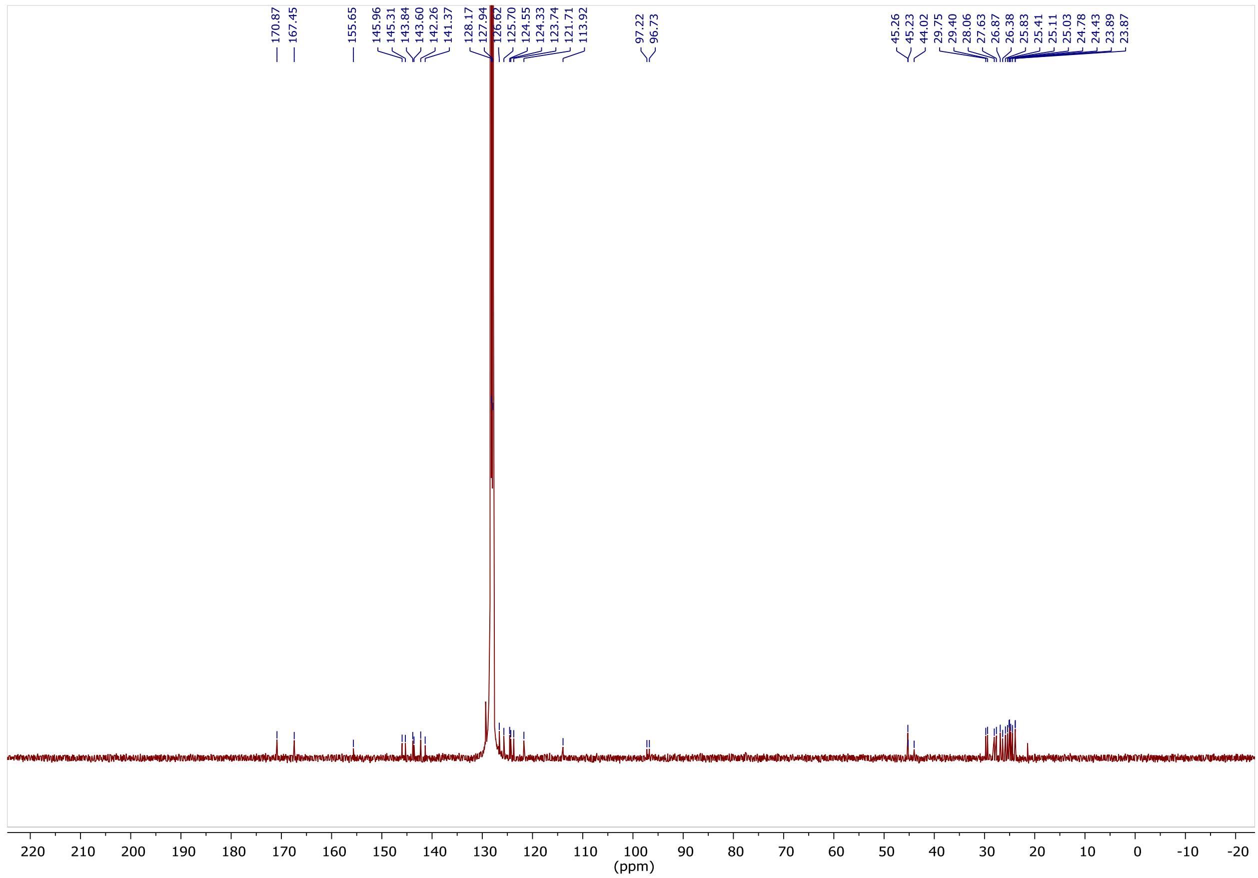

Figure 101: ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) of [L(Me$_2$N)Ga]SbSb[N(Ph)Ga(NMe$_2$)L] (**25**).

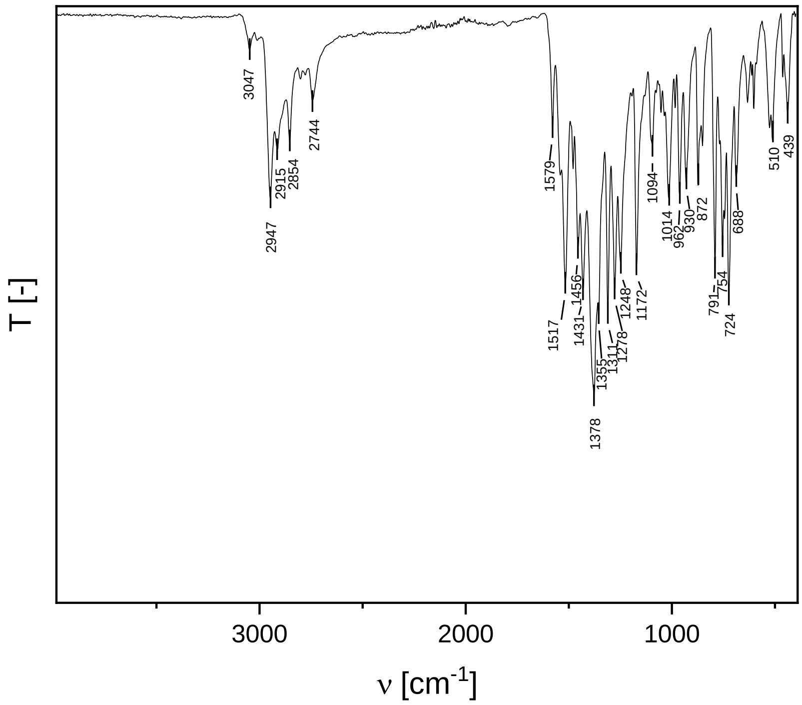

Figure 102: ATR-IR spectrum of [L(Me$_2$N)Ga]SbSb[N(Ph)Ga(NMe$_2$)L] (**25**).

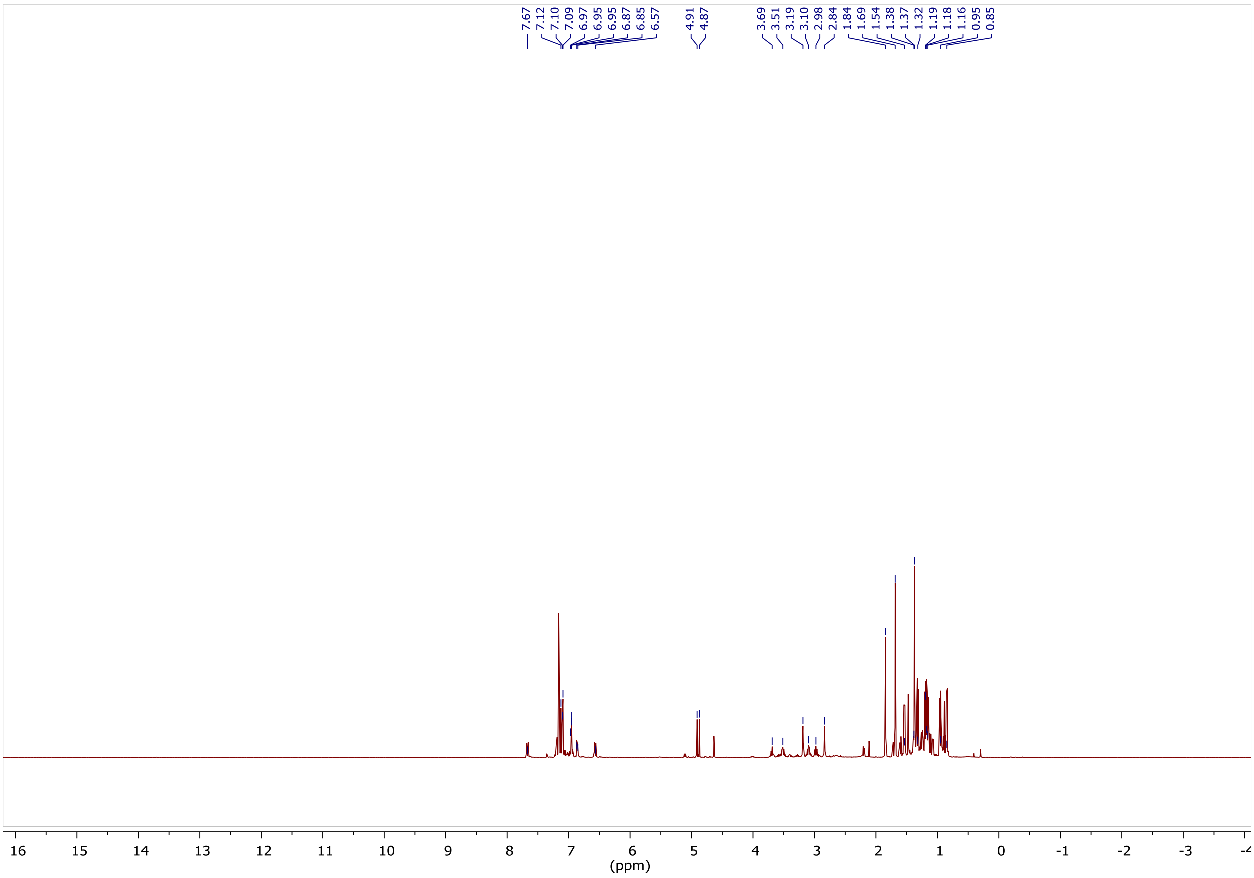

Figure 103: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of [L(Me$_2$N)Ga]SbSb[N(*p*-CF$_3$Ph)Ga(NMe$_2$)L] (**26**).

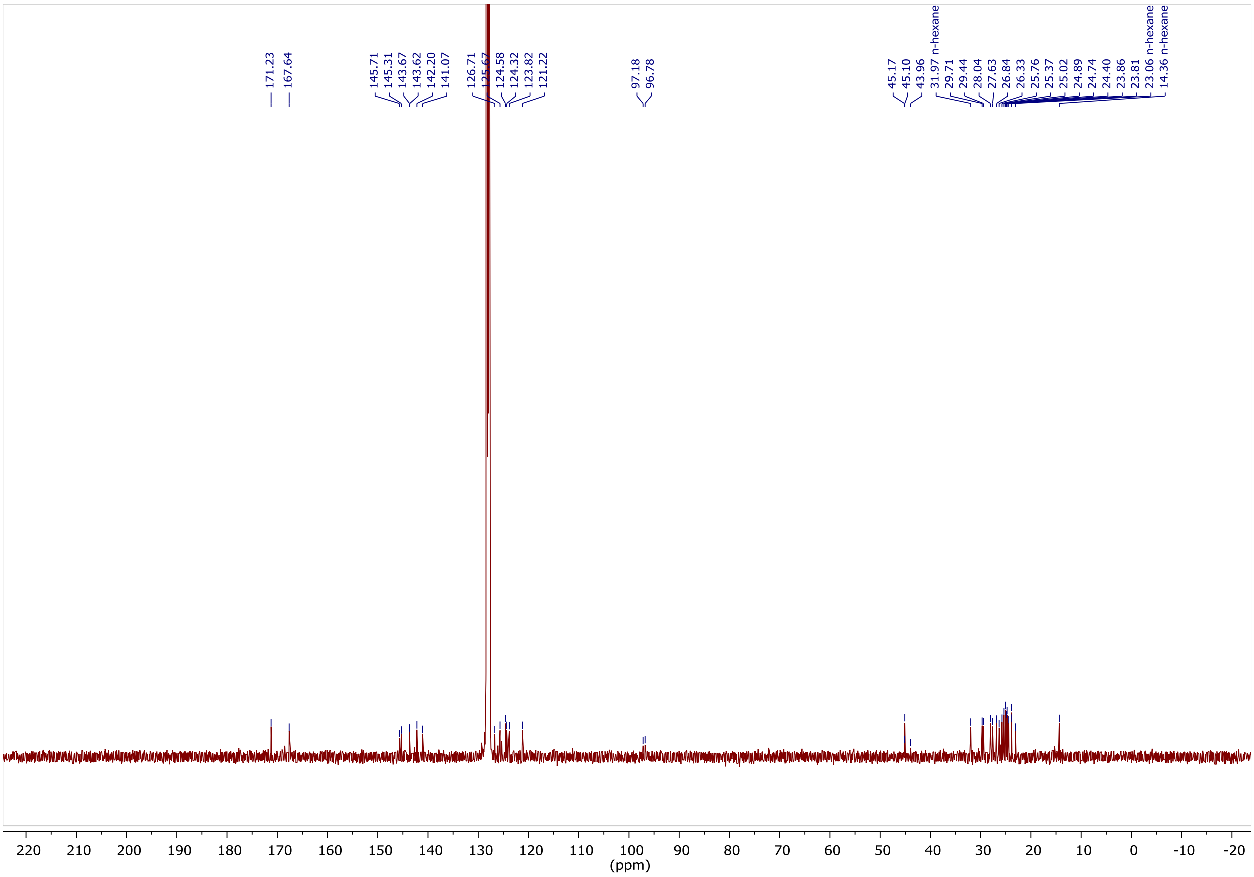

Figure 104: ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N(*p*-CF_3Ph)Ga(NMe_2)L] (**26**).

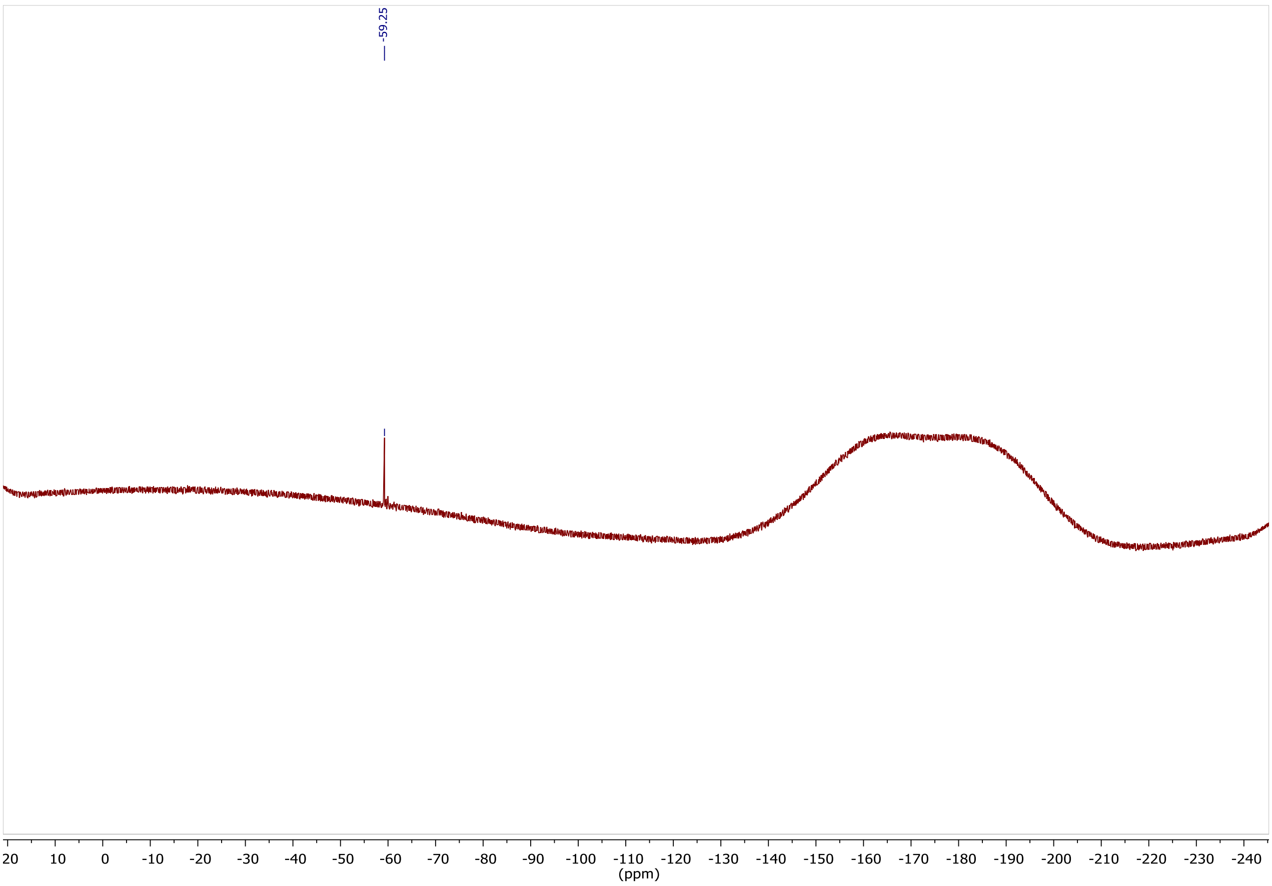

Figure 105: ^{19}F NMR spectrum (282.4 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N(*p*-CF_3Ph)Ga(NMe_2)L] (**26**).

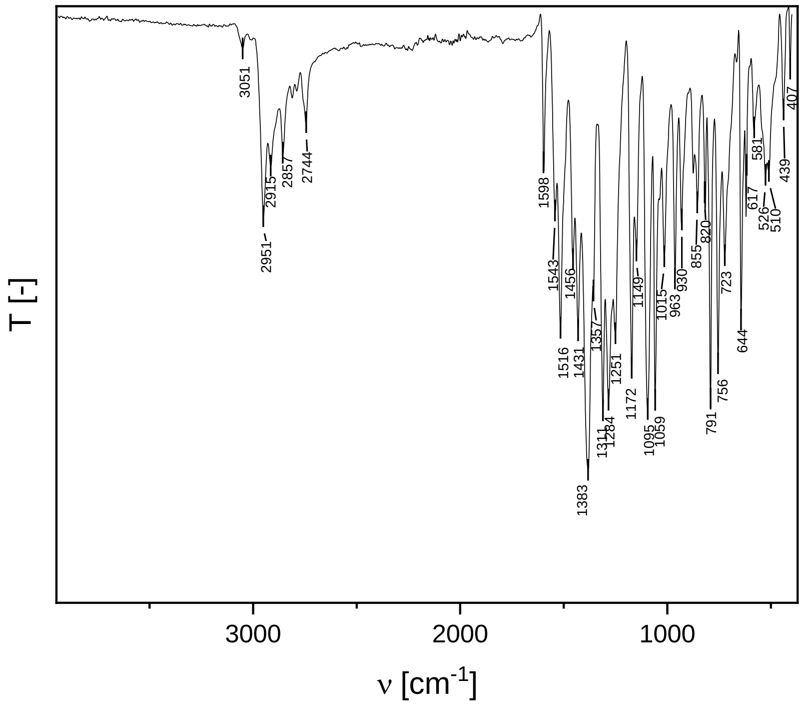

Figure 106: ATR-IR spectrum of [L(Me$_2$N)Ga]SbSb[N(*p*-CF$_3$Ph)Ga(NMe$_2$)L] (**26**).

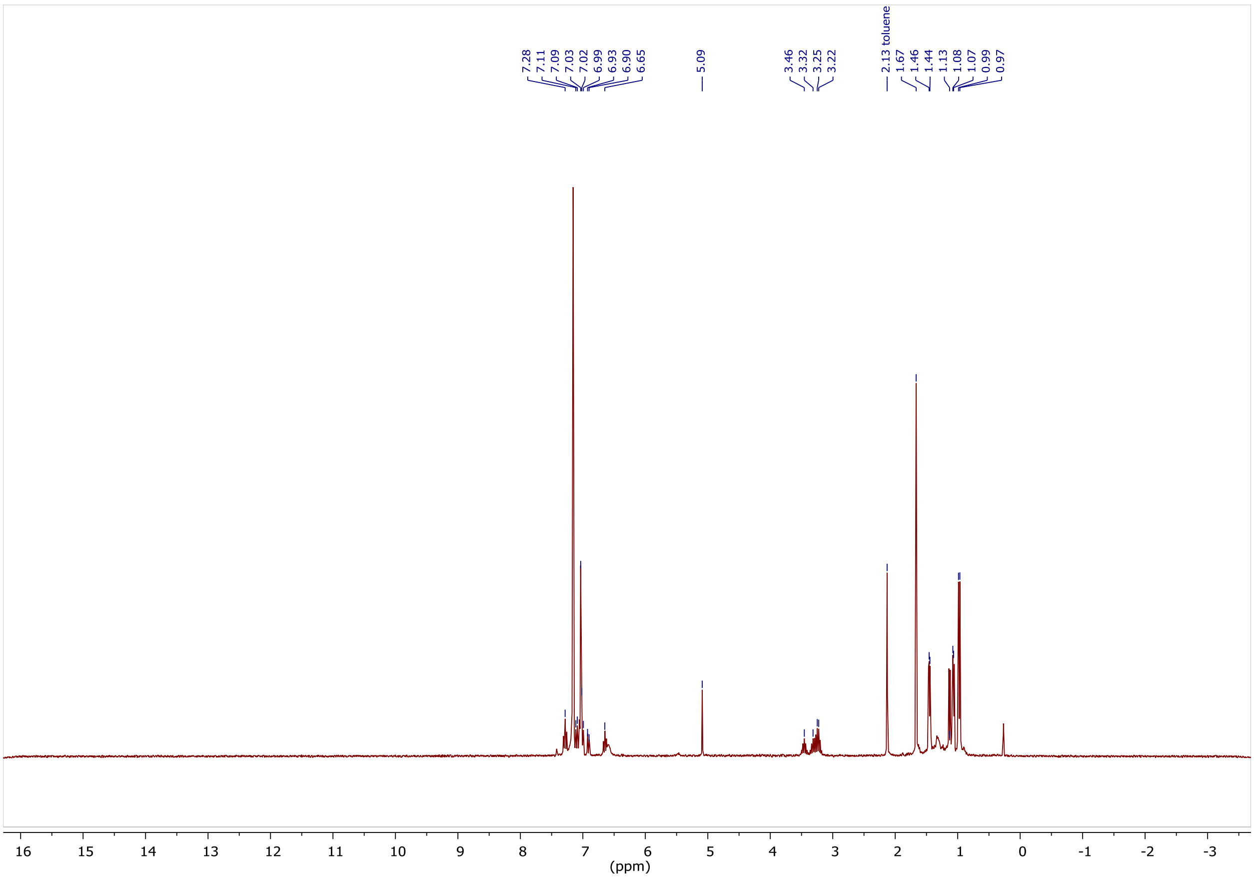

Figure 107: ^{1}H NMR spectrum (300 MHz, C_6D_6, 70 °C) of [(L(NPh)Ga-κ*Ga,*κ*N*)$_2$-(μ,η$^{1:1:1:1}$-Sb$_4$)] (**27**).

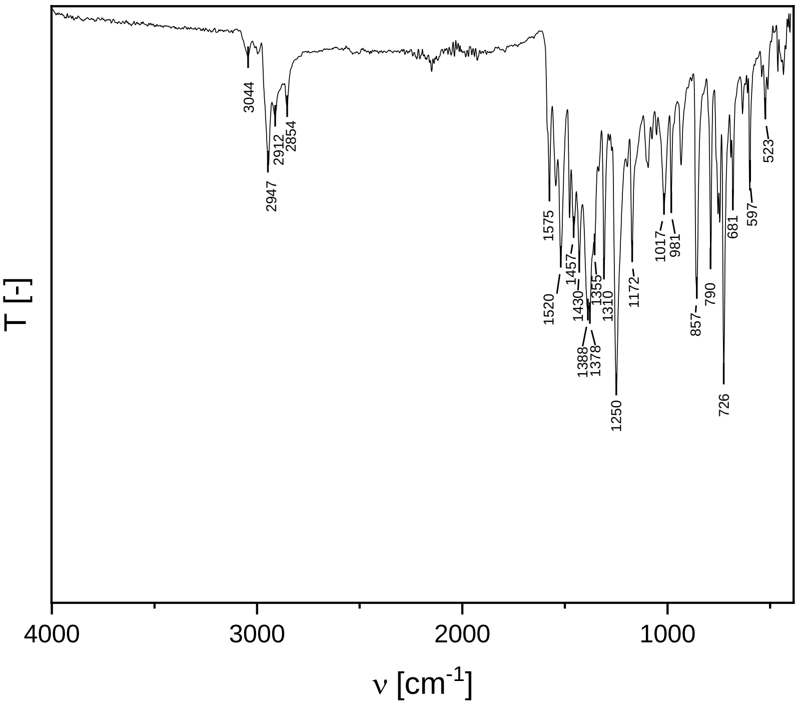

Figure 108: ATR-IR spectrum of [(L(NPh)Ga-κ*Ga,*κ*N*)$_2$-(μ,η$^{1:1:1:1}$-Sb$_4$)] (**27**).

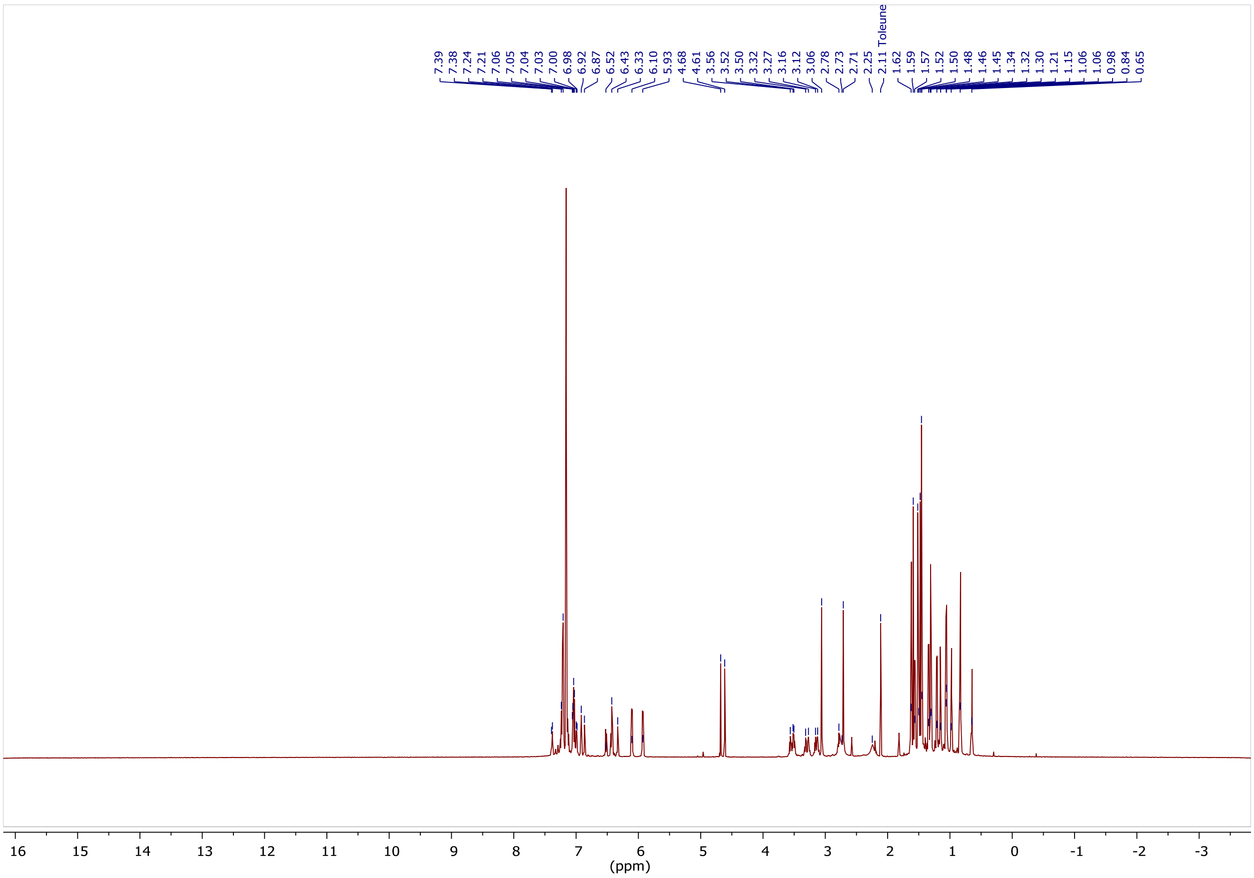

Figure 109: ^{1}H NMR spectrum (600 MHz, C$_6$D$_6$, 25 °C) of [L(Me$_2$N)GaSb][L(Me$_2$N)GaN(Ph)Sb]NPh (**28**).

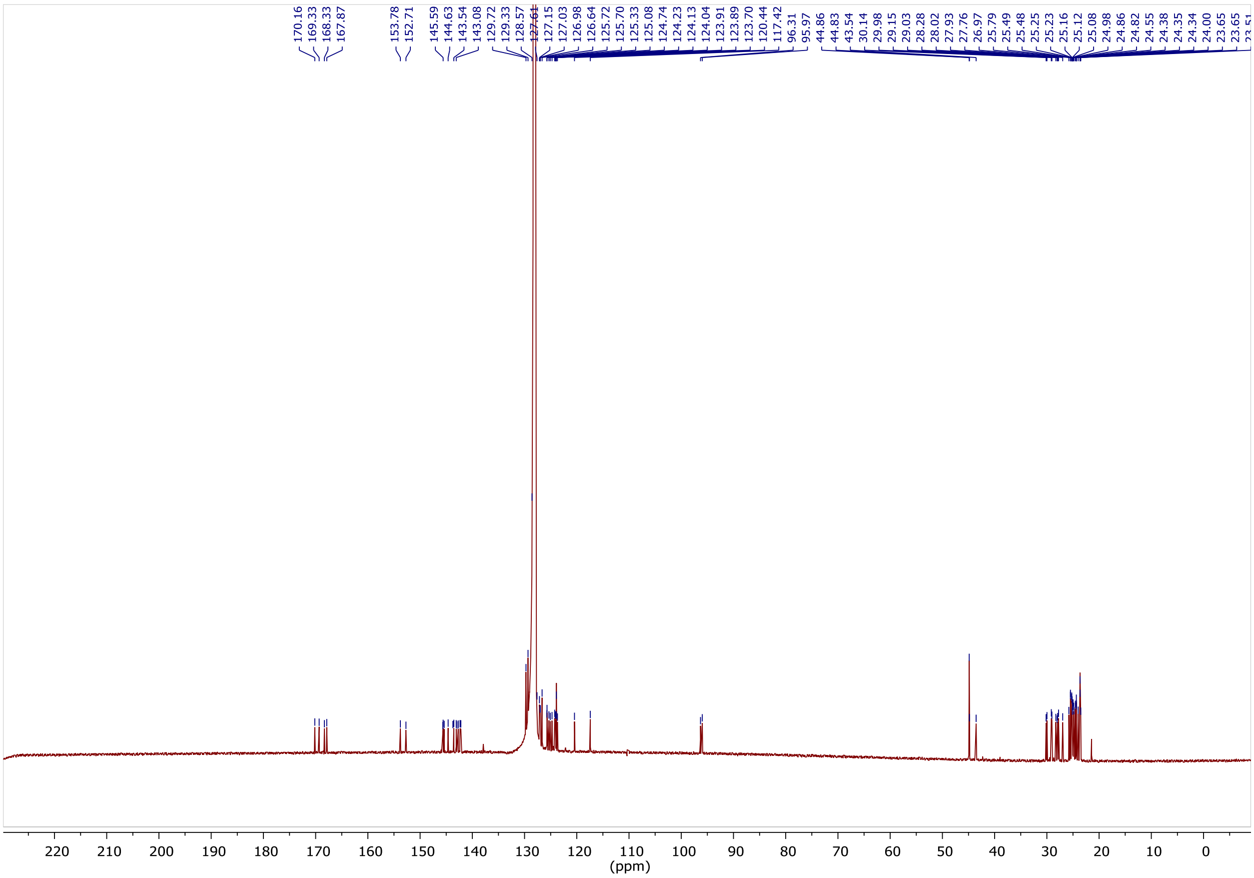

Figure 110: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of [L(Me_2N)GaSb][L(Me_2N)GaN(Ph)Sb]NPh (**28**).

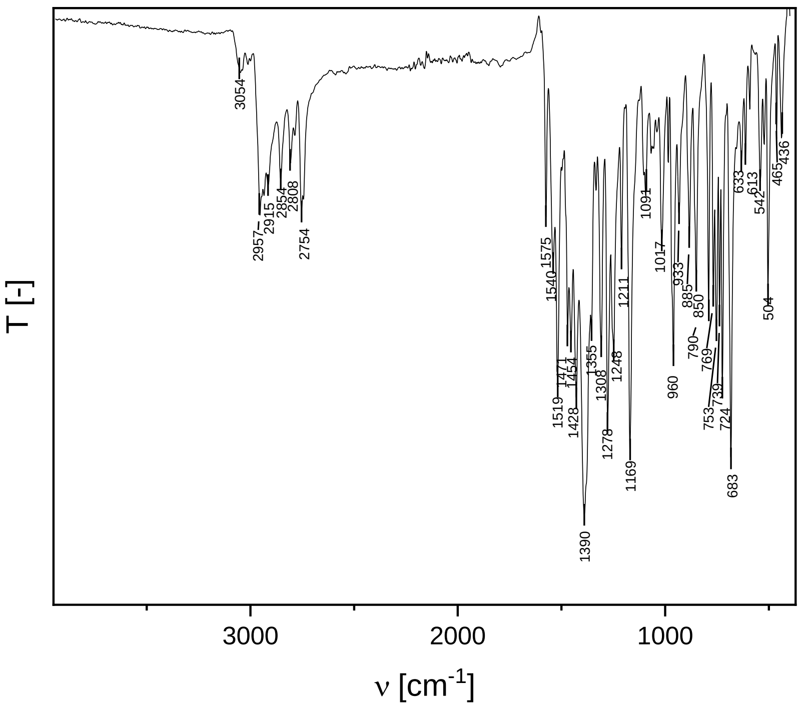

Figure 111: ATR-IR spectrum of [L(Me_2N)GaSb][L(Me_2N)GaN(Ph)Sb]NPh (**28**).

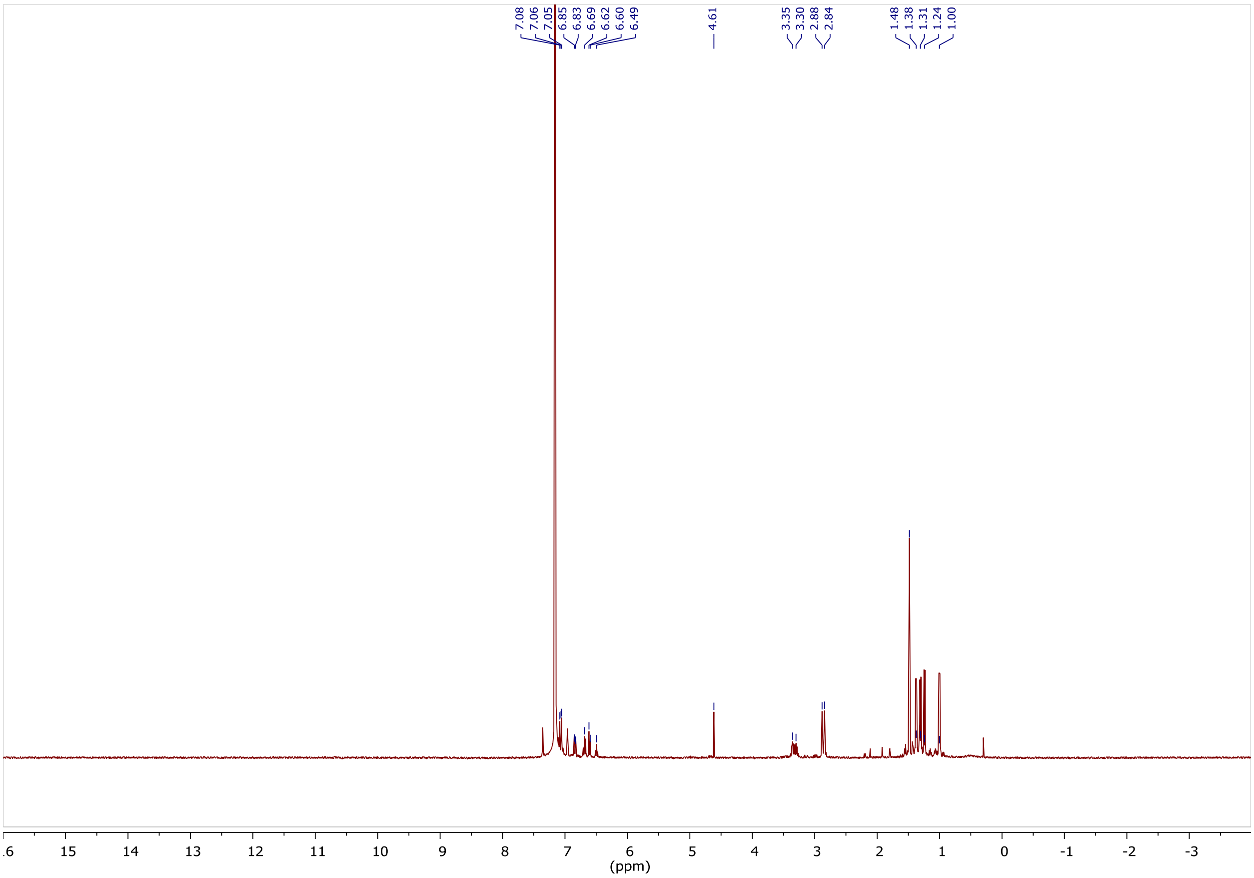

Figure 112: ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaN(Ph)Sb]_2$ (**29**).

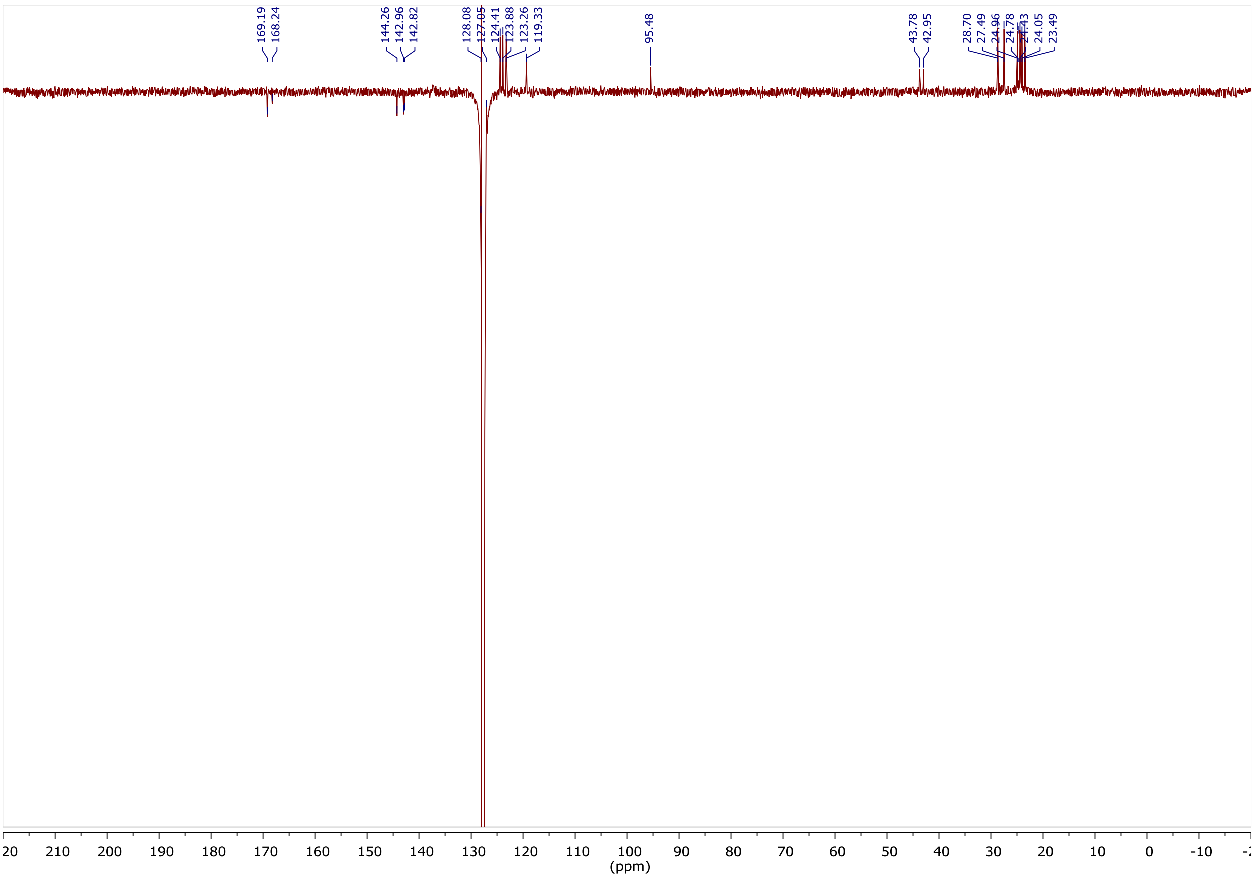

Figure 113: DEPTQ ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaN(Ph)Sb]_2$ (**29**).

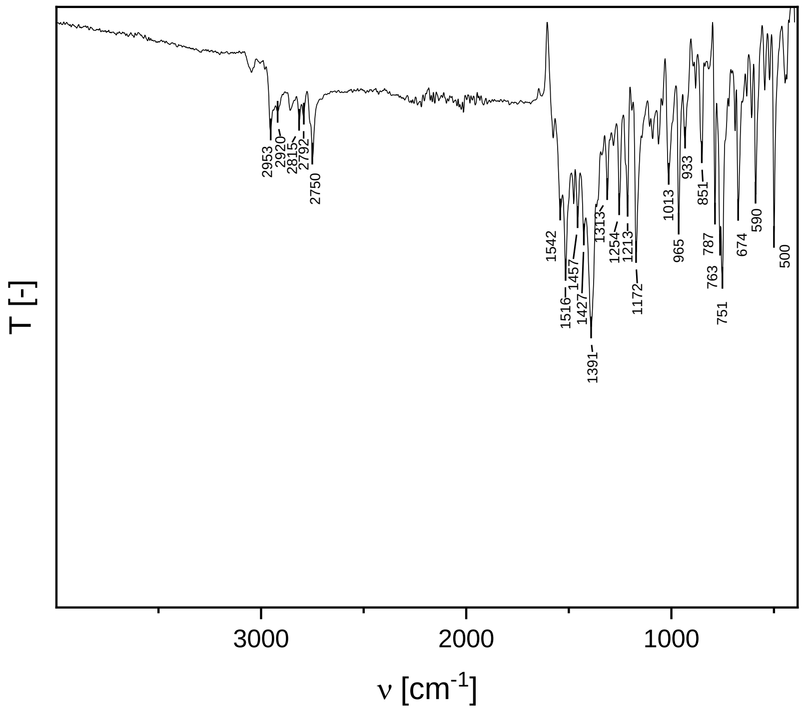

Figure 114: ATR-IR spectrum of $[L(Me_2N)GaN(Ph)Sb]_2$ (**29**).

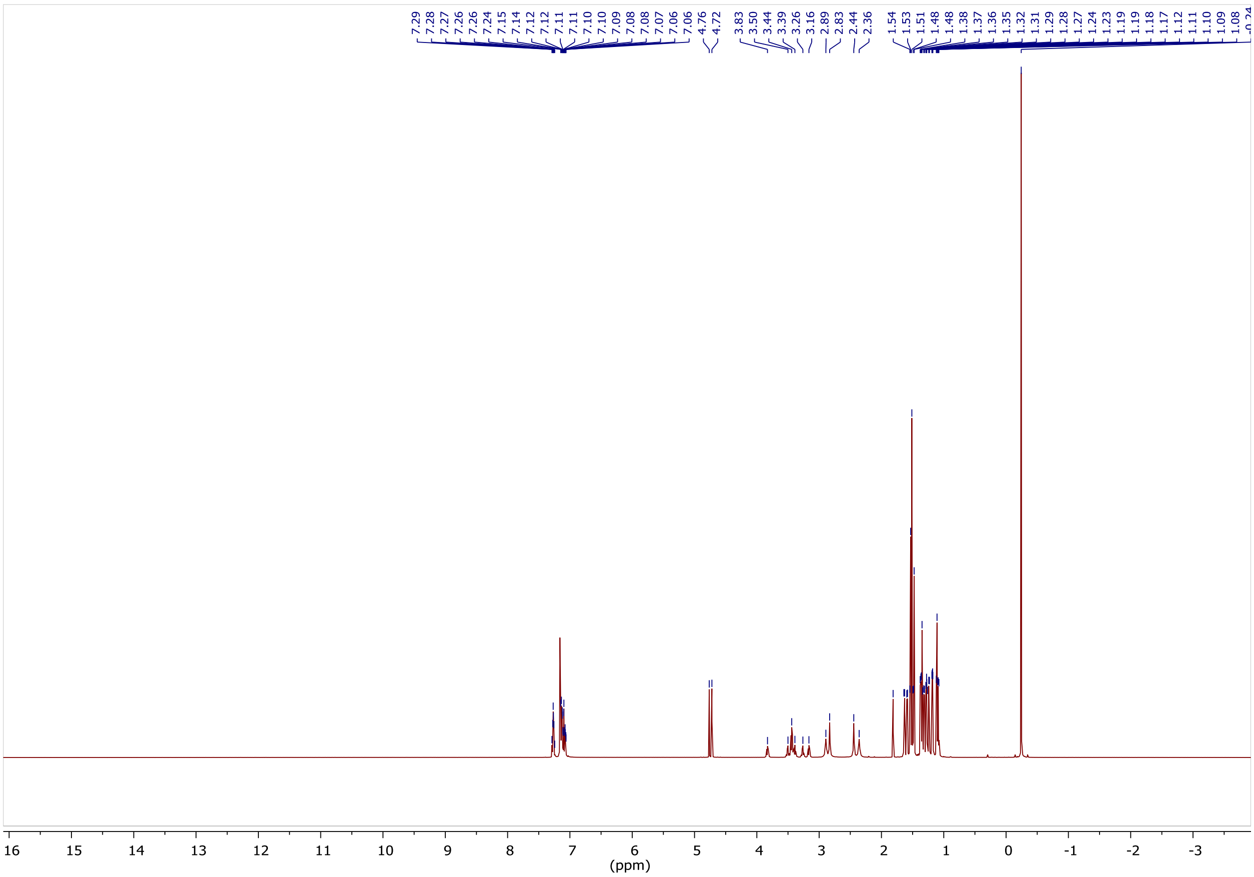

Figure 115: ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**30**).

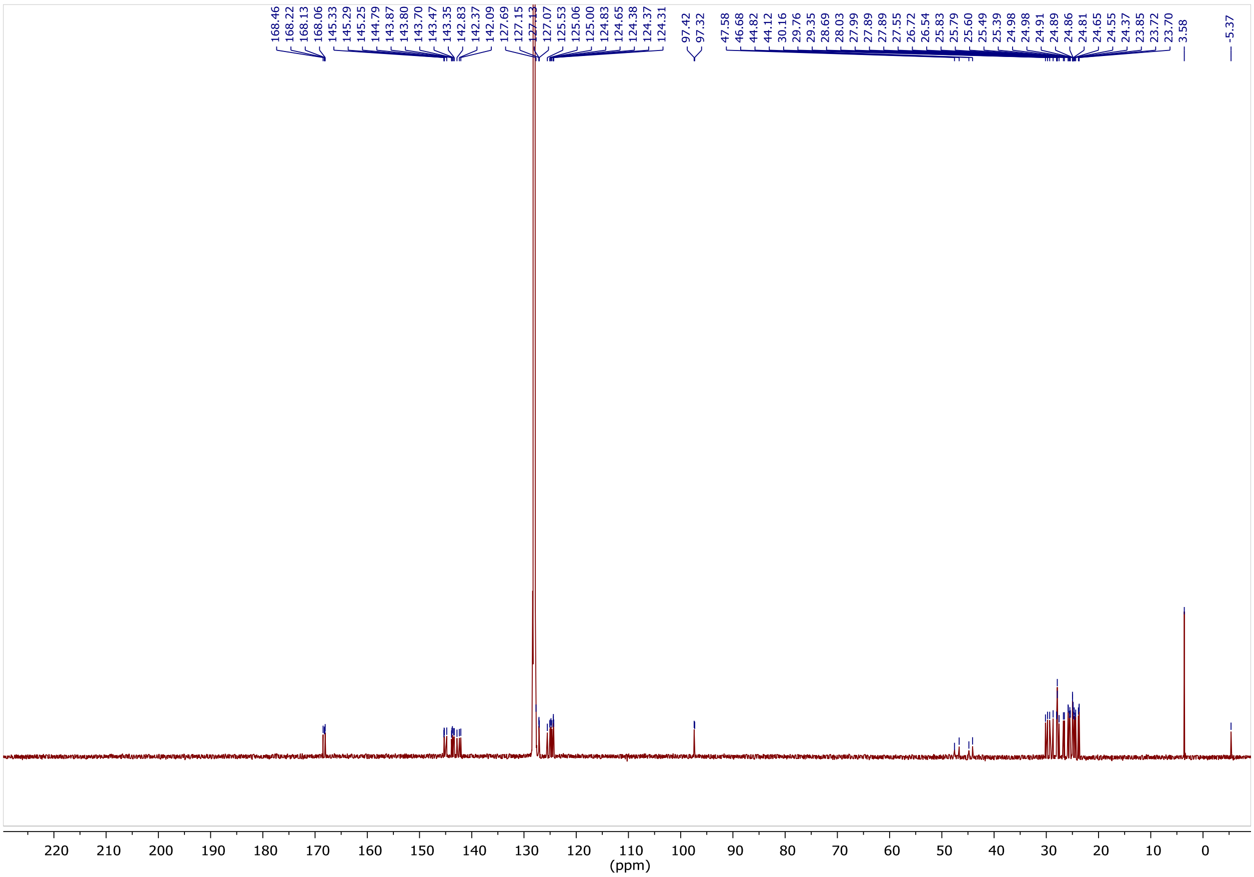

Figure 116: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**30**).

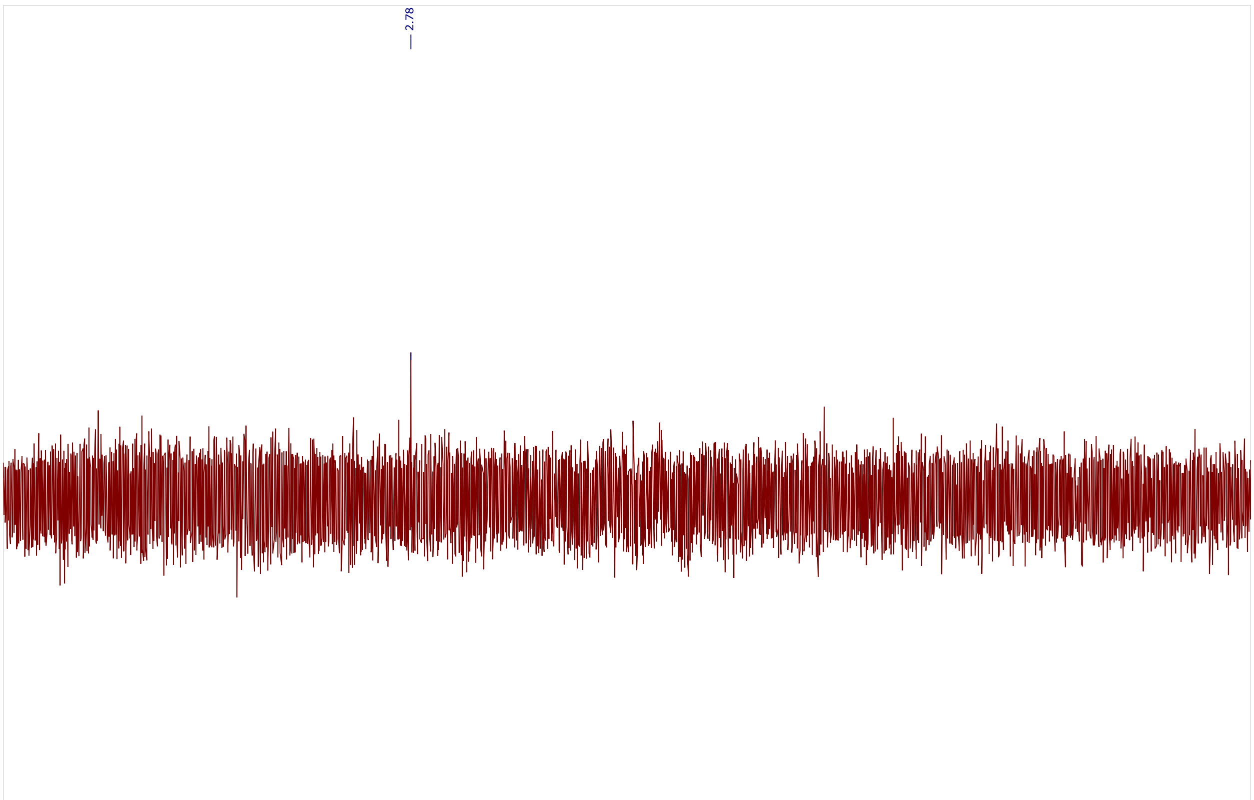

Figure 117: ^{29}Si NMR spectrum (79.5 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**30**).

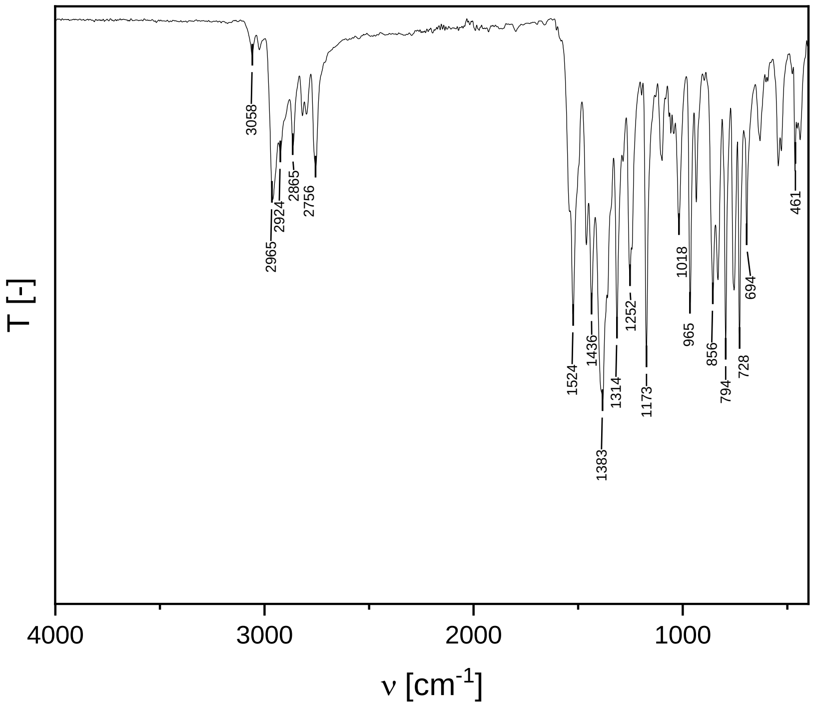

Figure 118: ATR-IR spectrum of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**30**).

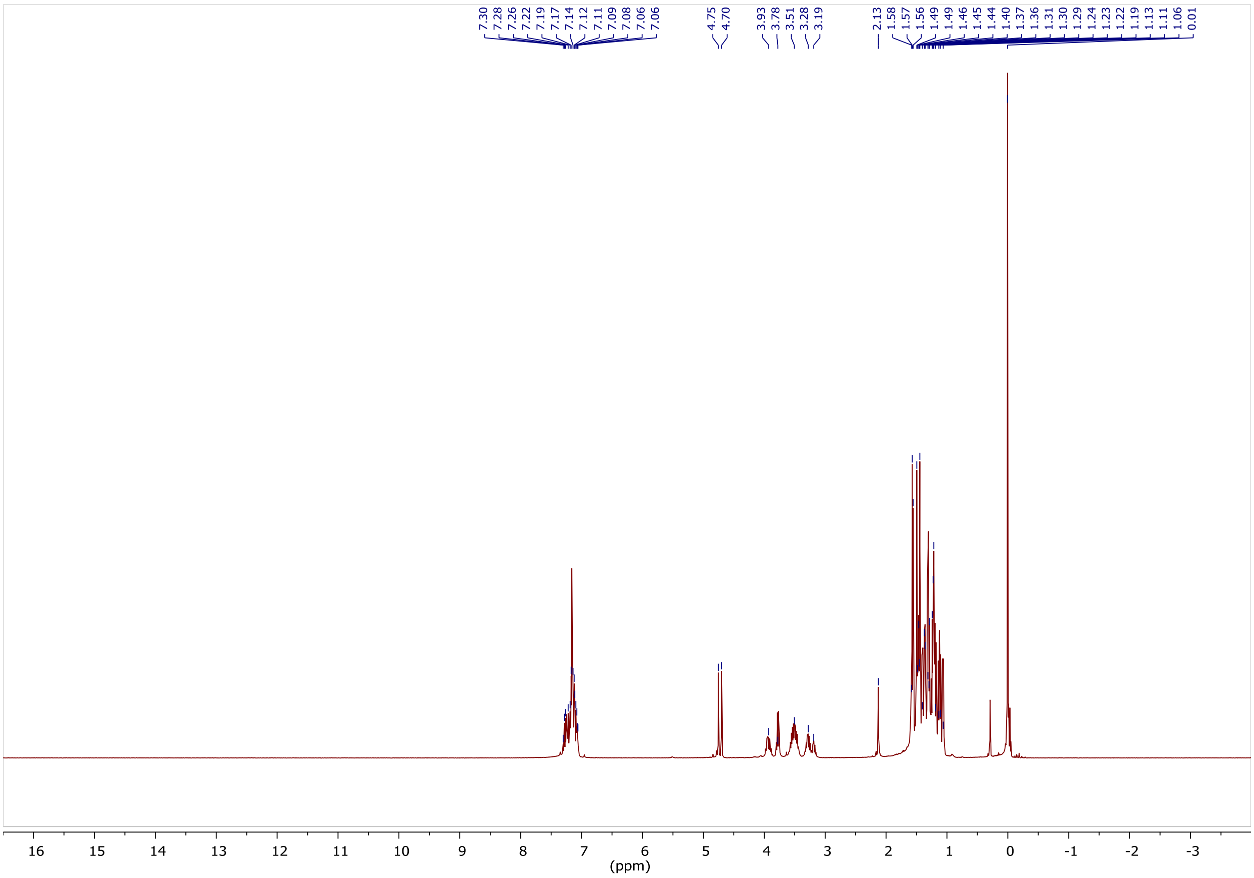

Figure 119: ^1H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $[L(EtO)GaSb]_2C(H)SiMe_3$ (**31**).

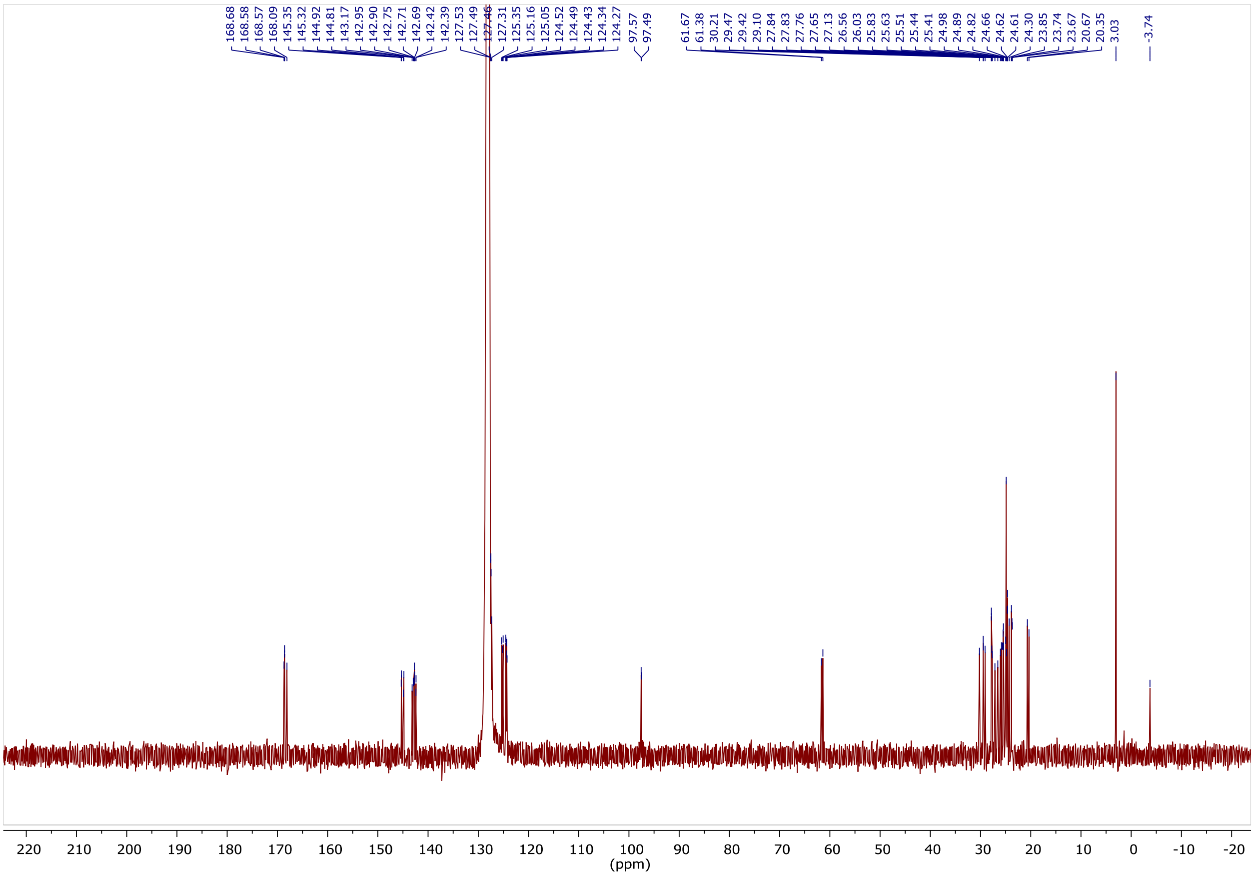

Figure 120: ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) of $[L(EtO)GaSb]_2C(H)SiMe_3$ (**31**).

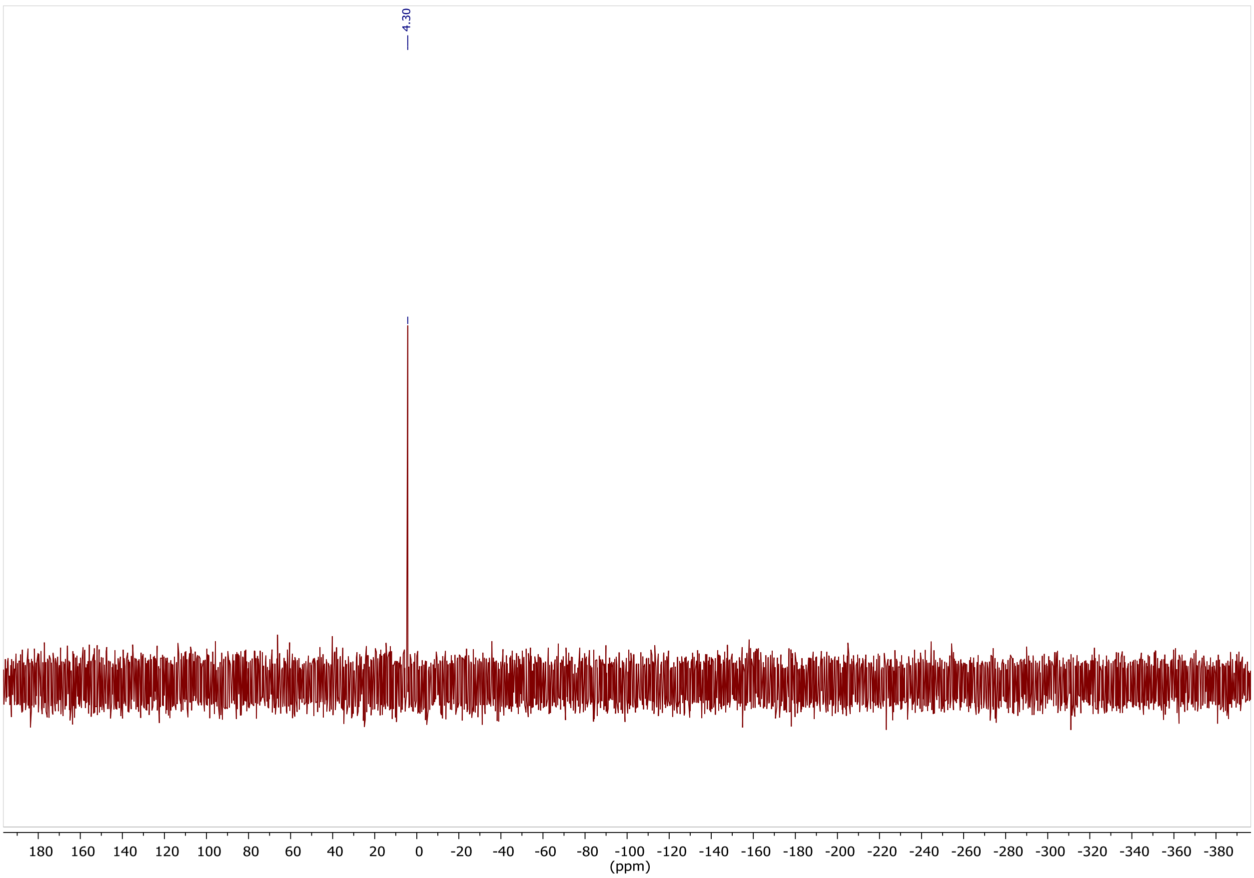

Figure 121: DEPT ^{29}Si NMR spectrum (79.5 MHz, C_6D_6, 25 °C) of $[L(EtO)GaSb]_2C(H)SiMe_3$ (**31**).

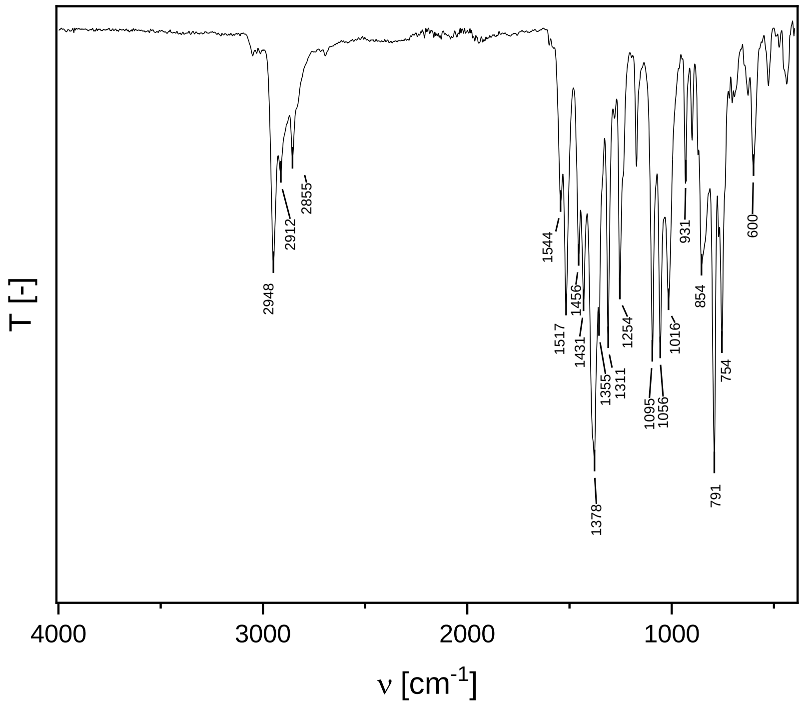

Figure 122: ATR-IR spectrum of $[L(EtO)GaSb]_2C(H)SiMe_3$ (**31**).

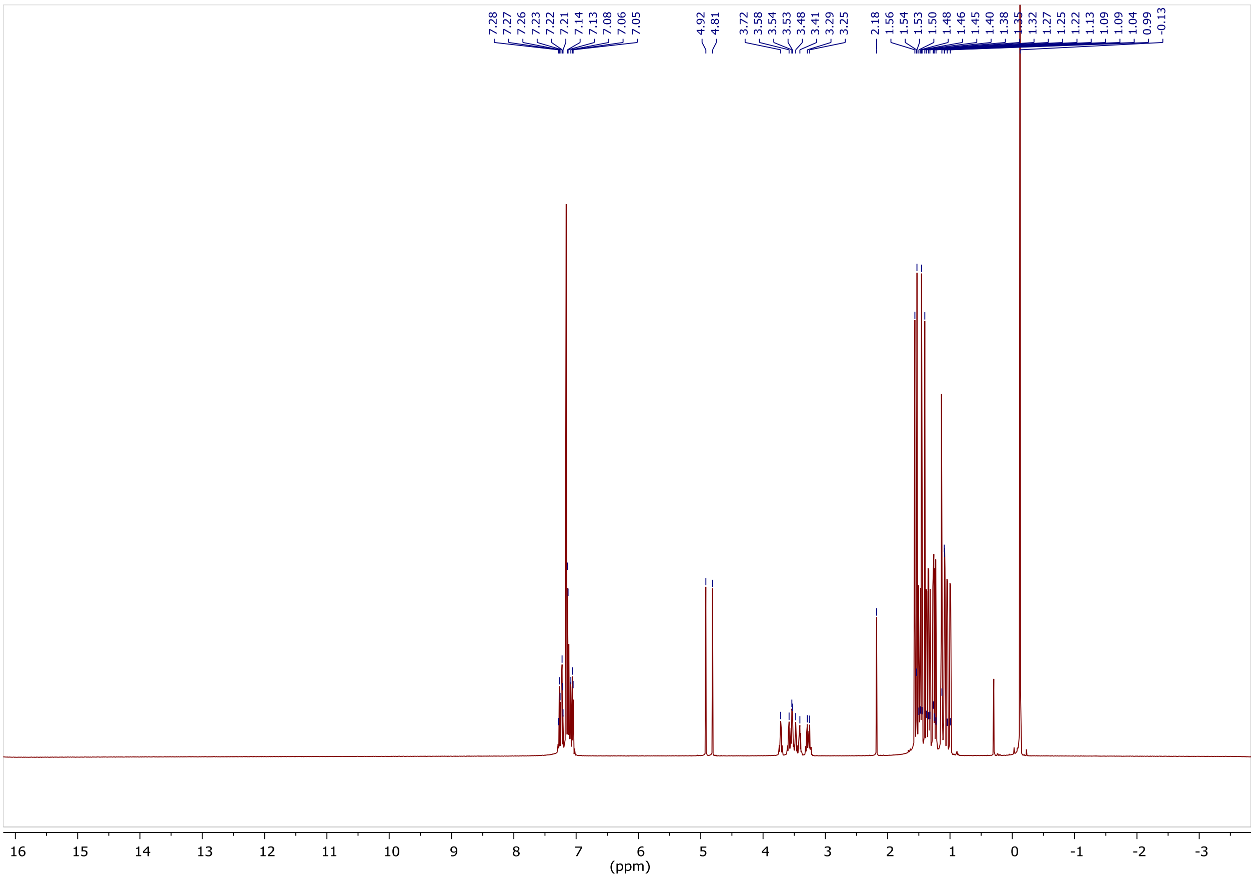

Figure 123: ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of $[L(Cl)GaSb]_2C(H)SiMe_3$ (**32**).

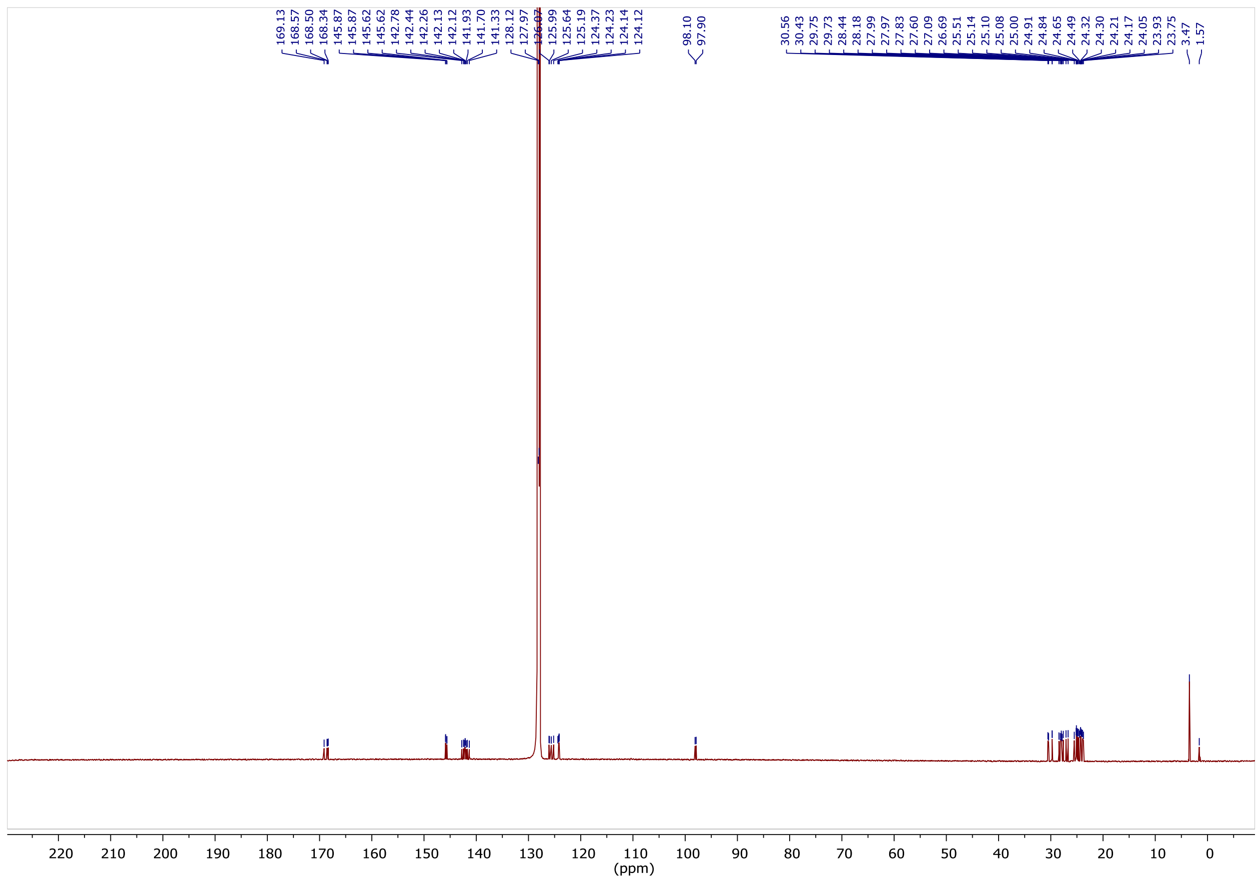

Figure 124: ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Cl)GaSb]_2C(H)SiMe_3$ (**32**).

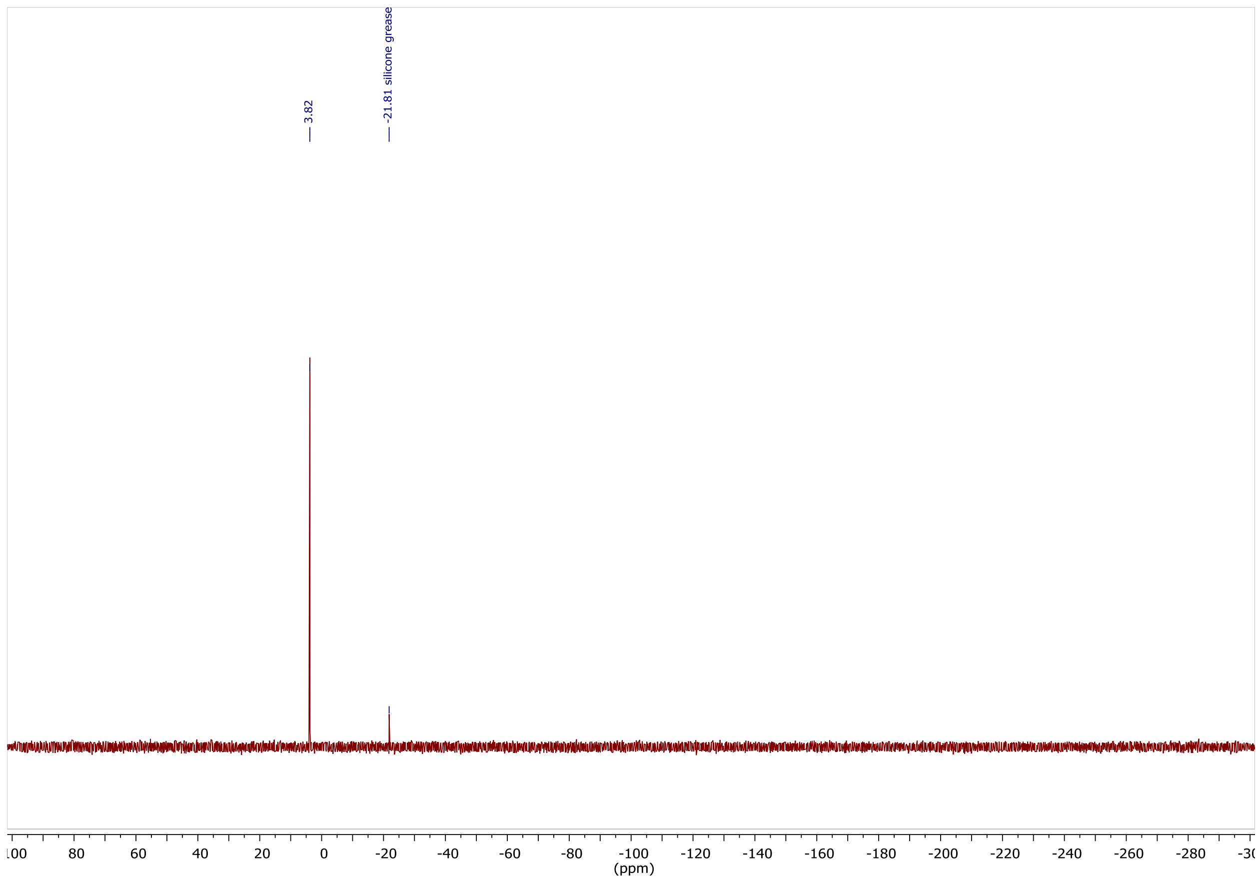

Figure 125: DEPT ^{29}Si NMR spectrum (79.5 MHz, C_6D_6, 25 °C) of $[L(Cl)GaSb]_2C(H)SiMe_3$ (**32**).

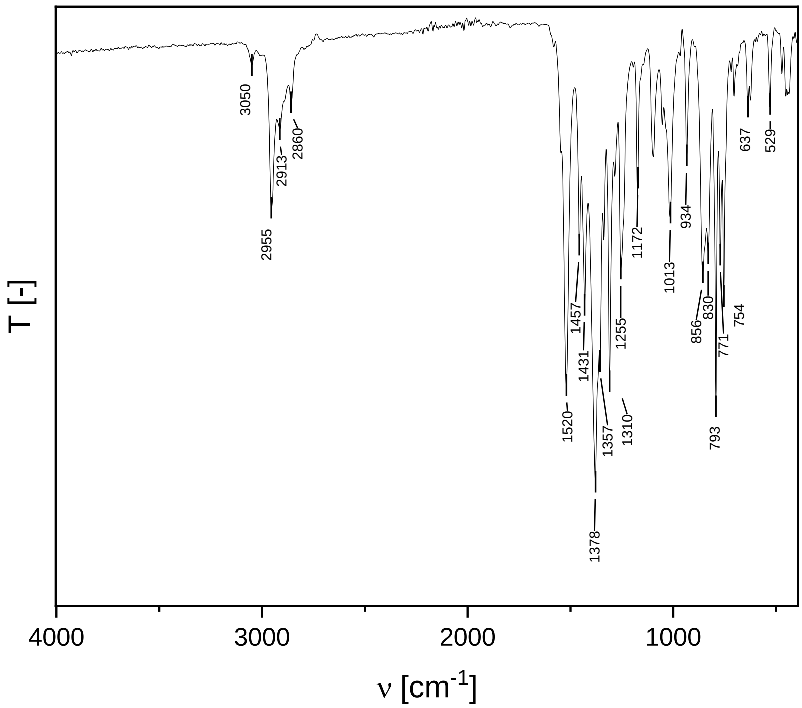

Figure 126: ATR-IR spectrum of [L(Cl)GaSb]$_2$C(H)SiMe$_3$ (**32**).

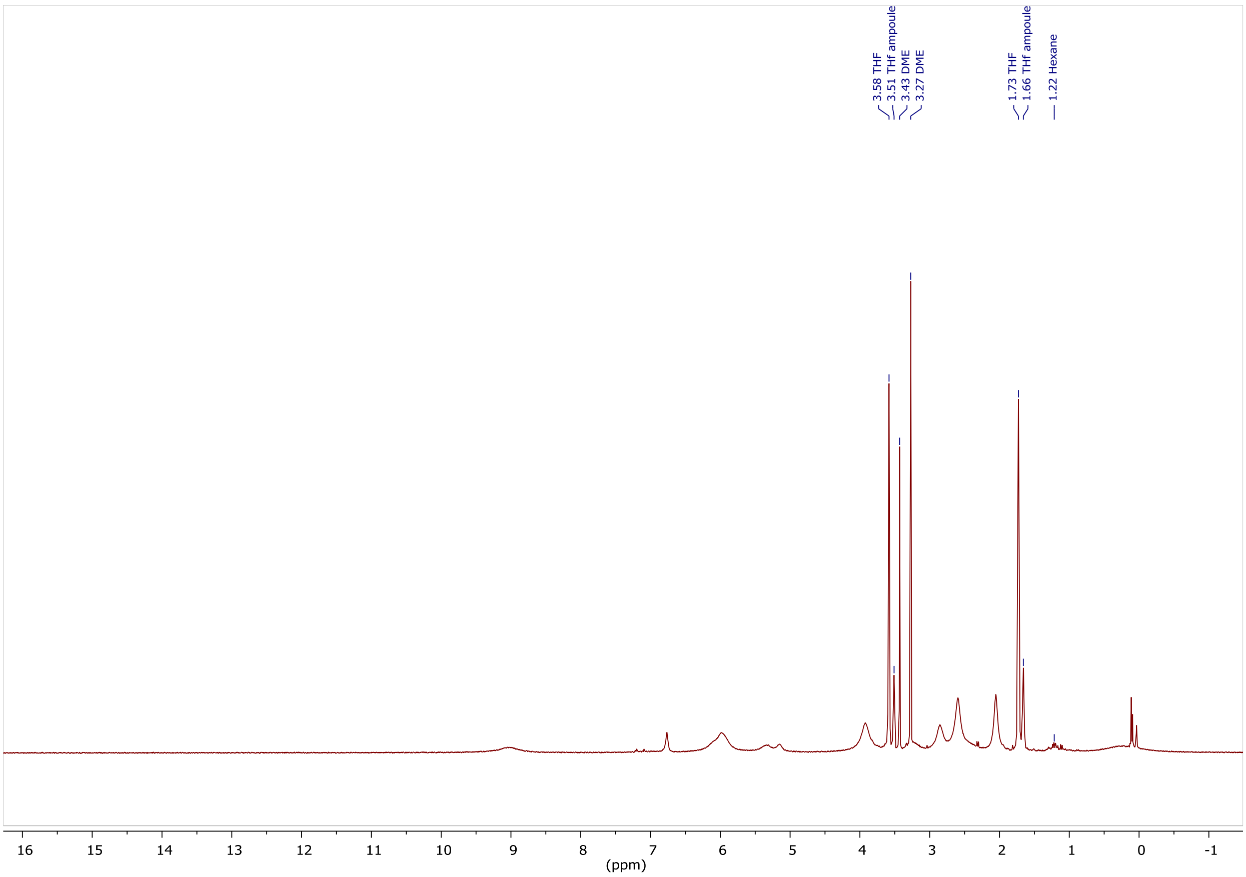

Figure 127: ^{1}H NMR (300 MHz thf-d$_8$, 25 °C) of (DME)[K(B-18-C-6)][L(Me$_2$N)GaSb]$_2$ (**33**) for Evans' method.

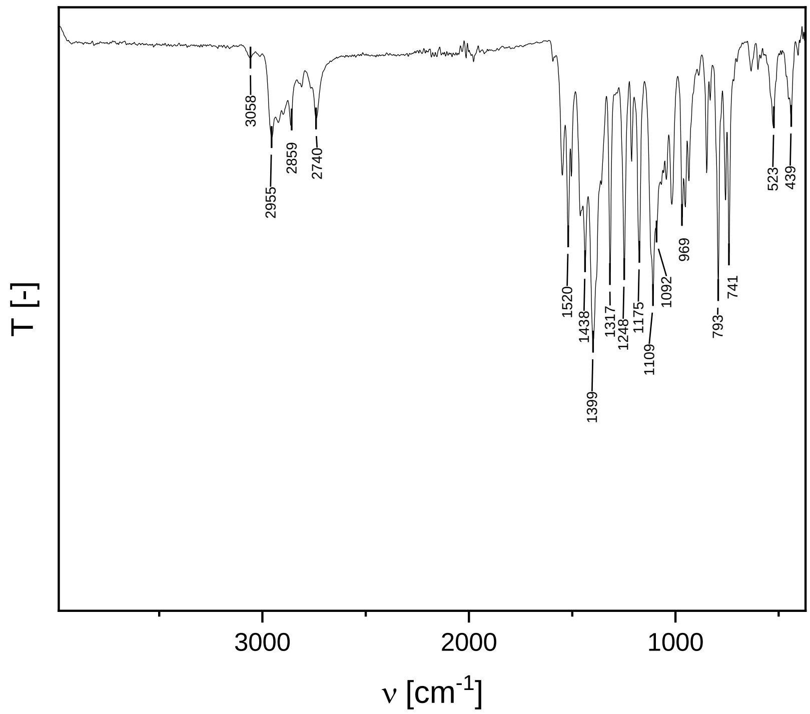

Figure 128: ATR-IR spectrum of (DME)[K(B-18-C-6)][L(Me_2N)GaSb]$_2$ (**33**).

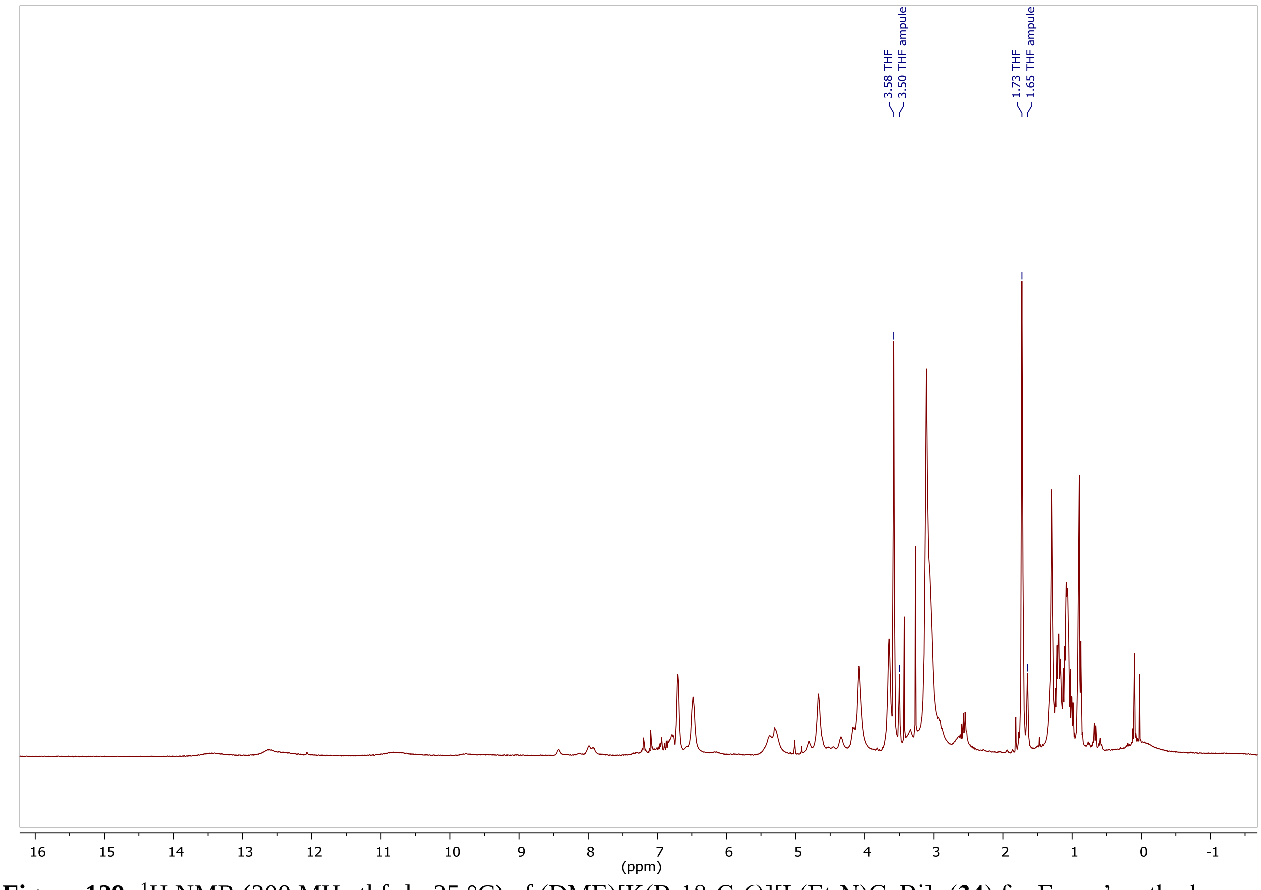

Figure 129: ^{1}H NMR (300 MHz thf-d_8, 25 °C) of (DME)[K(B-18-C-6)][L(Et_2N)GaBi]$_2$ (**34**) for Evans' method.

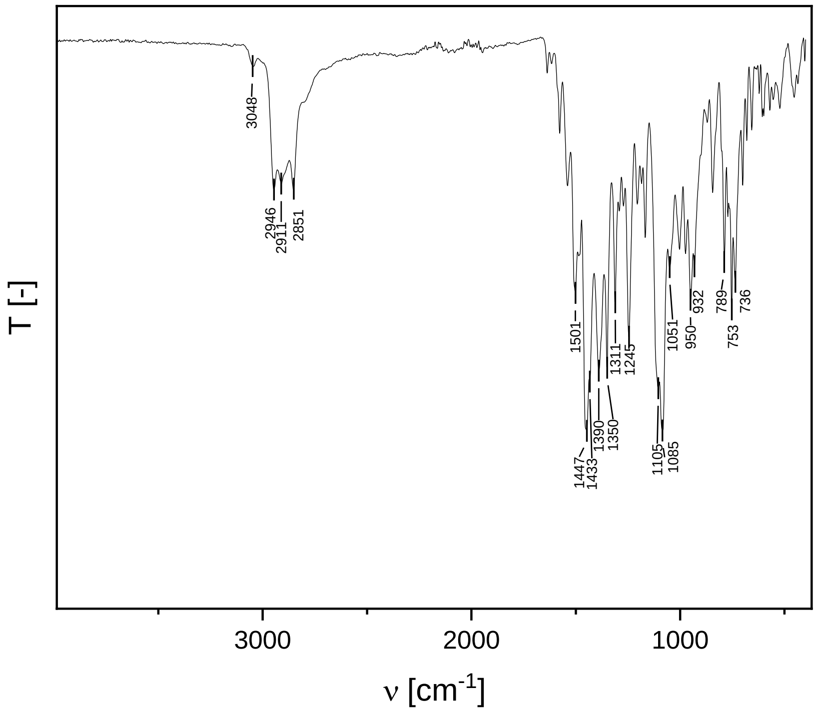

Figure 130: ATR-IR spectrum of (DME)[K(B-18-C-6)][L(Et_2N)GaBi]$_2$ (**34**).

Cyclic Voltammograms:

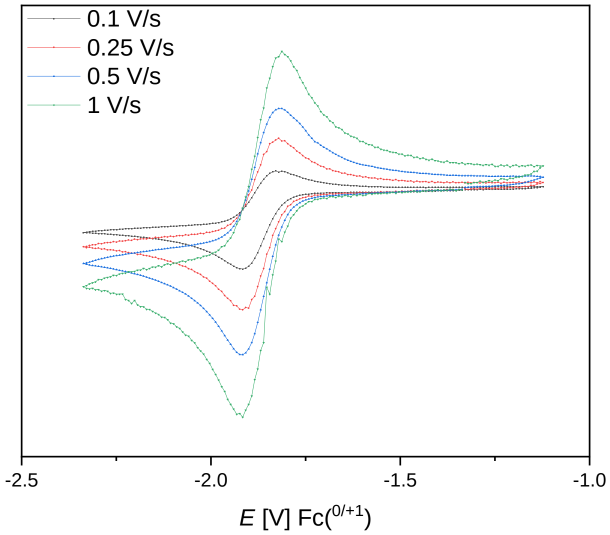

Figure 131: Cyclic voltammograms of [L(Cl)GaAs]$_2$ (**XXI**) in thf solution (1 mM) at ambient temperature containing [*n*-Bu$_4$N][PF$_6$] (100 mM) as electrolyte at varying scan rate showing the reversible reduction event.

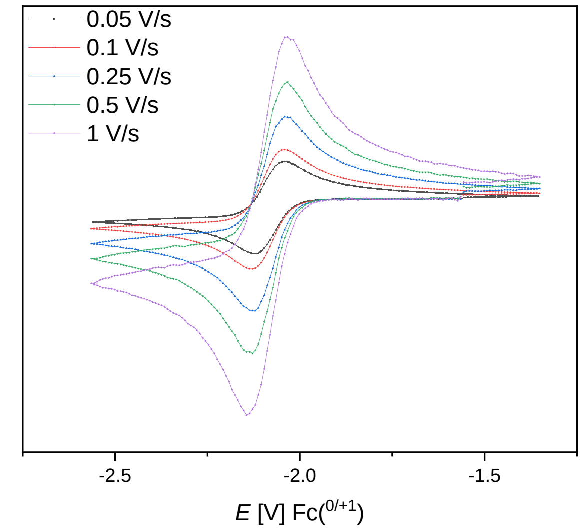

Figure 132: Cyclic voltammograms of [L(EtO)GaAs]$_2$ (**XXII**) in thf solution (1 mM) at ambient temperature containing [*n*-Bu$_4$N][PF$_6$] (100 mM) as electrolyte at varying scan rate showing the reversible reduction event.

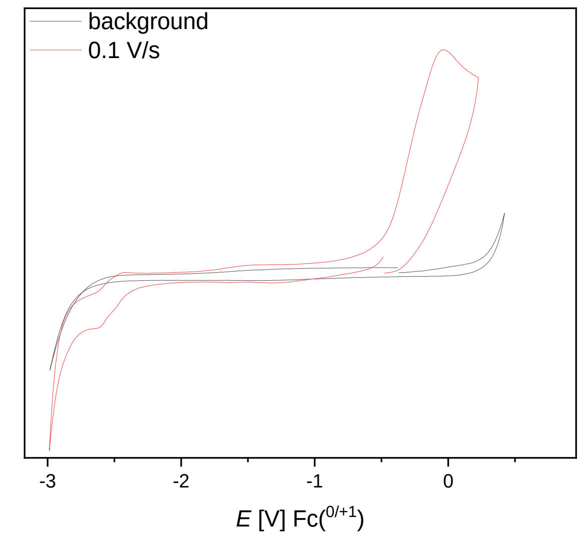

Figure 133: Cyclic voltammograms of [L(Me$_2$N)AlAs]$_2$ (**XXIII**) in thf solution (1 mM) at ambient temperature containing [*n*-Bu$_4$N][PF$_6$] (100 mM) as electrolyte.

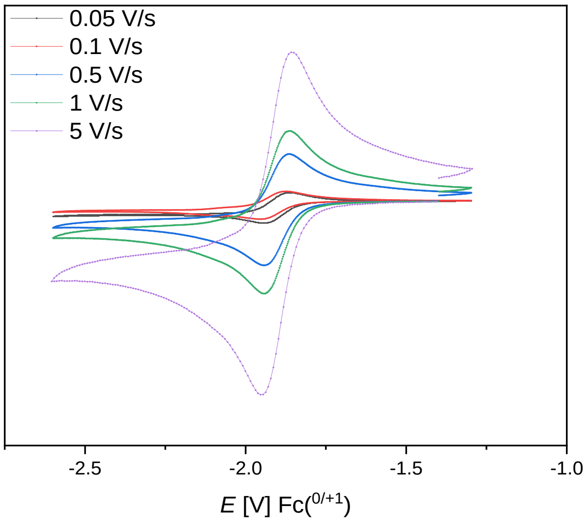

Figure 134: Cyclic voltammograms of $[L(Me_2N)GaSb]_2$ (**XXIV**) in thf solution (1 mM) at 45 °C containing $[n\text{-}Bu_4N][PF_6]$ (100 mM) as electrolyte at varying scan rate showing the reversible reduction event.

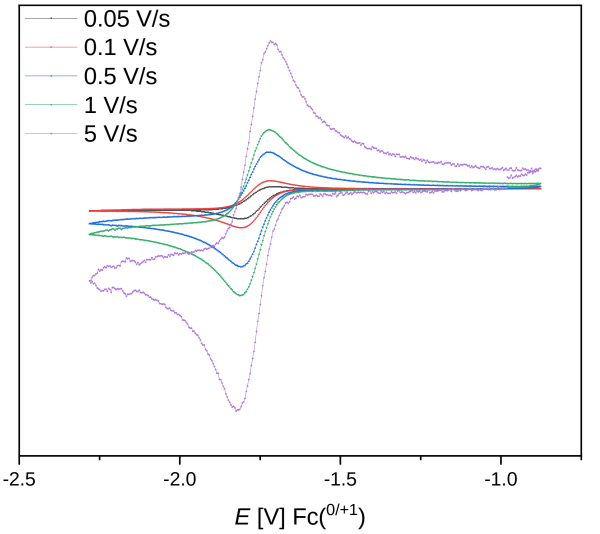

Figure 135: Cyclic voltammograms of $[L(Cl)GaSb]_2$ (**XXVI**) in thf solution (1 mM) at 45 °C containing $[n\text{-}Bu_4N][PF_6]$ (100 mM) as electrolyte at varying scan rates showing the reversible reduction event.

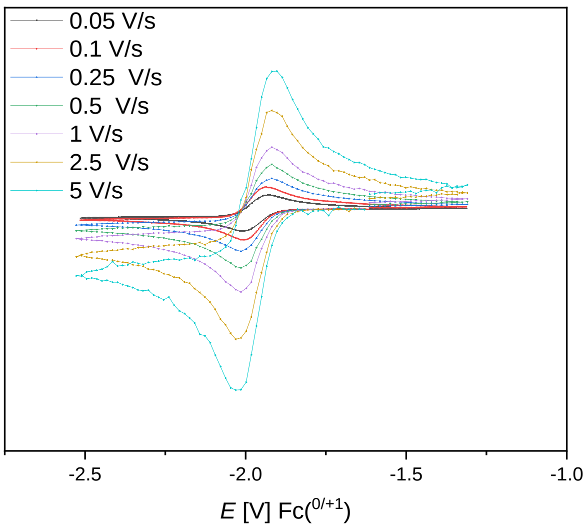

Figure 136: Cyclic voltammograms of $[L(EtO)GaSb]_2$ (**XXIX**) in thf solution (1 mM) at ambient temperature containing $[n\text{-}Bu_4N][PF_6]$ (100 mM) as electrolyte at varying scan rate showing the reversible reduction event.

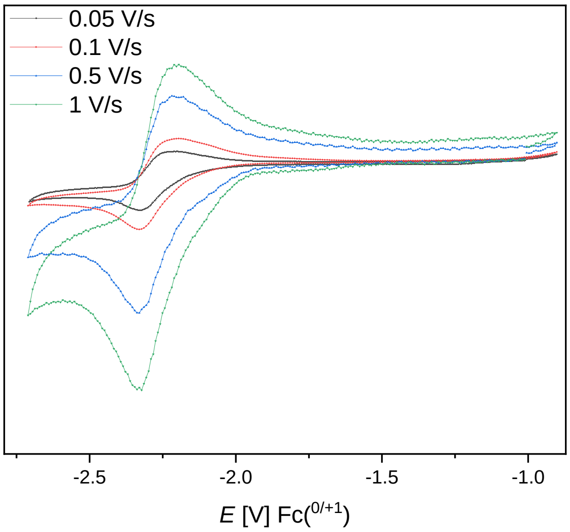

Figure 137: Cyclic voltammograms of $[L(Et_2N)GaBi]_2$ (**XXX**) in thf solution (1 mM) at 45 °C containing $[n\text{-}Bu_4N][PF_6]$ (100 mM) as electrolyte at varying scan rates showing the reversible reduction event.

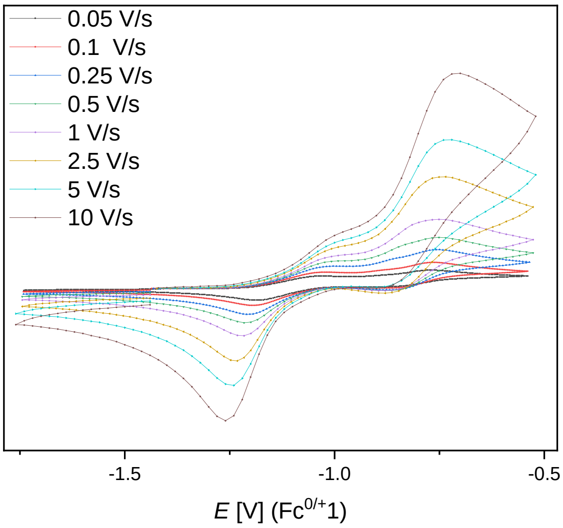

Figure 138: Cyclic voltammograms of $L(Me_2N)GaSbGaL$ (**5**) in 1,2-difluorobenzene solution (1 mM) at ambient temperature containing $[n\text{-}Bu_4N][BarF_{24}]$ (50 mM) as electrolyte at varying scan rate showing the pseudo reversible oxidation event.

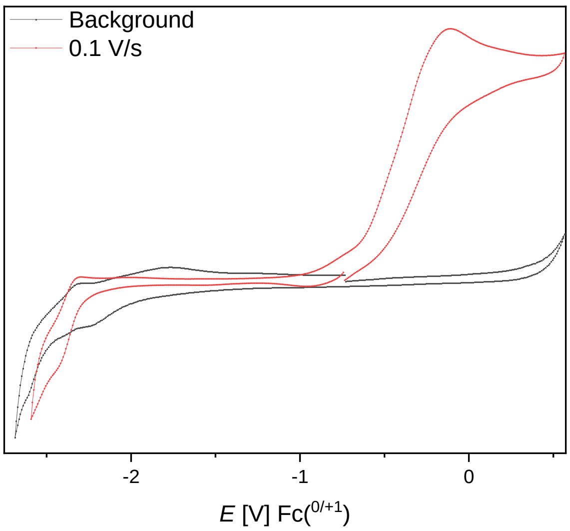

Figure 139: Cyclic voltammograms of $[L(Me_2N)AlSb]_2$ (**6**) in thf solution (1 mM) at ambient temperature containing $[n\text{-}Bu_4N][BarF_{24}]$ (50 mM) as electrolyte.

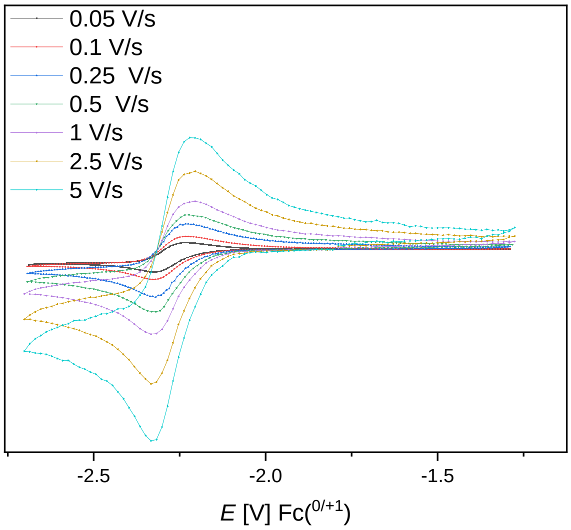

Figure 140: Cyclic voltammograms of [L(Me$_2$N)GaBi]$_2$ (**8**) in thf solution (1 mM) at 45 °C containing [*n*-Bu$_4$N][PF$_6$] (100 mM) as electrolyte at varying scan rates showing the reversible reduction event.

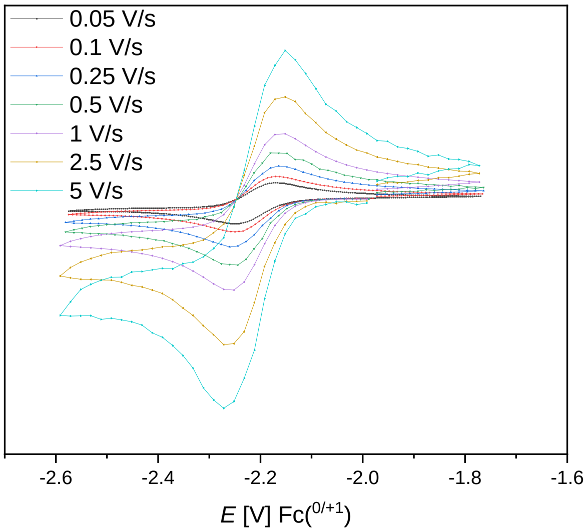

Figure 141: Cyclic voltammograms of [L(EtO)GaBi]$_2$ (**10**) in thf solution (1 mM) at ambient temperature containing [*n*-Bu$_4$N][PF$_6$] (100 mM) as electrolyte at varying scan rate showing the reversible reduction event.

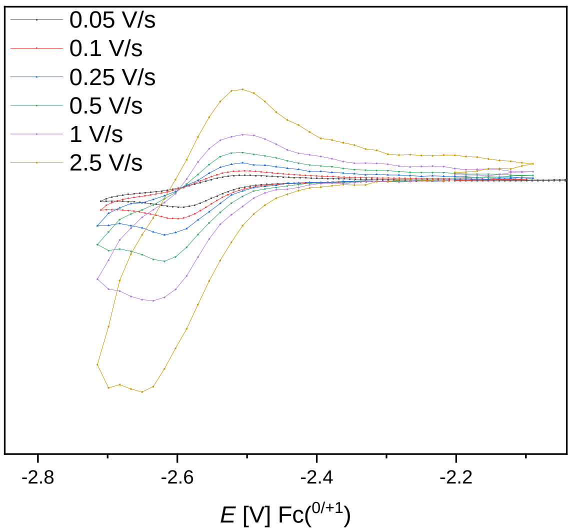

Figure 142: Cyclic voltammograms of [L(Et$_2$N)AlBi]$_2$ (**12**) in thf solution (1 mM) at ambient temperature containing [*n*-Bu$_4$N][PF$_6$] (100 mM) as electrolyte at varying scan rate showing the pseudo reversible reduction event.

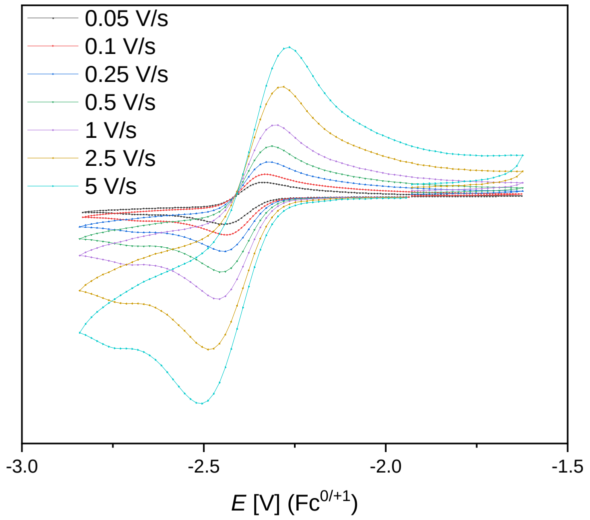

Figure 143: Cyclic voltammograms of [L(Me$_2$N)Ga]SbSb[N(SiMe$_3$)Ga(NMe$_2$)L] (**19**) in thf solution (1 mM) at ambient temperature containing [n-Bu$_4$N][PF$_6$] (100 mM) as electrolyte at varying scan rate showing the reversible reduction event.

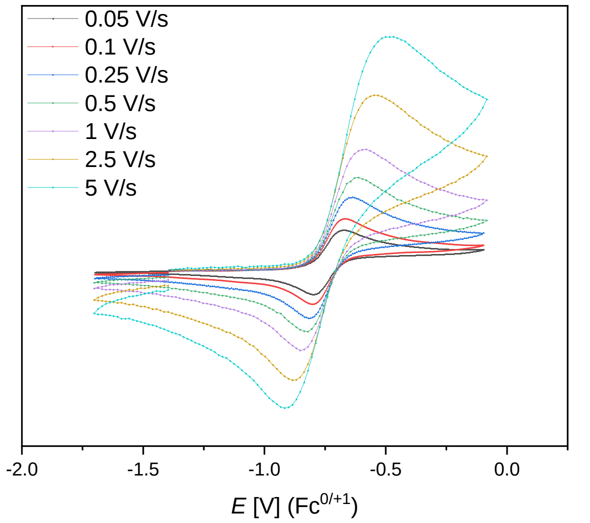

Figure 144: Cyclic voltammograms of [L(Me$_2$N)Ga]SbSb[N(SiMe$_3$)Ga(NMe$_2$)L] (**19**) in 1,2-difluorobenzene solution (1 mM) at ambient temperature containing [n-Bu$_4$N][BarF$_{24}$] (50 mM) as electrolyte at varying scan rate showing the reversible oxidation event.

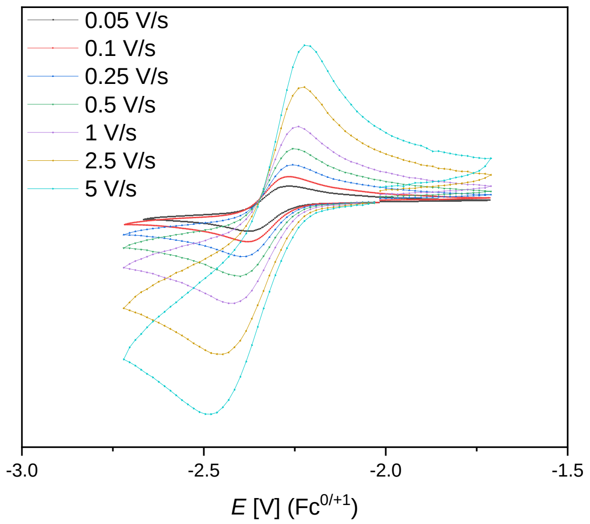

Figure 145: Cyclic voltammograms of [L(Me$_2$N)Ga]SbSb[N(Ph)Ga(NMe$_2$)L] (**25**) in thf solution (1 mM) at ambient temperature containing [n-Bu$_4$N][PF$_6$] (100 mM) as electrolyte at varying scan rate showing the reversible reduction event.

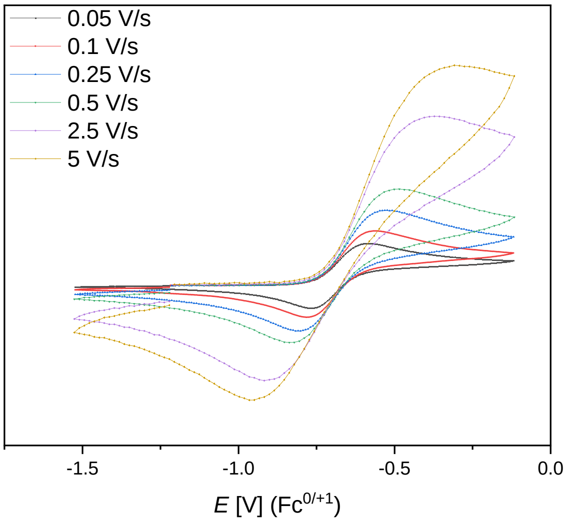

Figure 146: Cyclic voltammograms of [L(Me$_2$N)Ga]SbSb[N(Ph)Ga(NMe$_2$)L] (**25**) in 1,2-difluorobenzene solution (1 mM) at ambient temperature containing [*n*-Bu$_4$N][BarF$_{24}$] (50 mM) as electrolyte at varying scan rate showing the pseudo reversible oxidation event.

UV-Vis spectra:

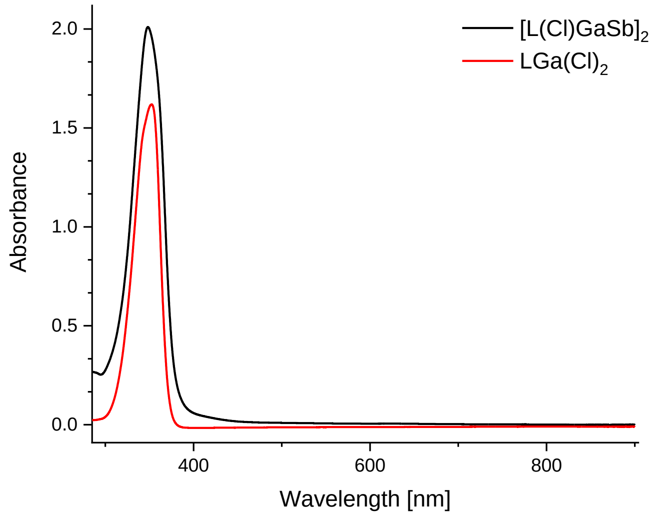

Figure 147: UV-Vis spectra of $[L(Cl)GaAs]_2$ (**XXI)** and $LGa(Cl)_2$.

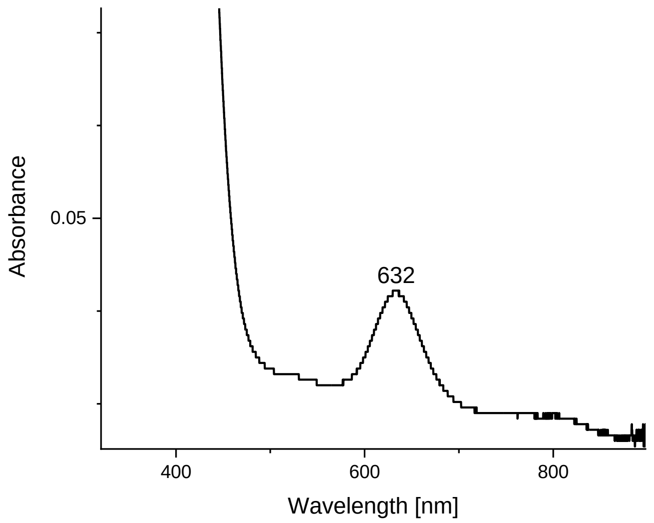

Figure 148: UV-Vis spectrum of $[L(Cl)GaAs]_2$ (**XXI**) in benzene.

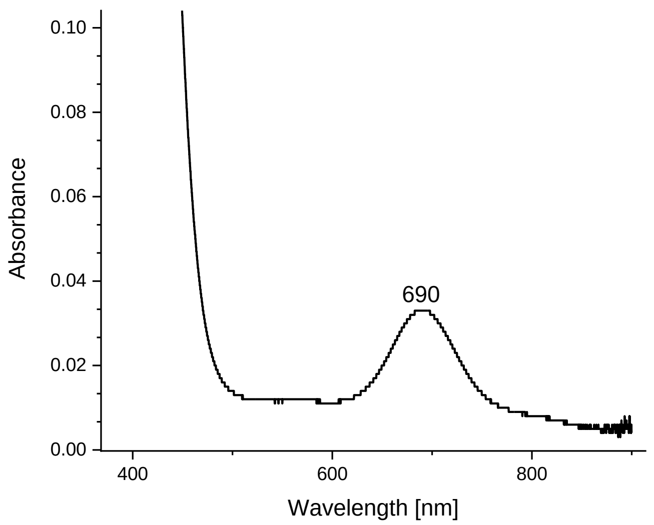

Figure 149: UV-Vis spectrum of $[L(EtO)GaAs]_2$ (**XXII**) in benzene.

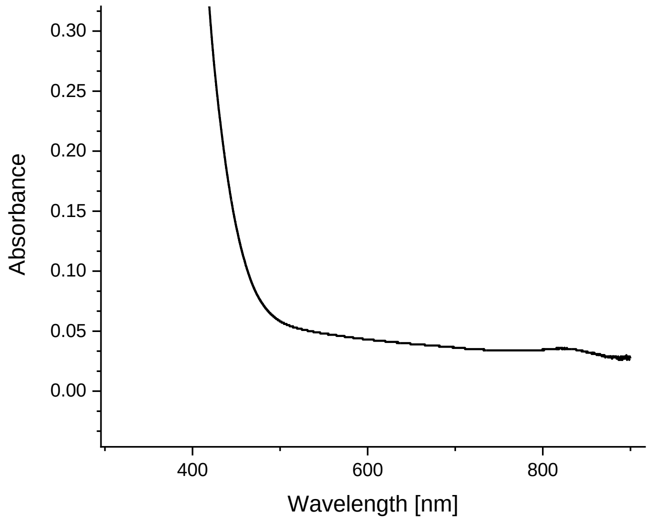

Figure 150: UV-Vis spectrum of $[L(Me_2N)AlAs]_2$ (**XXXIII**) in benzene.

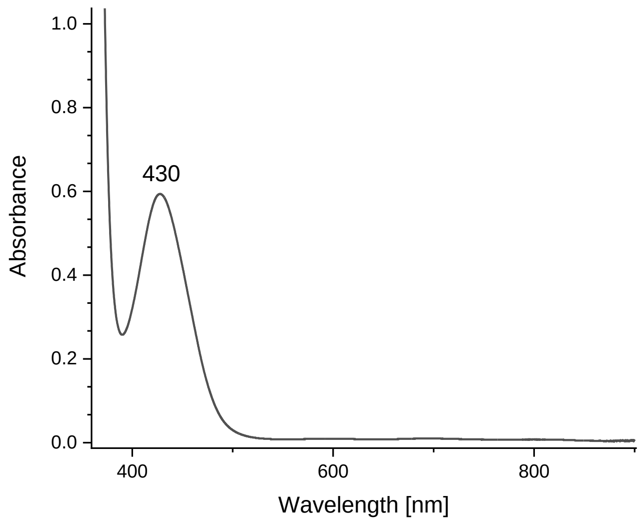

Figure 151: UV-Vis spectrum of $[L(Me_2N)GaSb]_2$ (**XXIV**) in benzene.

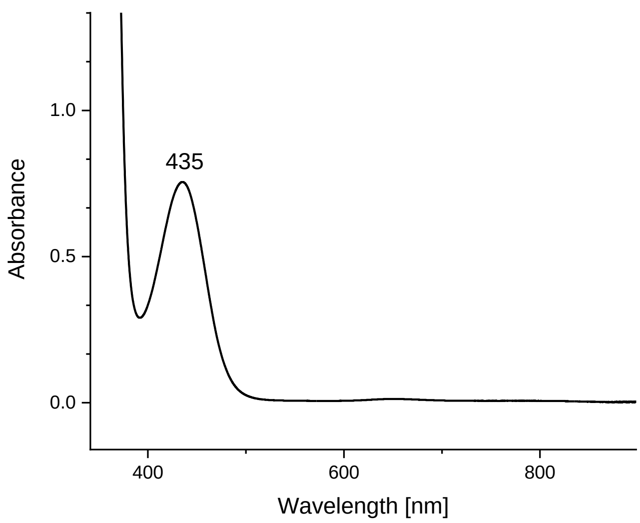

Figure 152: UV-Vis spectrum of $[L(Cl)GaSb]_2$ (**XXVI**) in benzene.

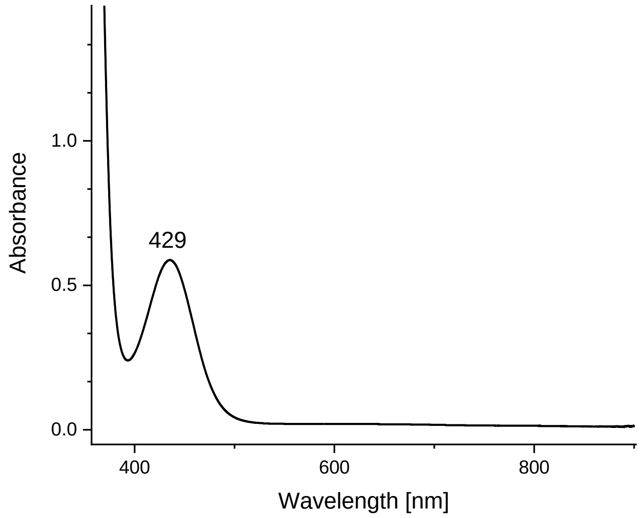

Figure 153: UV-Vis spectrum of $[L(EtO)GaSb]_2$ (**XXIX**) in benzene.

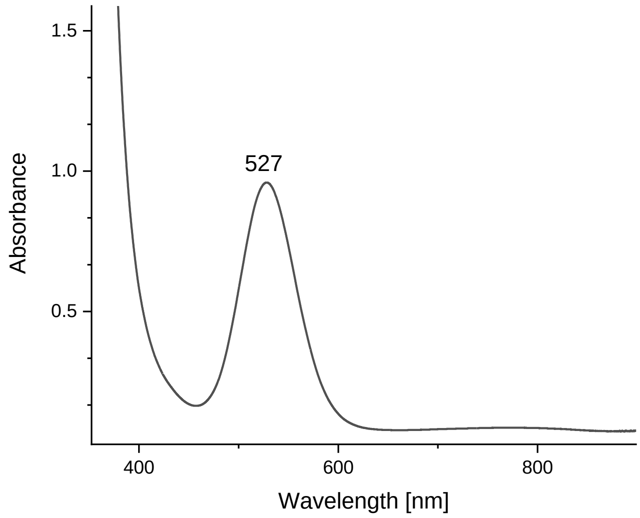

Figure 154: UV-Vis spectrum of $[L(Et_2N)GaBi]_2$ (**XXX**) in benzene.

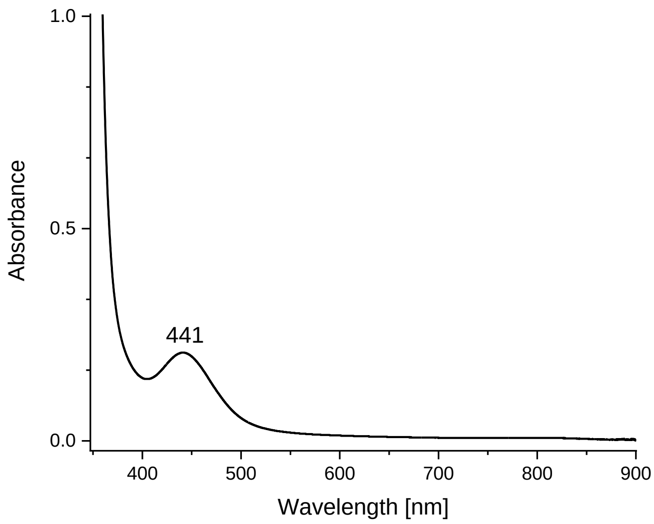

Figure 155: UV-Vis spectrum of $[L(Me_2N)AlSb]_2$ (**6**) in benzene. Decomposed during measurement.

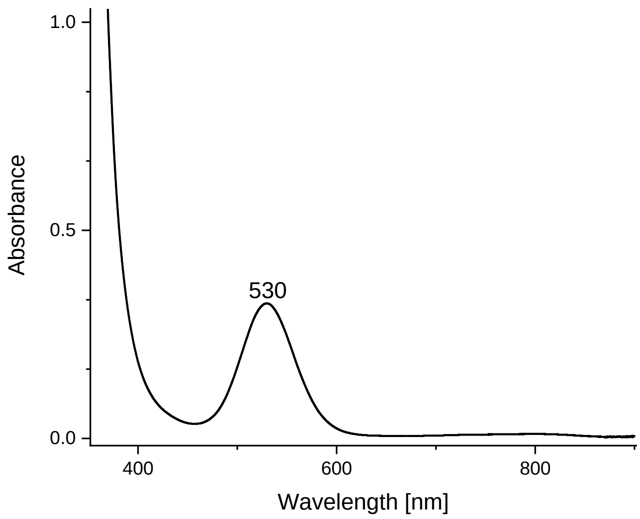

Figure 156: UV-Vis spectrum of $[L(Me_2N)GaBi]_2$ (**8**) in benzene.

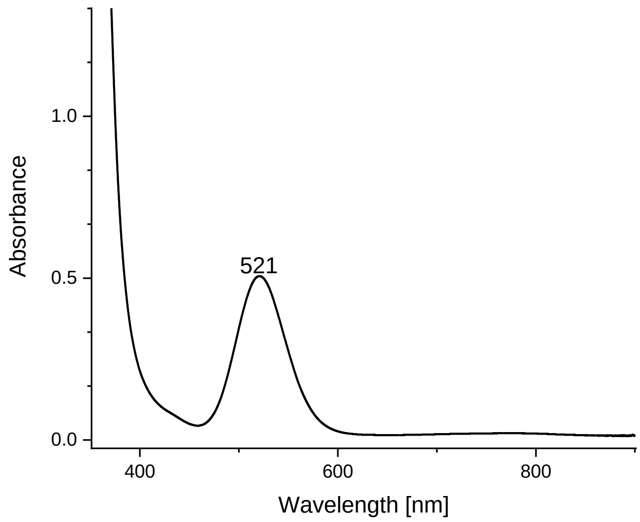

Figure 157: UV-Vis spectrum of $[L(EtO)GaBi]_2$ (**10**) in benzene.

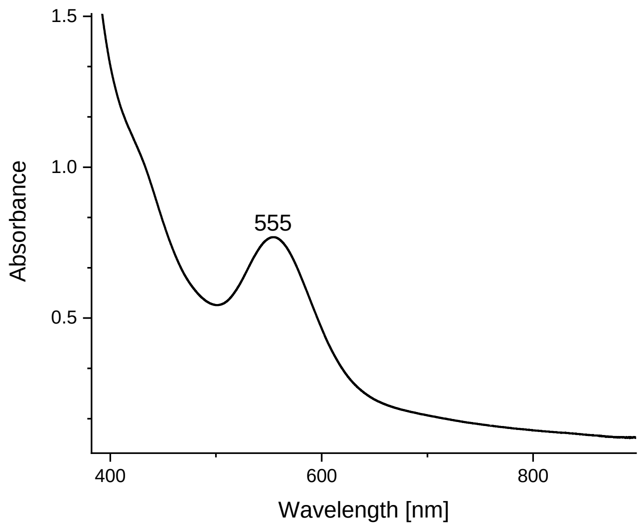

Figure 158: UV-Vis spectrum of $[L(Et_2N)AlBi]_2$ (**12**) in benzene.

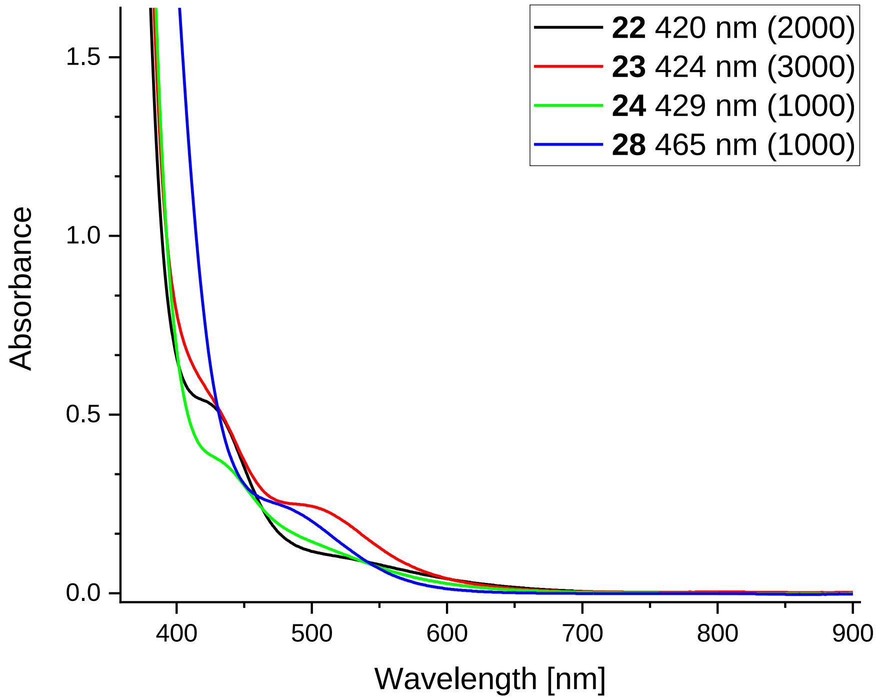

Figure 159: UV-vis spectra of azadistibirane **22**–**24** and **28** in toluene. Extinction coefficients are given in brackets, the wavelength refers to the inflection point.

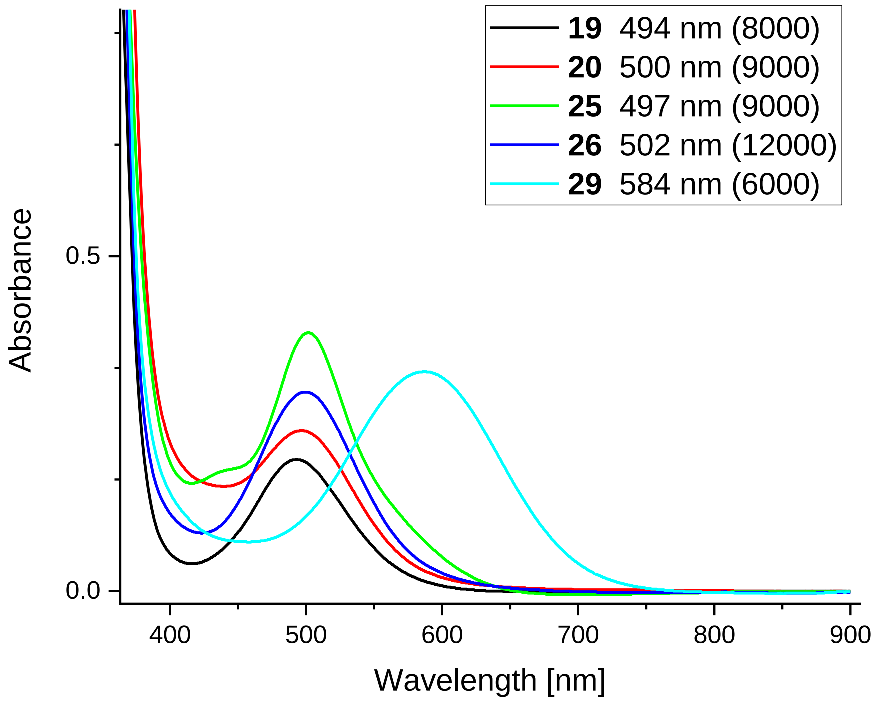

Figure 160: UV-vis spectra of distibenes **19**, **20**, **25**. **26** and **29** in toluene. Extinction coefficients are given in brackets.

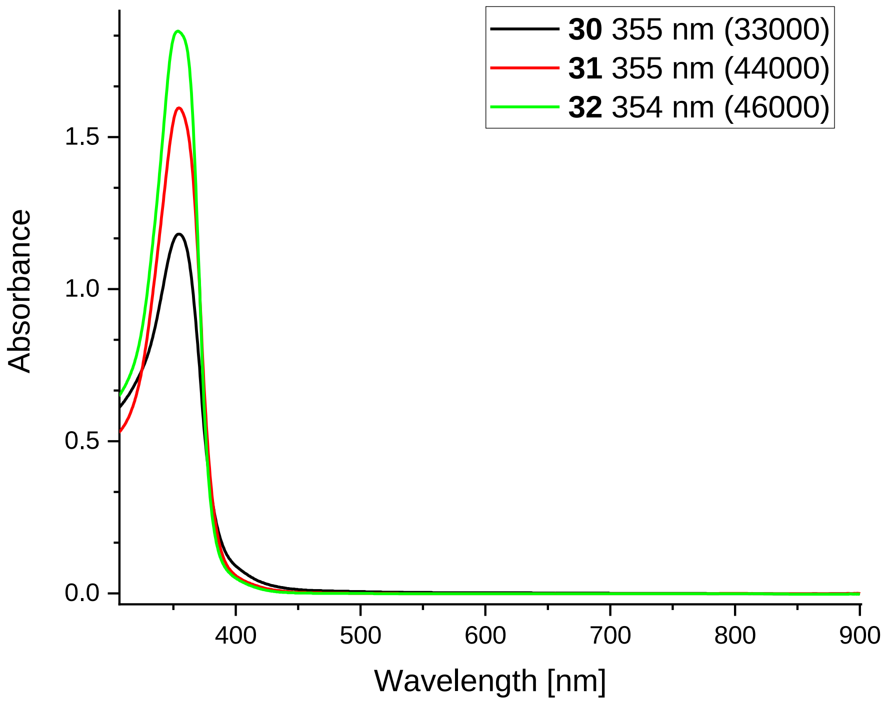

Figure 161: UV-vis spectra of distibirane **30**–**32** in toluene. Extinction coefficients are given in brackets.

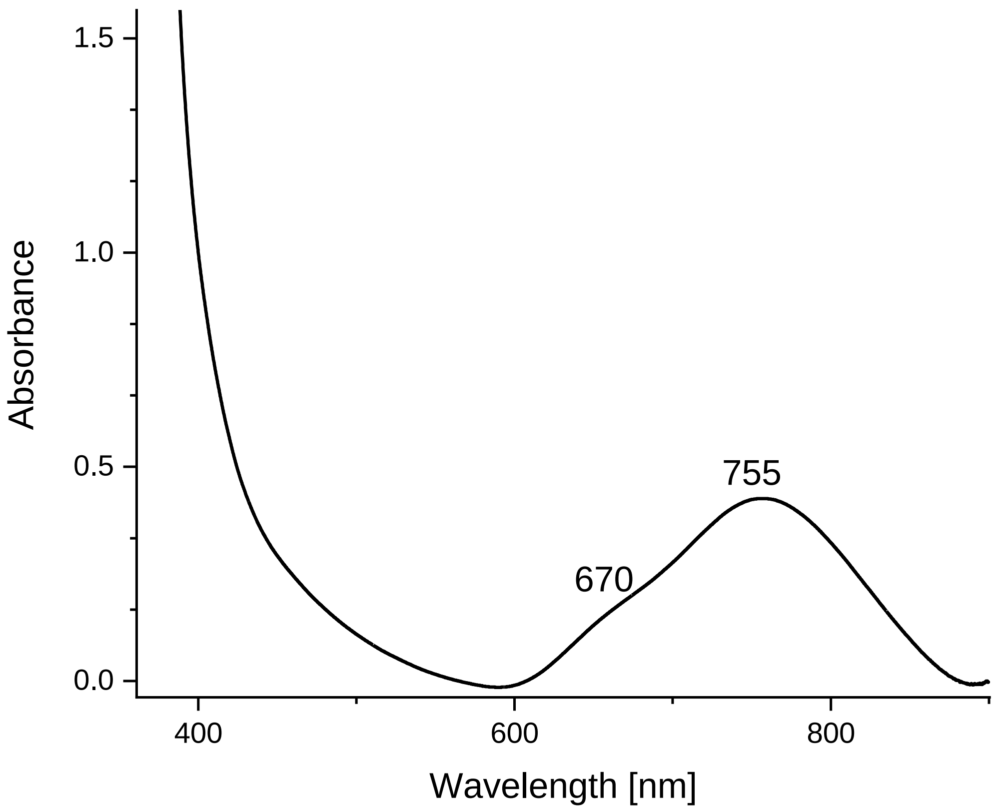

Figure 162: UV-Vis spectrum of (DME)[K(B-18-C-6)][L(Me$_2$N)GaSb]$_2$ (**33**) in thf solution.

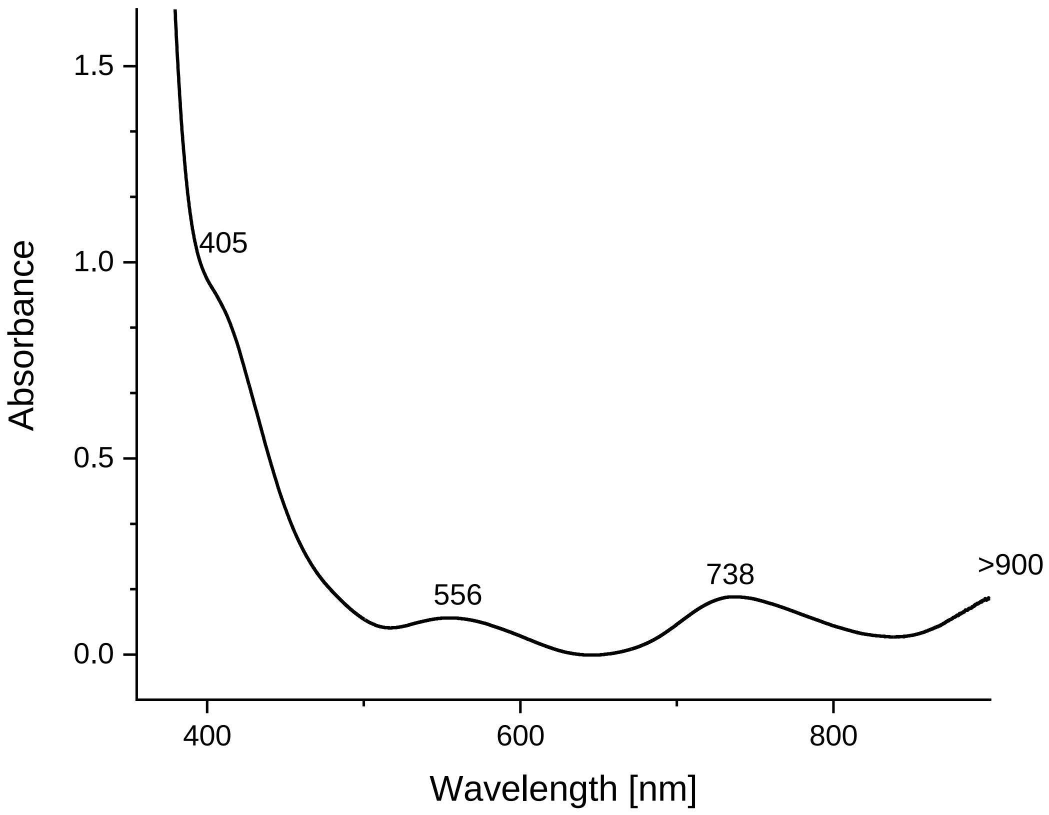

Figure 163: UV-Vis spectrum of (DME)[K(B-18-C-6)][L(Et_2N)GaBi]$_2$ (**34**) in thf solution.

Cartesian Coordinates from Geometry Optimization

Table 2: Cartesian coordinates of $[L(Me_2N)GaSb]_2$ (**XXIV**) [Å] for the optimized geometry. ORCA Version 4.2.1. Optimization: def2-SVP for H, C, N and def2-TZVP for Ga, Sb. Single-point: def2-TZVP for H, C, N and def2-QZVPP for Ga, Sb.

Sb	-2.88665266	7.222704001	0.019784319	Sb	-1.66968342	4.907113154	-0.171072979
Ga	-2.07422035	7.386233793	2.488356019	Ga	-2.24156069	4.574618883	-2.690562137
N	-3.19319325	8.705441787	3.476035536	N	-1.5356504	2.835866994	-3.345579495
N	-2.52950357	5.904361454	3.766235917	N	-1.00536655	5.647836787	-3.860513821
N	-0.27019253	7.794138561	2.766032219	N	-3.97753918	4.727296312	-3.36930266
C	-3.36394732	8.624357456	4.791494006	C	-1.04058117	2.710743653	-4.574412575
C	-3.09679303	7.460628558	5.529287206	C	-0.66021789	3.800605033	-5.37256607
H	-3.25004043	7.532162828	6.605123238	H	-0.28602596	3.554115641	-6.366060056
C	-2.81266635	6.171257803	5.036540236	C	-0.51968478	5.15053947	-4.987361745
C	-3.85675405	9.828832251	5.545203343	C	-0.87477902	1.334990393	-5.159350603
H	-3.04302636	10.56876593	5.61004173	H	-1.86283691	0.932942067	-5.432686349
H	-4.17013485	9.565761408	6.562476815	H	-0.24760786	1.356827538	-6.058494943
H	-4.68680467	10.32300522	5.023586489	H	-0.44195226	0.63674131	-4.430200436
C	-2.84186413	5.049491732	6.038479066	C	0.25984239	6.020907676	-5.937261377
H	-3.30523081	4.146890279	5.618335109	H	0.28922614	7.068870722	-5.617105957
H	-3.37829236	5.347171837	6.947276869	H	1.29019419	5.648136519	-6.029513179
H	-1.81307753	4.776106932	6.318146308	H	-0.19252589	5.963418584	-6.938492406
C	-3.80718922	9.75210268	2.730205087	C	-1.66890775	1.700044083	-2.493451427
C	-5.15621663	9.590155837	2.335710465	C	-0.60822934	1.393555152	-1.606827362
C	-5.76776643	10.6150852	1.61049079	C	-0.73434005	0.273655124	-0.781158034
H	-6.81252626	10.50766113	1.309847262	H	0.07671201	0.018772946	-0.097667534
C	-5.06861925	11.76298511	1.254402406	C	-1.87717266	-0.518575227	-0.804823471
H	-5.56385166	12.55422499	0.686656401	H	-1.95255797	-1.392848474	-0.153497967
C	-3.73260963	11.88859438	1.610793519	C	-2.92590394	-0.18219778	-1.648836457
H	-3.17786497	12.78212918	1.313196375	H	-3.83354556	-0.790984011	-1.651163957
C	-3.07733013	10.89304492	2.343135477	C	-2.84793101	0.926339701	-2.498613075
C	-5.94408368	8.340081424	2.681519218	C	0.64366033	2.25073053	-1.543756461
H	-5.21800918	7.583639144	3.014501233	H	0.3259362	3.282569803	-1.770378853
C	-6.67698998	7.772915277	1.468016957	C	1.27686254	2.259446802	-0.15627557
H	-7.4609373	8.454779387	1.103674017	H	1.72154104	1.284673113	0.099049195
H	-7.16964942	6.824453431	1.729241657	H	2.08526841	3.002167266	-0.11168768
H	-5.98333638	7.579580969	0.63501446	H	0.53859039	2.519172582	0.616531531
C	-6.91587182	8.58104219	3.83784296	C	1.67504137	1.858815111	-2.603527557
H	-6.39450512	8.899179955	4.751483007	H	1.28877455	1.983460006	-3.624017684
H	-7.47097816	7.659987394	4.075384693	H	2.5738138	2.489511884	-2.513432872
H	-7.65044318	9.361124588	3.580308873	H	1.98534347	0.80865346	-2.4802209
C	-1.61066657	11.06494387	2.679574485	C	-4.04372887	1.277441204	-3.358762254
H	-1.28389898	10.15536116	3.2029857	H	-3.76052992	2.136266686	-3.980882037
C	-0.77699157	11.17722593	1.403567367	C	-5.21254524	1.723430267	-2.480532362
H	-0.92763632	10.30134131	0.755207282	H	-4.91325052	2.551677131	-1.823705727
H	0.29515837	11.24259988	1.64405765	H	-6.05443866	2.070386011	-3.099715569
H	-1.0447178	12.07604876	0.825118161	H	-5.57618559	0.896115855	-1.849812523
C	-1.37032328	12.25977817	3.601715494	C	-4.45948292	0.133026886	-4.282350578
H	-1.64774395	13.20822994	3.114241136	H	-4.81610282	-0.740447758	-3.71376618
H	-0.30665432	12.32657197	3.879308066	H	-5.28062927	0.452413134	-4.94287743
H	-1.95844224	12.18287199	4.528511893	H	-3.6269345	-0.20725347	-4.916580165
C	-2.38630292	4.551357025	3.330870959	C	-0.62844324	6.93166452	-3.363630723
C	-3.47741347	3.930521675	2.673900122	C	0.61460446	7.083662308	-2.708958033
C	-3.31834999	2.62163288	2.209125235	C	0.91621191	8.318151419	-2.124049639
H	-4.13916199	2.13322046	1.6833246	H	1.87292734	8.446453242	-1.612249059
C	-2.12366569	1.931081818	2.384188246	C	0.0182373	9.374204157	-2.16500608
H	-2.01922564	0.915629331	1.996857964	H	0.26438037	10.32567489	-1.6882826
C	-1.06192606	2.555103354	3.021175399	C	-1.20267135	9.21130827	-2.811288113

H	-0.11700897	2.019743373	3.141968096	H	-1.90755839	10.04312182	-2.834580698
C	-1.16291118	3.86889281	3.492812394	C	-1.55022547	8.002889318	-3.421481114
C	-4.78419479	4.667896134	2.455728806	C	1.64484451	5.971987984	-2.626671178
H	-4.50960899	5.707741652	2.2022308	H	1.18736786	5.05559049	-3.029700385
C	-5.59129446	4.118370486	1.28556753	C	2.06416904	5.683399024	-1.186833775
H	-4.97793978	4.042171539	0.375462413	H	1.20125581	5.414929383	-0.558202112
H	-6.43790815	4.783416029	1.063627481	H	2.78378248	4.851263959	-1.157106975
H	-6.00819794	3.122394403	1.5028933	H	2.55064199	6.554638065	-0.722203478
C	-5.64390902	4.712687899	3.721077814	C	2.87810598	6.296800039	-3.473751076
H	-6.60025821	5.218645966	3.516686463	H	3.57822513	5.446461431	-3.482255067
H	-5.15476839	5.258088384	4.539029671	H	2.61445644	6.533777107	-4.513377303
H	-5.87214843	3.694301882	4.074075039	H	3.41560317	7.167148763	-3.064715999
C	0.06336739	4.51704516	4.102991915	C	-2.87869711	7.861442293	-4.141785722
H	-0.22689796	5.517239021	4.452149342	H	-3.23156017	6.835629774	-3.95301987
C	1.14510194	4.705057184	3.039758958	C	-3.95451501	8.814786158	-3.632160882
H	1.5228591	3.734579977	2.680861086	H	-3.7368927	9.863650794	-3.891573047
H	1.99899232	5.267889176	3.448167152	H	-4.92190476	8.564699634	-4.093112036
H	0.7505123	5.256651292	2.176330026	H	-4.0713122	8.747216338	-2.54000286
C	0.61310783	3.730448546	5.293194001	C	-2.70773505	8.023867323	-5.653726299
H	-0.15014068	3.554084862	6.065905716	H	-2.04360907	7.260133877	-6.077836366
H	1.44904494	4.275299842	5.758914086	H	-3.68081646	7.935086707	-6.161870254
H	0.99674411	2.74572384	4.982788273	H	-2.2867641	9.013232224	-5.896951442
C	0.68152549	7.984944222	1.712917182	C	-5.08502856	5.276335311	-2.645782806
H	1.06744957	9.025188293	1.667267054	H	-5.99290506	4.643601162	-2.733043218
H	0.23590859	7.758377367	0.73166851	H	-4.84890126	5.367032912	-1.574837653
H	1.57207102	7.330615824	1.825422444	H	-5.3745711	6.290080479	-2.998919882
C	0.24810302	8.115326642	4.061541997	C	-4.24486815	4.562967146	-4.767691106
H	1.14572653	7.512134932	4.319414252	H	-4.47538435	5.52278992	-5.28285926
H	-0.50002356	7.937667576	4.849912136	H	-3.38419543	4.119770833	-5.292489388
H	0.56330681	9.180291991	4.149027681	H	-5.11864843	3.900455323	-4.948614411

Table 3: Cartesian coordinates of $[L(Et_2N)GaBi]_2$ (**XXX**) [Å] for the optimized geometry. ORCA Version 4.2.1. Optimization: def2-SVP for H, C, N and def2-TZVP for Ga, Bi. Single-point: def2-TZVP for H, C, N and def2-QZVPP for Ga, Bi.

Bi	-0.09238185	-0.33990564	1.34046818	Bi	0.09301410	0.33874549	-1.33993510
Ga	2.56392709	-0.10043865	1.52796859	Ga	-2.56326763	0.09920268	-1.52763182
N	3.06136449	-0.99797020	3.24364338	N	-3.06056490	0.99665014	-3.24341698
N	3.74685199	-1.28062775	0.40483184	N	-3.74629638	1.27936749	-0.40464783
N	3.36885424	1.59512973	1.46569858	N	-3.36825657	-1.59635064	-1.46542027
C	4.30110419	-1.45354814	3.39693325	C	-4.30026316	1.45229974	-3.39680625
C	5.16494565	-1.71202479	2.31973138	C	-5.16418001	1.71083204	-2.31967745
H	6.15955420	-2.06760889	2.58777654	H	-6.15875866	2.06644175	-2.58780917
C	4.84939982	-1.78511447	0.94597795	C	-4.84879212	1.78386214	-0.94588911
C	4.81389836	-1.73561229	4.78253193	C	-4.81295522	1.73431988	-4.78245214
H	5.82807681	-2.15133246	4.75685575	H	-5.82705207	2.15024377	-4.75685952
H	4.15197724	-2.43367316	5.31443077	H	-4.15087415	2.43217743	-5.31441496
H	4.82055415	-0.80829262	5.37416352	H	-4.81978692	0.80692715	-5.37396875
C	5.84907410	-2.52465821	0.09570855	C	-5.84871516	2.52317188	-0.09569354
H	5.83222043	-3.59506692	0.34892388	H	-5.83343399	3.59330596	-0.35008258
H	6.86172941	-2.15854160	0.31803376	H	-6.86105993	2.15552961	-0.31692481
H	5.65262187	-2.41868811	-0.97719606	H	-5.65146176	2.41847917	0.97717849
C	2.14668010	-1.04020517	4.33697543	C	-2.14578084	1.03880864	-4.33666860
C	1.97495687	0.07037053	5.18948578	C	-1.97403192	-0.07180491	-5.18912105
C	1.14369161	-0.06315730	6.30723239	C	-1.14262529	0.06162879	-6.30677351
H	1.02468569	0.78672476	6.98403547	H	-1.02360098	-0.78828407	-6.98353150
C	0.46250057	-1.24318462	6.56453909	C	-0.46132209	1.24159808	-6.56404238
H	-0.17386866	-1.33321132	7.44808630	H	0.17516298	1.33154933	-7.44751330
C	0.56269136	-2.29790085	5.66406727	C	-0.56155637	2.29635553	-5.66362626

H	-0.02060581	-3.20298600	5.83859970	H	0.02182110	3.20139526	-5.83812268
C	1.37938251	-2.21475445	4.53374989	C	-1.37838940	2.21330578	-4.53340576
C	2.60660837	1.41859683	4.91239905	C	-2.60581420	-1.41997627	-4.91207268
H	3.14665416	1.34351367	3.95812786	H	-3.14595502	-1.34482911	-3.95786026
C	3.59969457	1.83810398	5.99424517	C	-3.59881183	-1.83943041	-5.99401777
H	4.06172438	2.80497954	5.74160288	H	-4.06094320	-2.80626469	-5.74140782
H	4.41078908	1.10429146	6.11355723	H	-4.40983706	-1.10556027	-6.11343516
H	3.10739568	1.94878882	6.97385062	H	-3.10641088	-1.95017042	-6.97356572
C	1.51921807	2.48001581	4.73174412	C	-1.51852468	-2.48147310	-4.73127950
H	1.96233928	3.44308076	4.43674091	H	-1.96175048	-3.44449085	-4.43628506
H	0.95440029	2.64384802	5.66366741	H	-0.95363365	-2.64538687	-5.66314401
H	0.79926917	2.18387028	3.95376636	H	-0.79862237	-2.18535719	-3.95324951
C	1.39037554	-3.34793102	3.52206618	C	-1.38945658	3.34654435	-3.52179430
H	1.58237798	-2.87934104	2.54155950	H	-1.58157738	2.87801671	-2.54128028
C	2.50737049	-4.36445828	3.76336837	C	-2.50639011	4.36309583	-3.76327484
H	2.44216856	-5.18540581	3.03163421	H	-2.44122431	5.18409036	-3.03159177
H	2.42706447	-4.80465657	4.77050463	H	-2.42596568	4.80322031	-4.77043368
H	3.50477822	-3.91585727	3.66208995	H	-3.50382674	3.91454667	-3.66206020
C	0.03773122	-4.05160192	3.44047025	C	-0.03680304	4.05018406	-3.44008501
H	0.02352875	-4.76145361	2.60283026	H	-0.02266718	4.76005037	-2.60245835
H	-0.78179509	-3.33349583	3.28593661	H	0.78269247	3.33206573	-3.28545669
H	-0.18209085	-4.62878652	4.35186691	H	0.18312136	4.62734257	-4.35147343
C	3.37134408	-1.60711199	-0.93736610	C	-3.37075934	1.60588017	0.93753566
C	3.55082075	-0.66575996	-1.98077734	C	-3.55019159	0.66458132	1.98099809
C	3.11967365	-1.00488578	-3.26655615	C	-3.11897921	1.00377450	3.26673979
H	3.24223075	-0.28537888	-4.07646148	H	-3.24152096	0.28431544	4.07669096
C	2.51877768	-2.22885178	-3.53550114	C	-2.51806812	2.22775409	3.53559464
H	2.17685436	-2.46371433	-4.54605748	H	-2.17611894	2.46267786	4.54612946
C	2.34764292	-3.14139034	-2.50600695	C	-2.34695901	3.14023404	2.50604212
H	1.87043547	-4.10219034	-2.71317705	H	-1.86973834	4.10104332	2.71314090
C	2.76416911	-2.85431613	-1.20140648	C	-2.76353418	2.85308373	1.20147523
C	4.21136860	0.67798078	-1.74059406	C	-4.21078852	-0.67915512	1.74092330
H	3.89188902	1.01388913	-0.74142756	H	-3.89139313	-1.01511182	0.74174574
C	5.73672911	0.55469752	-1.73681486	C	-5.73614338	-0.55581656	1.73725265
H	6.20134601	1.53774952	-1.56347010	H	-6.20081536	-1.53884035	1.56388730
H	6.09977233	0.17177308	-2.70470488	H	-6.09910558	-0.17291957	2.70518414
H	6.09600668	-0.12172441	-0.95085994	H	-6.09542898	0.12067209	0.95136257
C	3.78456915	1.74867965	-2.73938342	C	-3.78395039	-1.74982528	2.73972898
H	2.68904635	1.81404363	-2.82266103	H	-2.68842321	-1.81523485	2.82292615
H	4.19137297	1.56302466	-3.74631460	H	-4.19066920	-1.56410328	3.74668265
H	4.15800051	2.73154608	-2.41724493	H	-4.15744998	-2.73269278	2.41766867
C	2.53279005	-3.90436668	-0.13265990	C	-2.53225764	3.90306801	0.13264400
H	2.86519974	-3.48925656	0.83022134	H	-2.86431466	3.48770875	-0.83024889
C	3.34356438	-5.17351155	-0.40301185	C	-3.34358541	5.17192941	0.40265333
H	4.41336283	-4.95884167	-0.53428253	H	-4.41334884	4.95685229	0.53351620
H	2.99551731	-5.67928882	-1.31764524	H	-2.99605836	5.67784136	1.31741093
H	3.23726056	-5.88532547	0.43075262	H	-3.23723625	5.88376136	-0.43109103
C	1.04859552	-4.23791947	-0.00874434	C	-1.04815935	4.23712556	0.00897393
H	0.88642299	-5.00670889	0.76053330	H	-0.88611081	5.00580006	-0.76044616
H	0.64435648	-4.63086653	-0.95440463	H	-0.64422641	4.63043736	0.95461324
H	0.45804919	-3.34891205	0.25646814	H	-0.45725854	3.34826368	-0.25593939
C	4.80024204	1.78530640	1.45545960	C	-4.79965239	-1.78646194	-1.45521361
H	5.08119345	2.56505278	0.71808143	H	-5.08066592	-2.56616595	-0.71781405
H	5.28312938	0.86429564	1.09292908	H	-5.28251251	-0.86541783	-1.09273247
C	5.42819282	2.14946424	2.79845965	C	-5.42757286	-2.15064721	-2.79821906
H	6.50095132	2.37253347	2.68079245	H	-6.50034774	-2.37365450	-2.68058303
H	5.33531298	1.32068134	3.51556628	H	-5.33461778	-1.32190351	-3.51536089
H	4.95082042	3.03642365	3.24309960	H	-4.95023135	-3.03765295	-3.24279766
C	2.58138975	2.80438065	1.44681773	C	-2.58085036	-2.80563522	-1.44643840

H	2.91945773	3.50958836	2.23458269	H	-2.91893139	-3.51087607	-2.23416703
H	1.54050200	2.55176085	1.71358945	H	-1.53994679	-2.55307789	-1.71320402
C	2.56093731	3.54010169	0.11180495	C	-2.56046484	-3.54128071	-0.11138327
H	2.00379739	4.48690772	0.19043548	H	-2.00338648	-4.48812718	-0.18995074
H	2.07867798	2.92258880	-0.66144709	H	-2.07817994	-2.92375763	0.66184402
H	3.57624061	3.78251426	-0.23792680	H	-3.57578950	-3.78361110	0.23834239

Table 4: Cartesian coordinates of $[L(Me_2N)GaSb]_2^{\bullet -}$ (**33**) [Å] for the optimized geometry. ORCA Version 4.2.1. Optimization: def2-SVP for H, C, ma-def2-SVP for N and ma-def2-TZVP for Ga, Sb. Single-point: def2-SVP for H, C, ma-def2-SVP for N, and ma-def2-TZVP for Ga, Sb. Here AutoAux generation procedure for the auxiliary basis set.

Sb	-3.122680322	7.131654146	0.05273982	Sb	-1.901429282	4.69815312	-0.162183704
Ga	-2.197089361	7.346383863	2.433456398	Ga	-2.210124628	4.577069263	-2.700063905
N	-3.252632516	8.716139897	3.493544151	N	-1.491129792	2.835102213	-3.450912463
N	-2.523328523	5.945853615	3.881585023	N	-0.890209876	5.652008318	-3.851611734
N	-0.382786087	7.811558978	2.699116623	N	-3.870932083	4.796812227	-3.575740666
C	-3.30006832	8.709378847	4.819527094	C	-0.965534781	2.743239517	-4.666733479
C	-2.969212391	7.589388815	5.597701866	C	-0.540497649	3.849439371	-5.417725162
H	-3.030894325	7.719866804	6.677181725	H	-0.14033279	3.629471128	-6.407415846
C	-2.714566917	6.275269851	5.149189047	C	-0.38683577	5.183351132	-4.978145532
C	-3.734642875	9.956407829	5.544995705	C	-0.788088005	1.381577877	-5.287076273
H	-3.01356407	10.76469371	5.34770955	H	-1.769931283	0.921026788	-5.472017131
H	-3.794265795	9.789040182	6.627327921	H	-0.242405504	1.445526111	-6.236294653
H	-4.706899649	10.31585955	5.181531644	H	-0.251508711	0.704998458	-4.606637818
C	-2.674212891	5.202092439	6.206013737	C	0.449449733	6.061617301	-5.876112031
H	-3.277484564	4.333407532	5.907232795	H	0.446565907	7.1101201	-5.556652613
H	-3.036200139	5.582975743	7.168627266	H	1.488988914	5.702053603	-5.889093695
H	-1.645350345	4.836110198	6.335757789	H	0.072013736	5.99523039	-6.907354818
C	-3.951127644	9.722073296	2.774072709	C	-1.677470676	1.661760411	-2.668008261
C	-5.341952378	9.559958786	2.57218568	C	-0.669928771	1.296002028	-1.744035355
C	-6.045846508	10.57106635	1.91475322	C	-0.842478713	0.127138372	-0.998744458
H	-7.122579416	10.45961416	1.763512901	H	-0.073267361	-0.168352657	-0.283576915
C	-5.399457477	11.70404317	1.432446726	C	-1.983655441	-0.656830881	-1.133578758
H	-5.966400602	12.48563886	0.92012224	H	-2.097700099	-1.567605752	-0.539816627
C	-4.022914179	11.81799146	1.578283983	C	-2.988518936	-0.256734139	-2.003261825
H	-3.506997493	12.68900092	1.165425513	H	-3.904035938	-0.849313602	-2.080989294
C	-3.275639248	10.8348612	2.234903903	C	-2.862161107	0.90442476	-2.772447406
C	-6.073836257	8.31056708	3.027537377	C	0.562514403	2.159854409	-1.544801385
H	-5.30760881	7.582585969	3.331117884	H	0.233807376	3.201905604	-1.696987227
C	-6.86686621	7.683223664	1.882804217	C	1.113779878	2.07445968	-0.125706216
H	-7.670292143	8.347840171	1.52634017	H	1.559032263	1.088996796	0.089620906
H	-7.340126155	6.746449529	2.21518993	H	1.902371643	2.826574835	0.016599562
H	-6.203108039	7.450495225	1.035276586	H	0.324934439	2.278433138	0.613596611
C	-6.970822519	8.573364357	4.237700912	C	1.655886097	1.867647802	-2.573381326
H	-6.397465795	8.941269741	5.100936414	H	1.324037846	2.083002585	-3.598577692
H	-7.480493236	7.647125992	4.54770458	H	2.540771489	2.49443833	-2.377631542
H	-7.745680279	9.322073338	4.003243309	H	1.971735186	0.811952131	-2.526513851
C	-1.769858133	10.97797892	2.316271535	C	-4.026141998	1.353464395	-3.630508944
H	-1.379630694	10.07994904	2.817529264	H	-3.697963009	2.236767316	-4.194163474
C	-1.16227983	11.00515551	0.913365603	C	-5.18193954	1.80396988	-2.736973462
H	-1.426046054	10.09259177	0.356441867	H	-4.844267866	2.572294515	-2.027422376
H	-0.064534991	11.06378891	0.968596547	H	-5.995366113	2.234394016	-3.341299356
H	-1.517896262	11.87358832	0.334539115	H	-5.592926277	0.958061147	-2.161434147
C	-1.349888821	12.20112844	3.130238016	C	-4.483234593	0.288034302	-4.625291665
H	-1.688523426	13.13850442	2.658306197	H	-4.881954058	-0.603677481	-4.114718342
H	-0.252592756	12.24800882	3.216826482	H	-5.284864435	0.684519447	-5.268596304
H	-1.768044295	12.17422307	4.148509857	H	-3.661465003	-0.046964165	-5.277276936
C	-2.398324083	4.568465566	3.526337358	C	-0.482847319	6.916992638	-3.334694546
C	-3.5298476	3.89666786	3.010087514	C	0.752656867	7.023592849	-2.659781567

C	-3.408399712	2.545076074	2.680168236	C	1.110623468	8.258426295	-2.110691462
H	-4.267439788	2.017262861	2.264520767	H	2.058770663	8.34792645	-1.574361092
C	-2.201683357	1.870204633	2.823940868	C	0.275815662	9.362098343	-2.211966387
H	-2.123188881	0.820176776	2.531704467	H	0.563136244	10.31386203	-1.758964432
C	-1.087789221	2.554166848	3.290696224	C	-0.94387458	9.239982676	-2.866887016
H	-0.128261556	2.035723165	3.365054752	H	-1.60979162	10.10235458	-2.920527287
C	-1.158997719	3.905489383	3.642857732	C	-1.34947709	8.028878632	-3.43188967
C	-4.840640948	4.627712556	2.790447536	C	1.705007908	5.852548877	-2.501552307
H	-4.569905418	5.65527986	2.491640371	H	1.216658939	4.963519318	-2.927865895
C	-5.655587721	4.047121746	1.640247601	C	1.991303329	5.556481563	-1.031170188
H	-5.034666812	3.963029253	0.734663262	H	1.057776497	5.341201687	-0.487573341
H	-6.501571878	4.71051663	1.408165711	H	2.661487796	4.68735784	-0.938133435
H	-6.071410104	3.054664367	1.88044266	H	2.483523763	6.407937577	-0.535629743
C	-5.672644472	4.706728074	4.071550173	C	3.01198545	6.084249669	-3.263355094
H	-6.63414224	5.207875559	3.877526704	H	3.653442364	5.189368224	-3.21329828
H	-5.160812692	5.274591887	4.861592031	H	2.836732097	6.321195681	-4.322583565
H	-5.891861664	3.698199553	4.460297346	H	3.577763339	6.923839822	-2.827770291
C	0.108678162	4.62277483	4.060585351	C	-2.680850799	7.925486794	-4.151842546
H	-0.169355432	5.64513184	4.34898071	H	-3.050150213	6.901620116	-3.98303165
C	1.061533411	4.737662439	2.871445709	C	-3.737091074	8.884734641	-3.61305097
H	1.438157107	3.747659769	2.567692518	H	-3.504861255	9.936669905	-3.850222684
H	1.926697889	5.36978189	3.126494257	H	-4.713161441	8.658288574	-4.069221399
H	0.550434155	5.181805583	2.006588094	H	-3.839057363	8.788430144	-2.521143603
C	0.806495846	3.958622994	5.247169833	C	-2.508543662	8.11517215	-5.660559142
H	0.141074362	3.852391289	6.118031022	H	-1.859319171	7.345345004	-6.098775853
H	1.680153218	4.553277992	5.558831377	H	-3.483535141	8.055818628	-6.170357612
H	1.17029638	2.950975897	4.988715416	H	-2.066273432	9.100803846	-5.884323107
C	0.515826833	7.991299402	1.600151699	C	-5.025967753	5.295972256	-2.89289917
H	0.862034298	9.044279394	1.497581496	H	-5.925149713	4.669268271	-3.080970738
H	0.032349071	7.709237585	0.652073764	H	-4.856023324	5.319156985	-1.805172356
H	1.434664831	7.374248596	1.702107149	H	-5.297666867	6.330864686	-3.19963864
C	0.178683619	8.196424963	3.95319953	C	-4.050745473	4.696549392	-4.988892182
H	1.119905385	7.646227751	4.18457944	H	-4.288663553	5.67432726	-5.470329531
H	-0.518801963	8.010974892	4.783500533	H	-3.147322171	4.309642201	-5.483779271
H	0.448595373	9.280077285	3.994834551	H	-4.892303129	4.016581719	-5.258243012

Table 5: Cartesian coordinates of $[L(Et_2N)GaBi]_2^{\bullet-}$ (**34**) [Å] for the optimized geometry. ORCA Version 4.2.1. Optimization: def2-SVP for H, C, ma-def2-SVP for N and ma-def2-TZVP for Ga, Bi. Single-point: def2-SVP for H, C, ma-def2-SVP for N, and ma-def2-TZVP for Ga, Bi. Here AutoAux generation procedure for the auxiliary basis set.

Bi	1.98166003	3.85987069	10.17867004	H	2.30052511	3.00036734	5.32354455
Bi	3.10565550	6.51002283	9.92866696	H	5.19570218	8.62805159	13.36900844
Ga	3.88673060	3.21055727	11.88814603	C	3.11471791	8.32961781	13.80916864
Ga	1.86064872	6.77891806	7.61782889	H	6.08907277	5.05339126	12.82930426
N	3.96293196	4.19702321	13.69926284	C	7.07661600	6.22903046	14.33276849
N	3.50479514	1.45193228	12.78955771	C	6.69617325	6.90280592	11.95341572
N	5.72858069	3.09463694	11.43175667	H	1.07538134	7.74065323	14.12968041
N	-0.17696627	6.95737468	7.53097402	H	1.53142355	4.12671682	13.51827466
N	2.11305202	8.69974918	6.96453428	C	1.01932434	4.63212982	15.54029091
N	2.21336728	5.69175648	6.10066952	C	-0.06977453	5.51602938	13.44626372
C	4.35471371	3.56204181	14.78324967	H	2.59685952	-1.85266870	9.70060609
C	3.68849615	5.59608243	13.71777584	C	1.01500434	-1.52080978	11.11480857
C	4.03166630	1.18088277	13.98531261	H	4.80511696	0.96576834	10.73662705
C	2.66310660	0.48575643	12.17599313	C	5.45345368	-1.07289143	10.72909023
C	6.21973549	3.85476219	10.30511948	C	4.26172830	0.12848904	8.86055723
C	6.67772425	2.17758740	12.00221668	H	-0.43459101	-0.89266257	12.57413950
C	-0.75150632	7.79546655	6.68419550	H	1.52234025	1.95939730	14.00084234
C	-0.95770359	6.21054885	8.46372828	C	0.43805968	0.45119935	15.05881184
C	1.25169828	9.23174458	6.10717564	C	-0.46193634	1.91009161	13.21593906

C	3.28368457	9.43092132	7.30973025	H	-2.10122093	3.06051945	9.07157272
C	1.45957755	5.72136507	4.87503030	C	-2.41785105	4.74999782	10.35491753
C	3.32520784	4.77075289	6.11946948	H	0.27520156	4.56598233	6.75455034
C	4.52346240	2.15603544	14.85837771	C	-1.65048955	4.35159442	5.82963539
C	4.62678569	4.30116636	16.07128009	C	-0.47882060	2.62480802	7.20370134
C	4.71844119	6.53252787	13.47816867	H	-2.54611341	6.58942946	11.45603098
C	2.35802182	6.02453944	13.92139150	H	-0.57506896	8.72327883	9.10640719
C	4.09579476	-0.25317149	14.44614054	C	-2.50890267	9.11361681	9.94126181
C	3.09352328	-0.25565873	11.05389590	C	-0.43900777	8.50710478	11.22428470
C	1.36140389	0.28835464	12.69645023	H	6.50779901	9.96455497	6.34875518
H	7.24980730	4.21657118	10.50441649	C	5.48422099	11.06644104	7.88390095
H	5.60779413	4.76506363	10.18872294	H	3.75913137	7.55114454	5.56720705
C	6.19603190	3.12176612	8.96842524	C	5.02066615	8.63213104	4.20974335
H	7.25676027	1.66642462	11.20223902	C	5.78332253	7.17614140	6.11980463
H	6.14352061	1.36916936	12.52840000	H	4.27454132	11.88836938	9.45587311
C	7.66923266	2.80094472	12.98495781	H	1.56058371	9.39745309	9.27577512
C	-0.05067678	8.74360836	5.90731984	C	0.93422964	11.38689124	8.79553424
C	-2.25131902	7.81527228	6.51689159	C	2.38345847	10.70731133	10.73833412
C	-1.19398145	4.83080442	8.25384997	H	2.89025573	9.39845298	13.84585123
C	-1.44412580	6.85052897	9.62459620	H	8.09181443	5.90085908	14.05803573
C	1.65639911	10.44923863	5.31547080	H	6.74734379	5.61786224	15.18327240
C	4.49529203	9.24754669	6.61133629	H	7.14105842	7.27444531	14.67860878
C	3.21796570	10.34612747	8.38768676	H	6.00368949	6.89509180	11.09818645
H	0.46728693	6.15576265	5.06997246	H	7.65138130	6.46445942	11.62526297
H	1.25686092	4.68986592	4.51556869	H	6.89293195	7.95438096	12.22009508
C	2.09246610	6.50317233	3.72347059	H	0.76725904	5.51392774	16.15257218
H	3.93419114	4.98803283	7.01293182	H	1.91804495	4.16930287	15.97054438
C	2.95229619	3.29202649	6.16324176	H	0.19419984	3.90807858	15.63483301
H	3.99683534	4.93916290	5.24934857	H	0.09214753	5.77675768	12.39058160
H	4.95610150	1.78749875	15.78870172	H	-0.48667652	6.39083313	13.97127025
H	5.66630525	4.11836351	16.38341514	H	-0.83214492	4.72512985	13.47779172
H	3.97923867	3.91269657	16.87106445	H	0.38384105	-2.31786807	10.71352725
H	4.46702815	5.38131836	15.97803993	H	5.12413753	-2.07025343	10.39200996
C	4.40672917	7.89421333	13.54807863	H	5.62408486	-1.12548553	11.81488013
C	6.13455231	6.11051899	13.13417060	H	6.42113236	-0.85380187	10.25054188
C	2.09905424	7.39593246	13.97557096	H	3.92301088	-0.81190630	8.39642574
C	1.22724129	5.02644401	14.07782279	H	5.22185598	0.39784926	8.39679729
H	3.09126558	-0.67907196	14.57275079	H	3.53533617	0.91785763	8.61323246
H	4.63752083	-0.33864852	15.39605167	H	-0.31706485	-0.33414971	14.89056862
H	4.59541731	-0.87199843	13.68609673	H	0.03004046	1.15034685	15.80616908
C	2.25945623	-1.26165823	10.55518537	H	1.32532951	-0.02582586	15.50035474
C	4.42370391	-0.00048576	10.37382623	H	-0.20719777	2.50390305	12.32391264
C	0.56628872	-0.72965782	12.16509151	H	-0.88100932	2.58964177	13.97345990
C	0.77156885	1.19189508	13.76406018	H	-1.25292639	1.19508155	12.93811365
H	5.15545386	2.89562611	8.69089207	H	-2.97301663	4.17414049	11.09959978
H	6.75859020	2.17467048	9.00852365	H	-1.75178001	5.41603595	5.58195638
H	6.63310227	3.74292630	8.16878867	H	-2.65619687	3.95942242	6.05757052
H	8.21419438	3.64026484	12.52471498	H	-1.27889077	3.83690663	4.92954401
H	8.41441202	2.06072746	13.32376972	H	-1.42728530	2.07638226	7.32882742
H	7.14276931	3.18452363	13.87142140	H	0.15681848	2.42399400	8.07964188
H	-0.64799142	9.27637482	5.16740259	H	0.02509224	2.20524274	6.32018406
H	-2.50118951	7.79080620	5.44597496	H	-3.09248719	8.97838327	9.01931351
H	-2.65937462	8.75295373	6.92231964	H	-2.30546919	10.18983880	10.06317348
H	-2.74198600	6.97540792	7.02216895	H	-3.14626796	8.79872772	10.78346372
C	-1.92628316	4.12756665	9.21374981	H	0.53879828	8.00045823	11.19015135
C	-0.70057822	4.12063353	7.00726293	H	-1.00381484	8.10080728	12.07735661
C	-2.17641463	6.10150016	10.55059141	H	-0.27330727	9.57722785	11.41980722
C	-1.20138222	8.31944658	9.91520902	H	6.33348508	11.72265140	8.09107640
H	2.53529444	10.22105483	4.69472634	H	5.12859105	7.78735868	3.51154275

H	1.95737299	11.27052970	5.98180278	H	5.96415654	9.20232131	4.19260245
H	0.84019955	10.79300702	4.66849478	H	4.22905858	9.28815304	3.81619730
C	5.57299869	10.09113663	6.90124288	H	5.88977067	6.31363769	5.44479218
C	4.69560024	8.12622930	5.61342210	H	5.53116591	6.79602447	7.12183080
C	4.32045522	11.16622755	8.63887148	H	6.76190888	7.67968747	6.18323585
C	1.99956396	10.40886939	9.29153060	H	1.34425538	12.40677074	8.70501474
H	2.15070858	7.57506161	3.96252508	H	0.08927346	11.42473330	9.50209712
H	1.49686231	6.39491678	2.80113468	H	0.52946659	11.08987797	7.81783231
H	3.11199732	6.14885729	3.50629703	H	3.13998508	9.99384213	11.09806403
H	2.43196033	3.06285516	7.10567815	H	1.50477451	10.61608488	11.39159441
H	3.85632907	2.66302266	6.11626069	H	2.77440890	11.73000791	10.86327078

Table 6: Cartesian coordinates of $[L(TfO)GaSb]_2$ (**14**) [Å] for the optimized geometry. ORCA Version 5.0.0. Optimization: def2-SVP for H, C, F, N, O, S, and def2-TZVP for Ga, Sb. Single-point: def2-TZVP for H, C, F, N, O, S, and def2-QZVP for Ga, Sb.

Sb	8.47375728603033	6.66130135718944	7.76593989855310
Ga	6.39656877613931	5.21751842661895	7.24914189896088
S	6.04572963652690	3.02354207098028	4.87784992535688
F	7.50233945211107	3.98369981743321	2.92665845309266
F	8.44847979777197	2.39200922254205	4.03086527663604
F	6.85451563398451	1.94650246714196	2.65249619541271
O	6.78399327495966	4.08546397683512	5.69892592294131
O	5.97111423834658	1.73493500182483	5.55086678400245
O	4.85916646096725	3.53931569223493	4.20872300817760
N	4.58125233339181	5.77553147559884	6.87052615015405
N	5.94131526738201	3.83748119080532	8.53498162044997
C	3.69848003621865	4.77347026716274	6.75046511151446
C	3.87589608234788	3.51607142386680	7.34382873563638
H	3.11363436531546	2.77423646470049	7.11142613820426
C	4.86101036455077	3.10839418951556	8.26271773025146
C	2.50155968016675	4.95087299875653	5.86592099719661
H	1.66528983028797	4.31643796624753	6.18386152638115
H	2.82186081445050	4.61976133443025	4.86344249996886
H	2.17436414215284	5.99480025902548	5.79823246780399
C	4.69652265874933	1.75940613714672	8.89211244057897
H	5.17977123927120	1.02900419451268	8.22134595830864
H	3.63782896385190	1.48758000240716	8.98217980898966
H	5.18489598523314	1.69551295661316	9.87235618238183
C	4.22659674152732	7.11296285101651	6.51603277714347
C	4.63378576157031	7.65167207920646	5.27938808410729
C	4.25681203173199	8.96240274178490	4.96764884916807
H	4.55768427742737	9.38680925181243	4.00659356752024
C	3.50734167091797	9.72514484696180	5.85182771788486
H	3.21545811215169	10.74447495702646	5.58804121600493
C	3.14184142495450	9.19339689249377	7.08401626901648
H	2.58297251579208	9.81214769860977	7.78732537724855
C	3.49469605710900	7.89150524294324	7.44737592430008
C	5.44830739808010	6.85842753226386	4.27924669823167
H	5.60702955889697	5.85542752049981	4.68952246457776
C	4.70251604400039	6.66449104090247	2.96012864101275
H	5.27539811165347	5.99884090594792	2.29753978307188
H	4.54718173335696	7.62075179812574	2.43494002960830
H	3.71890734950836	6.20200000570719	3.12477126638969
C	6.82362889766697	7.48580936251806	4.05323273395799
H	7.43813479280294	6.83751100597269	3.41038672072801
H	7.36054033260422	7.62726694405939	5.00512131243339
H	6.74708802595962	8.47310177165502	3.56960189868122

C	3.10486083295241	7.35407554791430	8.81532747118685
H	3.88228367472590	6.62429429461030	9.09512387788258
C	1.76569506941919	6.61234660094719	8.80406261519642
H	1.78521182797323	5.71468565436759	8.17517493500683
H	0.96041440826166	7.26856781981420	8.43700648674601
H	1.50199442847769	6.29236607301952	9.82423564144793
C	3.07038714046991	8.43791656054518	9.89189920436544
H	2.19606968073833	9.09794104958447	9.77801935605854
H	3.97020313486460	9.06990924248183	9.87817360256477
H	2.99442392733611	7.97558149167762	10.88797597446617
C	6.83810897413673	3.50224175372858	9.59637108880170
C	7.91189971680257	2.61818544764375	9.37097549602238
C	8.75281601213369	2.31122240661038	10.44628271643366
H	9.58488450878060	1.62061188489407	10.28847133516871
C	8.54861495419765	2.86528412454524	11.70239157011299
H	9.21327496439026	2.60952858755427	12.53082127770092
C	7.51051532669479	3.77038440355753	11.89773870449997
H	7.37804873456967	4.22976821303241	12.87858106390991
C	6.64827449030328	4.11698616670867	10.85561188872025
C	8.19328461285041	2.02386473804941	8.00755302602367
H	7.36672751992397	2.28871638054342	7.33909936043495
C	9.46566989693922	2.62467366334176	7.40858045475556
H	9.61443123650021	2.26383590055279	6.38039114561169
H	10.35504053874877	2.35734867047845	8.00204109121501
H	9.41181304204665	3.72388047677861	7.37117921204275
C	8.26423141737461	0.49859131709032	8.03175444322083
H	8.34131228503655	0.11172202732412	7.00462487314020
H	7.36408639287917	0.06074574751644	8.48831770857284
H	9.13731899640760	0.13429087023946	8.59662812035134
C	5.53740548485627	5.12508907312911	11.07615032408204
H	5.39125060695247	5.63692127636577	10.10970538201020
C	5.89108406028058	6.19492450060230	12.10584898911510
H	5.14071644664227	6.99991478629435	12.08885254054110
H	6.87505174448451	6.64873821322790	11.91035896066683
H	5.90952381781191	5.79567956478553	13.13199949865145
C	4.21127390052632	4.45103510474783	11.43071502378908
H	3.87223071250307	3.76636210909563	10.64094195251831
H	3.42209691547890	5.20550521541913	11.57697260318677
H	4.30501744078950	3.87281944374670	12.36375138245462
C	7.29898000365178	2.82336871313416	3.53511443902615
Sb	6.75161648059339	8.14429232850076	9.07884352666754
Ga	8.54232829592702	9.59454442936486	10.20972293967172
S	9.18052858296458	9.83876140764495	13.37009200493906
F	9.07963824265819	7.38864265721759	14.30053281208390
F	7.27920633557510	8.52358040086719	14.62349387637382
F	9.03501553084775	8.93119340457245	15.80473830344433
O	8.46873051024703	9.26664774675260	12.13732601863763
O	8.62966902471326	11.11307623914884	13.80378131226530
O	10.62827367174912	9.68991082450072	13.32145047811364
N	10.43858455847648	9.71893229454728	9.93437985782598
N	8.12288716352224	11.47913546645316	10.16181577448881
C	11.04700623870614	10.78074240808542	10.47572417313313
C	10.37375824233017	11.95368717866467	10.85611991552182
H	10.99419658894887	12.71209595041462	11.33151516371884
C	9.03773452587196	12.33024015169113	10.61525704036553
C	12.51486282194916	10.71018565030445	10.76381565059907
H	12.99010930930510	11.69659508529365	10.69915909858583
H	12.60384703474686	10.35025330192220	11.80295386447114

H	13.03573692433867	9.99963783049574	10.11087779939610
C	8.64207454969734	13.74108911715220	10.92605546798381
H	8.27634706075555	13.77348683435921	11.96562244870441
H	9.49696943302319	14.42310733672481	10.84489038782784
H	7.82615217263842	14.08514141135098	10.27674603371208
C	11.15420524881846	8.68674226352214	9.24880512494424
C	11.42833204090715	7.45542841590619	9.87979763878730
C	12.08378614278261	6.46242194833554	9.14360227986880
H	12.30045061229080	5.50532238944059	9.62369287336798
C	12.46246058551230	6.66976652265687	7.82421429213951
H	12.97578401598498	5.88189397581793	7.26842033069277
C	12.17235580322633	7.88259765109239	7.21032129482265
H	12.45791308210806	8.03753032066885	6.16787297860697
C	11.50572238015737	8.90160510978866	7.89615385192326
C	11.05741733902688	7.17880481557633	11.31936660885941
H	10.49904375534418	8.04175829794145	11.69396420359793
C	12.30142217643136	7.05253143752044	12.19828916639789
H	12.00830536333813	6.95814445559640	13.25438737041717
H	12.89999156216554	6.16822561749445	11.92552094403270
H	12.94652774228965	7.93841770356156	12.11028847393043
C	10.15950220724433	5.95202301379788	11.45175460636290
H	9.85848017124531	5.80978016251342	12.49907999579887
H	9.24161723881391	6.05071948673230	10.85315100251069
H	10.66306543927234	5.02936528897716	11.12370795163629
C	11.18249436911841	10.19857633807673	7.17959723635886
H	10.41881955372820	10.71856390658119	7.77676173689739
C	12.40340550656110	11.11665557703444	7.10100474973972
H	12.79776918848598	11.35740842387894	8.09793846941128
H	13.21482765200745	10.64153150091373	6.52662166848808
H	12.14544326495020	12.06435027613064	6.60266141038554
C	10.59515818105316	9.95588625643791	5.79158254763905
H	11.32843569326384	9.50222677328924	5.10750432443926
H	9.72024327220646	9.28967686589140	5.83713114814231
H	10.27999590331906	10.90762910332363	5.33811239577320
C	6.80368857373020	11.84675273847464	9.75517699893004
C	5.77255446517259	11.99841293656590	10.70401980606959
C	4.48393846169070	12.29148783933151	10.24417707257473
H	3.67794446601688	12.41444169903880	10.97141610048013
C	4.21152987327829	12.41203720595801	8.88919660113545
H	3.19842511942596	12.64061358810654	8.54951347079206
C	5.23013090304702	12.22053418646144	7.96218499679451
H	5.00415904856824	12.28733847689103	6.89800241515684
C	6.53328954052830	11.92611078684217	8.36851322731594
C	6.00198940665501	11.79202519541755	12.18362093112310
H	7.07824566816973	11.68814466900062	12.35889708595833
C	5.35833713586924	10.48496715809000	12.64817479408520
H	5.59303192504127	10.29966588306909	13.70619617184549
H	4.26245833541810	10.51302983367714	12.53434921503992
H	5.73626686155229	9.62718948086374	12.07214919671215
C	5.52293734450679	12.97171433991691	13.02663430794614
H	5.82301100248409	12.82730131156538	14.07543309854997
H	5.95541214522257	13.92182763581672	12.67748109181653
H	4.42650345577723	13.07827656990909	13.00491882852936
C	7.62914943838535	11.71190550056759	7.34238660163842
H	8.30205923402419	10.93855583355999	7.75145062547899
C	7.10717525581228	11.18604486325940	6.01037912247695
H	7.94559557832176	10.91810869494983	5.35324172944833
H	6.48256585443478	10.29041140161603	6.14495388880687

H	6.50783130393438	11.93974371005234	5.47589680137566
C	8.46178060057090	12.98069224010062	7.15178845450239
H	8.92979273680619	13.30835089570110	8.09091388319834
H	9.26635978808146	12.81401791564024	6.41884646940243
H	7.83151062109154	13.80512018555751	6.78230135577710
C	8.60181102729102	8.58747541065305	14.60541413276868

Table 7: Cartesian coordinates of $[L(TfO)GaBi]_2$ (**XXXII**) [Å] for the optimized geometry. ORCA Version 5.0.0. Optimization: def2-SVP for H, C, F, N, O, S, and def2-TZVP for Ga, Bi. Single-point: def2-TZVP for H, C, F, N, O, S, and def2-QZVP for Ga, Bi.

Bi	6.02943262634699	8.65695855158125	9.63836065965616
Ga	8.06392717464773	10.21251102577149	10.34974594805054
S	8.24555844536580	12.08073558366164	13.01178467832779
F	7.04168108706099	10.65187959712811	14.84458874887560
F	7.41927730048954	12.69937463960841	15.40103281825969
F	5.82588016687855	12.23277843754843	14.02863047566142
O	7.59891608441470	11.08273039013283	12.04842483952655
O	9.51569042465682	11.61614776908079	13.55411510957213
O	8.13793356929079	13.45940085562473	12.55773470837516
N	9.94446683277541	9.84682352257114	10.62919045424447
N	8.32857553462506	11.80148008005970	9.26465040006853
C	10.72006214210003	10.91535465528090	10.85572659876229
C	10.38857824116842	12.20903447651998	10.42978851799200
H	11.07852745152362	12.99644004530403	10.72974867243279
C	9.33259595505680	12.60968387579901	9.58832532030017
C	11.95982014781088	10.76004426974840	11.68266915711825
H	12.35820267326002	9.73892093815970	11.65883523115691
H	11.65343372544433	10.98966113811764	12.71727715027117
H	12.73909496733191	11.47445995295288	11.38978485602676
C	9.33749433301311	14.02500071638930	9.09789042990644
H	10.36066298714264	14.40300488567888	8.98161491333196
H	8.83212212036056	14.64192272237403	9.85962302298357
H	8.78826422890859	14.13537006987875	8.15415412439617
C	10.43187320555251	8.51170548316345	10.75435083281636
C	10.08749292672083	7.73461771517885	11.87951367202814
C	10.52400986595519	6.40655312016066	11.92959486839560
H	10.26926006041915	5.79721311695519	12.80013162448202
C	11.27565417483590	5.85529268452510	10.90063590811943
H	11.60240393863238	4.81489601937698	10.95306594100391
C	11.60380614936915	6.63070549161702	9.79354112945314
H	12.17855898550100	6.18273452348653	8.98109653842473
C	11.18878965521633	7.96099961957457	9.68998379343977
C	9.29672502568267	8.30339747813393	13.03915109212015
H	9.02022407784546	9.33272563593001	12.78677037915598
C	10.15056110981526	8.39034093945408	14.30378650137767
H	10.43806525826763	7.39018250582715	14.66668747129438
H	9.59169720063698	8.90021438087326	15.10255100096017
H	11.07029145899130	8.96473147727483	14.12354636137730
C	8.00356945708336	7.53188049369096	13.29588087993143
H	7.39550917727036	7.45268137558970	12.38092600822613
H	7.40204912191454	8.04681934621063	14.05969109220061
H	8.19899613208638	6.50822966048090	13.65336998368439
C	11.54448072475662	8.77327442167582	8.45532512602116
H	10.78818004659620	9.56923721993772	8.37107818643225
C	12.91137832253747	9.44959200138731	8.58700766943871
H	13.70472323584036	8.69557647527549	8.71400015358650
H	12.95974599642334	10.13313379121871	9.44269087436265

H	13.13953075733372	10.03191153581767	7.68058260074838
C	11.50928342074302	7.95514310766540	7.16576434060146
H	11.62513604519046	8.61858002752859	6.29539970388480
H	10.56463516517744	7.40346598867379	7.04917118098698
H	12.33101028548587	7.22378415090170	7.12092759539534
H	4.59158178220725	12.78742580574641	5.63140745030639
H	6.90450191582567	13.21897037555720	10.62911426450140
C	4.85579490968247	12.67591796962227	10.74217637686790
H	3.89304276980798	12.85222111010293	10.23559084329312
H	4.76481638816606	13.01128679661627	11.78542563134226
H	5.03298400298091	11.58972650611764	10.75889576922959
H	8.91118985294683	10.11227882266608	7.54736444531265
C	9.88783546572627	11.55744849782911	6.31296999852033
H	10.75361427745381	10.92385826407227	6.06491454770599
H	10.17881495998781	12.20109537365675	7.15425626765344
H	9.68231219489623	12.20463288035433	5.44569547684053
C	7.05038460982541	11.90557924839885	14.41119199599528
Bi	7.92678053147320	7.02132648110803	8.44194283991995
Ga	6.04068413801308	5.48116139443439	7.38558679940395
S	5.21265525651930	4.84894316679813	4.31667189855202
F	5.32098791011557	7.15217975904916	3.07264590334112
F	5.18224454038814	5.43195791864912	1.78207068481497
F	7.04591497963600	5.90136169647837	2.75418221663232
O	5.98654644751935	5.57976432489503	5.42001129812228
O	3.76924547132041	5.02258683083851	4.40766643488760
O	5.73480076423589	3.51879227579537	4.03861929551810
N	4.14605531830875	5.35527506173826	7.74272001150120
N	6.46608643206330	3.59848753996411	7.57390534203281
C	3.52664816046917	4.24422137331333	7.32859205893260
C	4.19566582984251	3.05216085042541	7.00850607142412
H	3.56560433791940	2.25651289036426	6.61354251826864
C	5.54680265559859	2.71093534958795	7.20739847821508
C	2.04414081620371	4.26950097545250	7.11545923755713
H	1.54571390900019	5.03911378889653	7.71657798313037
H	1.89488222199839	4.51428149936541	6.05017322179156
H	1.59021751189174	3.29016738732082	7.31060411487598
C	5.95326080839432	1.29442273575722	6.94071263204839
H	5.11767679729955	0.60112459369427	7.09531111636578
H	6.25864314434965	1.23121192148183	5.88279490060637
H	6.81009109521768	0.99133036588958	7.55636945907411
C	3.43908968018710	6.43661247628778	8.35286991597866
C	3.13621648065220	7.60452241255437	7.62039983899504
C	2.48928638421100	8.65524878013390	8.28059078922000
H	2.25272000802870	9.56426577163920	7.72259356723932
C	2.14192488980303	8.56368694795761	9.62244306024951
H	1.63456826952317	9.39462864742183	10.11772499615348
C	2.45519682694466	7.41149404535906	10.33439158140437
H	2.19176053850749	7.34587977089501	11.39243250293487
C	3.11608285343636	6.33977528398219	9.72628329686446
C	3.46665891439773	7.74834469846683	6.15108096332247
H	4.01482276945445	6.85369621108715	5.84184181696423
C	2.19881100224029	7.79555852271300	5.29926806812702
H	1.60461687355404	8.69999938554279	5.50826509916847
H	2.46240583870748	7.79476037840280	4.23123956687759
H	1.56109615875868	6.91940668687996	5.48389471819508
C	4.36231732957262	8.95486149136464	5.88256081521741
H	5.28413869453361	8.91269389284427	6.48202874746937
H	4.65295178606747	8.98553191499218	4.82207799440197

H	3.86282871858932	9.90645131918960	6.12279361025014
C	3.46078039194148	5.11351370080319	10.54974690108280
H	4.14857922677164	4.49829597232077	9.95136117843889
C	2.22049547151161	4.26621254030071	10.83846790413990
H	1.48863285459457	4.82924666911489	11.43962767465868
H	1.71850454320580	3.95041219881794	9.91305389585568
H	2.49297429143100	3.35975632340097	11.40147170495244
C	4.18347345627345	5.48282489743968	11.84308034153288
H	4.47222438766190	4.57455854889591	12.39319823831340
H	5.09576300260011	6.06428033540580	11.63948049093188
H	3.54703092107734	6.07908161763720	12.51471972694206
C	7.79408309755904	3.25224011839843	7.96757428765074
C	8.81514190369124	3.09856714107763	7.00828567267518
C	10.10825966997902	2.80521014586661	7.45481987059692
H	10.90604060966037	2.67739461436301	6.71921403782648
C	10.39388931637659	2.68300015469094	8.80710990802067
H	11.40922478968210	2.44809428433980	9.13588186335764
C	9.38579196696482	2.88107788391090	9.74457714444180
H	9.62282687403359	2.81307238700361	10.80689273229949
C	8.07979213106677	3.18166401803105	9.35121517201345
C	8.56713789568900	3.29435073816936	5.52985488859899
H	7.48939658811231	3.40698544523997	5.37149106891610
C	9.22496857108930	4.58596296075452	5.04169447064283
H	10.32170237578331	4.54325325728339	5.14211911678124
H	8.98094653960824	4.76458203129557	3.98466411793153
H	8.86884768791922	5.45642811031799	5.61413077317578
C	9.01342804324169	2.09754966407860	4.69307107713013
H	8.56649861808712	1.16081067526584	5.05908287875301
H	8.69931145696814	2.23475964059681	3.64749031572331
H	10.10796577336030	1.97047146449968	4.70116476820704
C	6.99907148156730	3.42763129013254	10.38692028387242
H	6.32387019019273	4.19046028806447	9.96230758670118
C	7.54926586250729	3.99277165943860	11.69106109671156
H	8.15805164496660	3.25463448828103	12.23650318334597
H	8.17041982510710	4.88252504254120	11.51033734661576
H	6.72663315108740	4.28504180976766	12.35758230246674
C	6.16218076602174	2.17247826125315	10.63792530949050
H	5.37055096399116	2.37372914979469	11.37679755156999
H	5.67586834741527	1.81270455993011	9.72040504557831
H	6.79204516481979	1.35763209845633	11.02894977500762
C	5.72894907814706	5.90387092794168	2.88836226409539
C	7.33518577701517	12.11688758979573	8.29045578319931
C	6.20533749634472	12.88149410466154	8.64259971511906
C	5.23279310735628	13.11359624722645	7.66333058712362
H	4.35351216170863	13.70959058619859	7.91980661968805
C	5.36163899155254	12.59541041358827	6.38232479594349
C	6.46722548260787	11.81417335786801	6.05935383225825
H	6.54674809230378	11.38962349456153	5.05778378123951
C	7.46550334190710	11.55182063188824	6.99931254845690
C	5.99827328719408	13.41463479588513	10.04405103468938
C	5.76993056916880	14.92477435485320	10.06823050386903
H	6.57164804663888	15.46382908011273	9.54144354801060
H	5.74846821448662	15.28351777917757	11.10828645747619
H	4.81450768009695	15.20530773805546	9.59649242958000
C	8.66669297199770	10.69684171472645	6.64308746906779
C	8.39676661691673	9.69891691246328	5.52250617406620
H	8.26069013092513	10.19751044601367	4.54997235167377
H	7.50072164538529	9.09175704604125	5.71984595399507

H	9.25013202861329	9.01344813564223	5.41558456862298

Table 8: Cartesian coordinates of $[L(DMAP)GaSb]_2^{2+}$ (**15**) [Å] for the optimized geometry. ORCA Version 5.0.0. Optimization: def2-SVP for H, C, N and def2-TZVP for Ga, Sb. Single-point: def2-TZVP for H, C, N, and def2-QZVP for Ga, Sb.

Sb	-0.19368445784638	10.02499415547659	7.59686951757372
Ga	0.24073995393924	8.55622041125187	5.50894661035813
N	1.99200530469222	8.05027805820484	4.82685908661727
N	-0.52512082379522	6.78069094059933	5.58215064629615
N	-0.62929883951179	9.34914526823501	3.86441834283605
N	-2.44756143475095	10.92431610370271	0.45805222368093
C	2.15555533599262	6.87920770291682	4.20182452495930
C	1.16607426077952	5.88200988517948	4.12339255436569
H	1.43578161314448	5.00287951502831	3.54064318659998
C	-0.03928160502840	5.78456366065771	4.84347427025269
C	3.47068292530339	6.59104824987965	3.54078377886306
H	3.54615571032515	5.53779098620598	3.24882870999122
H	4.31106591968401	6.84625953752357	4.20092249068366
H	3.58261956627629	7.21201091366734	2.63937149000101
C	-0.80789240396997	4.50082463007247	4.75724398626449
H	-1.68573188423184	4.65014812332846	4.10764312564898
H	-1.19667105531812	4.19591989791281	5.73767344756993
H	-0.19900770754939	3.69280104904295	4.33636546257033
C	3.09662254064371	8.94897979171915	4.99047634226910
C	3.44295300294258	9.84732939624271	3.96065879962693
C	4.51027978225410	10.72802024112992	4.17442089792478
H	4.79330113848949	11.42374365962403	3.38129680957968
C	5.20710561882123	10.73972656033954	5.37270514918475
H	6.03065608461181	11.43919420181717	5.52733410952636
C	4.83798686178455	9.86721871772561	6.39183878118089
H	5.38399574183842	9.89894978646783	7.33470367483817
C	3.78510202477588	8.95969654259111	6.22984414009049
C	2.68031860169276	9.93758141411123	2.65383292581263
H	1.93989179810387	9.12499848536770	2.64321268988888
C	3.58064969384179	9.76529686671631	1.43014424044559
H	2.97775058654662	9.75085284055026	0.50952307223447
H	4.16295581997884	8.83303258418760	1.46810388156134
H	4.29850984444696	10.59415179237608	1.33625450030547
C	1.91797805083253	11.26162453694458	2.57333636358544
H	1.25869843827554	11.28101267191680	1.69188085389194
H	2.61192750220766	12.11258603481474	2.49154456334922
H	1.30248784777492	11.42910795069412	3.46845259200704
C	3.38434095471133	8.04025178524016	7.36847503192964
H	2.27807621798678	8.03656178535860	7.38876459743462
C	3.84439277210519	6.59523453555609	7.16173310370153
H	3.38172651010570	6.12679606216405	6.28365534639135
H	3.57578115133889	5.98173956390737	8.03502666069112
H	4.93760162464665	6.54554813157182	7.04261466873338
C	3.84764947764726	8.54609071958922	8.72986212072531
H	3.58175072998755	9.60326855372103	8.88193237439861
H	4.93726621382731	8.45471099538647	8.85474078422654
H	3.38115648675269	7.95507866465218	9.53101693925570
C	-1.57221067952952	6.56545272479549	6.53627644142311
C	-2.91623252082571	6.79791704510997	6.18726079666502
C	-3.89830410651510	6.60387239643613	7.16380081398015
H	-4.94738856242889	6.76980735236781	6.90768282563111
C	-3.56479255378498	6.19971157098777	8.44978812483649

H	-4.34718212428265	6.04266705647118	9.19538375622285
C	-2.23073112006532	5.99600812578754	8.78472688407793
H	-1.97656250731970	5.68057541843893	9.79879438630387
C	-1.21104883633972	6.18136177203444	7.84781785392543
C	-3.32383033236626	7.27429116327174	4.80862979909574
H	-2.41433723187243	7.31391599035029	4.19192579793337
C	-4.30052232668012	6.31819524563996	4.12481477969270
H	-4.52075371497217	6.65709843886910	3.10091621271326
H	-5.25781548480014	6.26208611268036	4.66499785406062
H	-3.89761772663773	5.29640535438127	4.06580274006020
C	-3.90012552554304	8.68945080999640	4.88099520191535
H	-4.07771045313757	9.09426520750459	3.87269377008062
H	-3.22290848829051	9.37443869712915	5.41369781911028
H	-4.86141038538025	8.69701068397557	5.41822754688712
C	0.23316357361370	5.93590255237090	8.24625462697919
H	0.87164543984502	6.39060147424846	7.47289520800340
C	0.55757312169198	4.44088407138836	8.28061776541675
H	0.39281630048179	3.96246658715975	7.30524791038764
H	-0.07156031754509	3.91847806373948	9.01811214900134
H	1.61000156688705	4.27617351078727	8.55816953546879
C	0.59109123972188	6.59534862659141	9.57675837925635
H	0.37153014503368	7.67535292118009	9.56382966805145
H	1.66283670422646	6.46271188035952	9.78838473775893
H	0.03886404486995	6.14995095552270	10.41809586416708
C	-0.64984056873169	8.66146033146563	2.70341450369703
H	-0.16753064466013	7.68024739642500	2.70987114036021
C	-1.23837694754490	9.13695371825368	1.55736187733712
H	-1.21038520602050	8.51642963874425	0.66387001150288
C	-1.86526918073517	10.41565314490243	1.55684770484142
C	-1.83516915795151	11.11788934964224	2.79257843358750
H	-2.28633645979432	12.10199700084566	2.89948086170615
C	-1.22303746655729	10.55674668035142	3.88683811459042
H	-1.19566237667439	11.09066742020762	4.84153034850345
C	-2.45973068853801	10.16890226368561	-0.77978768477782
H	-2.97407231182680	10.75024256098552	-1.55216439555496
H	-2.99345451349118	9.21161807633414	-0.66497788684581
H	-1.43812232065365	9.96116789602945	-1.13682496034799
C	-3.07604612154337	12.22947654912396	0.50611123714661
H	-3.48397278620785	12.47098760158346	-0.48126096874603
H	-2.35233505504290	13.01616524643810	0.77534000243276
H	-3.90641184198262	12.25259479206953	1.23095355057549
Sb	1.74115350152656	11.63284372182962	6.80083635525572
Ga	1.40577971365121	13.17602599324557	8.86361285033410
N	-0.21044943123282	14.25089273544773	8.98481634751992
N	2.68644803875956	14.60863510652890	9.11083156980478
N	1.41284454682157	12.26891064737909	10.66815393638135
N	1.33785701560542	10.50422716788686	14.44700286400513
C	-0.19321650689918	15.45816248890305	9.55039281720846
C	0.98851552345281	16.11260555968317	9.94223890172374
H	0.84772087065913	17.08237922260309	10.41806527758937
C	2.32469165645538	15.77049620724666	9.65539686393299
C	-1.48871642615666	16.16485302719537	9.82165187722139
H	-1.37721239806681	17.25166043342935	9.72152115606328
H	-2.29550879109415	15.81510003540163	9.16609665906283
H	-1.79402280843289	15.95929532564511	10.86062085913656
C	3.38196501750499	16.77404161464236	10.00758787635530
H	3.80926000409016	16.51796344398149	10.99038729115403
H	4.21032847149189	16.76302132230859	9.28763566369263

H	2.96522291240880	17.78576218760795	10.07391149200041
C	-1.37503461876995	13.67836541935641	8.37893226535001
C	-2.25600084734753	12.87750919118346	9.13262985355591
C	-3.28673751816047	12.21072179922120	8.45914011464040
H	-3.97316359616344	11.57850438385405	9.02681437131195
C	-3.46030140170114	12.34794122880953	7.08807587234950
H	-4.27631540286788	11.82474719961180	6.58447676323288
C	-2.60397100890789	13.17225070139016	6.36425159915512
H	-2.76666513919566	13.30231450305068	5.29279089923603
C	-1.54649290765439	13.84200853770135	6.98339397002467
C	-2.15044287081015	12.74022053152816	10.63855894257829
H	-1.26660673671106	13.31065032926520	10.95921313635684
C	-3.37300507373728	13.34527391295055	11.33245481050149
H	-3.24726756753906	13.32426849508074	12.42590626101810
H	-3.54590595723921	14.38715210463406	11.02803674304848
H	-4.28620585839053	12.77826661492590	11.09486215188522
C	-1.94881347657679	11.29014285571938	11.07466339745759
H	-1.77724491381911	11.23483478396026	12.16062259475316
H	-2.83388625353264	10.67545477449882	10.84886899801516
H	-1.09122406829213	10.82708168942970	10.56727866043726
C	-0.64338692219180	14.76070185420848	6.18208942922689
H	0.33209840075562	14.78175621603143	6.69441318415499
C	-1.17875241651444	16.19458346513348	6.17806815075819
H	-1.27902939173016	16.60129646430924	7.19269932538237
H	-0.50328430211928	16.85870590980964	5.61750594611841
H	-2.17111325057534	16.23870631370547	5.70257097294600
C	-0.39608746712332	14.28376984633267	4.75521956842707
H	-0.01064638637511	13.25271274032010	4.72823813800953
H	-1.30947603733401	14.32789304958608	4.14180801577241
H	0.34516965460024	14.93060854485834	4.26436441819007
C	4.02584456126232	14.36236756246274	8.66111800488135
C	4.99995814587358	13.87235468523677	9.55377173525709
C	6.28397257601976	13.61627310618001	9.06061978881901
H	7.05394310280611	13.24636075193120	9.74169851700726
C	6.59805290183393	13.82858102127760	7.72566277190417
H	7.60995355623598	13.63486316698563	7.36272160695894
C	5.61958608351532	14.29004097134054	6.85127556653383
H	5.87428716804263	14.44899106835061	5.80266098589356
C	4.32128721020449	14.55949306404068	7.29080800577486
C	4.70477806631167	13.58789427732468	11.01255355255032
H	3.66609192119454	13.89253094103340	11.20652093357764
C	5.60695949873220	14.38238199371586	11.95720646242498
H	5.31376520463824	14.21376396712395	13.00476744171517
H	6.65997377339133	14.07770822973288	11.85911897896811
H	5.56094169949805	15.46312056388807	11.75984154362931
C	4.81118421775876	12.08897495597816	11.29886627968535
H	4.45312129122603	11.85647176827860	12.31384294571331
H	4.22231433217802	11.49769240636079	10.58288567336604
H	5.85487954478552	11.74580006250013	11.22732270623749
C	3.27497869679311	15.07382011982731	6.31881129467244
H	2.30468072992467	14.66847795949333	6.65496283307738
C	3.15491655529516	16.59862134887141	6.35459306772732
H	2.85511718956075	16.97109706520624	7.34318942562438
H	4.11384665441269	17.07127549521472	6.09140197970759
H	2.40023666464474	16.94223517940323	5.63018444128780
C	3.49375724714904	14.58848624648559	4.88899255198835
H	3.61897771644522	13.49605474681930	4.84394428275386
H	2.63006971206128	14.85750474610713	4.26387090685046

H	4.37696382379392	15.05607779259973	4.42792176602526
C	1.22145488078878	13.00881998074695	11.78082096444095
H	1.08730244253769	14.08400162134397	11.63410695890629
C	1.19426644403055	12.47355094392073	13.04508510463616
H	1.03609415353755	13.14324932931737	13.88804364784406
C	1.36853819286630	11.07230649178380	13.23007074039828
C	1.57880862541075	10.31527591047618	12.04541644552068
H	1.73243087799512	9.23837530495942	12.07393889014951
C	1.59368419152305	10.94411971331264	10.82466577074911
H	1.75260116861177	10.37015151665113	9.90912088535423
C	1.13211453792912	11.31817768598990	15.62939469756867
H	1.13879800330863	10.67525111704536	16.51591141157214
H	1.93107444715113	12.06780717627040	15.74897418008266
H	0.16209963297734	11.84022315518293	15.59711335009839
C	1.52004360467287	9.07297085249726	14.58613223223303
H	1.44397413665993	8.80037939606206	15.64391813779925
H	0.74697436714917	8.51320897835989	14.03526437543729
H	2.51065588553329	8.75346042283098	14.22345633521347

Table 9: Cartesian coordinates of $[L(DMAP)GaBi]_2^{2+}$ (**16**) [Å] for the optimized geometry. ORCA Version 5.0.0. Optimization: def2-SVP for H, C, N, and def2-TZVP for Ga, Bi. Single-point: def2-TZVP for H, C, N and def2-QZVP for Ga, Bi.

Bi	-0.21153151342164	10.11492573110320	7.64896299549702
Ga	0.28701006935280	8.62096812727250	5.49883735707059
N	-0.48076055418506	6.83883780813947	5.53258447343047
N	2.04102026166628	8.11444391022951	4.80465403518505
C	-0.76989853385854	4.57498596799608	4.66624070052434
H	-1.64085075930991	4.73807296377128	4.01069086064053
H	-1.16891621553352	4.25681974679929	5.63817428017766
H	-0.16070853390682	3.77088409678377	4.23838966426618
C	0.00293371945761	5.85441255593349	4.77845179190959
C	1.21087566040894	5.96004411882900	4.06324170881238
H	1.47958897091218	5.08997847993873	3.46658182036845
C	2.20227645969059	6.95299558488275	4.16080032448502
C	3.51841040253919	6.67112336578467	3.49823663943266
H	3.58533245414322	5.62595725971344	3.17675440204164
H	4.35736432900872	6.89766446354963	4.17059810687792
H	3.64311229719620	7.31655944972440	2.61606586313153
C	-1.52998297774406	6.61026579548781	6.48064385829690
C	-1.17201686792098	6.20070707368152	7.78555396725226
C	-2.19338715408451	6.00328662032352	8.71829263619149
H	-1.94161413159361	5.66802635510871	9.72660915889462
C	-3.52624849620777	6.21957560832650	8.38609788569593
H	-4.31004733669270	6.05251984499003	9.12805398141346
C	-3.85650777078004	6.64917397917199	7.10748090137106
H	-4.90453214698043	6.82509163032897	6.85360169447471
C	-2.87259143506195	6.85633538706454	6.13537686699711
C	0.27089740747813	5.94176110144951	8.18000755320357
H	0.91126059960412	6.41268560637518	7.41800275698247
C	0.59093372308045	4.44535439323022	8.18004350777550
H	0.42695856934744	3.99037723786898	7.19343773814789
H	-0.04118863170931	3.90771649180720	8.90393480162352
H	1.64231081731025	4.27124728342243	8.45582122969302
C	0.62968944945325	6.56804911788068	9.52593600667511
H	0.41494431851622	7.64912665514969	9.53974626468054
H	1.70078791389926	6.42766491280812	9.73530846854402
H	0.07585139316375	6.10503096450176	10.35652988376563

C	-3.27671395068386	7.36016730107323	4.76543413259808
H	-2.36616877237858	7.40868831642002	4.15104344389489
C	-4.25517156660760	6.41977572151010	4.06255442934273
H	-4.47247919491561	6.77791994518691	3.04453034039433
H	-5.21359043545640	6.35670900973194	4.60006989905691
H	-3.85509516318298	5.39799271822246	3.98575963895237
C	-3.84916559607023	8.77546074416536	4.86315934074809
H	-4.02749772017881	9.19788979686544	3.86221707759022
H	-3.16838539757924	9.44957671286744	5.40545718689845
H	-4.80923641071365	8.77674056502670	5.40265263822536
C	3.15162214472308	9.00197315984803	4.98343538261810
C	3.50530486465402	9.91577207930080	3.96880087350460
C	4.58185183629138	10.78260598664868	4.19531381078779
H	4.86887639185298	11.49040927568887	3.41435964625855
C	5.28352400425473	10.76455296135840	5.39117072641414
H	6.11473486428787	11.45305706164568	5.55550562422166
C	4.90767881106418	9.87716699908039	6.39560691790651
H	5.45594686519025	9.88540544652530	7.33776133626345
C	3.84311320649152	8.98506040734853	6.22149817807954
C	2.74008603431276	10.03596810607120	2.66580896028280
H	1.99662438731029	9.22670207037257	2.64067869244126
C	3.63650417964601	9.88555691928053	1.43644809505401
H	3.03060768097201	9.89005580910904	0.51771330807555
H	4.21617061436608	8.95107264058684	1.45481325943241
H	4.35629334135709	10.71416602839136	1.35586270397605
C	1.98184186667962	11.36375171023803	2.61412146112653
H	1.32630274744168	11.40642758707916	1.73074438597811
H	2.67801677090026	12.21499735865599	2.55690746602275
H	1.35982927991568	11.50978296321221	3.50880646935022
C	3.43175508329887	8.05352925541541	7.34682863328813
H	2.32554726424587	8.05456043826296	7.35994132081623
C	3.88755556983744	6.60971246803844	7.12274319245303
H	3.42782595399966	6.15564359356240	6.23547732903935
H	3.61130829264804	5.98535240712888	7.98586890845796
H	4.98128962114379	6.55690010246330	7.00919933852566
C	3.88832856504366	8.53980224798057	8.71796577364916
H	3.61830795190789	9.59405151811170	8.88553934109953
H	4.97732439119301	8.44706799811232	8.84763348103430
H	3.41760364626713	7.93605417303334	9.50707687905422
N	-0.57226730775128	9.42031139875919	3.83872989786685
N	-2.37488230094632	11.00712548022480	0.42785842159177
C	-1.16928881659184	10.62573090906567	3.86212264122960
H	-1.14832760571402	11.15485114928306	4.81989709751175
C	-1.77610653637446	11.19158413922424	2.76694235301659
H	-2.23063385177453	12.17399393569756	2.87618085638855
C	-1.79695689169415	10.49520409774328	1.52786309401264
C	-1.16609389451164	9.21869534773627	1.52634514251743
H	-1.13073622647618	8.60247424294042	0.63011456780246
C	-0.58365766556212	8.73900649703644	2.67422079622028
H	-0.09898003905942	7.75897845823978	2.67864728501644
C	-3.00878699149061	12.30935552608838	0.47872029326439
H	-3.41196639917861	12.55408055292690	-0.50959896002649
H	-2.29013312817509	13.09777323086971	0.75593009636860
H	-3.84326876717360	12.32587597586547	1.19880544708169
C	-2.37851449552371	10.25681504610865	-0.81297293472573
H	-2.89015742772076	10.83999830467882	-1.58584988048896
H	-2.91036860056571	9.29761135732109	-0.70501129916023
H	-1.35449585228937	10.05297898533750	-1.16542836771888

Bi	1.88772505704154	11.74666214754185	6.80189956036970
Ga	1.49126744332445	13.36361053316591	8.88916024802398
N	2.75525980974663	14.82115129844231	9.12373600512363
N	-0.13886474893386	14.42752846995075	9.01037731812989
C	3.42842717354690	17.00396895644532	9.99662998242262
H	3.84312296539716	16.77530932612497	10.99158862220592
H	4.26661062665689	16.98156704070982	9.28847517387724
H	3.00375840952310	18.01401967889803	10.03309793540187
C	2.38254318419502	15.98430110194141	9.65592057099106
C	1.04285768030721	16.31482395989730	9.94102108432172
H	0.89212013638590	17.28882361379323	10.40508110086016
C	-0.13217097136262	15.64195438713110	9.56116440568904
C	-1.43425928862667	16.33880280139800	9.82852005617479
H	-1.33131894650603	17.42615650806315	9.72564296559999
H	-2.23716661677451	15.98135487447056	9.17221806129740
H	-1.74058941818525	16.13357557281060	10.86719923587768
C	4.09518739302100	14.58121532994078	8.67340938619920
C	4.38420930023606	14.75901129996331	7.29878280139133
C	5.68025487236321	14.48440578358061	6.85570673222825
H	5.92908782213182	14.62715066835047	5.80333647561517
C	6.66473453755683	14.03919145734934	7.73187755420616
H	7.67488097377360	13.84139704740377	7.36632853940015
C	6.35868655131696	13.84960774048129	9.07196159836153
H	7.13344302375019	13.49346847165312	9.75494806664739
C	5.07631483969436	14.10907766855490	9.56790795652177
C	3.33249385168176	15.26009205207002	6.32582452141161
H	2.36472511708100	14.85560497407407	6.67065972601309
C	3.20852504624251	16.78490523288832	6.34736779126163
H	2.91250314896267	17.16528147763522	7.33399919563314
H	4.16522245172158	17.25730425796494	6.07568080878697
H	2.44954431839236	17.12008767111232	5.62351001631940
C	3.54752214204102	14.76408278363392	4.89876088616105
H	3.68751895810846	13.67271193829151	4.85964393479598
H	2.67732166810170	15.01807940201612	4.27618448987933
H	4.42292278034981	15.23698413620375	4.42832005762802
C	4.79081839385662	13.84724262219533	11.03273394451043
H	3.74972790983830	14.14401588280886	11.22593521044302
C	5.68891438818820	14.66879936468911	11.95798437915456
H	5.40347150547653	14.51572937657776	13.01007220180376
H	6.74478689453185	14.37426396626495	11.85920394124565
H	5.62941738950972	15.74514647250541	11.74145289362787
C	4.91519223864848	12.35511001084242	11.34592854938970
H	4.56334162966392	12.13757457383099	12.36638385180955
H	4.33044687443624	11.74410865349762	10.64317538443296
H	5.96245041354030	12.02236322670663	11.27714260859135
C	-1.30372818121918	13.83716206841078	8.42341396906210
C	-2.17737940416349	13.04770913777430	9.19818602200763
C	-3.21446901925738	12.36935710080264	8.54584689729095
H	-3.89641733437420	11.74799578391450	9.13084237067081
C	-3.40108604906519	12.48281377578930	7.17415116788737
H	-4.22148309681909	11.95087250943357	6.68707067506857
C	-2.55040934382572	13.29317893518162	6.42828472018661
H	-2.72034456192339	13.40095523457172	5.35554931656409
C	-1.48795039729450	13.97409424351958	7.02645311798353
C	-2.05715584212568	12.93296847800814	10.70495561820604
H	-1.17737872000028	13.51786612718415	11.00999611757068
C	-3.28081202596301	13.53088902283779	11.40297564620335
H	-3.14267408928762	13.52922404884964	12.49510941734007

H	-3.47200228637332	14.56518339418988	11.08403442358336
H	-4.18848771984468	12.94739168043733	11.18498555913272
C	-1.83325322850500	11.49122084873108	11.15760464015341
H	-1.65988318961769	11.45015023296828	12.24387821489865
H	-2.70859641731215	10.86010511242002	10.93909513097117
H	-0.96639482535124	11.03683989539182	10.65764262303424
C	-0.58795230742078	14.87299946929225	6.20004244189284
H	0.39558751432156	14.88701583262501	6.69729687783865
C	-1.10431977074127	16.31360099005815	6.18652242723116
H	-1.17948773587920	16.73538103494939	7.19718575032241
H	-0.43062297734151	16.96095172370531	5.60458254085991
H	-2.10468514078217	16.36489556651351	5.72885271775745
C	-0.36916162171814	14.37499276768488	4.77560529546599
H	-0.00770955770038	13.33492925057636	4.75648388684997
H	-1.28944525217777	14.43104175348990	4.17346624797050
H	0.37938097649332	14.99973043206709	4.26736686758459
N	1.51237054276505	12.48945091300458	10.71766884588498
N	1.48532348226354	10.77552666896224	14.52054371345998
C	1.71114857417442	11.16967404620149	10.89048451797322
H	1.87168531042745	10.58627278226571	9.98013260842788
C	1.71165639113752	10.55665798541365	12.11969315615075
H	1.87992026251400	9.48241497841161	12.16230970171727
C	1.49976520303889	11.32712117511886	13.29545331007740
C	1.30580924468839	12.72309356530774	13.09280900567209
H	1.14443347262598	13.40196692424651	13.92781655260593
C	1.31851906154306	13.24155952813495	11.82098533330161
H	1.16995171634905	14.31288335505529	11.66039168464025
C	1.68879359297172	9.34920053431973	14.67836388370354
H	1.62722098912166	9.09095585691289	15.74077987661264
H	0.91814487890993	8.77057121831893	14.14363935086323
H	2.68016462666337	9.03810600331214	14.31032127429117
C	1.27646862119232	11.60311013283580	15.69274252146853
H	1.29671444745984	10.97272839331696	16.58794622123444
H	2.06632574047207	12.36456809172873	15.79708473444141
H	0.29972153480157	12.11234365365982	15.65950681981903

Table 10: Cartesian coordinates of $[LGaSb]_2^{2+}$ (**17**) [Å] for the optimized geometry. ORCA Version 5.0.0. Optimization: def2-SVP for H, C, N and def2-TZVP for Ga, Sb. Single-point: def2-TZVP for H, C, N and def2-QZVP for Ga, Sb.

Sb	10.75255527443637	3.30624158835253	7.66409725644245
Ga	9.26557820960564	4.97208091834930	6.38585697988910
N	9.47629945364847	6.83543627988903	6.50065568069158
N	7.80408369320973	4.89722602239657	5.20055330917968
C	8.70232679240763	7.70550692274852	5.83898694401301
C	7.63996847390417	7.29971524841010	5.01611461490454
H	7.07334692268417	8.10301294175002	4.54785794577175
C	7.20327463794286	6.00007079523230	4.72152168692379
C	8.98614921239468	9.16388030804598	5.99599303561863
H	10.02625065363608	9.38097304640034	5.70943564529997
H	8.88863581258273	9.46278705388146	7.05088226897443
H	8.30980794694323	9.77417693147166	5.38778092310706
C	6.02450017880705	5.83792837698270	3.81240280266283
H	5.44408678079391	6.76582569470354	3.75363135328523
H	5.37261543684835	5.01699674026515	4.14031932304979
H	6.36386092765259	5.58608918450653	2.79464897759104
C	10.53730181935441	7.24141651614900	7.37818571573947
C	11.85687721914102	7.26516733304272	6.88687670369011
C	12.88581322939830	7.52640931451328	7.79810622284864

H	13.91908353707900	7.56090207592431	7.44474488988845
C	12.61408038601155	7.75570341263716	9.14168074411531
H	13.43079884707691	7.96747591526853	9.83550938483812
C	11.30082959971879	7.73468823337541	9.60247725860714
H	11.10003480562958	7.92741158534180	10.65814601801839
C	10.23601152717745	7.47714476948648	8.73551335525046
C	12.18443235190427	7.02167614171508	5.42501227635818
H	11.23412979735614	6.91433780444187	4.87780753429167
C	12.96925376347385	5.72261053472284	5.23853914828122
H	12.42144467687047	4.85144298504367	5.63701285513372
H	13.93744502553668	5.76287179835873	5.76152392130122
H	13.17070618938590	5.53315467839001	4.17323302471808
C	12.92600643002118	8.20768475166718	4.80655387540360
H	13.91520110458234	8.35183571103767	5.26681112148089
H	12.36472238045341	9.14560999324482	4.93073822965724
H	13.08329939633885	8.04648203528920	3.72966736122856
C	8.81151708805091	7.41275106542012	9.25790172454246
H	8.13128534218105	7.52496548533781	8.39919084084444
C	8.52622915291852	6.04508958039116	9.88254394940210
H	7.48387667744236	5.97796651463189	10.22981544232632
H	9.18674870994952	5.85907343771101	10.74366719739056
H	8.69300870294378	5.22078357224837	9.16635042847413
C	8.48581426585520	8.54005228999179	10.23521303751862
H	9.04665915063552	8.44541348207410	11.17712082093297
H	7.41663461693359	8.52436878153154	10.49297117582094
H	8.71734657267296	9.52622430453688	9.80610660055356
C	7.34509475549256	3.57694441887180	4.89394560606795
C	7.70165884453739	2.98974544046391	3.66239088333637
C	7.28337803293841	1.67577117183516	3.42310428236559
H	7.53194800749172	1.19751836346566	2.47439771389967
C	6.56125039768563	0.96632616976942	4.37613132404426
H	6.24708696483891	-0.05868188712714	4.16932602912530
C	6.25635965473405	1.55076988208779	5.60249155234318
H	5.70441694337270	0.97560558625880	6.34691006345278
C	6.64628340818038	2.86298165361802	5.89413156420457
C	8.57132250227415	3.72356176267904	2.65648371520110
H	8.43392938225928	4.80356928599080	2.81492620826819
C	10.05197734858569	3.43131177644799	2.91431979927657
H	10.36218028147938	3.72638190379223	3.93106236603813
H	10.68788444550938	3.97861557134398	2.20243243188671
H	10.26761570670366	2.35634842987032	2.80573703345486
C	8.19746947212180	3.42821865599129	1.20704083264144
H	7.12530620731376	3.59163777558943	1.02177693819677
H	8.43355139860553	2.39170596339633	0.92234117943398
H	8.76302934492601	4.08329128466549	0.52858766801777
C	5.08459380165782	4.38494657413514	7.16549170150309
H	4.87497600583329	4.83464987246227	8.14749401669550
H	4.20393820320047	3.79487843852956	6.86922100194385
H	5.19995848795589	5.20369602405587	6.44222715509144
Sb	9.75770433239373	1.34983743488777	6.17730002626086
Ga	11.30807262235860	-0.29557507766201	7.41834412815939
N	11.17205836408699	-2.15946351923174	7.19581929355708
N	12.77891742038345	-0.23312938110861	8.58974909982816
C	11.97269203047120	-3.03667818534041	7.81228751806479
C	13.02215871316982	-2.63746697950650	8.65645182507114
H	13.61483487819744	-3.44360459213750	9.08554097916921
C	13.41629122871123	-1.34084332699360	9.01105744794018
C	11.73436491528998	-4.49393211143851	7.58510829620231

H	10.70762557698465	-4.75895345468996	7.88001908931718
H	11.81956983516091	-4.73686851519767	6.51504358272442
H	12.44133036684278	-5.11122035014930	8.14988428345032
C	14.60837497689110	-1.17118255834245	9.89806353505500
H	15.05071553499772	-2.13798800433878	10.16126222452450
H	15.36863198320924	-0.55344177485006	9.39742985783131
H	14.33736385625908	-0.63920132720565	10.82218435166256
C	10.12979017139416	-2.55234707947587	6.29050607372802
C	8.81078875249178	-2.65605235550397	6.77138459623587
C	7.79522317772859	-2.89445352170371	5.83879693007151
H	6.76260610636840	-2.98903818238706	6.18292797374115
C	8.08063465972162	-3.02630998182676	4.48531442752382
H	7.27495451843145	-3.22126055760062	3.77391240848215
C	9.39468834199450	-2.93243433813599	4.03510311341577
H	9.60591584974683	-3.05482431144078	2.97132124587427
C	10.44629627662129	-2.69414908823065	4.92315012657617
C	8.47017417059792	-2.52037451242578	8.24414524545454
H	9.41481506723294	-2.42502270370176	8.80327618504842
C	7.65129125008122	-1.25725873819042	8.51151359807950
H	8.18041008270464	-0.35051809602818	8.17160851912709
H	6.68595307890057	-1.28660396096543	7.98278825571827
H	7.44277693836575	-1.14165638871296	9.58589140444263
C	7.75685910704622	-3.76363757239585	8.77741381710917
H	6.77227940821957	-3.90034373776406	8.30525293797001
H	8.34131422770197	-4.67687920855504	8.59149841643860
H	7.59362754726115	-3.68004972792753	9.86218174069759
C	11.87416678336405	-2.56024062880677	4.42162738272520
H	12.54791301301066	-2.78927922762347	5.26245280935751
C	12.17073218067861	-1.12297302303612	3.98874314087441
H	13.20722004027543	-1.02222749688004	3.63285610310740
H	11.49636416037861	-0.80680725293631	3.17765896015268
H	12.03890327723333	-0.40203327019092	4.81605489329974
C	12.20865465083020	-3.54325452655076	3.30231606389300
H	11.66928104160378	-3.30998467009893	2.37198479849852
H	13.28292390701277	-3.50345301340338	3.07004437031714
H	11.96010581130173	-4.57695227405030	3.58463608064354
C	13.19614869621921	1.08148543081666	8.98557590615652
C	12.69816751286508	1.61358458568424	10.19594443407975
C	13.02760123987539	2.93517779461343	10.51056062563477
H	12.66271128413346	3.37285713320596	11.44109220749522
C	13.81317934962104	3.70417999155278	9.65593235953532
H	14.04910246684814	4.73819252208033	9.91576663127644
C	14.30024108952637	3.15650638002130	8.47473475524663
H	14.93029475128282	3.76305411955865	7.82019175548670
C	14.01064263201781	1.83384818561281	8.11460278257693
C	11.80788506604958	0.79122643488501	11.11224466867359
H	12.04520563495183	-0.27044942217130	10.94117611169377
C	10.33131132562572	0.97536832656937	10.75699084866525
H	10.11346226404932	0.69374019626027	9.71234312435484
H	9.69173096081728	0.35691437223774	11.40434102489744
H	10.02327769522292	2.02632896170009	10.87731326155015
C	12.05049027676487	1.07097944799724	12.59272770531231
H	13.11552232221122	0.98243245093612	12.85371875349050
H	11.71478849534257	2.07770213651400	12.88418063371751
H	11.48958703403485	0.35448866723426	13.21027566313907
C	14.60100164983805	1.25237725564243	6.84245802459566
H	14.22576493563047	0.22169368549410	6.73565354770300
C	14.17496135383503	2.02719489354367	5.59557590040569

H	14.57732354238041	1.54850062794033	4.69036600777142
H	13.07963463979378	2.07521551069371	5.49632740311608
H	14.55186517454843	3.06112433488451	5.61528441556447
C	16.12653435436017	1.16934243851388	6.93678886015320
H	16.54292443171221	0.67928415136361	6.04415901443643
H	16.57691141151079	2.17122013333925	7.00710364043985
H	16.45355350264681	0.59910598383772	7.81854821376088
C	6.32684430691836	3.49476656174996	7.23697351259096
H	7.17754861515231	4.15754060153143	7.49840264520610
C	6.21536834703219	2.48727863376156	8.37436481597637
H	6.12745282813649	3.01500387083530	9.33522809229306
H	7.09825329745155	1.83218436092886	8.42545439539131
H	5.32209490659131	1.85220413538055	8.27602042763667

Table 11: Cartesian coordinates of $[LGaBi]_2^{2+}$ (**18**) [Å] for the optimized geometry. ORCA Version 5.0.0. Optimization: def2-SVP for H, C, N and def2-TZVP for Ga, Bi. Single-point: def2-TZVP for H, C, N and def2-QZVP for Ga, Bi.

Bi	-1.14796508626029	1.10289221633125	13.52890708649197
Bi	0.37537989006493	-1.09949856883406	12.70056958690100
Ga	0.47890842063905	2.57959258424721	12.04415369058627
Ga	-1.14969162144264	-2.58615042587225	14.27566760834525
N	0.42983301844940	4.46707548948400	12.11417124897856
N	1.89157874672954	2.37390979738519	10.80923710569841
N	-1.15127627086127	-4.47054921448994	14.16536851171537
N	-2.35285903435644	-2.37846404053690	15.71360877240065
C	1.24370547823328	5.26127309482933	11.41255299680628
C	-0.57414101267078	4.96428919076442	13.00944003393162
C	2.50668897692951	3.42032845510773	10.22607638913969
C	2.27554973003079	1.02224390569347	10.52352500164598
C	-1.87337393866015	-5.26266570835294	14.96406784863897
C	-0.29733892027706	-4.96709226109616	13.12563306803903
C	-2.89890100024339	-3.42237333766387	16.36369759156511
C	-2.63762979971756	-1.02168579535274	16.07713705032831
C	2.20213498481348	4.75500050015029	10.51779946081154
C	1.12641237323979	6.74019672462950	11.59225674394248
C	-1.85206357338556	5.25979374044297	12.48945140392187
C	-0.29665088861075	5.00771759477717	14.38990026393286
C	3.57239465931973	3.13387944301526	9.21604287918507
C	1.54123727008270	0.28259242575312	9.57365145905097
C	3.33076742214234	0.44715434761489	11.26824313399300
C	-2.67714672487727	-4.75658319700412	15.99993464130934
C	-1.81582047259914	-6.73953816228238	14.74302870702797
C	1.03275796784660	-5.30708726822983	13.45011552674643
C	-0.76808377517778	-4.96291769404301	11.79752657440322
C	-3.78889502818259	-3.13772307921818	17.53228431748282
C	-1.70815359628158	-0.31005519491343	16.86404671587334
C	-3.79647610906077	-0.40921059499839	15.54780285994976
H	2.79022722953100	5.49993188166944	9.98445244544187
H	1.85621357240739	7.27986982763578	10.97905025683749
H	1.27784351056169	7.00470430938037	12.64959197740755
H	0.11407044193019	7.08354939956323	11.33083732256983
C	-2.85894523915567	5.60144818754668	13.39533004563264
C	-2.14044083164945	5.17077507768658	11.00043228447412
C	-1.34173859136544	5.35686887938706	15.25282671882630
C	1.08178915056567	4.71555254919352	14.95512092364034
H	3.17105652390100	2.50767378029106	8.40547982454771
H	4.39731714998257	2.56329952662824	9.66868437180909
H	3.97477063519384	4.05821194225100	8.78777850411216

C	1.86931334985992	-1.06939111061211	9.40361129677158
C	0.44806846674993	0.90442805534300	8.72344668958699
C	3.62179914386794	-0.90368494307604	11.05136121084865
C	4.11502511317722	1.25717356916432	12.28707486720836
H	-3.19799000418616	-5.50108008707157	16.59971531305019
H	-2.47673663563528	-7.27639375157122	15.43215216249208
H	-2.10131957242751	-6.97866714998963	13.70766638738548
H	-0.78734492428937	-7.10960127983614	14.87238761423258
C	1.89000354935094	-5.65122617660918	12.40206260260147
C	1.53925788181085	-5.25696057863443	14.88135727914202
C	0.13316545579374	-5.31407486464383	10.78619533385971
C	-2.20157104557411	-4.61276120103216	11.44092085475545
H	-3.26265274753512	-2.51542454092217	18.27063174819299
H	-4.67480227493040	-2.56468896480795	17.21965675744503
H	-4.12088893919184	-4.06324574034906	18.01496766806844
C	-1.96152653413381	1.04699702904334	17.10442391509075
C	-0.48688431169133	-0.96874875632687	17.48021555675423
C	-4.00388515037420	0.94523092994431	15.82602610517842
C	-4.76838623610448	-1.18323545250015	14.67309615021568
H	-3.85667219980879	5.84317975963504	13.02482722303580
C	-2.60989746564461	5.64630372390439	14.76450575122598
H	-1.18757400426181	5.30705577268170	10.46531657944571
C	-3.08832337435111	6.26144421566708	10.50812555383192
C	-2.66640565535895	3.78299362167035	10.62732520987899
H	-1.15324248511346	5.41341454582105	16.32761089655910
C	1.68203007362680	5.95566498550028	15.62114610207393
H	1.74351247851192	4.44598906442663	14.11580305985896
C	1.06410027009672	3.53152656153943	15.92181870760554
H	1.31755858216711	-1.66588526050334	8.67344917786565
C	2.89440927140802	-1.65922597938289	10.13477815493141
H	0.37078095909146	1.96820479381550	8.99947832802916
C	0.80819141823654	0.84776979760175	7.23715717824039
C	-0.91593787670189	0.26298844219160	8.98049484485434
H	4.43595124390331	-1.37318810497258	11.60612861129716
H	4.03577331937259	2.31719533229748	11.99986329967601
C	5.60095038096328	0.90851493013856	12.30797208685773
C	3.50478635032558	1.13222129380649	13.68442792463823
H	2.92284111816170	-5.92824716931623	12.62128428251162
C	1.44803083292445	-5.65256527759389	11.08186264750266
H	0.66905066130433	-5.34183363269821	15.55073166328871
C	2.47921690070468	-6.41065465503742	15.22256101762948
C	2.19945750287991	-3.90785285256612	15.17586173526022
H	-0.20677686327271	-5.33284717865375	9.74801766457237
C	-2.92910444753101	-5.81043575093875	10.82615126736199
H	-2.73130919273834	-4.35741022305422	12.37331423242926
C	-2.27868839832582	-3.39358142696893	10.52140595885595
H	-1.26180438642040	1.62083896962216	17.71601456315938
C	-3.09386568704503	1.67027358184859	16.59173934957405
H	-0.42799630117346	-1.99935334338472	17.09343948614065
C	-0.63084138912943	-1.06525868406076	19.00132798929216
C	0.81450422610321	-0.26184679067456	17.10215835047368
H	-4.89339138208196	1.44381493395074	15.43761773966060
H	-4.68879262371912	-2.24659237797539	14.94656894682093
C	-6.22304672301699	-0.77344228979086	14.88465638740117
C	-4.38087008247585	-1.08001477138934	13.19660378318599
H	-3.41040255268900	5.92442819293765	15.45367871022145
H	-3.15647130012221	6.23842945736278	9.41069066963931
H	-2.74285036049992	7.26245011228563	10.80611166635585

H	-4.10934299633001	6.12878115891797	10.89648903811386
H	-3.60434044373365	3.55968615576426	11.15928912479946
H	-1.94964665033294	2.98226992044863	10.88533802583673
H	-2.86049260641629	3.71145175423091	9.54645165749407
H	1.09197230236504	6.26435585293898	16.49745735119633
H	1.71728392344821	6.81132974245601	14.93100801689192
H	2.70784795915999	5.75457410272431	15.96441309976444
H	2.07893870336692	3.30818337602716	16.28423551196069
H	0.67046314998936	2.61805842132632	15.44487402840092
H	0.43468072733296	3.73857443689687	16.80105159334549
H	3.13343983781455	-2.71434141649855	9.98608151553318
H	0.05162697680519	1.37538964745215	6.63762410179497
H	0.85385273936963	-0.19015233616863	6.87371118063022
H	1.78453861898466	1.31174123741337	7.03332838044800
H	-0.91258788904838	-0.80724366832733	8.72091955205662
H	-1.69139646708844	0.74816243407580	8.36919066868997
H	-1.21558842699081	0.34631346385069	10.03663894590916
H	6.04300549575886	0.95244325370015	11.30150156027451
H	5.78463030823577	-0.09829363314905	12.71271737678353
H	6.14659367120966	1.61629950393591	12.94880073700068
H	2.45563919686863	1.47114247601466	13.71559719276548
H	4.06829979373777	1.73453173788742	14.41274401696806
H	3.51559281006266	0.08557900530635	14.02970178986445
H	2.13306473881477	-5.93397691021217	10.27886135294444
H	2.71281888458564	-6.40603668696132	16.29729577295185
H	2.03007965432918	-7.38432958626938	14.97661792188645
H	3.43639851245260	-6.33765037977488	14.68463075845158
H	3.05748288295339	-3.73431146116511	14.50758230217012
H	1.50039601971945	-3.06439773091402	15.03185386362647
H	2.55964441369073	-3.86222991647532	16.21483104782482
H	-2.47660661227560	-6.10518910802154	9.86712597807472
H	-2.89812270043233	-6.68829825558101	11.48820645438350
H	-3.98494080659190	-5.56708665659744	10.63490350139164
H	-3.32601256695463	-3.12961517233366	10.31060133145671
H	-1.79453582072919	-2.51010193104714	10.97119778383719
H	-1.78369459011641	-3.58360244289060	9.55656170918014
H	-3.27240950371616	2.72894078418694	16.79134986329600
H	0.22576664345919	-1.60005710002100	19.43793425298922
H	-0.66967611091125	-0.06532804116786	19.46006788752384
H	-1.54643655920314	-1.59851409779843	19.29559068835527
H	0.85164261053257	0.76199275914772	17.50467814440264
H	1.67791750004664	-0.80519263230351	17.51423591716177
H	0.94215580545400	-0.19636917357834	16.01067999806848
H	-6.50338430642439	-0.80440237470072	15.94803400686220
H	-6.42537835844347	0.24217662766470	14.51217341019721
H	-6.89145271924655	-1.45444781706437	14.33810148190592
H	-3.35827568582260	-1.44811297449144	13.00432753798038
H	-5.06528347235062	-1.67032406516125	12.56909328463341
H	-4.42008964798470	-0.03506391751921	12.84878001364707

Crystallographic Appendix

Crystal structure of mw_129_3m

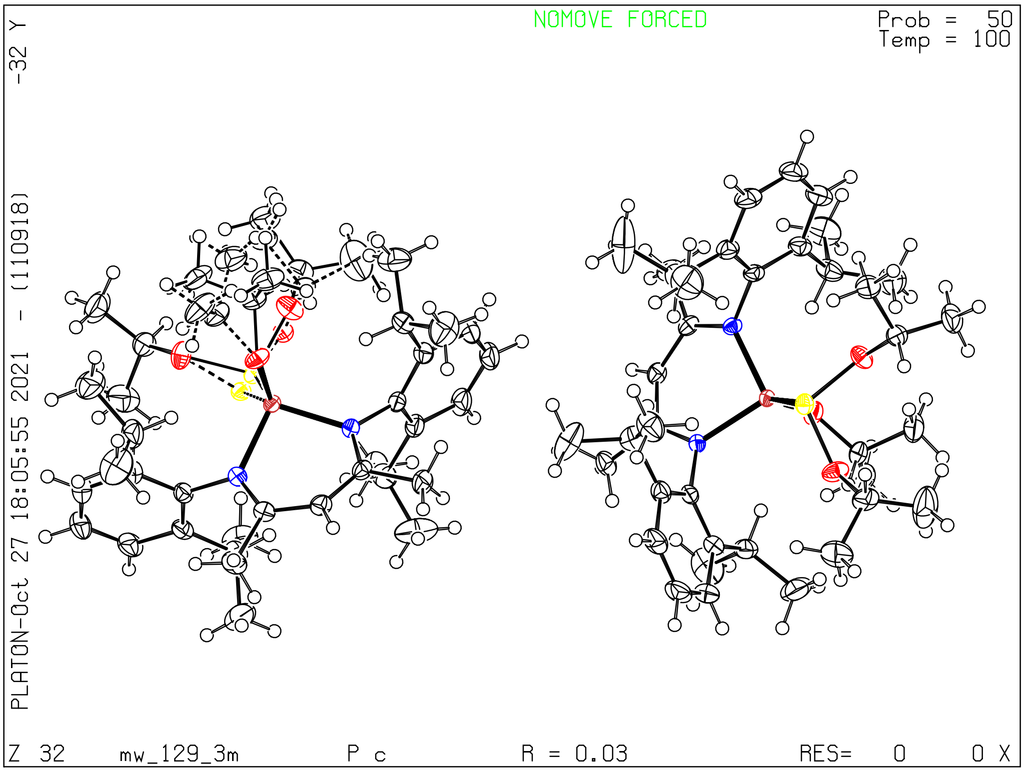

Table 1: Crystal data and structure refinement for mw_129_3m.

Identification code	mw_129_3m
Empirical Formula	$C_{38}H_{62}AsGaN_2O_3$
Formula weight	739.53 Da
Density (calculated)	$1.247\,g \cdot cm^{-3}$
$F(000)$	1568
Temperature	100(2) K
Crystal size	0.543 × 0.316 × 0.229 mm
Crystal appearance	pale yellow tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	Pc
Unit cell dimensions	$a = 17.612(8)$ Å
	$b = 12.131(6)$ Å
	$c = 18.479(9)$ Å
	$\alpha = 90°$
	$\beta = 94.032(10)°$
	$\gamma = 90°$
Unit cell volume	3939(3) $Å^3$
Z	4
Cell measurement refections used	9185
θ range for cell measurement	2.78° to 32.27°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	2.359° to 33.421°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.3%)
Index ranges	$-27 \leq h \leq 27$
	$-18 \leq k \leq 18$
	$-28 \leq l \leq 28$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.567\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.52
R_{merg} before/after correction	0.1016/0.0706
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	154109
Independent reflections	30297 ($R_{int} = 0.0477$)
Reflections with $I > 2\sigma(I)$	25979
Data / retraints / parameter	30297 / 81 / 922
Goodness-of-fit on F^2	1.008
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 0.5351P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0306$
	$wR2 = 0.0699$
R indices [all data]	$R1 = 0.0436$
	$wR2 = 0.0755$
Absolute structure parameter	0.075(5)
Largest diff. peak and hole	0.819 and -0.429 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

An isopropyl group and part of the –As(O–iPr)$_2$) moiety are disordered over two positions. All corresponding bond lengths and the bond angles of the isopropyl groups were restrained to be equal (`SADI`). `RIGU` restraints were applied to the displacement parameters of the isopropyl groups. Due to the close proximity of the alternate positions additional `SIMU` restraints were used for C37_2 and C37'_2.

Twinning

The model was refined as a 2-component inversion twin.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_129_3m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
As11	7506(1)	5915(1)	7494(1)	21(1)
Ga11	7690(1)	5637(1)	6212(1)	16(1)
O11	8619(1)	5870(2)	5885(1)	26(1)
O21	8335(1)	5110(2)	7750(1)	30(1)
O31	7911(1)	7279(1)	7450(1)	27(1)
N11	7312(1)	4174(1)	5886(1)	18(1)
N21	7009(1)	6480(2)	5544(1)	19(1)
C11	7014(1)	4044(2)	5209(1)	21(1)
C21	6848(1)	4925(2)	4737(1)	23(1)
C31	6782(1)	6044(2)	4902(1)	23(1)
C41	6811(2)	2913(2)	4916(2)	30(1)
C51	6417(2)	6774(3)	4315(2)	37(1)
C61	7352(1)	3248(2)	6383(1)	22(1)
C71	8036(2)	2652(2)	6485(2)	28(1)
C81	8056(2)	1779(2)	6983(2)	37(1)
C91	7445(2)	1515(2)	7364(2)	40(1)
C101	6781(2)	2116(2)	7258(2)	35(1)
C111	6723(2)	2991(2)	6771(2)	27(1)
C121	8727(2)	2921(2)	6078(2)	35(1)
C131	8757(3)	2247(4)	5379(3)	62(1)
C141	9468(2)	2767(3)	6546(3)	60(1)
C151	5976(2)	3604(3)	6666(2)	38(1)
C161	5365(2)	2886(4)	6259(2)	57(1)
C171	5686(2)	3963(3)	7394(2)	47(1)
C181	6757(1)	7578(2)	5719(1)	22(1)
C191	7217(2)	8494(2)	5608(1)	27(1)
C201	6947(2)	9532(2)	5790(2)	36(1)
C211	6250(2)	9666(2)	6066(2)	38(1)
C221	5804(2)	8754(2)	6173(2)	35(1)
C231	6045(2)	7700(2)	6010(1)	28(1)
C241	7990(2)	8405(2)	5299(2)	34(1)
C251	8001(3)	8993(3)	4567(2)	52(1)
C261	8607(2)	8870(3)	5835(2)	50(1)
C271	5535(2)	6727(3)	6144(2)	42(1)
C281	4844(3)	6710(6)	5594(3)	101(2)
C291	5263(3)	6734(4)	6900(2)	63(1)
C301	9324(1)	5663(2)	6286(1)	26(1)
C311	9892(2)	5317(3)	5746(2)	37(1)
C321	9611(2)	6652(3)	6716(2)	41(1)
C331	8531(2)	4957(2)	8516(2)	34(1)
C341	8501(3)	3753(3)	8687(2)	54(1)
C351	9306(3)	5438(5)	8675(3)	77(2)
C361	7853(2)	7995(2)	8066(1)	26(1)
C371	7074(2)	8503(2)	8046(2)	35(1)
C381	8471(2)	8843(3)	8030(2)	45(1)
As12	2669(1)	798(1)	2597(1)	21(1)
O32	2532(2)	2258(2)	2727(1)	32(1)
C362	2694(2)	2986(3)	2147(2)	32(1)
C372	3269(5)	3819(6)	2446(6)	44(1)
C382	1965(3)	3490(4)	1843(3)	48(1)

Table 2: (continued)

	x	y	z	U_{eq}
As1'2	2697(1)	379(5)	2500(2)	22(1)
O3'2	2931(6)	1789(8)	2226(6)	25(3)
C36'2	2645(9)	2726(16)	2559(9)	25(3)
C37'2	3140(40)	3730(40)	2540(40)	68(13)
C38'2	1916(13)	3131(18)	2187(14)	47(5)
Ga12	2444(1)	483(1)	3856(1)	18(1)
O12	1635(1)	1077(2)	4263(1)	28(1)
O22	1722(1)	360(2)	2278(1)	30(1)
N12	2428(1)	−1080(2)	4124(1)	20(1)
N22	3328(1)	881(2)	4508(1)	20(1)
C12	2704(1)	−1390(2)	4778(1)	22(1)
C22	3137(2)	−705(2)	5256(1)	25(1)
C32	3478(1)	301(2)	5116(1)	22(1)
C42	2573(2)	−2547(2)	5046(2)	34(1)
C52	4063(2)	716(2)	5687(2)	33(1)
C62	2130(2)	−1904(2)	3612(1)	23(1)
C72	1344(2)	−2079(2)	3508(2)	32(1)
C82	1085(2)	−2885(3)	3014(2)	44(1)
C92	1582(2)	−3490(3)	2631(2)	46(1)
C102	2351(2)	−3303(2)	2730(2)	38(1)
C112	2644(2)	−2512(2)	3222(1)	26(1)
C122	778(2)	−1449(3)	3929(2)	43(1)
C132	486(3)	−2158(4)	4536(2)	63(1)
C142	91(2)	−1068(4)	3428(3)	56(1)
C152	3498(2)	−2355(2)	3323(2)	31(1)
C162	3889(2)	−3376(3)	3661(2)	54(1)
C172	3844(2)	−2084(3)	2612(2)	51(1)
C182	3820(1)	1793(2)	4353(1)	23(1)
C192	4469(2)	1580(2)	3975(2)	28(1)
C202	4960(2)	2454(2)	3863(2)	36(1)
C212	4820(2)	3500(3)	4105(2)	40(1)
C222	4164(2)	3706(2)	4448(2)	36(1)
C232	3646(2)	2872(2)	4571(1)	28(1)
C242	4645(2)	440(2)	3686(2)	34(1)
C252	5248(3)	−148(4)	4168(2)	68(1)
C262	4893(2)	496(3)	2912(2)	44(1)
C272	2921(2)	3164(2)	4921(2)	32(1)
C282	2517(2)	4122(3)	4515(2)	53(1)
C292	3062(2)	3470(4)	5723(2)	56(1)
C302	1235(2)	2021(3)	4044(2)	28(1)
C312	641(3)	1811(5)	3432(3)	45(1)
C322	874(3)	2498(4)	4700(2)	41(1)
C30'2	942(6)	1397(10)	3886(6)	32(3)
C31'2	900(9)	2463(13)	3494(9)	49(4)
C32'2	352(7)	1323(14)	4445(6)	46(4)
C332	1576(2)	172(2)	1512(2)	33(1)
C342	1857(3)	−942(3)	1306(2)	55(1)
C352	731(2)	305(4)	1345(2)	56(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_129_3m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
As11	22(1)	24(1)	16(1)	−1(1)	1(1)	−2(1)
Ga11	17(1)	16(1)	15(1)	0(1)	−2(1)	−1(1)
O11	20(1)	34(1)	25(1)	5(1)	−1(1)	−5(1)
O21	37(1)	35(1)	18(1)	2(1)	−1(1)	12(1)
O31	37(1)	22(1)	22(1)	−5(1)	6(1)	−3(1)
N11	18(1)	18(1)	18(1)	−1(1)	0(1)	−1(1)
N21	21(1)	20(1)	16(1)	1(1)	−1(1)	3(1)
C11	21(1)	23(1)	19(1)	−5(1)	2(1)	−1(1)
C21	25(1)	28(1)	15(1)	−4(1)	−1(1)	1(1)
C31	21(1)	29(1)	17(1)	2(1)	−1(1)	3(1)
C41	38(1)	26(1)	26(1)	−9(1)	0(1)	−5(1)
C51	50(2)	38(1)	23(1)	3(1)	−11(1)	11(1)
C61	26(1)	17(1)	22(1)	−1(1)	−2(1)	−3(1)
C71	29(1)	19(1)	34(1)	0(1)	−3(1)	−1(1)
C81	42(2)	22(1)	46(2)	5(1)	−5(1)	3(1)
C91	58(2)	22(1)	39(2)	10(1)	−4(1)	−4(1)
C101	46(2)	28(1)	33(1)	6(1)	5(1)	−11(1)
C111	30(1)	24(1)	27(1)	2(1)	1(1)	−6(1)
C121	26(1)	24(1)	54(2)	5(1)	2(1)	3(1)
C131	55(2)	61(2)	75(3)	−14(2)	31(2)	−9(2)
C141	31(2)	53(2)	95(3)	29(2)	−10(2)	5(1)
C151	31(1)	43(2)	42(2)	15(1)	12(1)	0(1)
C161	30(2)	105(3)	37(2)	3(2)	−1(1)	−3(2)
C171	40(2)	42(2)	61(2)	−5(2)	18(2)	−7(1)
C181	28(1)	21(1)	17(1)	0(1)	−3(1)	6(1)
C191	34(1)	24(1)	24(1)	3(1)	0(1)	3(1)
C201	48(2)	23(1)	38(2)	3(1)	1(1)	5(1)
C211	50(2)	26(1)	38(2)	−4(1)	−1(1)	15(1)
C221	33(1)	34(1)	36(1)	−3(1)	2(1)	15(1)
C231	27(1)	27(1)	30(1)	−3(1)	0(1)	7(1)
C241	39(2)	24(1)	41(2)	7(1)	12(1)	−1(1)
C251	67(2)	48(2)	43(2)	13(2)	18(2)	0(2)
C261	38(2)	48(2)	63(2)	9(2)	6(2)	−5(1)
C271	28(2)	35(1)	66(2)	−9(1)	16(1)	0(1)
C281	78(3)	152(6)	71(3)	−21(3)	−2(3)	−70(4)
C291	60(2)	66(3)	63(3)	15(2)	12(2)	−14(2)
C301	18(1)	32(1)	28(1)	0(1)	0(1)	−3(1)
C311	26(1)	47(2)	38(2)	−3(1)	7(1)	1(1)
C321	27(2)	47(2)	49(2)	−14(1)	−2(1)	−6(1)
C331	44(2)	37(1)	19(1)	7(1)	−3(1)	5(1)
C341	69(3)	41(2)	51(2)	23(2)	0(2)	−4(2)
C351	82(3)	94(3)	50(3)	25(2)	−31(2)	−43(3)
C361	30(1)	26(1)	22(1)	−7(1)	−1(1)	4(1)
C371	30(1)	33(1)	43(2)	−5(1)	5(1)	5(1)
C381	34(2)	39(2)	64(2)	−26(2)	1(2)	−2(1)
As12	21(1)	25(1)	17(1)	2(1)	1(1)	1(1)
O32	51(2)	25(1)	22(1)	1(1)	9(1)	−2(1)
C362	45(2)	28(2)	25(2)	1(1)	5(1)	3(1)
C372	40(4)	44(3)	50(3)	3(2)	12(3)	−15(2)
C382	54(3)	46(2)	43(2)	3(2)	−5(2)	10(2)
As1'2	24(1)	21(2)	21(1)	−4(1)	−1(1)	5(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O3'2	20(5)	24(5)	31(6)	−1(4)	2(4)	2(4)
C36'2	29(8)	33(8)	16(8)	8(7)	4(5)	2(6)
C37'2	53(19)	76(19)	80(30)	10(18)	34(16)	−30(15)
C38'2	59(11)	34(10)	44(12)	5(9)	−18(10)	9(8)
Ga12	15(1)	19(1)	18(1)	0(1)	0(1)	1(1)
O12	20(1)	35(1)	29(1)	0(1)	3(1)	10(1)
O22	27(1)	43(1)	21(1)	−5(1)	1(1)	−6(1)
N12	21(1)	20(1)	19(1)	−1(1)	3(1)	−1(1)
N22	17(1)	20(1)	20(1)	−1(1)	0(1)	−1(1)
C12	25(1)	22(1)	20(1)	2(1)	6(1)	0(1)
C22	30(1)	27(1)	17(1)	2(1)	−1(1)	2(1)
C32	22(1)	26(1)	19(1)	−2(1)	−1(1)	3(1)
C42	46(2)	27(1)	29(1)	9(1)	0(1)	−4(1)
C52	38(2)	34(1)	26(1)	0(1)	−10(1)	−4(1)
C62	28(1)	21(1)	20(1)	1(1)	−1(1)	−2(1)
C72	26(1)	29(1)	40(2)	−2(1)	−2(1)	−5(1)
C82	36(2)	38(2)	57(2)	−8(1)	−11(1)	−8(1)
C92	57(2)	32(1)	46(2)	−14(1)	−15(2)	−5(1)
C102	50(2)	28(1)	34(2)	−10(1)	−2(1)	4(1)
C112	33(1)	20(1)	25(1)	−2(1)	2(1)	1(1)
C122	24(1)	42(2)	63(2)	−10(2)	4(1)	−6(1)
C132	50(2)	88(3)	54(2)	0(2)	10(2)	−1(2)
C142	31(2)	58(2)	78(3)	7(2)	3(2)	4(2)
C152	31(1)	29(1)	33(1)	−7(1)	8(1)	0(1)
C162	39(2)	61(2)	59(2)	17(2)	−4(2)	6(2)
C172	46(2)	60(2)	49(2)	14(2)	19(2)	12(2)
C182	21(1)	24(1)	24(1)	1(1)	−4(1)	−3(1)
C192	22(1)	31(1)	31(1)	2(1)	−2(1)	−4(1)
C202	24(1)	42(2)	40(2)	4(1)	1(1)	−11(1)
C212	36(2)	36(1)	47(2)	6(1)	−6(1)	−16(1)
C222	40(2)	25(1)	42(2)	1(1)	−10(1)	−9(1)
C232	31(1)	25(1)	27(1)	−1(1)	−5(1)	−1(1)
C242	28(1)	33(1)	43(2)	−1(1)	12(1)	−1(1)
C252	82(3)	67(3)	55(2)	10(2)	9(2)	39(2)
C262	34(2)	54(2)	46(2)	−9(1)	12(1)	−4(1)
C272	34(1)	25(1)	36(1)	−7(1)	0(1)	2(1)
C282	49(2)	45(2)	65(2)	6(2)	5(2)	17(2)
C292	58(2)	73(3)	38(2)	−14(2)	2(2)	2(2)
C302	23(2)	31(2)	30(2)	0(1)	4(1)	9(1)
C312	34(2)	56(3)	44(3)	−5(2)	−10(2)	21(2)
C322	41(2)	48(2)	35(2)	−1(2)	8(2)	22(2)
C30'2	23(5)	44(6)	30(5)	−4(4)	4(4)	9(5)
C31'2	34(7)	53(8)	59(9)	10(7)	8(6)	12(6)
C32'2	27(6)	80(10)	31(6)	0(6)	3(4)	15(6)
C332	41(2)	34(1)	24(1)	0(1)	−4(1)	0(1)
C342	85(3)	43(2)	34(2)	−9(1)	−7(2)	13(2)
C352	45(2)	69(2)	51(2)	−8(2)	−20(2)	4(2)

Table 4: Bond lengths [Å] for mw_129_3m.

As11–O21	1.791(2)
As11–O31	1.8058(19)
As11–Ga11	2.4364(12)
Ga11–O11	1.807(2)
Ga11–N21	1.9500(19)
Ga11–N11	1.9752(19)
O11–C301	1.423(3)
O21–C331	1.445(3)
O31–C361	1.442(3)
N11–C11	1.332(3)
N11–C61	1.449(3)
N21–C31	1.333(3)
N21–C181	1.448(3)
C11–C21	1.396(3)
C11–C41	1.508(3)
C21–C31	1.398(4)
C31–C51	1.509(3)
C61–C111	1.397(4)
C61–C71	1.406(4)
C71–C81	1.401(4)
C71–C121	1.511(4)
C81–C91	1.364(5)
C91–C101	1.380(5)
C101–C111	1.392(4)
C111–C151	1.511(4)
C121–C141	1.526(5)
C121–C131	1.532(5)
C151–C171	1.534(5)
C151–C161	1.540(5)
C181–C191	1.399(4)
C181–C231	1.406(4)
C191–C201	1.396(4)
C191–C241	1.517(4)
C201–C211	1.372(5)
C211–C221	1.379(5)
C221–C231	1.387(4)
C231–C271	1.514(4)
C241–C261	1.526(5)
C241–C251	1.531(4)
C271–C291	1.509(6)
C271–C281	1.530(7)
C301–C321	1.507(4)
C301–C311	1.521(4)
C331–C351	1.495(6)
C331–C341	1.495(5)
C361–C371	1.502(4)
C361–C381	1.503(4)
As12–O32	1.805(3)
As12–O22	1.810(2)
As12–Ga12	2.4172(12)
O32–C362	1.434(4)
C362–C382	1.495(6)
C362–C372	1.507(7)

Table 4: (continued)

As1'2–O22	1.738(3)
As1'2–O3'2	1.838(11)
As1'2–Ga12	2.579(3)
O3'2–C36'2	1.40(2)
C36'2–C38'2	1.497(17)
C36'2–C37'2	1.50(2)
Ga12–O12	1.808(2)
Ga12–N12	1.960(2)
Ga12–N22	1.961(2)
O12–C302	1.390(4)
O12–C30'2	1.416(11)
O22–C332	1.439(4)
N12–C12	1.326(3)
N12–C62	1.448(3)
N22–C32	1.336(3)
N22–C182	1.447(3)
C12–C22	1.398(4)
C12–C42	1.512(3)
C22–C32	1.393(4)
C32–C52	1.508(4)
C62–C72	1.401(4)
C62–C112	1.406(4)
C72–C82	1.393(4)
C72–C122	1.513(4)
C82–C92	1.376(5)
C92–C102	1.372(5)
C102–C112	1.394(4)
C112–C152	1.515(4)
C122–C132	1.532(6)
C122–C142	1.541(5)
C152–C172	1.523(4)
C152–C162	1.528(5)
C182–C192	1.405(4)
C182–C232	1.408(4)
C192–C202	1.394(4)
C192–C242	1.522(4)
C202–C212	1.373(5)
C212–C222	1.380(5)
C222–C232	1.391(4)
C232–C272	1.515(4)
C242–C252	1.517(5)
C242–C262	1.526(5)
C272–C292	1.531(5)
C272–C282	1.531(4)
C302–C312	1.507(6)
C302–C322	1.522(5)
C30'2–C31'2	1.481(14)
C30'2–C32'2	1.519(13)
C332–C342	1.497(5)
C332–C352	1.508(5)

Table 5: Bond angles [°] for mw_129_3m.

O21–As11–O31	101.23(10)
O21–As11–Ga11	91.13(6)
O31–As11–Ga11	90.16(6)
O11–Ga11–N21	103.68(9)
O11–Ga11–N11	109.36(9)
N21–Ga11–N11	95.66(8)
O11–Ga11–As11	119.30(7)
N21–Ga11–As11	115.20(6)
N11–Ga11–As11	110.91(6)
C301–O11–Ga11	125.12(17)
C331–O21–As11	117.58(18)
C361–O31–As11	117.75(16)
C11–N11–C61	120.21(19)
C11–N11–Ga11	119.66(15)
C61–N11–Ga11	120.12(14)
C31–N21–C181	119.10(19)
C31–N21–Ga11	119.21(16)
C181–N21–Ga11	121.68(15)
N11–C11–C21	123.2(2)
N11–C11–C41	120.7(2)
C21–C11–C41	116.1(2)
C11–C21–C31	128.6(2)
N21–C31–C21	123.7(2)
N21–C31–C51	119.5(2)
C21–C31–C51	116.8(2)
C111–C61–C71	121.3(2)
C111–C61–N11	119.5(2)
C71–C61–N11	119.2(2)
C81–C71–C61	117.3(3)
C81–C71–C121	120.4(3)
C61–C71–C121	122.2(2)
C91–C81–C71	122.1(3)
C81–C91–C101	119.7(3)
C91–C101–C111	121.1(3)
C101–C111–C61	118.5(3)
C101–C111–C151	118.8(3)
C61–C111–C151	122.7(2)
C71–C121–C141	112.1(3)
C71–C121–C131	112.4(3)
C141–C121–C131	109.5(3)
C111–C151–C171	111.6(3)
C111–C151–C161	110.9(3)
C171–C151–C161	109.0(3)
C191–C181–C231	120.9(2)
C191–C181–N21	120.6(2)
C231–C181–N21	118.5(2)
C201–C191–C181	118.1(3)
C201–C191–C241	119.0(2)
C181–C191–C241	122.9(2)
C211–C201–C191	121.6(3)
C201–C211–C221	119.5(3)
C211–C221–C231	121.5(3)
C221–C231–C181	118.4(3)

Table 5: (continued)

C221–C231–C271	119.2(3)
C181–C231–C271	122.4(2)
C191–C241–C261	110.2(3)
C191–C241–C251	111.5(3)
C261–C241–C251	110.4(3)
C291–C271–C231	112.2(3)
C291–C271–C281	109.0(3)
C231–C271–C281	110.8(4)
O11–C301–C321	112.4(2)
O11–C301–C311	107.3(2)
C321–C301–C311	110.8(2)
O21–C331–C351	107.2(3)
O21–C331–C341	108.8(3)
C351–C331–C341	112.7(3)
O31–C361–C371	110.1(2)
O31–C361–C381	106.6(2)
C371–C361–C381	112.4(2)
O32–As12–O22	101.70(12)
O32–As12–Ga12	89.71(9)
O22–As12–Ga12	93.27(7)
C362–O32–As12	118.0(2)
O32–C362–C382	108.8(3)
O32–C362–C372	107.6(5)
C382–C362–C372	113.6(5)
O22–As1'2–O3'2	100.7(4)
O22–As1'2–Ga12	89.65(14)
O3'2–As1'2–Ga12	106.2(4)
C36'2–O3'2–As1'2	122.6(11)
O3'2–C36'2–C38'2	112.8(15)
O3'2–C36'2–C37'2	115(3)
C38'2–C36'2–C37'2	102(4)
O12–Ga12–N12	104.81(9)
O12–Ga12–N22	105.11(9)
N12–Ga12–N22	96.19(8)
O12–Ga12–As12	121.67(7)
N12–Ga12–As12	113.71(7)
N22–Ga12–As12	112.04(7)
O12–Ga12–As1'2	128.27(10)
N12–Ga12–As1'2	101.80(15)
N22–Ga12–As1'2	115.15(9)
C302–O12–Ga12	127.3(2)
C30'2–O12–Ga12	125.5(4)
C332–O22–As1'2	109.8(2)
C332–O22–As12	117.61(19)
C12–N12–C62	119.6(2)
C12–N12–Ga12	119.53(16)
C62–N12–Ga12	120.90(15)
C32–N22–C182	118.87(19)
C32–N22–Ga12	119.30(16)
C182–N22–Ga12	121.83(15)
N12–C12–C22	123.9(2)
N12–C12–C42	120.4(2)
C22–C12–C42	115.8(2)

Table 5: (continued)

C32–C22–C12	128.7(2)
N22–C32–C22	123.7(2)
N22–C32–C52	119.9(2)
C22–C32–C52	116.4(2)
C72–C62–C112	121.0(2)
C72–C62–N12	120.2(2)
C112–C62–N12	118.7(2)
C82–C72–C62	118.1(3)
C82–C72–C122	119.6(3)
C62–C72–C122	122.2(2)
C92–C82–C72	121.4(3)
C102–C92–C82	120.0(3)
C92–C102–C112	121.2(3)
C102–C112–C62	118.3(3)
C102–C112–C152	119.1(2)
C62–C112–C152	122.6(2)
C72–C122–C132	111.1(3)
C72–C122–C142	111.1(3)
C132–C122–C142	108.5(3)
C112–C152–C172	111.9(3)
C112–C152–C162	111.3(3)
C172–C152–C162	109.4(3)
C192–C182–C232	120.9(2)
C192–C182–N22	118.5(2)
C232–C182–N22	120.6(2)
C202–C192–C182	118.0(3)
C202–C192–C242	119.6(3)
C182–C192–C242	122.4(2)
C212–C202–C192	121.8(3)
C202–C212–C222	119.5(3)
C212–C222–C232	121.5(3)
C222–C232–C182	118.2(3)
C222–C232–C272	118.8(2)
C182–C232–C272	123.1(2)
C252–C242–C192	111.8(3)
C252–C242–C262	109.7(3)
C192–C242–C262	111.6(3)
C232–C272–C292	112.7(3)
C232–C272–C282	110.2(3)
C292–C272–C282	109.2(3)
O12–C302–C312	112.9(3)
O12–C302–C322	108.2(3)
C312–C302–C322	110.8(3)
O12–C30'2–C31'2	119.5(11)
O12–C30'2–C32'2	104.8(8)
C31'2–C30'2–C32'2	111.8(10)
O22–C332–C342	110.8(3)
O22–C332–C352	106.8(3)
C342–C332–C352	112.6(3)

Crystal structure of mw_024_fillm

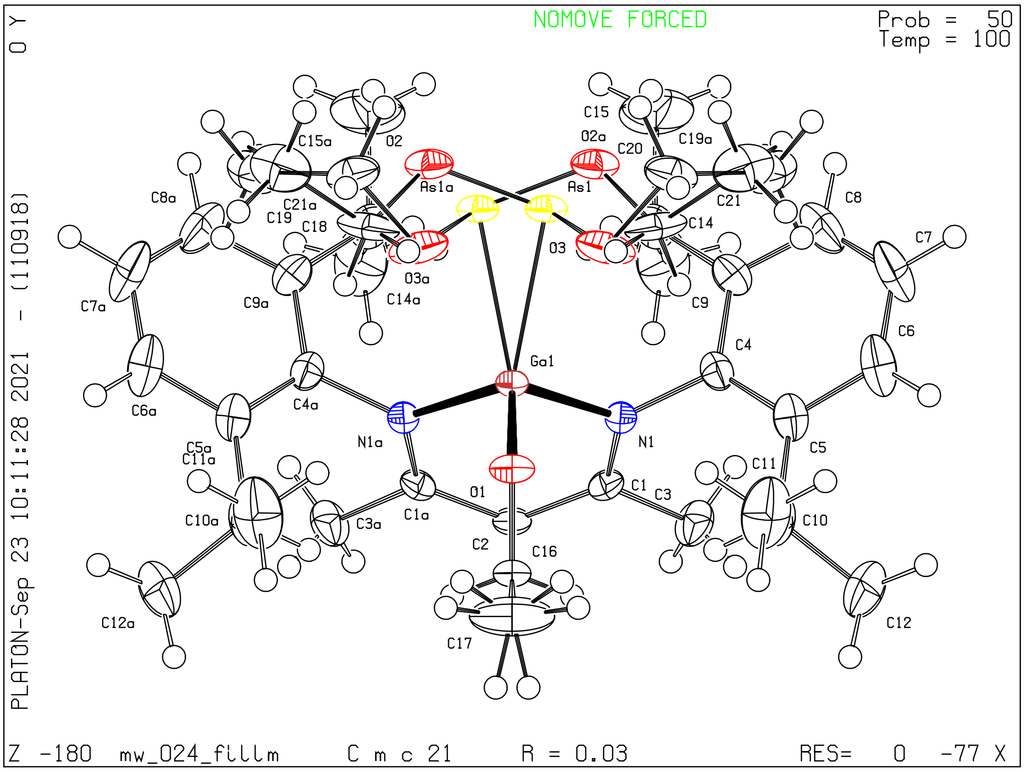

Table 1: Crystal data and structure refinement for mw_024_fillm.

Identification code	mw_024_fillm
Empirical Formula	$C_{35}H_{56}AsGaN_2O_3$
Formula weight	697.45 Da
Density (calculated)	$1.332\,g\cdot cm^{-3}$
$F(000)$	1472
Temperature	100(2) K
Crystal size	$0.330 \times 0.134 \times 0.070$ mm
Crystal appearance	colourless tablet
Wavelength (CuK_α)	1.54178 Å
Crystal system	Orthorhombic
Space group	$Cmc2_1$
Unit cell dimensions	$a = 22.1286(9)$ Å
	$b = 9.1624(4)$ Å
	$c = 17.1571(7)$ Å
	$\alpha = 90°$
	$\beta = 90°$
	$\gamma = 90°$
Unit cell volume	3478.6(3) $Å^3$
Z	4
Cell measurement refections used	9404
θ range for cell measurement	4.00° to 79.62°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	3.995° to 80.375°
Completeness to $\theta = 67.679°$ (to θ_{max})	100.0% (100.0%)
Index ranges	$-28 \leq h \leq 28$
	$-11 \leq k \leq 11$
	$-21 \leq l \leq 18$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$2.406\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.53
R_{merg} before/after correction	0.1446/0.0651
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	75266
Independent reflections	3805 ($R_{int} = 0.0415$)
Reflections with $I > 2\sigma(I)$	3767
Data / retraints / parameter	3805 / 5 / 237
Goodness-of-fit on F^2	1.063
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 2.9102P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0282$
	$wR2 = 0.0767$
R indices [all data]	$R1 = 0.0287$
	$wR2 = 0.0774$
Absolute structure parameter	0.004(11)
Largest diff. peak and hole	1.119 and -0.591 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

The $As(OEt)_2$ moiety is disordered over a mirror plane. Its corresponding bond lengths and angles were restrained to be equal (`SADI`). The local symmetry was ignored in its refinement (negative `PART`).

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_024_fillm. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
As(1)	4793(1)	6935(1)	6228(1)	23(1)
O(2)	5502(2)	7470(5)	6650(2)	30(1)
O(3)	4434(3)	8689(7)	6127(4)	42(2)
C(18)	5869(5)	8547(9)	6280(5)	39(2)
C(19)	6400(7)	8894(16)	6788(9)	52(3)
C(20)	4038(4)	9068(8)	6762(4)	40(2)
C(21)	3437(6)	8407(18)	6698(8)	52(3)
Ga(1)	5000	6796(1)	4814(1)	17(1)
O(1)	5000	8558(3)	4339(2)	25(1)
N(1)	4342(1)	5589(2)	4394(1)	20(1)
C(1)	4430(1)	4780(3)	3756(2)	21(1)
C(2)	5000	4513(4)	3433(2)	22(1)
C(3)	3896(1)	4070(4)	3363(2)	34(1)
C(4)	3760(1)	5638(3)	4771(2)	24(1)
C(5)	3313(1)	6622(3)	4518(2)	31(1)
C(6)	2780(2)	6716(4)	4945(3)	47(1)
C(7)	2687(2)	5856(6)	5596(3)	60(1)
C(8)	3121(2)	4880(6)	5826(3)	56(1)
C(9)	3669(2)	4741(4)	5434(2)	36(1)
C(10)	3392(1)	7596(4)	3813(2)	40(1)
C(11)	3463(2)	9190(4)	4062(4)	62(1)
C(12)	2865(2)	7446(6)	3239(3)	56(1)
C(13)	4137(2)	3647(5)	5690(3)	50(1)
C(14)	4087(2)	2220(5)	5244(4)	71(2)
C(15)	4126(4)	3367(9)	6577(4)	100(3)
C(16)	5000	8761(5)	3525(2)	25(1)
C(17)	5000	10384(7)	3376(4)	71(2)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_024_fillm.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
As(1)	33(1)	24(1)	13(1)	1(1)	1(1)	4(1)
O(2)	44(2)	30(2)	16(2)	−1(2)	−3(2)	−8(2)
O(3)	66(4)	35(3)	24(3)	8(2)	18(3)	20(3)
C(18)	74(6)	32(3)	13(4)	−2(3)	6(4)	−22(5)
C(19)	70(10)	45(7)	40(6)	−7(5)	4(6)	−21(6)
C(20)	53(5)	39(4)	26(4)	4(3)	12(3)	13(3)
C(21)	53(6)	73(10)	31(5)	−5(6)	−4(5)	34(6)
Ga(1)	20(1)	19(1)	13(1)	−1(1)	0	0
O(1)	38(2)	22(1)	16(1)	2(1)	0	0
N(1)	19(1)	23(1)	18(1)	−1(1)	0(1)	0(1)
C(1)	24(1)	22(1)	18(1)	−1(1)	−5(1)	−1(1)
C(2)	28(2)	25(2)	12(2)	−5(1)	0	0
C(3)	28(1)	38(2)	34(2)	−13(1)	−9(1)	−1(1)
C(4)	21(1)	27(1)	26(1)	−5(1)	3(1)	−4(1)
C(5)	23(1)	28(1)	42(2)	−4(1)	2(1)	−2(1)
C(6)	25(1)	44(2)	71(3)	−7(2)	11(2)	1(1)
C(7)	32(2)	78(3)	70(3)	2(2)	28(2)	−3(2)
C(8)	38(2)	74(3)	55(2)	17(2)	20(2)	−10(2)
C(9)	30(2)	44(2)	35(2)	8(1)	6(1)	−8(1)
C(10)	23(1)	39(2)	56(2)	10(2)	−5(1)	5(1)
C(11)	46(2)	31(2)	108(4)	14(2)	−9(2)	5(2)
C(12)	34(2)	68(3)	64(3)	9(2)	−12(2)	14(2)
C(13)	32(2)	63(2)	55(3)	41(2)	2(2)	−10(2)
C(14)	54(3)	48(2)	111(5)	31(3)	11(3)	17(2)
C(15)	105(5)	131(6)	64(4)	67(4)	−11(3)	−22(4)
C(16)	27(2)	34(2)	15(2)	6(2)	0	0
C(17)	138(7)	40(3)	35(3)	16(3)	0	0

Table 4: Bond lengths [Å] for mw_024_fillm.

As(1)–O(2)	1.796(4)
As(1)–O(3)	1.801(6)
As(1)–Ga(1)	2.4732(7)
O(2)–C(18)	1.427(8)
O(3)–C(20)	1.440(8)
C(18)–C(19)	1.497(16)
C(20)–C(21)	1.467(13)
Ga(1)–O(1)	1.808(3)
Ga(1)–N(1)#1	1.965(2)
Ga(1)–N(1)	1.966(2)
O(1)–C(16)	1.410(5)
N(1)–C(1)	1.335(3)
N(1)–C(4)	1.443(3)
C(1)–C(2)	1.399(3)
C(1)–C(3)	1.510(4)
C(4)–C(5)	1.407(4)
C(4)–C(9)	1.417(5)
C(5)–C(6)	1.390(5)
C(5)–C(10)	1.513(5)
C(6)–C(7)	1.382(7)
C(7)–C(8)	1.370(7)
C(8)–C(9)	1.394(5)
C(9)–C(13)	1.508(5)
C(10)–C(11)	1.530(6)
C(10)–C(12)	1.532(5)
C(13)–C(14)	1.519(8)
C(13)–C(15)	1.544(7)
C(16)–C(17)	1.509(7)

#1 -x+1,y,z

Table 5: Bond angles [°] for mw_024_fillm.

O(2)–As(1)–O(3)	100.4(3)
O(2)–As(1)–Ga(1)	104.36(13)
O(3)–As(1)–Ga(1)	91.90(19)
C(18)–O(2)–As(1)	120.4(5)
C(20)–O(3)–As(1)	114.3(5)
O(2)–C(18)–C(19)	109.6(9)
O(3)–C(20)–C(21)	113.4(8)
O(1)–Ga(1)–N(1)#1	109.74(9)
O(1)–Ga(1)–N(1)	109.74(9)
N(1)#1–Ga(1)–N(1)	95.61(13)
O(1)–Ga(1)–As(1)	113.31(9)
N(1)#1–Ga(1)–As(1)	121.71(7)
N(1)–Ga(1)–As(1)	104.57(7)
C(16)–O(1)–Ga(1)	124.3(3)
C(1)–N(1)–C(4)	121.1(2)
C(1)–N(1)–Ga(1)	120.24(18)
C(4)–N(1)–Ga(1)	118.64(18)
N(1)–C(1)–C(2)	123.7(3)
N(1)–C(1)–C(3)	119.4(2)
C(2)–C(1)–C(3)	117.0(3)
C(1)–C(2)–C(1)#1	128.6(3)
C(5)–C(4)–C(9)	121.3(3)
C(5)–C(4)–N(1)	120.6(3)
C(9)–C(4)–N(1)	118.0(3)
C(6)–C(5)–C(4)	118.2(3)
C(6)–C(5)–C(10)	118.9(3)
C(4)–C(5)–C(10)	122.9(3)
C(7)–C(6)–C(5)	121.2(4)
C(8)–C(7)–C(6)	120.0(3)
C(7)–C(8)–C(9)	122.0(4)
C(8)–C(9)–C(4)	117.3(3)
C(8)–C(9)–C(13)	121.2(3)
C(4)–C(9)–C(13)	121.5(3)
C(5)–C(10)–C(11)	110.6(4)
C(5)–C(10)–C(12)	111.9(3)
C(11)–C(10)–C(12)	110.1(3)
C(9)–C(13)–C(14)	112.0(3)
C(9)–C(13)–C(15)	112.8(5)
C(14)–C(13)–C(15)	110.6(5)
O(1)–C(16)–C(17)	107.3(4)

#1 -x+1,y,z

Crystal structure of mw_138m

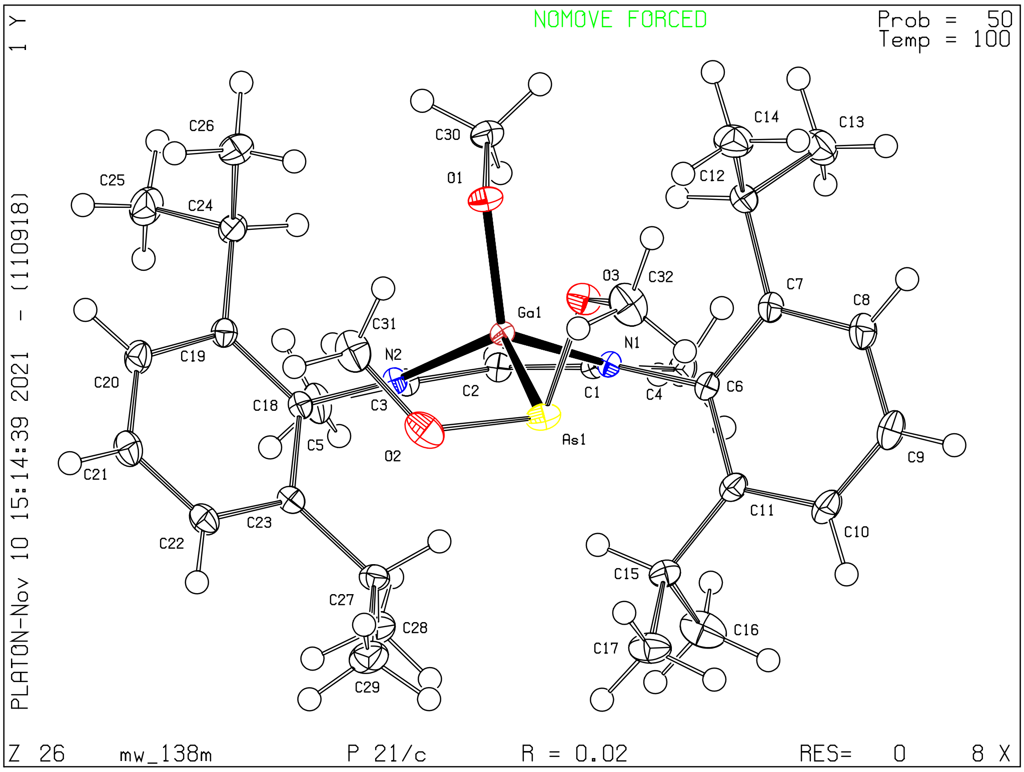

Table 1: Crystal data and structure refinement for mw_138m.

Identification code	mw_138m
Empirical Formula	$C_{32}\,H_{50}\,As\,Ga\,N_2\,O_3$
Formula weight	655.38 Da
Density (calculated)	$1.350\,g \cdot cm^{-3}$
$F(000)$	1376
Temperature	100(2) K
Crystal size	$0.35 \times 0.31 \times 0.20$ mm
Crystal appearance	colourless block
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 13.5685(12)$ Å
	$b = 12.1896(11)$ Å
	$c = 19.5758(16)$ Å
	$\alpha = 90°$
	$\beta = 95.013(4)°$
	$\gamma = 90°$
Unit cell volume	$3225.3(5)$ Å^3
Z	4
Cell measurement refections used	9758
θ range for cell measurement	2.54° to 33.51°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.970° to 34.127°
Completeness to $\theta = 25.242°$ (to θ_{max})	100.0% (97.2%)
Index ranges	$-21 \leq h \leq 21$
	$-19 \leq k \leq 19$
	$-30 \leq l \leq 30$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.904\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.59
R_{merg} before/after correction	0.0778/0.0412
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	268513
Independent reflections	12923 ($R_{int} = 0.0315$)
Reflections with $I > 2\sigma(I)$	11552
Data / retraints / parameter	12923 / 0 / 365
Goodness-of-fit on F^2	1.101
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0307P)^2 + 1.1929P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0218$
	$wR2 = 0.0584$
R indices [all data]	$R1 = 0.0279$
	$wR2 = 0.0620$
Largest diff. peak and hole	0.672 and -0.399 Å^{-3}

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_138m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
As(1)	2819(1)	2424(1)	2477(1)	16(1)
Ga(1)	1955(1)	3300(1)	1455(1)	10(1)
O(1)	1264(1)	4512(1)	1661(1)	17(1)
O(2)	1876(1)	1641(1)	2838(1)	23(1)
O(3)	2746(1)	3685(1)	2950(1)	18(1)
N(1)	2946(1)	3649(1)	824(1)	11(1)
N(2)	1107(1)	2471(1)	777(1)	11(1)
C(1)	2722(1)	3709(1)	148(1)	12(1)
C(2)	1830(1)	3320(1)	−178(1)	13(1)
C(3)	1117(1)	2664(1)	108(1)	12(1)
C(4)	3452(1)	4205(1)	−300(1)	17(1)
C(5)	344(1)	2143(1)	−387(1)	19(1)
C(6)	3946(1)	3828(1)	1117(1)	12(1)
C(7)	4218(1)	4854(1)	1401(1)	15(1)
C(8)	5181(1)	4981(1)	1708(1)	20(1)
C(9)	5854(1)	4124(1)	1732(1)	22(1)
C(10)	5572(1)	3115(1)	1454(1)	20(1)
C(11)	4616(1)	2938(1)	1145(1)	15(1)
C(12)	3511(1)	5819(1)	1373(1)	17(1)
C(13)	3913(1)	6786(1)	983(1)	24(1)
C(14)	3278(1)	6176(1)	2092(1)	25(1)
C(15)	4333(1)	1816(1)	849(1)	18(1)
C(16)	4817(1)	1593(1)	187(1)	28(1)
C(17)	4591(1)	883(1)	1355(1)	24(1)
C(18)	410(1)	1716(1)	1034(1)	12(1)
C(19)	−562(1)	2054(1)	1123(1)	14(1)
C(20)	−1174(1)	1327(1)	1441(1)	18(1)
C(21)	−840(1)	312(1)	1675(1)	20(1)
C(22)	123(1)	−9(1)	1579(1)	17(1)
C(23)	763(1)	675(1)	1256(1)	13(1)
C(24)	−959(1)	3184(1)	919(1)	16(1)
C(25)	−1893(1)	3110(1)	415(1)	26(1)
C(26)	−1176(1)	3844(1)	1554(1)	23(1)
C(27)	1820(1)	317(1)	1163(1)	15(1)
C(28)	1953(1)	6(1)	416(1)	22(1)
C(29)	2178(1)	−618(1)	1642(1)	26(1)
C(30)	929(1)	5284(1)	1158(1)	20(1)
C(31)	905(1)	2090(1)	2828(1)	24(1)
C(32)	3259(1)	3686(1)	3617(1)	26(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_138m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
As(1)	19(1)	17(1)	11(1)	1(1)	0(1)	6(1)
Ga(1)	10(1)	11(1)	8(1)	0(1)	1(1)	1(1)
O(1)	19(1)	16(1)	16(1)	−2(1)	3(1)	6(1)
O(2)	34(1)	18(1)	18(1)	5(1)	1(1)	−3(1)
O(3)	22(1)	18(1)	12(1)	−2(1)	−3(1)	1(1)
N(1)	10(1)	13(1)	11(1)	0(1)	1(1)	0(1)
N(2)	12(1)	12(1)	9(1)	0(1)	1(1)	−1(1)
C(1)	12(1)	12(1)	11(1)	2(1)	3(1)	2(1)
C(2)	14(1)	15(1)	10(1)	2(1)	1(1)	0(1)
C(3)	13(1)	13(1)	9(1)	0(1)	0(1)	−1(1)
C(4)	15(1)	21(1)	15(1)	5(1)	5(1)	−1(1)
C(5)	21(1)	25(1)	11(1)	0(1)	−2(1)	−8(1)
C(6)	10(1)	16(1)	12(1)	1(1)	1(1)	0(1)
C(7)	12(1)	17(1)	15(1)	−1(1)	1(1)	−2(1)
C(8)	15(1)	24(1)	20(1)	−2(1)	−1(1)	−4(1)
C(9)	12(1)	30(1)	22(1)	1(1)	−3(1)	−1(1)
C(10)	12(1)	25(1)	21(1)	4(1)	0(1)	3(1)
C(11)	12(1)	17(1)	16(1)	2(1)	1(1)	2(1)
C(12)	16(1)	14(1)	21(1)	−2(1)	0(1)	−1(1)
C(13)	26(1)	19(1)	29(1)	3(1)	1(1)	−3(1)
C(14)	29(1)	22(1)	25(1)	−5(1)	5(1)	2(1)
C(15)	16(1)	16(1)	22(1)	2(1)	0(1)	3(1)
C(16)	43(1)	23(1)	19(1)	−1(1)	4(1)	1(1)
C(17)	32(1)	19(1)	23(1)	4(1)	6(1)	6(1)
C(18)	13(1)	13(1)	10(1)	0(1)	2(1)	−2(1)
C(19)	13(1)	15(1)	13(1)	0(1)	2(1)	−1(1)
C(20)	15(1)	21(1)	19(1)	2(1)	5(1)	−2(1)
C(21)	20(1)	20(1)	20(1)	3(1)	6(1)	−5(1)
C(22)	20(1)	14(1)	17(1)	2(1)	3(1)	−3(1)
C(23)	16(1)	12(1)	12(1)	0(1)	2(1)	−1(1)
C(24)	14(1)	17(1)	19(1)	2(1)	2(1)	1(1)
C(25)	18(1)	28(1)	30(1)	5(1)	−4(1)	2(1)
C(26)	21(1)	22(1)	28(1)	−4(1)	8(1)	3(1)
C(27)	17(1)	12(1)	17(1)	1(1)	3(1)	1(1)
C(28)	22(1)	23(1)	21(1)	−5(1)	6(1)	2(1)
C(29)	25(1)	21(1)	32(1)	10(1)	5(1)	7(1)
C(30)	18(1)	16(1)	26(1)	2(1)	2(1)	4(1)
C(31)	30(1)	29(1)	16(1)	−2(1)	8(1)	−7(1)
C(32)	31(1)	29(1)	15(1)	−1(1)	−6(1)	−5(1)

Table 4: Bond lengths [Å] for mw_138m.

As(1)–O(2)	1.7897(8)
As(1)–O(3)	1.8022(7)
As(1)–Ga(1)	2.4713(2)
Ga(1)–O(1)	1.8146(7)
Ga(1)–N(1)	1.9499(7)
Ga(1)–N(2)	1.9598(7)
O(1)–C(30)	1.4078(12)
O(2)–C(31)	1.4253(15)
O(3)–C(32)	1.4252(12)
N(1)–C(1)	1.3355(11)
N(1)–C(6)	1.4424(11)
N(2)–C(3)	1.3309(11)
N(2)–C(18)	1.4412(11)
C(1)–C(2)	1.4004(12)
C(1)–C(4)	1.5054(12)
C(2)–C(3)	1.4078(12)
C(3)–C(5)	1.5061(13)
C(6)–C(7)	1.4050(13)
C(6)–C(11)	1.4133(13)
C(7)–C(8)	1.3987(13)
C(7)–C(12)	1.5155(13)
C(8)–C(9)	1.3862(15)
C(9)–C(10)	1.3850(16)
C(10)–C(11)	1.3989(13)
C(11)–C(15)	1.5217(14)
C(12)–C(13)	1.5303(15)
C(12)–C(14)	1.5328(15)
C(15)–C(16)	1.5277(16)
C(15)–C(17)	1.5287(14)
C(18)–C(19)	1.4073(12)
C(18)–C(23)	1.4116(12)
C(19)–C(20)	1.3986(13)
C(19)–C(24)	1.5195(13)
C(20)–C(21)	1.3819(15)
C(21)–C(22)	1.3913(14)
C(22)–C(23)	1.3935(12)
C(23)–C(27)	1.5250(13)
C(24)–C(26)	1.5317(15)
C(24)–C(25)	1.5387(15)
C(27)–C(29)	1.5282(14)
C(27)–C(28)	1.5360(14)

Table 5: Bond angles [°] for mw_138m.

O(2)–As(1)–O(3)	100.26(4)
O(2)–As(1)–Ga(1)	104.19(3)
O(3)–As(1)–Ga(1)	90.23(2)
O(1)–Ga(1)–N(1)	111.21(3)
O(1)–Ga(1)–N(2)	106.62(3)
N(1)–Ga(1)–N(2)	94.62(3)
O(1)–Ga(1)–As(1)	112.97(2)
N(1)–Ga(1)–As(1)	107.57(2)
N(2)–Ga(1)–As(1)	122.28(2)
C(30)–O(1)–Ga(1)	122.04(6)
C(31)–O(2)–As(1)	118.81(7)
C(32)–O(3)–As(1)	115.31(7)
C(1)–N(1)–C(6)	120.66(7)
C(1)–N(1)–Ga(1)	122.02(6)
C(6)–N(1)–Ga(1)	117.32(5)
C(3)–N(2)–C(18)	121.30(7)
C(3)–N(2)–Ga(1)	121.24(6)
C(18)–N(2)–Ga(1)	117.23(6)
N(1)–C(1)–C(2)	123.03(8)
N(1)–C(1)–C(4)	119.67(8)
C(2)–C(1)–C(4)	117.29(8)
C(1)–C(2)–C(3)	127.46(8)
N(2)–C(3)–C(2)	123.91(8)
N(2)–C(3)–C(5)	119.50(8)
C(2)–C(3)–C(5)	116.57(8)
C(7)–C(6)–C(11)	121.49(8)
C(7)–C(6)–N(1)	119.83(8)
C(11)–C(6)–N(1)	118.58(8)
C(8)–C(7)–C(6)	118.18(9)
C(8)–C(7)–C(12)	119.60(8)
C(6)–C(7)–C(12)	122.22(8)
C(9)–C(8)–C(7)	121.21(9)
C(10)–C(9)–C(8)	119.88(9)
C(9)–C(10)–C(11)	121.37(9)
C(10)–C(11)–C(6)	117.85(9)
C(10)–C(11)–C(15)	119.80(8)
C(6)–C(11)–C(15)	122.35(8)
C(7)–C(12)–C(13)	111.28(8)
C(7)–C(12)–C(14)	111.66(8)
C(13)–C(12)–C(14)	110.53(9)
C(11)–C(15)–C(16)	111.75(9)
C(11)–C(15)–C(17)	112.64(9)
C(16)–C(15)–C(17)	109.05(9)
C(19)–C(18)–C(23)	121.42(8)
C(19)–C(18)–N(2)	120.42(8)
C(23)–C(18)–N(2)	117.84(8)
C(20)–C(19)–C(18)	117.95(8)
C(20)–C(19)–C(24)	118.75(8)
C(18)–C(19)–C(24)	123.24(8)
C(21)–C(20)–C(19)	121.65(9)
C(20)–C(21)–C(22)	119.44(9)
C(21)–C(22)–C(23)	121.51(9)
C(22)–C(23)–C(18)	118.01(8)

Table 5: (continued)

C(22)–C(23)–C(27)	120.86(8)
C(18)–C(23)–C(27)	121.11(8)
C(19)–C(24)–C(26)	110.59(8)
C(19)–C(24)–C(25)	111.65(8)
C(26)–C(24)–C(25)	110.18(9)
C(23)–C(27)–C(29)	113.07(8)
C(23)–C(27)–C(28)	111.99(8)
C(29)–C(27)–C(28)	110.00(8)

Crystal structure of mw_141_4m

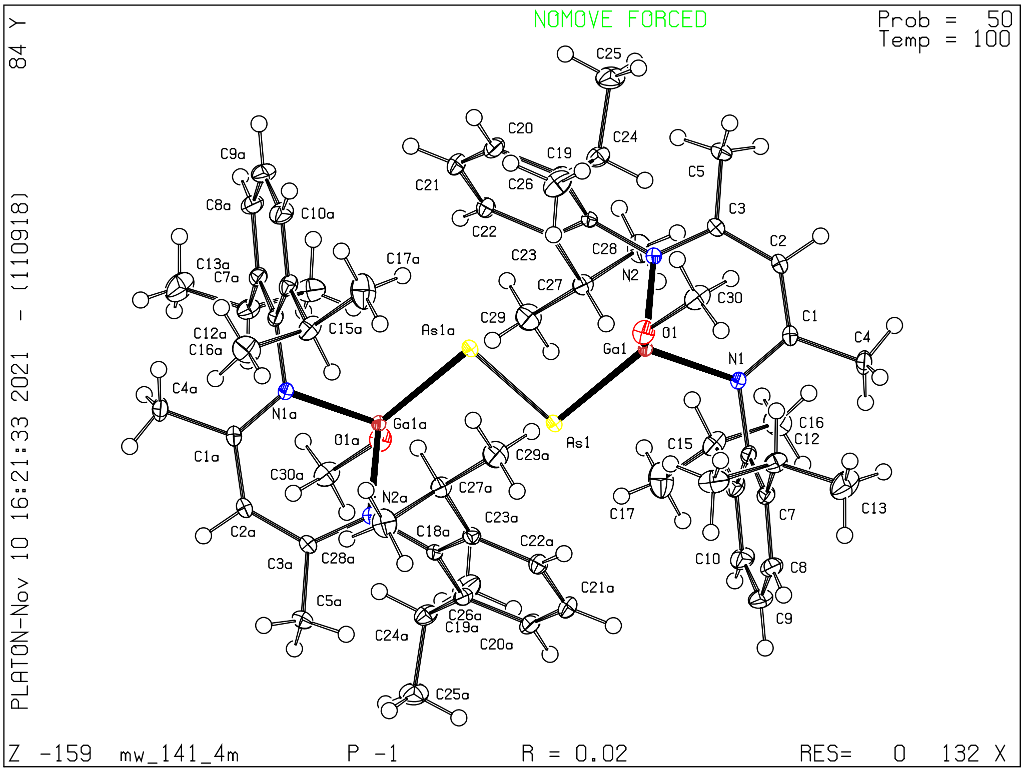

Table 1: Crystal data and structure refinement for mw_141_4m.

Identification code	mw_141_4m
Empirical Formula	$C_{60}\,H_{88}\,As_2\,Ga_2\,N_4\,O_2$
Formula weight	1186.62 Da
Density (calculated)	$1.365\,g \cdot cm^{-3}$
$F(000)$	620
Temperature	100(2) K
Crystal size	0.275 × 0.187 × 0.122 mm
Crystal appearance	pale green tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 10.4846(8)$ Å
	$b = 11.9639(8)$ Å
	$c = 13.0692(8)$ Å
	$\alpha = 91.924(2)°$
	$\beta = 109.372(2)°$
	$\gamma = 108.984(2)°$
Unit cell volume	1443.91(16) $Å^3$
Z	1
Cell measurement refections used	9251
θ range for cell measurement	2.23° to 33.53°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	2.204° to 33.552°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.4%)
Index ranges	$-16 \le h \le 16$
	$-18 \le k \le 18$
	$-20 \le l \le 20$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$2.114\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.63
R_{merg} before/after correction	0.0642/0.0379
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	127387
Independent reflections	11320 ($R_{int} = 0.0265$)
Reflections with $I > 2\sigma(I)$	10065
Data / retraints / parameter	11320 / 0 / 327
Goodness-of-fit on F^2	1.054
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0292P)^2 + 0.3698P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0191$
	$wR2 = 0.0521$
R indices [all data]	$R1 = 0.0237$
	$wR2 = 0.0538$
Largest diff. peak and hole	0.555 and -0.255 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_141_4m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
As(1)	4114(1)	4085(1)	9709(1)	13(1)
Ga(1)	4000(1)	4128(1)	7846(1)	10(1)
O(1)	5669(1)	4221(1)	7648(1)	17(1)
N(1)	2379(1)	2785(1)	6820(1)	11(1)
N(2)	3389(1)	5380(1)	7108(1)	10(1)
C(1)	1711(1)	2894(1)	5785(1)	12(1)
C(2)	1891(1)	4002(1)	5417(1)	14(1)
C(3)	2582(1)	5160(1)	6044(1)	12(1)
C(4)	714(1)	1784(1)	4960(1)	18(1)
C(5)	2360(1)	6175(1)	5443(1)	18(1)
C(6)	1949(1)	1669(1)	7224(1)	12(1)
C(7)	2649(1)	850(1)	7208(1)	13(1)
C(8)	2249(1)	−190(1)	7663(1)	18(1)
C(9)	1194(1)	−414(1)	8121(1)	21(1)
C(10)	523(1)	410(1)	8144(1)	20(1)
C(11)	889(1)	1466(1)	7708(1)	15(1)
C(12)	3856(1)	1085(1)	6758(1)	17(1)
C(13)	3590(2)	31(1)	5922(1)	31(1)
C(14)	5314(1)	1381(1)	7703(1)	25(1)
C(15)	163(1)	2367(1)	7763(1)	19(1)
C(16)	−1244(1)	2085(1)	6777(1)	26(1)
C(17)	−127(1)	2476(1)	8826(1)	32(1)
C(18)	3985(1)	6558(1)	7751(1)	11(1)
C(19)	5303(1)	7382(1)	7768(1)	13(1)
C(20)	5938(1)	8450(1)	8512(1)	18(1)
C(21)	5300(1)	8696(1)	9221(1)	19(1)
C(22)	3986(1)	7879(1)	9184(1)	16(1)
C(23)	3304(1)	6804(1)	8456(1)	12(1)
C(24)	6086(1)	7150(1)	7039(1)	17(1)
C(25)	6271(1)	8103(1)	6290(1)	26(1)
C(26)	7559(1)	7093(1)	7732(1)	24(1)
C(27)	1889(1)	5904(1)	8445(1)	15(1)
C(28)	603(1)	5895(1)	7445(1)	23(1)
C(29)	1590(1)	6084(1)	9494(1)	25(1)
C(30)	5776(1)	4100(1)	6609(1)	21(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_141_4m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
As(1)	15(1)	12(1)	9(1)	2(1)	2(1)	2(1)
Ga(1)	10(1)	9(1)	9(1)	0(1)	2(1)	3(1)
O(1)	12(1)	20(1)	20(1)	1(1)	6(1)	6(1)
N(1)	11(1)	10(1)	10(1)	0(1)	3(1)	2(1)
N(2)	11(1)	10(1)	9(1)	1(1)	3(1)	4(1)
C(1)	11(1)	14(1)	10(1)	−1(1)	3(1)	3(1)
C(2)	15(1)	15(1)	9(1)	1(1)	2(1)	5(1)
C(3)	12(1)	14(1)	10(1)	3(1)	4(1)	5(1)
C(4)	18(1)	17(1)	13(1)	−4(1)	2(1)	1(1)
C(5)	23(1)	17(1)	14(1)	6(1)	4(1)	8(1)
C(6)	12(1)	10(1)	11(1)	−1(1)	3(1)	2(1)
C(7)	13(1)	12(1)	14(1)	1(1)	4(1)	3(1)
C(8)	17(1)	12(1)	21(1)	4(1)	5(1)	4(1)
C(9)	21(1)	15(1)	24(1)	6(1)	9(1)	2(1)
C(10)	19(1)	17(1)	24(1)	3(1)	12(1)	1(1)
C(11)	13(1)	14(1)	17(1)	−1(1)	7(1)	1(1)
C(12)	17(1)	14(1)	22(1)	3(1)	10(1)	7(1)
C(13)	40(1)	22(1)	39(1)	−2(1)	25(1)	10(1)
C(14)	16(1)	25(1)	36(1)	12(1)	8(1)	8(1)
C(15)	18(1)	16(1)	26(1)	−1(1)	14(1)	3(1)
C(16)	28(1)	30(1)	27(1)	6(1)	12(1)	17(1)
C(17)	30(1)	42(1)	26(1)	−6(1)	15(1)	13(1)
C(18)	13(1)	10(1)	10(1)	2(1)	3(1)	5(1)
C(19)	14(1)	11(1)	15(1)	3(1)	5(1)	4(1)
C(20)	18(1)	11(1)	21(1)	1(1)	6(1)	2(1)
C(21)	23(1)	12(1)	17(1)	−2(1)	5(1)	5(1)
C(22)	22(1)	14(1)	14(1)	1(1)	6(1)	8(1)
C(23)	15(1)	12(1)	12(1)	2(1)	5(1)	6(1)
C(24)	16(1)	15(1)	22(1)	3(1)	11(1)	4(1)
C(25)	31(1)	24(1)	30(1)	10(1)	20(1)	7(1)
C(26)	15(1)	20(1)	37(1)	2(1)	11(1)	5(1)
C(27)	16(1)	15(1)	16(1)	2(1)	8(1)	6(1)
C(28)	14(1)	30(1)	24(1)	2(1)	6(1)	9(1)
C(29)	29(1)	27(1)	24(1)	3(1)	18(1)	7(1)
C(30)	21(1)	19(1)	28(1)	2(1)	15(1)	7(1)

Table 4: Bond lengths [Å] for mw_141_4m.

As(1)–As(1)#1	2.2646(2)
As(1)–Ga(1)	2.40030(19)
Ga(1)–O(1)	1.8212(7)
Ga(1)–N(1)	1.9588(7)
Ga(1)–N(2)	1.9745(7)
O(1)–C(30)	1.4058(12)
N(1)–C(1)	1.3339(10)
N(1)–C(6)	1.4408(11)
N(2)–C(3)	1.3299(10)
N(2)–C(18)	1.4427(10)
C(1)–C(2)	1.4018(12)
C(1)–C(4)	1.5071(12)
C(2)–C(3)	1.4110(12)
C(3)–C(5)	1.5079(12)
C(6)–C(7)	1.4050(12)
C(6)–C(11)	1.4128(12)
C(7)–C(8)	1.3981(12)
C(7)–C(12)	1.5170(12)
C(8)–C(9)	1.3825(14)
C(9)–C(10)	1.3902(15)
C(10)–C(11)	1.3949(13)
C(11)–C(15)	1.5202(13)
C(12)–C(13)	1.5289(14)
C(12)–C(14)	1.5341(14)
C(15)–C(17)	1.5276(15)
C(15)–C(16)	1.5281(15)
C(18)–C(19)	1.4050(12)
C(18)–C(23)	1.4148(11)
C(19)–C(20)	1.3982(12)
C(19)–C(24)	1.5189(13)
C(20)–C(21)	1.3836(14)
C(21)–C(22)	1.3894(14)
C(22)–C(23)	1.3927(12)
C(23)–C(27)	1.5184(12)
C(24)–C(26)	1.5340(14)
C(24)–C(25)	1.5347(14)
C(27)–C(29)	1.5278(13)
C(27)–C(28)	1.5319(14)

#1 -x+1,-y+1,-z+2

Table 5: Bond angles [°] for mw_141_4m.

As(1)#1–As(1)–Ga(1)	92.121(6)
O(1)–Ga(1)–N(1)	109.77(3)
O(1)–Ga(1)–N(2)	106.35(3)
N(1)–Ga(1)–N(2)	95.10(3)
O(1)–Ga(1)–As(1)	114.54(2)
N(1)–Ga(1)–As(1)	112.47(2)
N(2)–Ga(1)–As(1)	116.82(2)
C(30)–O(1)–Ga(1)	123.48(6)
C(1)–N(1)–C(6)	121.36(7)
C(1)–N(1)–Ga(1)	121.34(6)
C(6)–N(1)–Ga(1)	117.30(5)
C(3)–N(2)–C(18)	122.48(7)
C(3)–N(2)–Ga(1)	120.71(6)
C(18)–N(2)–Ga(1)	116.49(5)
N(1)–C(1)–C(2)	123.09(7)
N(1)–C(1)–C(4)	119.31(8)
C(2)–C(1)–C(4)	117.59(7)
C(1)–C(2)–C(3)	128.51(8)
N(2)–C(3)–C(2)	123.59(8)
N(2)–C(3)–C(5)	120.08(7)
C(2)–C(3)–C(5)	116.33(7)
C(7)–C(6)–C(11)	121.17(8)
C(7)–C(6)–N(1)	120.45(7)
C(11)–C(6)–N(1)	118.21(7)
C(8)–C(7)–C(6)	118.46(8)
C(8)–C(7)–C(12)	119.32(8)
C(6)–C(7)–C(12)	122.17(8)
C(9)–C(8)–C(7)	121.12(9)
C(8)–C(9)–C(10)	119.87(9)
C(9)–C(10)–C(11)	121.26(9)
C(10)–C(11)–C(6)	118.11(8)
C(10)–C(11)–C(15)	120.35(8)
C(6)–C(11)–C(15)	121.54(8)
C(7)–C(12)–C(13)	112.07(8)
C(7)–C(12)–C(14)	110.04(8)
C(13)–C(12)–C(14)	110.71(9)
C(11)–C(15)–C(17)	113.26(9)
C(11)–C(15)–C(16)	111.66(8)
C(17)–C(15)–C(16)	109.67(8)
C(19)–C(18)–C(23)	121.13(7)
C(19)–C(18)–N(2)	120.20(7)
C(23)–C(18)–N(2)	118.25(7)
C(20)–C(19)–C(18)	118.24(8)
C(20)–C(19)–C(24)	118.72(8)
C(18)–C(19)–C(24)	123.01(8)
C(21)–C(20)–C(19)	121.41(8)
C(20)–C(21)–C(22)	119.66(8)
C(21)–C(22)–C(23)	121.32(8)
C(22)–C(23)–C(18)	118.22(8)
C(22)–C(23)–C(27)	120.80(8)
C(18)–C(23)–C(27)	120.96(7)
C(19)–C(24)–C(26)	110.89(8)
C(19)–C(24)–C(25)	111.19(8)

Table 5: (continued)

C(26)–C(24)–C(25)	110.56(8)
C(23)–C(27)–C(29)	113.63(8)
C(23)–C(27)–C(28)	111.61(8)
C(29)–C(27)–C(28)	109.73(8)

#1 -x+1,-y+1,-z+2

Crystal structure of mw_017m

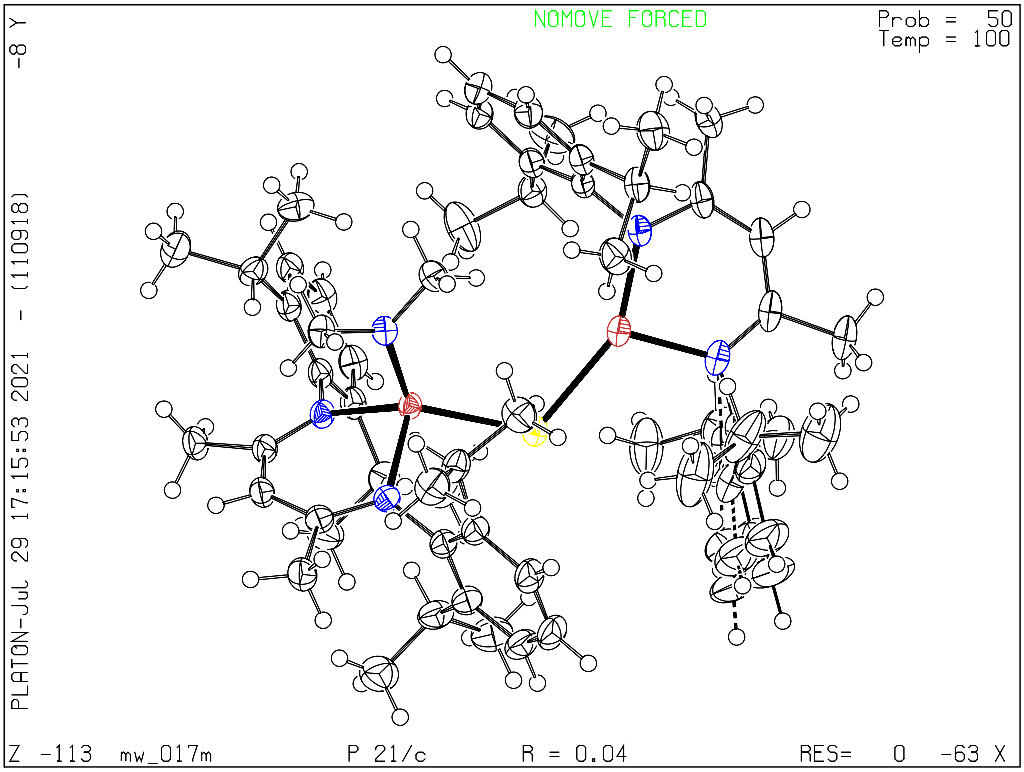

Table 1: Crystal data and structure refinement for mw_017m.

Identification code	mw_017m
Empirical Formula	$C_{60}H_{88}Ga_2N_5Sb$
Formula weight	1140.54 Da
Density (calculated)	$1.276\,g\cdot cm^{-3}$
$F(000)$	2384
Temperature	100(2) K
Crystal size	0.200 × 0.157 × 0.060 mm
Crystal appearance	orange tablet
Wavelength (CuK_α)	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 13.1548(12)$ Å
	$b = 17.1106(15)$ Å
	$c = 26.409(2)$ Å
	$\alpha = 90°$
	$\beta = 93.231(4)°$
	$\gamma = 90°$
Unit cell volume	$5934.8(9)\,Å^3$
Z	4
Cell measurement refections used	9609
θ range for cell measurement	3.08° to 79.15°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	3.079° to 79.610°
Completeness to $\theta = 67.679°$ (to θ_{max})	100.0% (99.5%)
Index ranges	$-16 \leq h \leq 16$
	$-21 \leq k \leq 21$
	$-25 \leq l \leq 33$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$4.933\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.54
R_{merg} before/after correction	0.1172/0.0803
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	186706
Independent reflections	12848 ($R_{int} = 0.0949$)
Reflections with $I > 2\sigma(I)$	10386
Data / retraints / parameter	12848 / 252 / 678
Goodness-of-fit on F^2	1.040
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 5.1505P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0379$
	$wR2 = 0.0922$
R indices [all data]	$R1 = 0.0532$
	$wR2 = 0.1040$
Largest diff. peak and hole	1.333 and $-0.852\,Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

A phenyl ring is disorderd over two positions. `RIGU` and `SIMU` restraints were applied to the anisotropic displacement parameters of the corresponding atoms. Due to their close proximity C47 and C47' as well as C48 and C48' were refined with common displacement parameters (`EADP`).

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_017m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	2350(1)	1942(1)	1081(1)	33(1)
Ga(1)	3226(1)	3075(1)	622(1)	23(1)
Ga(2)	3250(1)	1507(1)	1871(1)	28(1)
N(1)	3652(2)	2919(1)	−99(1)	26(1)
N(2)	2033(2)	3729(2)	375(1)	28(1)
N(3)	4461(2)	1447(1)	2324(1)	28(1)
N(4)	2440(2)	793(2)	2271(1)	32(1)
N(5)	4257(2)	3727(1)	892(1)	28(1)
C(1)	3445(2)	3448(2)	−456(1)	28(1)
C(2)	2784(2)	4082(2)	−403(1)	32(1)
C(3)	2082(2)	4191(2)	−32(1)	31(1)
C(4)	3929(3)	3399(2)	−962(1)	36(1)
C(5)	1345(3)	4864(2)	−110(1)	40(1)
C(6)	4304(2)	2264(2)	−200(1)	27(1)
C(7)	5365(2)	2354(2)	−188(1)	29(1)
C(8)	5961(2)	1698(2)	−277(1)	33(1)
C(9)	5518(3)	972(2)	−372(1)	35(1)
C(10)	4476(3)	895(2)	−381(1)	34(1)
C(11)	3843(2)	1528(2)	−299(1)	31(1)
C(12)	5900(2)	3130(2)	−81(1)	32(1)
C(13)	6607(3)	3359(2)	−504(1)	42(1)
C(14)	6506(2)	3111(2)	430(1)	40(1)
C(15)	2691(2)	1434(2)	−344(1)	34(1)
C(16)	2255(3)	1669(2)	−873(1)	46(1)
C(17)	2331(3)	610(2)	−216(1)	46(1)
C(18)	1109(2)	3735(2)	647(1)	31(1)
C(19)	1027(2)	4200(2)	1080(1)	33(1)
C(20)	114(3)	4185(2)	1325(1)	39(1)
C(21)	−688(3)	3722(2)	1157(1)	43(1)
C(22)	−589(2)	3247(2)	736(1)	40(1)
C(23)	306(2)	3242(2)	477(1)	35(1)
C(24)	1907(2)	4688(2)	1304(1)	34(1)
C(25)	1633(3)	5557(2)	1354(1)	46(1)
C(26)	2264(3)	4367(2)	1823(1)	44(1)
C(27)	385(2)	2701(2)	21(1)	40(1)
C(28)	−120(3)	3068(3)	−460(1)	54(1)
C(29)	−67(3)	1896(2)	104(2)	51(1)
C(30)	4587(3)	937(2)	2708(1)	32(1)
C(31)	3823(3)	445(2)	2863(1)	36(1)
C(32)	2810(3)	400(2)	2676(1)	36(1)
C(33)	5608(3)	894(2)	2997(1)	38(1)
C(34)	2112(3)	−114(2)	2965(1)	46(1)
C(35)	5329(2)	1921(2)	2213(1)	26(1)
C(36)	5943(2)	1682(2)	1826(1)	30(1)
C(37)	6818(2)	2120(2)	1743(1)	34(1)
C(38)	7058(3)	2774(2)	2033(1)	37(1)
C(39)	6419(3)	3016(2)	2405(1)	35(1)
C(40)	5545(2)	2597(2)	2505(1)	30(1)
C(41)	5684(2)	966(2)	1503(1)	33(1)
C(42)	6422(4)	297(2)	1604(2)	56(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(43)	5587(4)	1173(2)	944(1)	58(1)
C(44)	4854(3)	2851(2)	2917(1)	33(1)
C(45)	5399(3)	3292(2)	3351(1)	46(1)
C(46)	3958(3)	3340(2)	2692(1)	42(1)
C(47)	1415(7)	722(6)	2157(4)	31(1)
C(48)	1029(9)	113(7)	1840(4)	40(2)
C(49)	3(7)	61(7)	1719(4)	62(2)
C(50)	−656(6)	606(7)	1908(5)	79(3)
C(51)	−287(6)	1214(6)	2201(5)	66(2)
C(52)	738(7)	1294(7)	2335(4)	45(2)
C(47')	1312(17)	731(13)	2016(6)	31(1)
C(48')	1080(20)	96(15)	1701(7)	40(2)
C(49')	33(12)	125(11)	1498(8)	55(3)
C(50')	−647(11)	702(11)	1626(10)	69(4)
C(51')	−362(13)	1269(12)	1937(10)	67(4)
C(52')	641(16)	1324(13)	2155(8)	46(3)
C(53)	1748(3)	−523(2)	1615(1)	47(1)
C(54)	1385(4)	−1349(3)	1741(2)	59(1)
C(55)	1883(5)	−468(3)	1047(2)	72(2)
C(56)	1052(4)	1975(2)	2615(2)	69(1)
C(57)	716(5)	2766(3)	2391(2)	88(2)
C(58)	676(5)	1898(3)	3152(2)	84(2)
C(59)	4495(2)	4482(2)	676(1)	32(1)
C(60)	4704(2)	3647(2)	1397(1)	32(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_017m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	33(1)	34(1)	32(1)	8(1)	2(1)	−7(1)
Ga(1)	24(1)	25(1)	22(1)	1(1)	6(1)	2(1)
Ga(2)	31(1)	27(1)	26(1)	2(1)	8(1)	−1(1)
N(1)	27(1)	29(1)	23(1)	0(1)	6(1)	2(1)
N(2)	24(1)	34(1)	27(1)	3(1)	5(1)	4(1)
N(3)	34(1)	27(1)	22(1)	2(1)	6(1)	1(1)
N(4)	37(1)	29(1)	33(1)	2(1)	14(1)	−3(1)
N(5)	30(1)	27(1)	26(1)	2(1)	3(1)	−1(1)
C(1)	29(1)	34(1)	23(1)	2(1)	6(1)	3(1)
C(2)	32(1)	37(2)	26(1)	8(1)	7(1)	7(1)
C(3)	27(1)	35(2)	31(1)	3(1)	5(1)	8(1)
C(4)	40(2)	44(2)	25(1)	6(1)	10(1)	9(1)
C(5)	38(2)	42(2)	40(1)	12(1)	10(1)	14(1)
C(6)	32(1)	30(1)	20(1)	0(1)	7(1)	5(1)
C(7)	34(1)	31(1)	23(1)	3(1)	7(1)	5(1)
C(8)	33(1)	40(2)	27(1)	3(1)	8(1)	7(1)
C(9)	45(2)	32(2)	28(1)	−1(1)	9(1)	11(1)
C(10)	46(2)	30(1)	28(1)	−3(1)	7(1)	3(1)
C(11)	38(2)	31(1)	23(1)	0(1)	9(1)	4(1)
C(12)	26(1)	34(2)	36(1)	0(1)	8(1)	3(1)
C(13)	39(2)	39(2)	51(2)	7(1)	15(1)	1(1)
C(14)	30(2)	44(2)	46(2)	−6(1)	1(1)	4(1)
C(15)	38(2)	33(2)	33(1)	−6(1)	6(1)	−1(1)
C(16)	40(2)	55(2)	41(2)	−2(1)	−5(1)	−1(2)
C(17)	43(2)	41(2)	55(2)	−6(1)	11(2)	−6(2)
C(18)	27(1)	35(2)	32(1)	5(1)	7(1)	7(1)
C(19)	29(1)	38(2)	32(1)	4(1)	8(1)	6(1)
C(20)	37(2)	45(2)	37(1)	3(1)	15(1)	8(1)
C(21)	33(2)	51(2)	46(2)	7(1)	18(1)	6(1)
C(22)	26(1)	44(2)	49(2)	2(1)	8(1)	1(1)
C(23)	28(1)	40(2)	38(1)	3(1)	5(1)	6(1)
C(24)	35(2)	34(2)	36(1)	−1(1)	12(1)	2(1)
C(25)	46(2)	36(2)	57(2)	4(1)	9(2)	4(2)
C(26)	51(2)	36(2)	44(2)	0(1)	−2(1)	−2(2)
C(27)	28(1)	50(2)	42(2)	−7(1)	3(1)	3(1)
C(28)	48(2)	69(3)	44(2)	−4(2)	1(2)	4(2)
C(29)	44(2)	50(2)	58(2)	−11(2)	−1(2)	0(2)
C(30)	48(2)	26(1)	22(1)	2(1)	11(1)	4(1)
C(31)	54(2)	29(1)	28(1)	3(1)	13(1)	0(1)
C(32)	52(2)	24(1)	33(1)	1(1)	22(1)	−2(1)
C(33)	50(2)	36(2)	29(1)	10(1)	4(1)	7(1)
C(34)	59(2)	37(2)	45(2)	8(1)	25(2)	−7(2)
C(35)	29(1)	28(1)	21(1)	4(1)	4(1)	3(1)
C(36)	33(1)	31(1)	25(1)	4(1)	4(1)	4(1)
C(37)	31(1)	43(2)	29(1)	4(1)	7(1)	4(1)
C(38)	34(2)	41(2)	38(1)	8(1)	6(1)	−5(1)
C(39)	41(2)	34(2)	31(1)	2(1)	3(1)	−5(1)
C(40)	36(2)	30(1)	24(1)	4(1)	4(1)	2(1)
C(41)	38(2)	35(2)	27(1)	−2(1)	7(1)	4(1)
C(42)	67(3)	34(2)	65(2)	−2(2)	−18(2)	9(2)
C(43)	104(4)	40(2)	30(2)	−5(1)	3(2)	8(2)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(44)	45(2)	31(1)	25(1)	1(1)	8(1)	−1(1)
C(45)	58(2)	50(2)	29(1)	−7(1)	7(1)	0(2)
C(46)	49(2)	48(2)	31(1)	−2(1)	10(1)	12(2)
C(47)	35(3)	38(2)	22(4)	8(3)	7(3)	−3(2)
C(48)	37(2)	53(2)	33(5)	−3(4)	15(4)	−11(2)
C(49)	45(3)	84(5)	58(5)	−6(4)	0(4)	−22(3)
C(50)	30(3)	115(7)	91(7)	−6(5)	−3(4)	−8(3)
C(51)	37(3)	76(5)	85(6)	3(4)	15(4)	10(3)
C(52)	36(3)	51(3)	50(5)	10(4)	16(3)	6(2)
C(47')	35(3)	38(2)	22(4)	8(3)	7(3)	−3(2)
C(48')	37(2)	53(2)	33(5)	−3(4)	15(4)	−11(2)
C(49')	36(5)	65(7)	66(9)	6(7)	6(6)	−7(4)
C(50')	29(5)	88(8)	91(10)	3(7)	4(6)	−2(5)
C(51')	43(5)	70(8)	90(10)	6(7)	15(7)	6(5)
C(52')	46(6)	40(5)	54(9)	1(7)	25(6)	−6(4)
C(53)	47(2)	44(2)	51(2)	−6(2)	13(2)	−16(2)
C(54)	64(3)	51(2)	62(2)	3(2)	12(2)	−18(2)
C(55)	118(5)	49(2)	52(2)	−6(2)	25(2)	−30(3)
C(56)	63(3)	40(2)	109(4)	−6(2)	53(3)	2(2)
C(57)	118(5)	48(3)	104(4)	7(3)	69(4)	9(3)
C(58)	97(4)	50(3)	109(4)	4(3)	51(4)	0(3)
C(59)	38(2)	29(1)	31(1)	2(1)	6(1)	−4(1)
C(60)	37(2)	32(2)	28(1)	0(1)	0(1)	0(1)

Table 4: Bond lengths [Å] for mw_017m.

Sb(1)–Ga(2)	2.4540(4)
Sb(1)–Ga(1)	2.5914(4)
Ga(1)–N(5)	1.865(2)
Ga(1)–N(2)	2.007(2)
Ga(1)–N(1)	2.033(2)
Ga(2)–N(3)	1.940(2)
Ga(2)–N(4)	1.968(2)
N(1)–C(1)	1.325(4)
N(1)–C(6)	1.445(3)
N(2)–C(3)	1.338(4)
N(2)–C(18)	1.447(3)
N(3)–C(30)	1.342(3)
N(3)–C(35)	1.443(4)
N(4)–C(32)	1.332(4)
N(4)–C(47)	1.370(10)
N(4)–C(47')	1.60(2)
N(5)–C(60)	1.434(3)
N(5)–C(59)	1.454(4)
C(1)–C(2)	1.402(4)
C(1)–C(4)	1.516(3)
C(2)–C(3)	1.396(4)
C(3)–C(5)	1.513(4)
C(6)–C(7)	1.402(4)
C(6)–C(11)	1.415(4)
C(7)–C(8)	1.397(4)
C(7)–C(12)	1.522(4)
C(8)–C(9)	1.389(5)
C(9)–C(10)	1.376(5)
C(10)–C(11)	1.390(4)
C(11)–C(15)	1.523(4)
C(12)–C(14)	1.529(4)
C(12)–C(13)	1.543(4)
C(15)–C(17)	1.531(5)
C(15)–C(16)	1.534(4)
C(18)–C(19)	1.400(4)
C(18)–C(23)	1.406(5)
C(19)–C(20)	1.396(4)
C(19)–C(24)	1.520(4)
C(20)–C(21)	1.373(5)
C(21)–C(22)	1.389(5)
C(22)–C(23)	1.395(4)
C(23)–C(27)	1.527(4)
C(24)–C(26)	1.527(4)
C(24)–C(25)	1.538(5)
C(27)–C(29)	1.523(5)
C(27)–C(28)	1.533(5)
C(30)–C(31)	1.389(4)
C(30)–C(33)	1.509(5)
C(31)–C(32)	1.397(5)
C(32)–C(34)	1.509(4)
C(35)–C(36)	1.401(4)
C(35)–C(40)	1.409(4)
C(36)–C(37)	1.401(4)

Table 4: (continued)

C(36)–C(41)	1.520(4)
C(37)–C(38)	1.382(5)
C(38)–C(39)	1.393(4)
C(39)–C(40)	1.393(4)
C(40)–C(44)	1.519(4)
C(41)–C(42)	1.514(5)
C(41)–C(43)	1.516(4)
C(44)–C(45)	1.520(4)
C(44)–C(46)	1.538(5)
C(47)–C(48)	1.413(11)
C(47)–C(52)	1.421(14)
C(48)–C(49)	1.371(14)
C(48)–C(53)	1.579(12)
C(49)–C(50)	1.386(14)
C(50)–C(51)	1.368(14)
C(51)–C(52)	1.382(11)
C(52)–C(56)	1.430(13)
C(47')–C(48')	1.39(2)
C(47')–C(52')	1.41(3)
C(48')–C(53)	1.40(3)
C(48')–C(49')	1.46(3)
C(49')–C(50')	1.39(2)
C(50')–C(51')	1.31(3)
C(51')–C(52')	1.41(3)
C(52')–C(56)	1.71(2)
C(53)–C(55)	1.524(5)
C(53)–C(54)	1.535(5)
C(56)–C(57)	1.532(7)
C(56)–C(58)	1.533(7)

Table 5: Bond angles [°] for mw_017m.

Ga(2)–Sb(1)–Ga(1)	114.699(14)
N(5)–Ga(1)–N(2)	109.27(10)
N(5)–Ga(1)–N(1)	101.69(10)
N(2)–Ga(1)–N(1)	91.14(9)
N(5)–Ga(1)–Sb(1)	127.02(7)
N(2)–Ga(1)–Sb(1)	102.08(7)
N(1)–Ga(1)–Sb(1)	119.52(7)
N(3)–Ga(2)–N(4)	94.98(11)
N(3)–Ga(2)–Sb(1)	151.60(7)
N(4)–Ga(2)–Sb(1)	113.24(8)
C(1)–N(1)–C(6)	120.0(2)
C(1)–N(1)–Ga(1)	121.28(18)
C(6)–N(1)–Ga(1)	118.27(16)
C(3)–N(2)–C(18)	118.3(2)
C(3)–N(2)–Ga(1)	121.25(19)
C(18)–N(2)–Ga(1)	120.36(17)
C(30)–N(3)–C(35)	116.9(2)
C(30)–N(3)–Ga(2)	124.2(2)
C(35)–N(3)–Ga(2)	118.51(16)
C(32)–N(4)–C(47)	116.3(5)
C(32)–N(4)–C(47')	126.4(7)
C(32)–N(4)–Ga(2)	124.1(2)
C(47)–N(4)–Ga(2)	119.5(4)
C(47')–N(4)–Ga(2)	109.4(7)
C(60)–N(5)–C(59)	111.3(2)
C(60)–N(5)–Ga(1)	123.27(19)
C(59)–N(5)–Ga(1)	123.35(18)
N(1)–C(1)–C(2)	124.3(2)
N(1)–C(1)–C(4)	120.6(3)
C(2)–C(1)–C(4)	115.1(2)
C(3)–C(2)–C(1)	127.6(3)
N(2)–C(3)–C(2)	123.3(3)
N(2)–C(3)–C(5)	120.0(2)
C(2)–C(3)–C(5)	116.7(3)
C(7)–C(6)–C(11)	121.2(3)
C(7)–C(6)–N(1)	120.6(3)
C(11)–C(6)–N(1)	118.1(3)
C(8)–C(7)–C(6)	118.3(3)
C(8)–C(7)–C(12)	118.3(3)
C(6)–C(7)–C(12)	123.4(3)
C(9)–C(8)–C(7)	121.0(3)
C(10)–C(9)–C(8)	119.7(3)
C(9)–C(10)–C(11)	121.9(3)
C(10)–C(11)–C(6)	117.8(3)
C(10)–C(11)–C(15)	120.5(3)
C(6)–C(11)–C(15)	121.6(3)
C(7)–C(12)–C(14)	110.9(3)
C(7)–C(12)–C(13)	112.3(2)
C(14)–C(12)–C(13)	109.7(3)
C(11)–C(15)–C(17)	113.6(3)
C(11)–C(15)–C(16)	111.3(3)
C(17)–C(15)–C(16)	109.8(3)
C(19)–C(18)–C(23)	120.7(3)

Table 5: (continued)

C(19)–C(18)–N(2)	121.1(3)
C(23)–C(18)–N(2)	118.2(3)
C(20)–C(19)–C(18)	118.5(3)
C(20)–C(19)–C(24)	119.0(3)
C(18)–C(19)–C(24)	122.4(3)
C(21)–C(20)–C(19)	121.7(3)
C(20)–C(21)–C(22)	119.4(3)
C(21)–C(22)–C(23)	121.1(3)
C(22)–C(23)–C(18)	118.6(3)
C(22)–C(23)–C(27)	119.2(3)
C(18)–C(23)–C(27)	122.2(3)
C(19)–C(24)–C(26)	109.9(3)
C(19)–C(24)–C(25)	112.8(3)
C(26)–C(24)–C(25)	109.4(3)
C(29)–C(27)–C(23)	112.9(3)
C(29)–C(27)–C(28)	109.7(3)
C(23)–C(27)–C(28)	111.0(3)
N(3)–C(30)–C(31)	123.8(3)
N(3)–C(30)–C(33)	118.9(3)
C(31)–C(30)–C(33)	117.3(3)
C(30)–C(31)–C(32)	128.4(3)
N(4)–C(32)–C(31)	123.6(3)
N(4)–C(32)–C(34)	119.7(3)
C(31)–C(32)–C(34)	116.7(3)
C(36)–C(35)–C(40)	122.2(3)
C(36)–C(35)–N(3)	118.6(2)
C(40)–C(35)–N(3)	119.2(2)
C(37)–C(36)–C(35)	118.0(3)
C(37)–C(36)–C(41)	120.3(3)
C(35)–C(36)–C(41)	121.7(3)
C(38)–C(37)–C(36)	120.8(3)
C(37)–C(38)–C(39)	120.2(3)
C(38)–C(39)–C(40)	121.2(3)
C(39)–C(40)–C(35)	117.5(3)
C(39)–C(40)–C(44)	121.4(3)
C(35)–C(40)–C(44)	121.0(3)
C(42)–C(41)–C(43)	111.5(3)
C(42)–C(41)–C(36)	112.9(3)
C(43)–C(41)–C(36)	111.2(3)
C(40)–C(44)–C(45)	114.1(3)
C(40)–C(44)–C(46)	110.8(2)
C(45)–C(44)–C(46)	109.9(3)
N(4)–C(47)–C(48)	120.8(8)
N(4)–C(47)–C(52)	119.6(8)
C(48)–C(47)–C(52)	119.5(9)
C(49)–C(48)–C(47)	120.2(10)
C(49)–C(48)–C(53)	118.0(8)
C(47)–C(48)–C(53)	121.8(9)
C(48)–C(49)–C(50)	119.9(8)
C(51)–C(50)–C(49)	120.5(7)
C(50)–C(51)–C(52)	121.9(9)
C(51)–C(52)–C(47)	117.9(9)
C(51)–C(52)–C(56)	117.5(9)

Table 5: (continued)

C(47)–C(52)–C(56)	124.4(8)
C(48')–C(47')–C(52')	127(2)
C(48')–C(47')–N(4)	117.9(19)
C(52')–C(47')–N(4)	115.0(15)
C(47')–C(48')–C(53)	125(2)
C(47')–C(48')–C(49')	111(2)
C(53)–C(48')–C(49')	123.7(17)
C(50')–C(49')–C(48')	123.1(17)
C(51')–C(50')–C(49')	120.9(16)
C(50')–C(51')–C(52')	122.1(17)
C(47')–C(52')–C(51')	115.5(17)
C(47')–C(52')–C(56)	118.5(15)
C(51')–C(52')–C(56)	125.7(16)
C(48')–C(53)–C(55)	102.8(9)
C(48')–C(53)–C(54)	117.2(10)
C(55)–C(53)–C(54)	109.0(3)
C(55)–C(53)–C(48)	115.7(5)
C(54)–C(53)–C(48)	110.7(5)
C(52)–C(56)–C(57)	116.8(6)
C(52)–C(56)–C(58)	108.0(6)
C(57)–C(56)–C(58)	109.4(4)
C(57)–C(56)–C(52')	103.1(9)
C(58)–C(56)–C(52')	119.6(7)

Crystal structure of mw_031_1m

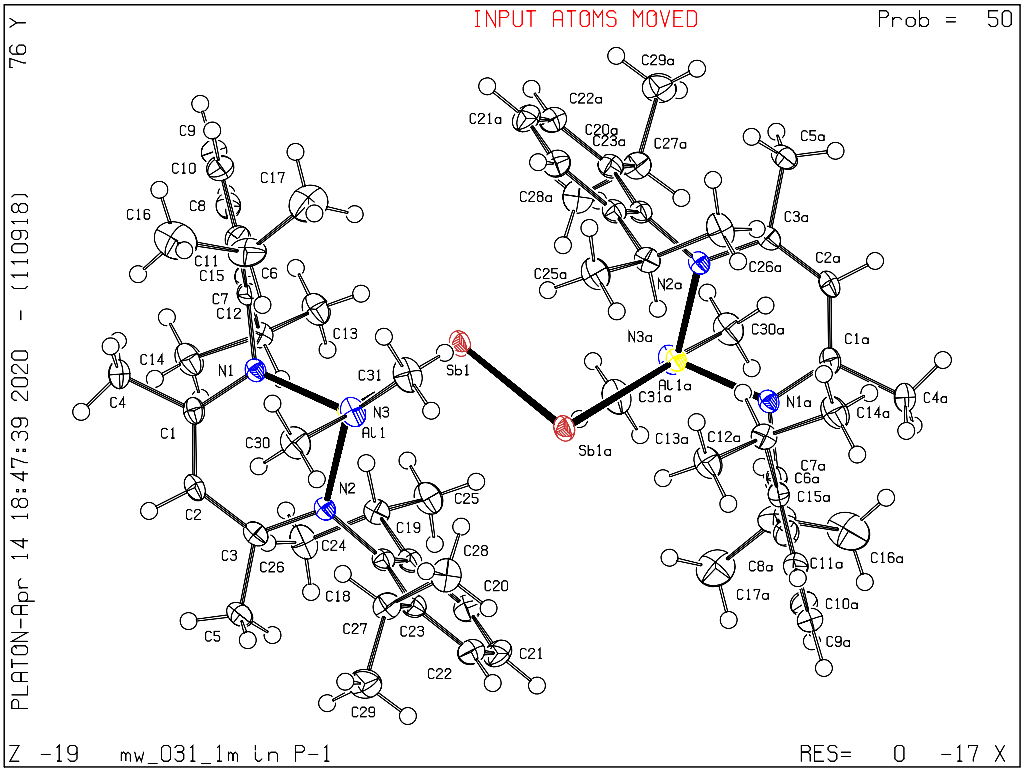

Table 1: Crystal data and structure refinement for mw_031_1m.

Identification code	mw_031_1m
Empirical Formula	$C_{62}H_{94}Al_2N_6Sb_2$
Formula weight	1220.89 Da
Density (calculated)	$1.317\,g\cdot cm^{-3}$
$F(000)$	636
Temperature	100(2) K
Crystal size	0.293 × 0.171 × 0.087 mm
Crystal appearance	orange block
Wavelength (CuK_α)	1.54178 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 10.5975(14)$ Å
	$b = 12.2926(16)$ Å
	$c = 14.1227(19)$ Å
	$\alpha = 107.189(3)°$
	$\beta = 103.366(3)°$
	$\gamma = 109.673(3)°$
Unit cell volume	$1539.2(4)\,Å^3$
Z	1
Cell measurement refections used	9522
θ range for cell measurement	3.52° to 80.26°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	3.522° to 81.153°
Completeness to $\theta = 67.679°$ (to θ_{max})	99.9% (98.7%)
Index ranges	$-13 \leq h \leq 11$
	$-15 \leq k \leq 15$
	$-17 \leq l \leq 18$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$7.544\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.47
R_{merg} before/after correction	0.1197/0.0660
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	148073
Independent reflections	6690 ($R_{int} = 0.0446$)
Reflections with $I > 2\sigma(I)$	6677
Data / retraints / parameter	6690 / 0 / 337
Goodness-of-fit on F^2	1.041
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 0.9583P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0209$
	$wR2 = 0.0569$
R indices [all data]	$R1 = 0.0209$
	$wR2 = 0.0570$
Largest diff. peak and hole	0.656 and $-0.914\,Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_031_1m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	5171(1)	3949(1)	9866(1)	21(1)
Al(1)	3507(1)	2716(1)	7799(1)	15(1)
N(1)	3497(1)	1088(1)	7208(1)	16(1)
N(2)	4241(1)	3315(1)	6837(1)	16(1)
N(3)	1673(1)	2517(1)	7516(1)	22(1)
C(1)	3254(2)	535(1)	6168(1)	19(1)
C(2)	3352(2)	1201(2)	5516(1)	20(1)
C(3)	3927(2)	2517(2)	5842(1)	18(1)
C(4)	2863(2)	−862(2)	5648(1)	26(1)
C(5)	4199(2)	3008(2)	5013(1)	24(1)
C(6)	3682(2)	367(1)	7832(1)	18(1)
C(7)	5053(2)	406(1)	8211(1)	20(1)
C(8)	5199(2)	−404(2)	8693(1)	25(1)
C(9)	4037(2)	−1224(2)	8810(1)	29(1)
C(10)	2720(2)	−1200(2)	8489(1)	29(1)
C(11)	2512(2)	−398(2)	8009(1)	24(1)
C(12)	6356(2)	1285(2)	8088(1)	21(1)
C(13)	7658(2)	2042(2)	9135(1)	29(1)
C(14)	6757(2)	563(2)	7212(2)	31(1)
C(15)	1055(2)	−369(2)	7718(2)	34(1)
C(16)	−144(2)	−1639(2)	6865(2)	51(1)
C(17)	680(2)	16(2)	8717(2)	44(1)
C(18)	4998(2)	4663(1)	7131(1)	17(1)
C(19)	6508(2)	5262(2)	7673(1)	19(1)
C(20)	7227(2)	6563(2)	7979(1)	24(1)
C(21)	6488(2)	7251(2)	7758(2)	26(1)
C(22)	5011(2)	6650(2)	7227(1)	24(1)
C(23)	4236(2)	5349(2)	6898(1)	20(1)
C(24)	7344(2)	4522(2)	7915(1)	20(1)
C(25)	8799(2)	5342(2)	8835(1)	28(1)
C(26)	7581(2)	3795(2)	6935(1)	29(1)
C(27)	2609(2)	4743(2)	6321(1)	24(1)
C(28)	1877(2)	5196(2)	7072(2)	30(1)
C(29)	2194(2)	5019(2)	5329(2)	33(1)
C(30)	585(2)	1814(2)	6450(1)	28(1)
C(31)	1037(2)	2871(2)	8292(2)	30(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_031_1m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	23(1)	20(1)	14(1)	4(1)	2(1)	9(1)
Al(1)	11(1)	16(1)	14(1)	4(1)	4(1)	4(1)
N(1)	13(1)	16(1)	14(1)	4(1)	4(1)	4(1)
N(2)	12(1)	17(1)	14(1)	5(1)	4(1)	4(1)
N(3)	13(1)	27(1)	20(1)	5(1)	6(1)	6(1)
C(1)	14(1)	18(1)	16(1)	2(1)	3(1)	4(1)
C(2)	18(1)	22(1)	13(1)	2(1)	4(1)	6(1)
C(3)	14(1)	24(1)	16(1)	7(1)	5(1)	7(1)
C(4)	28(1)	19(1)	19(1)	2(1)	5(1)	7(1)
C(5)	24(1)	28(1)	16(1)	9(1)	8(1)	9(1)
C(6)	20(1)	16(1)	15(1)	4(1)	5(1)	4(1)
C(7)	22(1)	18(1)	17(1)	5(1)	7(1)	8(1)
C(8)	31(1)	24(1)	22(1)	9(1)	9(1)	14(1)
C(9)	42(1)	21(1)	23(1)	11(1)	12(1)	12(1)
C(10)	33(1)	21(1)	26(1)	10(1)	12(1)	4(1)
C(11)	22(1)	20(1)	23(1)	7(1)	6(1)	2(1)
C(12)	19(1)	24(1)	22(1)	10(1)	8(1)	10(1)
C(13)	22(1)	33(1)	24(1)	7(1)	7(1)	8(1)
C(14)	28(1)	38(1)	25(1)	9(1)	13(1)	14(1)
C(15)	18(1)	37(1)	43(1)	23(1)	10(1)	3(1)
C(16)	25(1)	58(1)	44(1)	19(1)	5(1)	−6(1)
C(17)	31(1)	45(1)	59(1)	23(1)	24(1)	14(1)
C(18)	16(1)	18(1)	16(1)	7(1)	7(1)	5(1)
C(19)	16(1)	21(1)	18(1)	7(1)	7(1)	6(1)
C(20)	17(1)	22(1)	27(1)	9(1)	9(1)	4(1)
C(21)	25(1)	20(1)	34(1)	12(1)	13(1)	6(1)
C(22)	25(1)	23(1)	28(1)	12(1)	11(1)	11(1)
C(23)	18(1)	23(1)	20(1)	9(1)	8(1)	8(1)
C(24)	14(1)	24(1)	20(1)	9(1)	5(1)	6(1)
C(25)	19(1)	34(1)	23(1)	7(1)	2(1)	10(1)
C(26)	23(1)	38(1)	24(1)	7(1)	6(1)	17(1)
C(27)	18(1)	25(1)	26(1)	11(1)	4(1)	10(1)
C(28)	20(1)	33(1)	35(1)	11(1)	9(1)	13(1)
C(29)	30(1)	38(1)	30(1)	17(1)	3(1)	15(1)
C(30)	14(1)	34(1)	27(1)	8(1)	3(1)	6(1)
C(31)	19(1)	36(1)	31(1)	8(1)	13(1)	10(1)

Table 4: Bond lengths [Å] for mw_031_1m.

Sb(1)–Sb(1)#1	2.6596(4)
Sb(1)–Al(1)	2.6708(6)
Al(1)–N(3)	1.8061(14)
Al(1)–N(2)	1.9202(13)
Al(1)–N(1)	1.9217(14)
N(1)–C(1)	1.343(2)
N(1)–C(6)	1.4490(19)
N(2)–C(3)	1.340(2)
N(2)–C(18)	1.4516(19)
N(3)–C(30)	1.449(2)
N(3)–C(31)	1.449(2)
C(1)–C(2)	1.401(2)
C(1)–C(4)	1.515(2)
C(2)–C(3)	1.402(2)
C(3)–C(5)	1.509(2)
C(6)–C(7)	1.407(2)
C(6)–C(11)	1.407(2)
C(7)–C(8)	1.390(2)
C(7)–C(12)	1.524(2)
C(8)–C(9)	1.385(3)
C(9)–C(10)	1.378(3)
C(10)–C(11)	1.397(2)
C(11)–C(15)	1.518(3)
C(12)–C(13)	1.527(2)
C(12)–C(14)	1.532(2)
C(15)–C(16)	1.532(3)
C(15)–C(17)	1.537(3)
C(18)–C(23)	1.403(2)
C(18)–C(19)	1.413(2)
C(19)–C(20)	1.395(2)
C(19)–C(24)	1.521(2)
C(20)–C(21)	1.384(3)
C(21)–C(22)	1.382(2)
C(22)–C(23)	1.396(2)
C(23)–C(27)	1.523(2)
C(24)–C(25)	1.528(2)
C(24)–C(26)	1.536(2)
C(27)–C(28)	1.536(2)
C(27)–C(29)	1.538(2)

#1 -x+1,-y+1,-z+2

Table 5: Bond angles [°] for mw_031_1m.

Sb(1)#1–Sb(1)–Al(1)	95.859(12)
N(3)–Al(1)–N(2)	109.40(6)
N(3)–Al(1)–N(1)	109.16(6)
N(2)–Al(1)–N(1)	94.64(6)
N(3)–Al(1)–Sb(1)	114.03(5)
N(2)–Al(1)–Sb(1)	116.77(4)
N(1)–Al(1)–Sb(1)	111.07(4)
C(1)–N(1)–C(6)	116.32(13)
C(1)–N(1)–Al(1)	120.83(11)
C(6)–N(1)–Al(1)	122.80(10)
C(3)–N(2)–C(18)	118.38(12)
C(3)–N(2)–Al(1)	121.01(10)
C(18)–N(2)–Al(1)	120.18(10)
C(30)–N(3)–C(31)	110.77(13)
C(30)–N(3)–Al(1)	122.33(11)
C(31)–N(3)–Al(1)	126.47(11)
N(1)–C(1)–C(2)	122.67(14)
N(1)–C(1)–C(4)	120.50(14)
C(2)–C(1)–C(4)	116.83(14)
C(1)–C(2)–C(3)	127.11(14)
N(2)–C(3)–C(2)	122.77(14)
N(2)–C(3)–C(5)	120.76(14)
C(2)–C(3)–C(5)	116.46(14)
C(7)–C(6)–C(11)	120.96(15)
C(7)–C(6)–N(1)	117.84(13)
C(11)–C(6)–N(1)	121.12(14)
C(8)–C(7)–C(6)	118.26(15)
C(8)–C(7)–C(12)	119.83(15)
C(6)–C(7)–C(12)	121.91(14)
C(9)–C(8)–C(7)	121.48(16)
C(10)–C(9)–C(8)	119.45(16)
C(9)–C(10)–C(11)	121.58(16)
C(10)–C(11)–C(6)	118.01(16)
C(10)–C(11)–C(15)	119.11(15)
C(6)–C(11)–C(15)	122.87(15)
C(7)–C(12)–C(13)	112.17(14)
C(7)–C(12)–C(14)	111.63(14)
C(13)–C(12)–C(14)	110.31(14)
C(11)–C(15)–C(16)	112.17(19)
C(11)–C(15)–C(17)	110.31(17)
C(16)–C(15)–C(17)	110.31(17)
C(23)–C(18)–C(19)	121.41(14)
C(23)–C(18)–N(2)	120.40(13)
C(19)–C(18)–N(2)	118.18(13)
C(20)–C(19)–C(18)	118.02(15)
C(20)–C(19)–C(24)	120.25(14)
C(18)–C(19)–C(24)	121.73(14)
C(21)–C(20)–C(19)	121.14(15)
C(22)–C(21)–C(20)	120.05(16)
C(21)–C(22)–C(23)	121.29(16)
C(22)–C(23)–C(18)	118.08(15)
C(22)–C(23)–C(27)	118.80(14)
C(18)–C(23)–C(27)	123.11(14)

Table 5: (continued)

C(19)–C(24)–C(25)	113.46(14)
C(19)–C(24)–C(26)	112.38(13)
C(25)–C(24)–C(26)	108.90(13)
C(23)–C(27)–C(28)	110.84(14)
C(23)–C(27)–C(29)	111.68(14)
C(28)–C(27)–C(29)	109.93(15)

#1 -x+1,-y+1,-z+2

Crystal structure of mw_096m

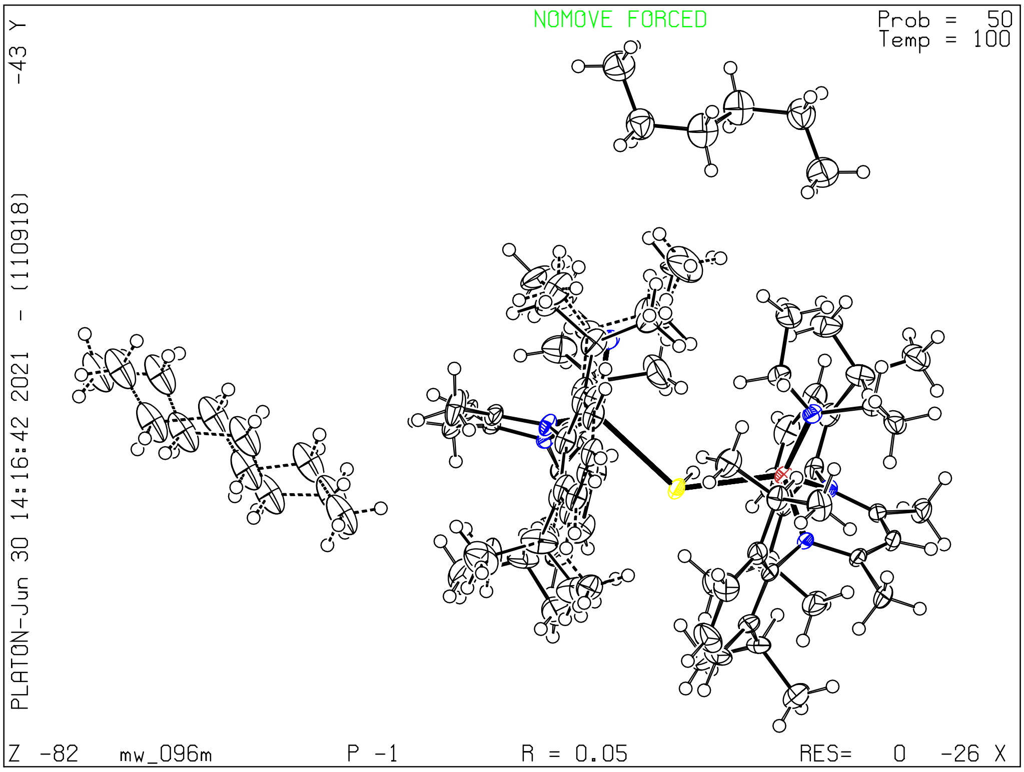

Table 1: Crystal data and structure refinement for mw_096m.

Identification code	mw_096m
Empirical Formula	$C_{72}H_{117}Al_2N_6Sb$
Formula weight	1242.42 Da
Density (calculated)	$1.174\,g\cdot cm^{-3}$
$F(000)$	1336
Temperature	100(2) K
Crystal size	$0.165 \times 0.089 \times 0.045$ mm
Crystal appearance	orange tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 12.6715(11)$ Å
	$b = 14.0133(12)$ Å
	$c = 22.717(2)$ Å
	$\alpha = 86.217(5)°$
	$\beta = 75.012(5)°$
	$\gamma = 64.550(5)°$
Unit cell volume	3513.8(6) $Å^3$
Z	2
Cell measurement refections used	9847
θ range for cell measurement	2.26° to 27.12°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.841° to 27.219°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.7% (99.0%)
Index ranges	$-16 \leq h \leq 16$
	$-18 \leq k \leq 18$
	$-29 \leq l \leq 29$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$0.461\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.70
R_{merg} before/after correction	0.0713/0.0583
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	81969
Independent reflections	15523 ($R_{int} = 0.0746$)
Reflections with $I > 2\sigma(I)$	11345
Data / retraints / parameter	15523 / 495 / 822
Goodness-of-fit on F^2	1.036
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0590P)^2 + 2.2198P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0483$
	$wR2 = 0.1118$
R indices [all data]	$R1 = 0.0775$
	$wR2 = 0.1234$
Largest diff. peak and hole	2.257 and -0.783 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The hydrogen bonded the Sb is refined freely with its Sb–H bond length restrained to be equal to 1.7 Å (`DFIX`).

Disorder

A diisopropyl phenyl group is disordered over two positions. The bond lengths and angles of its isopropyl groups were restrained to be equal (`SADI`). The phenyl ring's atoms were refined with common anisotropic displacement parameters (`EADP`) and the ring was constrained to a regular hexagon of 1.39 Å (`AFIX 66`). `RIGU` restraints were applied to all atoms of the diisopropyl phenyl group and additional `SIMU` restrints were used for the isopropyl groups. An ethyl group of the amide group is disordered over two positions. `RIGU` and `SIMU` restraints were applied to the corresponding atoms. The displacement parameters of the minor component suggest that there might be more orientations, however identifing them in the residual electron density failed.

Disordered solvent

An n-hexane molecule is disordered over a centre of inversion. It was modelled using two alternate positions and ignoring the local symmetry (negative `PART`). All of these atoms were refined with common displacement parameters (`EADP`). The bond lengths and angles of all solvent molecules were restrained to be equal (`SADI`) and `RIGU` and `SIMU` restraints were applied to the displacement parameters

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_096m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	2754(1)	2311(1)	2299(1)	27(1)
Al(1)	2715(1)	4198(1)	2296(1)	19(1)
Al(2)	3135(1)	919(1)	3151(1)	18(1)
N(1)	1100(2)	5311(2)	2402(1)	22(1)
N(2)	3268(2)	4420(2)	1446(1)	18(1)
N(3)	4592(2)	−352(2)	2857(1)	21(1)
N(4)	2057(2)	276(2)	3163(1)	20(1)
N(5)	3494(3)	4598(2)	2742(1)	32(1)
N(6)	3077(2)	1218(2)	3933(1)	22(1)
C(1)	959(3)	6187(2)	2099(1)	26(1)
C(2)	1853(3)	6247(2)	1607(1)	25(1)
C(3)	2885(3)	5418(2)	1274(1)	22(1)
C(4)	−205(3)	7188(3)	2277(2)	48(1)
C(5)	3578(3)	5692(3)	694(1)	32(1)
C(6)	59(8)	5304(11)	2852(5)	31(1)
C(7)	−773(10)	5053(9)	2683(4)	31(1)
C(8)	−1836(8)	5169(7)	3108(4)	31(1)
C(9)	−2066(6)	5536(6)	3702(4)	31(1)
C(10)	−1233(8)	5786(7)	3872(4)	31(1)
C(11)	−171(8)	5670(9)	3447(6)	31(1)
C(12)	−390(20)	4556(16)	2010(9)	38(4)
C(13)	−990(20)	5343(15)	1564(11)	60(5)
C(14)	−640(30)	3584(17)	1994(11)	42(4)
C(15)	689(15)	5968(11)	3697(6)	24(3)
C(16)	40(20)	7045(10)	4047(8)	49(5)
C(17)	1316(18)	5135(9)	4103(7)	61(4)
C(6')	16(7)	5288(9)	2819(4)	31(1)
C(7')	−729(8)	5028(8)	2573(3)	31(1)
C(8')	−1829(6)	5101(6)	2938(4)	31(1)
C(9')	−2184(5)	5434(5)	3550(4)	31(1)
C(10')	−1439(6)	5694(6)	3796(3)	31(1)
C(11')	−339(6)	5621(7)	3431(5)	31(1)
C(12')	−512(17)	4707(13)	1930(8)	48(4)
C(13')	−630(20)	3695(14)	1871(12)	80(6)
C(14')	−1361(19)	5594(15)	1619(9)	73(5)
C(15')	484(13)	5815(11)	3714(6)	35(3)
C(16')	120(19)	6999(10)	3828(7)	48(4)
C(17')	650(9)	5269(6)	4303(4)	37(2)
C(18)	4129(3)	3596(2)	986(1)	21(1)
C(19)	3696(3)	3279(2)	560(1)	27(1)
C(20)	4537(4)	2523(3)	103(1)	40(1)
C(21)	5750(4)	2087(3)	63(2)	43(1)
C(22)	6160(3)	2376(3)	494(2)	38(1)
C(23)	5367(3)	3140(2)	961(1)	27(1)
C(24)	2365(3)	3719(3)	579(2)	39(1)
C(25)	2026(4)	4465(4)	75(3)	70(1)
C(26)	1977(5)	2851(4)	543(2)	73(2)
C(27)	5887(3)	3449(3)	1405(2)	36(1)
C(28)	6650(4)	4034(4)	1088(2)	54(1)
C(29)	6643(4)	2488(4)	1702(2)	66(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(30)	4612(3)	−1277(2)	3047(1)	24(1)
C(31)	3575(3)	−1414(2)	3317(1)	26(1)
C(32)	2381(3)	−721(2)	3332(1)	25(1)
C(33)	5806(3)	−2255(2)	2983(2)	33(1)
C(34)	1449(3)	−1154(3)	3548(2)	35(1)
C(35)	5707(3)	−332(2)	2501(1)	24(1)
C(36)	5969(3)	−417(2)	1860(1)	29(1)
C(37)	7063(3)	−408(3)	1524(2)	39(1)
C(38)	7846(3)	−305(3)	1810(2)	40(1)
C(39)	7570(3)	−209(3)	2433(2)	35(1)
C(40)	6505(3)	−223(2)	2790(2)	29(1)
C(41)	5123(3)	−534(3)	1535(1)	34(1)
C(42)	5331(4)	−1691(3)	1489(2)	46(1)
C(43)	5186(4)	−77(3)	906(2)	46(1)
C(44)	6258(3)	−115(3)	3476(2)	35(1)
C(45)	7258(4)	−1014(3)	3714(2)	49(1)
C(46)	6143(4)	937(3)	3680(2)	50(1)
C(47)	873(3)	817(2)	3041(1)	25(1)
C(48)	744(3)	577(3)	2477(2)	34(1)
C(49)	−412(4)	1045(3)	2382(2)	47(1)
C(50)	−1390(4)	1719(4)	2810(2)	54(1)
C(51)	−1245(3)	1979(3)	3343(2)	43(1)
C(52)	−109(3)	1539(3)	3468(2)	28(1)
C(53)	1799(3)	−157(3)	1982(2)	38(1)
C(54)	1710(4)	−1186(3)	1886(2)	56(1)
C(55)	1904(4)	383(3)	1383(2)	52(1)
C(56)	−16(3)	1847(3)	4072(1)	30(1)
C(57)	−718(3)	1457(3)	4611(2)	43(1)
C(58)	−479(4)	3047(3)	4143(2)	46(1)
C(59)	3349(4)	5689(3)	2778(2)	43(1)
C(60)	4358(5)	5924(3)	2368(2)	61(1)
C(61)	3942(9)	4005(7)	3231(5)	37(2)
C(62)	5115(6)	3933(7)	3282(4)	37(2)
C(61')	4532(16)	3786(10)	2982(6)	39(3)
C(62')	4690(30)	3991(16)	3572(9)	124(11)
C(63)	3374(3)	400(2)	4378(1)	26(1)
C(64)	2301(3)	302(3)	4824(2)	34(1)
C(65)	2521(4)	2277(3)	4198(2)	38(1)
C(66)	3098(4)	2601(3)	4574(2)	47(1)
C11	5538(4)	2872(3)	5178(2)	59(1)
C21	5808(4)	3701(3)	5403(2)	53(1)
C31	5636(4)	4661(3)	5010(2)	60(1)
C32	110(80)	9560(30)	190(30)	60(2)
C42	−130(80)	10510(30)	−190(30)	60(2)
C22	−20(30)	8650(30)	−61(12)	60(2)
C52	150(30)	11350(30)	10(12)	60(2)
C62	−40(20)	12270(30)	−405(10)	60(2)
C12	328(18)	7680(30)	315(11)	60(2)
C13	−120(30)	12040(20)	−166(14)	60(2)
C63	80(50)	7420(30)	321(19)	60(2)
C23	−390(20)	11122(19)	−267(12)	60(2)
C53	440(20)	8310(20)	363(12)	60(2)

Table 2: (continued)

	x	y	z	U_{eq}
C33	220(20)	10147(17)	65(14)	60(2)
C43	−70(30)	9234(19)	−22(14)	60(2)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_096m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	43(1)	18(1)	26(1)	5(1)	−11(1)	−17(1)
Al(1)	26(1)	17(1)	14(1)	0(1)	−2(1)	−9(1)
Al(2)	20(1)	13(1)	21(1)	0(1)	−4(1)	−9(1)
N(1)	26(1)	14(1)	19(1)	−1(1)	3(1)	−8(1)
N(2)	24(1)	19(1)	13(1)	1(1)	−3(1)	−12(1)
N(3)	26(1)	18(1)	17(1)	−1(1)	−3(1)	−8(1)
N(4)	28(1)	17(1)	20(1)	4(1)	−8(1)	−14(1)
N(5)	51(2)	31(2)	24(1)	3(1)	−11(1)	−26(1)
N(6)	25(1)	21(1)	21(1)	0(1)	−4(1)	−11(1)
C(1)	36(2)	15(1)	26(2)	−1(1)	−7(1)	−9(1)
C(2)	39(2)	14(1)	24(2)	4(1)	−6(1)	−15(1)
C(3)	36(2)	22(2)	16(1)	5(1)	−8(1)	−21(1)
C(4)	51(2)	18(2)	47(2)	5(2)	6(2)	−2(2)
C(5)	44(2)	29(2)	26(2)	6(1)	−1(2)	−23(2)
C(6)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(7)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(8)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(9)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(10)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(11)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(12)	35(7)	40(6)	54(8)	32(6)	−25(5)	−27(5)
C(13)	54(10)	39(7)	69(10)	23(7)	−6(8)	−12(7)
C(14)	50(10)	53(8)	39(6)	13(6)	−10(6)	−39(7)
C(15)	26(6)	32(6)	17(4)	−6(4)	4(4)	−18(4)
C(16)	46(6)	31(6)	49(11)	−11(5)	14(9)	−12(5)
C(17)	90(11)	56(7)	50(8)	19(6)	−25(8)	−41(8)
C(6’)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(7’)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(8’)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(9’)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(10’)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(11’)	28(1)	22(1)	33(1)	1(1)	4(1)	−7(1)
C(12’)	32(6)	69(9)	40(5)	−22(6)	3(5)	−21(6)
C(13’)	55(10)	71(9)	116(17)	−32(9)	−37(11)	−14(8)
C(14’)	91(13)	85(11)	39(6)	3(6)	−16(7)	−35(10)
C(15’)	32(5)	36(5)	27(4)	−3(3)	13(3)	−17(4)
C(16’)	60(8)	45(5)	50(9)	9(5)	−8(8)	−36(5)
C(17’)	43(5)	34(4)	30(4)	−5(3)	3(3)	−19(4)
C(18)	28(2)	20(1)	12(1)	0(1)	1(1)	−12(1)
C(19)	40(2)	31(2)	14(1)	1(1)	−1(1)	−22(2)
C(20)	66(3)	42(2)	16(2)	−7(1)	2(2)	−33(2)
C(21)	59(3)	34(2)	25(2)	−9(2)	13(2)	−22(2)
C(22)	33(2)	31(2)	34(2)	0(2)	6(2)	−6(2)
C(23)	33(2)	22(2)	22(2)	2(1)	−1(1)	−13(1)
C(24)	47(2)	60(2)	22(2)	−9(2)	−4(2)	−35(2)
C(25)	63(3)	54(3)	111(4)	24(3)	−42(3)	−32(2)
C(26)	95(4)	88(4)	91(4)	50(3)	−62(3)	−75(3)
C(27)	31(2)	41(2)	35(2)	2(2)	−11(2)	−14(2)
C(28)	42(2)	72(3)	56(3)	−4(2)	−5(2)	−34(2)
C(29)	68(3)	61(3)	58(3)	11(2)	−36(2)	−10(2)
C(30)	37(2)	16(1)	19(2)	−2(1)	−11(1)	−8(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(31)	40(2)	16(2)	25(2)	5(1)	−11(1)	−13(1)
C(32)	43(2)	20(2)	18(2)	4(1)	−9(1)	−19(1)
C(33)	40(2)	18(2)	35(2)	−1(1)	−10(2)	−5(1)
C(34)	47(2)	28(2)	41(2)	14(2)	−16(2)	−26(2)
C(35)	25(2)	14(1)	23(2)	−4(1)	1(1)	−1(1)
C(36)	33(2)	17(2)	28(2)	−2(1)	−3(1)	−5(1)
C(37)	43(2)	28(2)	27(2)	−3(1)	9(2)	−7(2)
C(38)	28(2)	33(2)	48(2)	1(2)	4(2)	−10(2)
C(39)	25(2)	30(2)	42(2)	−1(2)	−2(2)	−7(1)
C(40)	27(2)	21(2)	33(2)	−2(1)	−3(1)	−7(1)
C(41)	48(2)	28(2)	20(2)	−6(1)	−1(2)	−15(2)
C(42)	79(3)	36(2)	29(2)	−1(2)	−13(2)	−30(2)
C(43)	68(3)	43(2)	28(2)	5(2)	−11(2)	−25(2)
C(44)	25(2)	46(2)	32(2)	−8(2)	−4(1)	−15(2)
C(45)	54(2)	48(2)	41(2)	−1(2)	−20(2)	−15(2)
C(46)	49(2)	46(2)	47(2)	−16(2)	−8(2)	−14(2)
C(47)	32(2)	23(2)	31(2)	11(1)	−15(1)	−21(1)
C(48)	49(2)	37(2)	38(2)	13(2)	−22(2)	−34(2)
C(49)	59(3)	66(3)	48(2)	19(2)	−34(2)	−48(2)
C(50)	40(2)	75(3)	62(3)	25(2)	−31(2)	−33(2)
C(51)	31(2)	48(2)	56(2)	14(2)	−15(2)	−21(2)
C(52)	26(2)	31(2)	35(2)	11(1)	−11(1)	−18(1)
C(53)	59(2)	40(2)	34(2)	5(2)	−24(2)	−33(2)
C(54)	93(3)	41(2)	55(3)	8(2)	−29(2)	−42(2)
C(55)	96(3)	45(2)	33(2)	3(2)	−18(2)	−45(2)
C(56)	25(2)	30(2)	31(2)	4(1)	−2(1)	−13(1)
C(57)	34(2)	48(2)	41(2)	12(2)	−3(2)	−18(2)
C(58)	47(2)	33(2)	51(2)	0(2)	−8(2)	−14(2)
C(59)	75(3)	39(2)	31(2)	−1(2)	−12(2)	−40(2)
C(60)	104(4)	58(3)	49(2)	2(2)	−14(2)	−64(3)
C(61)	53(5)	40(4)	35(5)	6(3)	−20(4)	−30(4)
C(62)	49(4)	42(4)	29(4)	−6(4)	−24(3)	−19(3)
C(61')	54(9)	43(6)	26(6)	4(5)	−11(5)	−25(6)
C(62')	230(30)	76(11)	60(11)	−10(11)	−86(15)	−34(15)
C(63)	34(2)	23(2)	23(2)	1(1)	−10(1)	−12(1)
C(64)	40(2)	41(2)	27(2)	8(1)	−12(2)	−21(2)
C(65)	59(2)	30(2)	35(2)	2(2)	−19(2)	−23(2)
C(66)	65(3)	33(2)	38(2)	−7(2)	−22(2)	−11(2)
C11	65(3)	55(3)	57(3)	−4(2)	−16(2)	−23(2)
C21	55(3)	48(2)	49(2)	2(2)	−12(2)	−17(2)
C31	51(2)	62(3)	57(3)	7(2)	−6(2)	−23(2)
C32	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C42	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C22	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C52	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C62	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C12	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C13	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C63	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C23	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C53	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)
C33	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C43	35(3)	84(6)	30(3)	8(3)	−2(2)	0(4)

Table 4: Bond lengths [Å] for mw_096m.

Sb(1)–Al(1)	2.6232(9)
Sb(1)–Al(2)	2.6385(9)
Al(1)–N(5)	1.838(3)
Al(1)–N(2)	1.930(2)
Al(1)–N(1)	1.931(2)
Al(2)–N(6)	1.829(2)
Al(2)–N(4)	1.928(2)
Al(2)–N(3)	1.928(2)
N(1)–C(1)	1.333(4)
N(1)–C(6)	1.448(5)
N(1)–C(6')	1.465(5)
N(2)–C(3)	1.337(4)
N(2)–C(18)	1.450(3)
N(3)–C(30)	1.331(4)
N(3)–C(35)	1.447(4)
N(4)–C(32)	1.336(4)
N(4)–C(47)	1.453(4)
N(5)–C(61)	1.431(8)
N(5)–C(59)	1.465(4)
N(5)–C(61')	1.525(13)
N(6)–C(65)	1.435(4)
N(6)–C(63)	1.467(4)
C(1)–C(2)	1.398(4)
C(1)–C(4)	1.515(4)
C(2)–C(3)	1.390(4)
C(3)–C(5)	1.510(4)
C(6)–C(7)	1.3900
C(6)–C(11)	1.3900
C(7)–C(8)	1.3900
C(7)–C(12)	1.59(2)
C(8)–C(9)	1.3900
C(9)–C(10)	1.3900
C(10)–C(11)	1.3900
C(11)–C(15)	1.557(13)
C(12)–C(14)	1.530(11)
C(12)–C(13)	1.532(11)
C(15)–C(17)	1.511(11)
C(15)–C(16)	1.530(11)
C(6')–C(7')	1.3900
C(6')–C(11')	1.3900
C(7')–C(8')	1.3900
C(7')–C(12')	1.477(17)
C(8')–C(9')	1.3900
C(9')–C(10')	1.3900
C(10')–C(11')	1.3900
C(11')–C(15')	1.479(13)
C(12')–C(13')	1.509(11)
C(12')–C(14')	1.526(11)
C(15')–C(17')	1.515(11)
C(15')–C(16')	1.539(10)
C(18)–C(23)	1.402(4)
C(18)–C(19)	1.406(4)
C(19)–C(20)	1.393(4)

Table 4: (continued)

C(19)–C(24)	1.516(5)
C(20)–C(21)	1.368(5)
C(21)–C(22)	1.376(5)
C(22)–C(23)	1.397(4)
C(23)–C(27)	1.513(4)
C(24)–C(26)	1.509(5)
C(24)–C(25)	1.515(6)
C(27)–C(29)	1.514(5)
C(27)–C(28)	1.540(5)
C(30)–C(31)	1.387(4)
C(30)–C(33)	1.523(4)
C(31)–C(32)	1.397(4)
C(32)–C(34)	1.509(4)
C(35)–C(40)	1.403(4)
C(35)–C(36)	1.408(4)
C(36)–C(37)	1.404(5)
C(36)–C(41)	1.516(5)
C(37)–C(38)	1.377(5)
C(38)–C(39)	1.368(5)
C(39)–C(40)	1.391(5)
C(40)–C(44)	1.512(5)
C(41)–C(43)	1.525(5)
C(41)–C(42)	1.533(5)
C(44)–C(46)	1.511(5)
C(44)–C(45)	1.541(5)
C(47)–C(52)	1.392(5)
C(47)–C(48)	1.412(4)
C(48)–C(49)	1.394(5)
C(48)–C(53)	1.517(5)
C(49)–C(50)	1.366(6)
C(50)–C(51)	1.364(6)
C(51)–C(52)	1.400(5)
C(52)–C(56)	1.512(5)
C(53)–C(55)	1.516(5)
C(53)–C(54)	1.528(5)
C(56)–C(58)	1.529(5)
C(56)–C(57)	1.535(5)
C(59)–C(60)	1.522(5)
C(61)–C(62)	1.480(9)
C(61')–C(62')	1.471(14)
C(63)–C(64)	1.526(4)
C(65)–C(66)	1.460(5)
C11–C21	1.497(5)
C21–C31	1.532(5)
C31–C31#1	1.489(8)
C32–C42	1.502(9)
C32–C22	1.518(13)
C42–C52	1.514(13)
C22–C12	1.516(12)
C52–C62	1.516(12)
C13–C23	1.512(14)
C63–C53	1.510(14)
C23–C33	1.516(14)

Table 4: (continued)

C53–C43	1.514(14)
C33–C43	1.514(14)

#1 -x+1,-y+1,-z+1

Table 5: Bond angles [°] for mw_096m.

Al(1)–Sb(1)–Al(2)	128.31(3)
N(5)–Al(1)–N(2)	108.91(12)
N(5)–Al(1)–N(1)	107.99(12)
N(2)–Al(1)–N(1)	95.31(10)
N(5)–Al(1)–Sb(1)	124.03(9)
N(2)–Al(1)–Sb(1)	104.55(7)
N(1)–Al(1)–Sb(1)	112.09(8)
N(6)–Al(2)–N(4)	109.51(11)
N(6)–Al(2)–N(3)	107.30(11)
N(4)–Al(2)–N(3)	94.93(10)
N(6)–Al(2)–Sb(1)	124.66(8)
N(4)–Al(2)–Sb(1)	104.95(8)
N(3)–Al(2)–Sb(1)	111.38(8)
C(1)–N(1)–C(6)	117.9(6)
C(1)–N(1)–C(6')	117.1(5)
C(1)–N(1)–Al(1)	118.2(2)
C(6)–N(1)–Al(1)	123.3(6)
C(6')–N(1)–Al(1)	124.6(5)
C(3)–N(2)–C(18)	117.1(2)
C(3)–N(2)–Al(1)	117.50(19)
C(18)–N(2)–Al(1)	125.23(18)
C(30)–N(3)–C(35)	118.4(2)
C(30)–N(3)–Al(2)	118.6(2)
C(35)–N(3)–Al(2)	122.60(18)
C(32)–N(4)–C(47)	117.0(2)
C(32)–N(4)–Al(2)	118.1(2)
C(47)–N(4)–Al(2)	124.79(18)
C(61)–N(5)–C(59)	111.8(4)
C(59)–N(5)–C(61')	114.6(5)
C(61)–N(5)–Al(1)	122.7(3)
C(59)–N(5)–Al(1)	122.3(2)
C(61')–N(5)–Al(1)	121.7(4)
C(65)–N(6)–C(63)	113.6(2)
C(65)–N(6)–Al(2)	122.9(2)
C(63)–N(6)–Al(2)	122.46(19)
N(1)–C(1)–C(2)	123.1(3)
N(1)–C(1)–C(4)	120.8(3)
C(2)–C(1)–C(4)	116.1(3)
C(3)–C(2)–C(1)	127.9(3)
N(2)–C(3)–C(2)	123.0(3)
N(2)–C(3)–C(5)	120.3(3)
C(2)–C(3)–C(5)	116.7(3)
C(7)–C(6)–C(11)	120.0
C(7)–C(6)–N(1)	120.9(9)
C(11)–C(6)–N(1)	118.7(9)
C(8)–C(7)–C(6)	120.0
C(8)–C(7)–C(12)	123.3(10)
C(6)–C(7)–C(12)	116.5(10)
C(7)–C(8)–C(9)	120.0
C(10)–C(9)–C(8)	120.0
C(11)–C(10)–C(9)	120.0
C(10)–C(11)–C(6)	120.0
C(10)–C(11)–C(15)	114.9(9)

Table 5: (continued)

C(6)–C(11)–C(15)	125.1(9)
C(14)–C(12)–C(13)	108.7(10)
C(14)–C(12)–C(7)	112.3(16)
C(13)–C(12)–C(7)	113.6(17)
C(17)–C(15)–C(16)	109.0(9)
C(17)–C(15)–C(11)	111.4(10)
C(16)–C(15)–C(11)	112.9(15)
C(7')–C(6')–C(11')	120.0
C(7')–C(6')–N(1)	117.9(7)
C(11')–C(6')–N(1)	121.8(7)
C(8')–C(7')–C(6')	120.0
C(8')–C(7')–C(12')	113.2(9)
C(6')–C(7')–C(12')	126.7(9)
C(7')–C(8')–C(9')	120.0
C(8')–C(9')–C(10')	120.0
C(11')–C(10')–C(9')	120.0
C(10')–C(11')–C(6')	120.0
C(10')–C(11')–C(15')	119.0(8)
C(6')–C(11')–C(15')	120.8(8)
C(7')–C(12')–C(13')	112.3(16)
C(7')–C(12')–C(14')	110.5(13)
C(13')–C(12')–C(14')	110.5(10)
C(11')–C(15')–C(17')	114.9(9)
C(11')–C(15')–C(16')	113.1(12)
C(17')–C(15')–C(16')	108.2(9)
C(23)–C(18)–C(19)	120.8(3)
C(23)–C(18)–N(2)	120.8(3)
C(19)–C(18)–N(2)	118.4(3)
C(20)–C(19)–C(18)	117.9(3)
C(20)–C(19)–C(24)	119.0(3)
C(18)–C(19)–C(24)	123.0(3)
C(21)–C(20)–C(19)	122.0(3)
C(20)–C(21)–C(22)	119.6(3)
C(21)–C(22)–C(23)	121.3(3)
C(22)–C(23)–C(18)	118.3(3)
C(22)–C(23)–C(27)	118.4(3)
C(18)–C(23)–C(27)	123.3(3)
C(26)–C(24)–C(25)	108.5(3)
C(26)–C(24)–C(19)	111.8(3)
C(25)–C(24)–C(19)	113.1(3)
C(23)–C(27)–C(29)	111.1(3)
C(23)–C(27)–C(28)	111.2(3)
C(29)–C(27)–C(28)	109.9(3)
N(3)–C(30)–C(31)	123.1(3)
N(3)–C(30)–C(33)	120.7(3)
C(31)–C(30)–C(33)	116.1(3)
C(30)–C(31)–C(32)	127.8(3)
N(4)–C(32)–C(31)	122.8(3)
N(4)–C(32)–C(34)	120.6(3)
C(31)–C(32)–C(34)	116.6(3)
C(40)–C(35)–C(36)	120.9(3)
C(40)–C(35)–N(3)	120.5(3)
C(36)–C(35)–N(3)	118.6(3)

Table 5: (continued)

C(37)–C(36)–C(35)	117.6(3)
C(37)–C(36)–C(41)	120.3(3)
C(35)–C(36)–C(41)	122.1(3)
C(38)–C(37)–C(36)	121.3(3)
C(39)–C(38)–C(37)	120.3(3)
C(38)–C(39)–C(40)	121.1(3)
C(39)–C(40)–C(35)	118.8(3)
C(39)–C(40)–C(44)	118.4(3)
C(35)–C(40)–C(44)	122.9(3)
C(36)–C(41)–C(43)	113.7(3)
C(36)–C(41)–C(42)	111.4(3)
C(43)–C(41)–C(42)	110.1(3)
C(46)–C(44)–C(40)	111.6(3)
C(46)–C(44)–C(45)	109.1(3)
C(40)–C(44)–C(45)	111.4(3)
C(52)–C(47)–C(48)	120.8(3)
C(52)–C(47)–N(4)	121.3(3)
C(48)–C(47)–N(4)	117.9(3)
C(49)–C(48)–C(47)	117.4(3)
C(49)–C(48)–C(53)	119.7(3)
C(47)–C(48)–C(53)	122.9(3)
C(50)–C(49)–C(48)	122.0(3)
C(51)–C(50)–C(49)	120.0(3)
C(50)–C(51)–C(52)	121.0(4)
C(47)–C(52)–C(51)	118.6(3)
C(47)–C(52)–C(56)	123.1(3)
C(51)–C(52)–C(56)	118.3(3)
C(55)–C(53)–C(48)	111.2(3)
C(55)–C(53)–C(54)	109.6(3)
C(48)–C(53)–C(54)	112.3(3)
C(52)–C(56)–C(58)	110.4(3)
C(52)–C(56)–C(57)	111.6(3)
C(58)–C(56)–C(57)	109.8(3)
N(5)–C(59)–C(60)	116.3(3)
N(5)–C(61)–C(62)	116.1(8)
C(62')–C(61')–N(5)	120.2(16)
N(6)–C(63)–C(64)	115.8(3)
N(6)–C(65)–C(66)	120.5(3)
C11–C21–C31	115.6(4)
C31#1–C31–C21	115.0(5)
C42–C32–C22	114.6(11)
C32–C42–C52	114.8(11)
C12–C22–C32	112.9(11)
C42–C52–C62	113.7(12)
C13–C23–C33	114.0(14)
C63–C53–C43	114.9(15)
C43–C33–C23	114.4(13)
C53–C43–C33	113.9(14)

#1 -x+1,-y+1,-z+1

Crystal structure of mw_060m

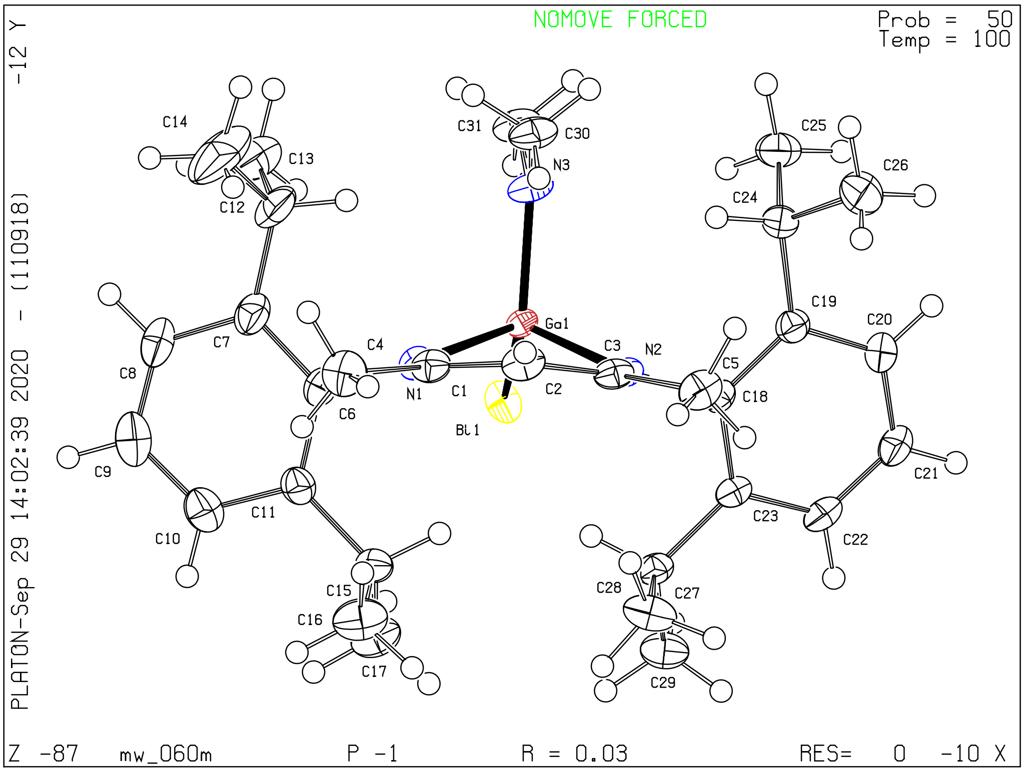

Table 1: Crystal data and structure refinement for mw_060m.

Identification code	mw_060m
Empirical Formula	$C_{62}\,H_{94}\,Bi_2\,Ga_2\,N_6$
Formula weight	1480.83 Da
Density (calculated)	$1.587\,g\cdot cm^{-3}$
$F(000)$	736
Temperature	100(2) K
Crystal size	0.304 × 0.287 × 0.152 mm
Crystal appearance	red block
Wavelength (CuK_α)	1.54178 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 10.6015(7)$ Å
	$b = 12.3243(8)$ Å
	$c = 14.1072(9)$ Å
	$\alpha = 106.8132(11)°$
	$\beta = 103.0605(12)°$
	$\gamma = 109.7870(12)°$
Unit cell volume	$1549.17(17)\,Å^3$
Z	1
Cell measurement refections used	9709
θ range for cell measurement	4.16° to 80.58°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	4.157° to 80.795°
Completeness to $\theta = 67.679°$ (to θ_{max})	99.9% (99.0%)
Index ranges	$-13 \leq h \leq 13$
	$-14 \leq k \leq 15$
	$-18 \leq l \leq 18$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$12.242\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.35
R_{merg} before/after correction	0.1475/0.0823
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	72163
Independent reflections	6737 ($R_{int} = 0.0473$)
Reflections with $I > 2\sigma(I)$	6729
Data / retraints / parameter	6737 / 0 / 337
Goodness-of-fit on F^2	1.043
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 6.3234P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0286$
	$wR2 = 0.0745$
R indices [all data]	$R1 = 0.0287$
	$wR2 = 0.0745$
Largest diff. peak and hole	2.104 and $-1.551\,Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_060m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Bi(1)	4818(1)	6101(1)	73(1)	26(1)
Ga(1)	6452(1)	7301(1)	2156(1)	17(1)
N(1)	6486(3)	8977(3)	2820(2)	21(1)
N(2)	5743(3)	6686(3)	3181(2)	18(1)
N(3)	8353(3)	7517(3)	2495(3)	28(1)
C(1)	6711(4)	9478(3)	3853(3)	24(1)
C(2)	6624(4)	8788(4)	4488(3)	25(1)
C(3)	6063(4)	7481(4)	4162(3)	22(1)
C(4)	7075(5)	10858(4)	4386(3)	34(1)
C(5)	5801(4)	6981(4)	4997(3)	30(1)
C(6)	6307(4)	9698(3)	2195(3)	24(1)
C(7)	7478(4)	10462(4)	2032(3)	32(1)
C(8)	7268(5)	11242(4)	1526(4)	37(1)
C(9)	5944(6)	11239(4)	1179(4)	41(1)
C(10)	4781(5)	10419(4)	1295(4)	36(1)
C(11)	4929(4)	9632(3)	1794(3)	26(1)
C(12)	8937(5)	10466(5)	2347(5)	48(1)
C(13)	9358(6)	10085(6)	1367(6)	60(2)
C(14)	10091(6)	11731(7)	3197(6)	77(2)
C(15)	3627(4)	8745(4)	1917(3)	28(1)
C(16)	3215(5)	9445(5)	2783(4)	42(1)
C(17)	2341(5)	7997(4)	882(4)	38(1)
C(18)	4999(4)	5348(3)	2878(3)	19(1)
C(19)	5759(4)	4666(4)	3093(3)	24(1)
C(20)	4989(4)	3363(4)	2749(3)	30(1)
C(21)	3519(4)	2776(4)	2219(4)	32(1)
C(22)	2787(4)	3463(4)	2013(3)	29(1)
C(23)	3496(4)	4757(3)	2332(3)	22(1)
C(24)	7385(4)	5268(4)	3669(3)	28(1)
C(25)	8128(4)	4847(4)	2918(4)	37(1)
C(26)	7786(5)	4957(5)	4643(4)	42(1)
C(27)	2662(4)	5499(4)	2104(3)	24(1)
C(28)	2382(5)	6164(5)	3073(3)	36(1)
C(29)	1239(4)	4708(4)	1165(3)	35(1)
C(30)	9406(4)	8224(4)	3560(3)	35(1)
C(31)	9000(4)	7208(4)	1721(4)	35(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_060m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi(1)	33(1)	23(1)	17(1)	4(1)	2(1)	13(1)
Ga(1)	14(1)	16(1)	15(1)	3(1)	4(1)	3(1)
N(1)	20(1)	16(1)	17(1)	2(1)	4(1)	4(1)
N(2)	14(1)	21(1)	14(1)	5(1)	3(1)	5(1)
N(3)	16(1)	34(2)	26(2)	6(1)	8(1)	7(1)
C(1)	19(2)	20(2)	21(2)	0(1)	3(1)	5(1)
C(2)	22(2)	28(2)	14(2)	0(1)	4(1)	6(1)
C(3)	16(2)	30(2)	15(2)	6(1)	3(1)	7(1)
C(4)	38(2)	23(2)	25(2)	−3(2)	6(2)	9(2)
C(5)	28(2)	37(2)	18(2)	10(2)	7(2)	9(2)
C(6)	27(2)	17(2)	23(2)	4(1)	8(1)	5(1)
C(7)	29(2)	22(2)	34(2)	11(2)	8(2)	3(2)
C(8)	42(2)	24(2)	38(2)	16(2)	14(2)	6(2)
C(9)	58(3)	29(2)	38(2)	16(2)	18(2)	20(2)
C(10)	42(2)	33(2)	38(2)	15(2)	15(2)	22(2)
C(11)	30(2)	23(2)	27(2)	9(2)	11(2)	14(2)
C(12)	25(2)	43(3)	67(3)	33(3)	11(2)	0(2)
C(13)	40(3)	53(3)	93(5)	36(3)	34(3)	17(2)
C(14)	37(3)	78(5)	67(4)	32(4)	−2(3)	−20(3)
C(15)	25(2)	32(2)	33(2)	16(2)	14(2)	15(2)
C(16)	35(2)	52(3)	32(2)	10(2)	14(2)	17(2)
C(17)	31(2)	39(2)	33(2)	7(2)	13(2)	10(2)
C(18)	20(2)	21(2)	17(2)	9(1)	7(1)	6(1)
C(19)	21(2)	26(2)	23(2)	12(1)	7(1)	8(1)
C(20)	31(2)	26(2)	37(2)	18(2)	14(2)	12(2)
C(21)	29(2)	22(2)	41(2)	14(2)	13(2)	5(2)
C(22)	20(2)	27(2)	33(2)	11(2)	10(2)	3(2)
C(23)	18(2)	25(2)	21(2)	9(1)	7(1)	6(1)
C(24)	20(2)	29(2)	33(2)	15(2)	4(2)	9(2)
C(25)	24(2)	38(2)	47(3)	15(2)	11(2)	14(2)
C(26)	35(2)	48(3)	40(2)	25(2)	3(2)	16(2)
C(27)	17(2)	26(2)	24(2)	9(1)	4(1)	6(1)
C(28)	30(2)	50(3)	28(2)	8(2)	7(2)	23(2)
C(29)	24(2)	41(2)	27(2)	8(2)	0(2)	12(2)
C(30)	18(2)	42(2)	32(2)	10(2)	2(2)	7(2)
C(31)	24(2)	40(2)	40(2)	10(2)	17(2)	12(2)

Table 4: Bond lengths [Å] for mw_060m.

Bi(1)–Ga(1)	2.6963(4)
Bi(1)–Bi(1)#1	2.8235(3)
Ga(1)–N(3)	1.867(3)
Ga(1)–N(1)	1.991(3)
Ga(1)–N(2)	1.993(3)
N(1)–C(1)	1.336(5)
N(1)–C(6)	1.447(5)
N(2)–C(3)	1.330(4)
N(2)–C(18)	1.443(4)
N(3)–C(31)	1.443(5)
N(3)–C(30)	1.445(5)
C(1)–C(2)	1.400(6)
C(1)–C(4)	1.514(5)
C(2)–C(3)	1.400(5)
C(3)–C(5)	1.515(5)
C(6)–C(7)	1.394(5)
C(6)–C(11)	1.407(5)
C(7)–C(8)	1.397(6)
C(7)–C(12)	1.509(7)
C(8)–C(9)	1.376(7)
C(9)–C(10)	1.383(7)
C(10)–C(11)	1.382(6)
C(11)–C(15)	1.525(5)
C(12)–C(14)	1.526(8)
C(12)–C(13)	1.541(9)
C(15)–C(17)	1.521(6)
C(15)–C(16)	1.521(6)
C(18)–C(19)	1.395(5)
C(18)–C(23)	1.413(5)
C(19)–C(20)	1.401(5)
C(19)–C(24)	1.527(5)
C(20)–C(21)	1.381(6)
C(21)–C(22)	1.375(6)
C(22)–C(23)	1.390(5)
C(23)–C(27)	1.520(5)
C(24)–C(25)	1.533(6)
C(24)–C(26)	1.538(6)
C(27)–C(28)	1.526(6)
C(27)–C(29)	1.528(5)

#1 -x+1,-y+1,-z

Table 5: Bond angles [°] for mw_060m.

Ga(1)–Bi(1)–Bi(1)#1	92.509(11)
N(3)–Ga(1)–N(1)	107.69(14)
N(3)–Ga(1)–N(2)	105.96(13)
N(1)–Ga(1)–N(2)	93.06(12)
N(3)–Ga(1)–Bi(1)	115.55(10)
N(1)–Ga(1)–Bi(1)	112.96(9)
N(2)–Ga(1)–Bi(1)	119.01(8)
C(1)–N(1)–C(6)	118.5(3)
C(1)–N(1)–Ga(1)	121.1(3)
C(6)–N(1)–Ga(1)	120.4(2)
C(3)–N(2)–C(18)	120.1(3)
C(3)–N(2)–Ga(1)	120.8(2)
C(18)–N(2)–Ga(1)	118.8(2)
C(31)–N(3)–C(30)	112.0(3)
C(31)–N(3)–Ga(1)	124.2(3)
C(30)–N(3)–Ga(1)	122.9(3)
N(1)–C(1)–C(2)	123.4(3)
N(1)–C(1)–C(4)	119.7(3)
C(2)–C(1)–C(4)	117.0(3)
C(3)–C(2)–C(1)	128.0(3)
N(2)–C(3)–C(2)	123.9(3)
N(2)–C(3)–C(5)	119.9(3)
C(2)–C(3)–C(5)	116.2(3)
C(7)–C(6)–C(11)	121.6(4)
C(7)–C(6)–N(1)	120.7(3)
C(11)–C(6)–N(1)	117.7(3)
C(6)–C(7)–C(8)	117.8(4)
C(6)–C(7)–C(12)	123.5(4)
C(8)–C(7)–C(12)	118.6(4)
C(9)–C(8)–C(7)	121.3(4)
C(8)–C(9)–C(10)	119.8(4)
C(11)–C(10)–C(9)	121.3(4)
C(10)–C(11)–C(6)	118.0(4)
C(10)–C(11)–C(15)	120.1(4)
C(6)–C(11)–C(15)	121.9(3)
C(7)–C(12)–C(14)	112.2(5)
C(7)–C(12)–C(13)	110.6(4)
C(14)–C(12)–C(13)	110.9(5)
C(17)–C(15)–C(16)	110.2(3)
C(17)–C(15)–C(11)	112.4(3)
C(16)–C(15)–C(11)	111.6(3)
C(19)–C(18)–C(23)	121.7(3)
C(19)–C(18)–N(2)	120.4(3)
C(23)–C(18)–N(2)	117.9(3)
C(18)–C(19)–C(20)	118.0(3)
C(18)–C(19)–C(24)	123.2(3)
C(20)–C(19)–C(24)	118.8(3)
C(21)–C(20)–C(19)	120.9(4)
C(22)–C(21)–C(20)	120.4(4)
C(21)–C(22)–C(23)	121.3(4)
C(22)–C(23)–C(18)	117.8(3)
C(22)–C(23)–C(27)	120.4(3)
C(18)–C(23)–C(27)	121.8(3)

Table 5: (continued)

C(19)–C(24)–C(25)	110.8(3)
C(19)–C(24)–C(26)	111.6(3)
C(25)–C(24)–C(26)	109.8(4)
C(23)–C(27)–C(28)	112.2(3)
C(23)–C(27)–C(29)	113.5(3)
C(28)–C(27)–C(29)	109.2(3)

#1 -x+1,-y+1,-z

Crystal structure of mw_117_10m

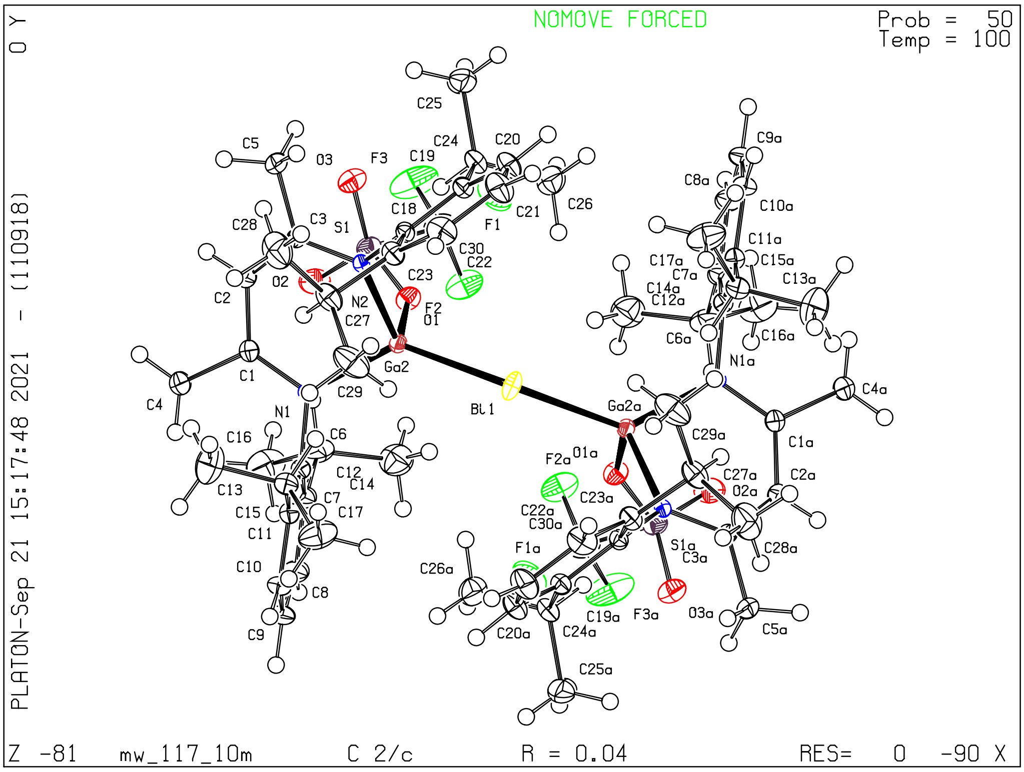

Table 1: Crystal data and structure refinement for mw_117_10m.

Identification code	mw_117_10m
Empirical Formula	$C_{60}\,H_{82}\,Bi\,F_6\,Ga_2\,N_4\,O_6\,S_2$
Formula weight	1481.83 Da
Density (calculated)	$1.501\,\mathrm{g\cdot cm^{-3}}$
$F(000)$	2996
Temperature	100(2) K
Crystal size	0.148 × 0.141 × 0.108 mm
Crystal appearance	orange tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$C2/c$
Unit cell dimensions	$a = 21.384(4)$ Å
	$b = 12.297(2)$ Å
	$c = 25.544(5)$ Å
	$\alpha = 90°$
	$\beta = 102.543(4)°$
	$\gamma = 90°$
Unit cell volume	6557(2) $Å^3$
Z	4
Cell measurement refections used	9909
θ range for cell measurement	2.17° to 28.98°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.922° to 33.353°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.7%)
Index ranges	$-33 \leq h \leq 32$
	$-18 \leq k \leq 18$
	$-38 \leq l \leq 39$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$3.623\,\mathrm{mm^{-1}}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.60
R_{merg} before/after correction	0.0812/0.0596
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	120726
Independent reflections	12655 ($R_{int} = 0.0715$)
Reflections with $I > 2\sigma(I)$	10474
Data / retraints / parameter	12655 / 0 / 376
Goodness-of-fit on F^2	1.107
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 29.9284P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0396$
	$wR2 = 0.0913$
R indices [all data]	$R1 = 0.0544$
	$wR2 = 0.0962$
Largest diff. peak and hole	1.889 and -1.449 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_117_10m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Bi(1)	5000	8177(1)	7500	19(1)
Ga(2)	4973(1)	7013(1)	6607(1)	12(1)
S(1)	5673(1)	4828(1)	6275(1)	19(1)
F(1)	6533(1)	4345(2)	7141(1)	40(1)
F(2)	5682(1)	3358(2)	7026(1)	34(1)
F(3)	6367(1)	3103(2)	6530(1)	48(1)
O(1)	5381(1)	5549(2)	6628(1)	19(1)
O(2)	5213(1)	4181(2)	5915(1)	32(1)
O(3)	6175(1)	5327(2)	6071(1)	24(1)
N(1)	4269(1)	6802(2)	5997(1)	16(1)
N(2)	5518(1)	7835(2)	6239(1)	13(1)
C(1)	4418(1)	6711(2)	5515(1)	18(1)
C(2)	5020(1)	6977(2)	5410(1)	16(1)
C(3)	5512(1)	7573(2)	5728(1)	15(1)
C(4)	3920(2)	6293(3)	5044(1)	26(1)
C(5)	6067(2)	7919(3)	5489(1)	22(1)
C(6)	3607(1)	6640(3)	6039(1)	19(1)
C(7)	3383(2)	5580(3)	6102(1)	23(1)
C(8)	2738(2)	5455(3)	6125(1)	29(1)
C(9)	2333(2)	6338(4)	6081(1)	32(1)
C(10)	2563(2)	7375(3)	6021(1)	28(1)
C(11)	3202(2)	7556(3)	6008(1)	22(1)
C(12)	3817(2)	4596(3)	6148(2)	28(1)
C(13)	3521(2)	3665(3)	5776(2)	43(1)
C(14)	3999(2)	4201(4)	6733(2)	39(1)
C(15)	3436(2)	8708(3)	5949(1)	24(1)
C(16)	3346(3)	9024(4)	5360(2)	45(1)
C(17)	3115(2)	9547(4)	6245(2)	42(1)
C(18)	5923(1)	8678(2)	6525(1)	14(1)
C(19)	6487(1)	8403(2)	6899(1)	17(1)
C(20)	6823(2)	9232(3)	7212(1)	24(1)
C(21)	6606(2)	10294(3)	7168(2)	29(1)
C(22)	6054(2)	10552(3)	6795(2)	26(1)
C(23)	5706(1)	9766(2)	6462(1)	18(1)
C(24)	6744(1)	7254(3)	6962(1)	20(1)
C(25)	7366(2)	7156(3)	6762(2)	32(1)
C(26)	6838(2)	6859(3)	7541(2)	31(1)
C(27)	5127(2)	10126(3)	6041(1)	24(1)
C(28)	5347(2)	10784(3)	5602(2)	40(1)
C(29)	4665(2)	10798(3)	6284(2)	39(1)
C(30)	6088(2)	3860(3)	6779(2)	27(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_117_10m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi(1)	33(1)	13(1)	12(1)	0	8(1)	0
Ga(2)	13(1)	13(1)	11(1)	−1(1)	3(1)	−1(1)
S(1)	20(1)	17(1)	21(1)	−5(1)	7(1)	0(1)
F(1)	28(1)	41(1)	47(1)	12(1)	−4(1)	4(1)
F(2)	42(1)	21(1)	45(1)	4(1)	23(1)	0(1)
F(3)	61(2)	22(1)	76(2)	7(1)	44(2)	18(1)
O(1)	22(1)	16(1)	21(1)	−1(1)	7(1)	4(1)
O(2)	25(1)	37(1)	35(1)	−19(1)	11(1)	−8(1)
O(3)	26(1)	22(1)	27(1)	−3(1)	12(1)	−2(1)
N(1)	13(1)	22(1)	13(1)	−2(1)	3(1)	−2(1)
N(2)	11(1)	16(1)	10(1)	0(1)	1(1)	−1(1)
C(1)	16(1)	22(1)	15(1)	−3(1)	2(1)	−1(1)
C(2)	16(1)	20(1)	13(1)	−2(1)	4(1)	−1(1)
C(3)	14(1)	17(1)	14(1)	3(1)	4(1)	1(1)
C(4)	19(1)	42(2)	17(1)	−7(1)	3(1)	−7(1)
C(5)	18(1)	31(2)	17(1)	0(1)	6(1)	−4(1)
C(6)	13(1)	29(1)	14(1)	−3(1)	3(1)	−2(1)
C(7)	18(1)	32(2)	20(1)	−6(1)	6(1)	−8(1)
C(8)	20(2)	43(2)	26(2)	−7(1)	8(1)	−13(1)
C(9)	13(1)	59(2)	23(2)	−7(2)	5(1)	−8(1)
C(10)	12(1)	52(2)	21(2)	−3(1)	4(1)	2(1)
C(11)	15(1)	35(2)	14(1)	−3(1)	2(1)	2(1)
C(12)	26(2)	27(2)	34(2)	−5(1)	14(1)	−8(1)
C(13)	46(2)	35(2)	53(3)	−17(2)	22(2)	−16(2)
C(14)	38(2)	39(2)	42(2)	9(2)	11(2)	−4(2)
C(15)	17(1)	33(2)	21(1)	0(1)	4(1)	5(1)
C(16)	62(3)	46(2)	28(2)	8(2)	10(2)	2(2)
C(17)	41(2)	39(2)	51(3)	−8(2)	24(2)	6(2)
C(18)	14(1)	16(1)	13(1)	−1(1)	2(1)	−4(1)
C(19)	15(1)	20(1)	16(1)	0(1)	2(1)	−2(1)
C(20)	18(1)	26(1)	24(2)	−2(1)	−3(1)	−5(1)
C(21)	27(2)	24(2)	32(2)	−5(1)	−2(1)	−10(1)
C(22)	28(2)	17(1)	34(2)	1(1)	5(1)	−4(1)
C(23)	18(1)	17(1)	20(1)	4(1)	1(1)	−2(1)
C(24)	15(1)	22(1)	20(1)	0(1)	−2(1)	1(1)
C(25)	25(2)	42(2)	30(2)	6(2)	9(1)	11(1)
C(26)	33(2)	33(2)	28(2)	9(1)	9(1)	9(2)
C(27)	23(2)	18(1)	28(2)	4(1)	−2(1)	0(1)
C(28)	43(2)	37(2)	36(2)	17(2)	−2(2)	−3(2)
C(29)	28(2)	32(2)	52(3)	−1(2)	−2(2)	7(2)
C(30)	29(2)	16(1)	39(2)	4(1)	16(2)	4(1)

Table 4: Bond lengths [Å] for mw_117_10m.

Bi(1)–Ga(2)#1	2.6817(5)
Bi(1)–Ga(2)	2.6817(5)
Ga(2)–N(2)	1.933(2)
Ga(2)–N(1)	1.936(2)
Ga(2)–O(1)	1.996(2)
S(1)–O(3)	1.430(2)
S(1)–O(2)	1.432(2)
S(1)–O(1)	1.494(2)
S(1)–C(30)	1.835(4)
F(1)–C(30)	1.317(4)
F(2)–C(30)	1.329(4)
F(3)–C(30)	1.339(4)
N(1)–C(1)	1.341(4)
N(1)–C(6)	1.457(4)
N(2)–C(3)	1.341(4)
N(2)–C(18)	1.445(3)
C(1)–C(2)	1.410(4)
C(1)–C(4)	1.514(4)
C(2)–C(3)	1.388(4)
C(3)–C(5)	1.509(4)
C(6)–C(7)	1.409(4)
C(6)–C(11)	1.412(4)
C(7)–C(8)	1.402(4)
C(7)–C(12)	1.513(5)
C(8)–C(9)	1.378(6)
C(9)–C(10)	1.387(6)
C(10)–C(11)	1.392(4)
C(11)–C(15)	1.520(5)
C(12)–C(13)	1.534(5)
C(12)–C(14)	1.540(6)
C(15)–C(16)	1.525(5)
C(15)–C(17)	1.527(5)
C(18)–C(19)	1.407(4)
C(18)–C(23)	1.414(4)
C(19)–C(20)	1.394(4)
C(19)–C(24)	1.512(4)
C(20)–C(21)	1.384(5)
C(21)–C(22)	1.383(5)
C(22)–C(23)	1.392(4)
C(23)–C(27)	1.519(4)
C(24)–C(26)	1.529(5)
C(24)–C(25)	1.531(5)
C(27)–C(29)	1.519(5)
C(27)–C(28)	1.538(5)

#1 -x+1,y,-z+3/2

Table 5: Bond angles [°] for mw_117_10m.

Ga(2)#1–Bi(1)–Ga(2)	115.54(2)
N(2)–Ga(2)–N(1)	97.07(10)
N(2)–Ga(2)–O(1)	100.25(9)
N(1)–Ga(2)–O(1)	99.15(10)
N(2)–Ga(2)–Bi(1)	103.40(7)
N(1)–Ga(2)–Bi(1)	128.73(7)
O(1)–Ga(2)–Bi(1)	122.02(6)
O(3)–S(1)–O(2)	117.90(15)
O(3)–S(1)–O(1)	114.17(13)
O(2)–S(1)–O(1)	113.56(14)
O(3)–S(1)–C(30)	104.32(15)
O(2)–S(1)–C(30)	104.53(17)
O(1)–S(1)–C(30)	99.45(14)
S(1)–O(1)–Ga(2)	139.21(14)
C(1)–N(1)–C(6)	119.0(2)
C(1)–N(1)–Ga(2)	116.87(19)
C(6)–N(1)–Ga(2)	123.85(18)
C(3)–N(2)–C(18)	122.9(2)
C(3)–N(2)–Ga(2)	117.95(18)
C(18)–N(2)–Ga(2)	119.10(17)
N(1)–C(1)–C(2)	124.3(3)
N(1)–C(1)–C(4)	119.4(3)
C(2)–C(1)–C(4)	116.3(3)
C(3)–C(2)–C(1)	128.1(3)
N(2)–C(3)–C(2)	122.8(3)
N(2)–C(3)–C(5)	118.9(3)
C(2)–C(3)–C(5)	118.3(3)
C(7)–C(6)–C(11)	121.7(3)
C(7)–C(6)–N(1)	119.7(3)
C(11)–C(6)–N(1)	118.6(3)
C(8)–C(7)–C(6)	117.9(3)
C(8)–C(7)–C(12)	120.1(3)
C(6)–C(7)–C(12)	122.0(3)
C(9)–C(8)–C(7)	121.1(3)
C(8)–C(9)–C(10)	120.1(3)
C(9)–C(10)–C(11)	121.5(3)
C(10)–C(11)–C(6)	117.6(3)
C(10)–C(11)–C(15)	119.8(3)
C(6)–C(11)–C(15)	122.6(3)
C(7)–C(12)–C(13)	112.7(3)
C(7)–C(12)–C(14)	110.4(3)
C(13)–C(12)–C(14)	110.5(3)
C(11)–C(15)–C(16)	111.2(3)
C(11)–C(15)–C(17)	112.8(3)
C(16)–C(15)–C(17)	110.0(3)
C(19)–C(18)–C(23)	121.1(3)
C(19)–C(18)–N(2)	120.2(2)
C(23)–C(18)–N(2)	118.4(2)
C(20)–C(19)–C(18)	118.2(3)
C(20)–C(19)–C(24)	119.5(3)
C(18)–C(19)–C(24)	122.3(3)
C(21)–C(20)–C(19)	121.5(3)
C(22)–C(21)–C(20)	119.6(3)

Table 5: (continued)

C(21)–C(22)–C(23)	121.6(3)
C(22)–C(23)–C(18)	118.0(3)
C(22)–C(23)–C(27)	118.3(3)
C(18)–C(23)–C(27)	123.6(3)
C(19)–C(24)–C(26)	111.6(3)
C(19)–C(24)–C(25)	111.1(3)
C(26)–C(24)–C(25)	110.9(3)
C(29)–C(27)–C(23)	111.9(3)
C(29)–C(27)–C(28)	109.9(3)
C(23)–C(27)–C(28)	109.8(3)
F(1)–C(30)–F(2)	108.9(3)
F(1)–C(30)–F(3)	108.7(3)
F(2)–C(30)–F(3)	107.9(3)
F(1)–C(30)–S(1)	111.4(2)
F(2)–C(30)–S(1)	111.6(2)
F(3)–C(30)–S(1)	108.4(3)

#1 -x+1,y,-z+3/2

Crystal structure of mw_117_1film

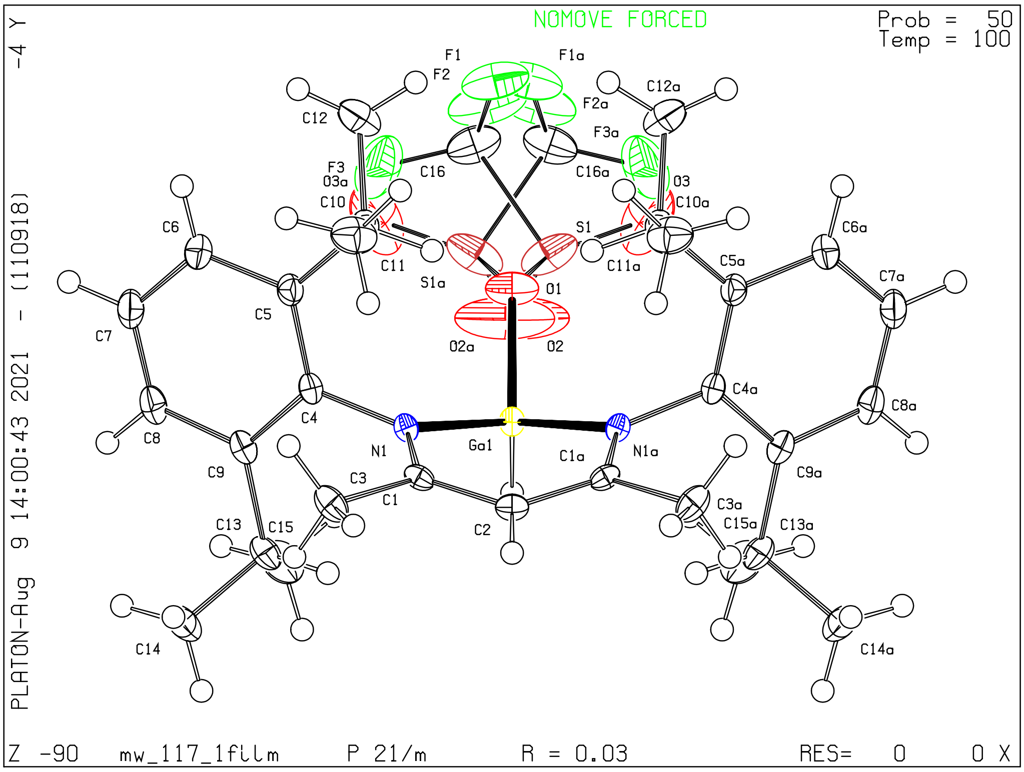

Table 1: Crystal data and structure refinement for mw_117_1film.

Identification code	mw_117_1film
Empirical Formula	$C_{30}\,H_{42}\,F_3\,Ga\,N_2\,O_3\,S$
Formula weight	637.43 Da
Density (calculated)	$1.346\,g\cdot cm^{-3}$
$F(000)$	668
Temperature	100(2) K
Crystal size	$0.305\times0.240\times0.182$ mm
Crystal appearance	colourless block
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/m$
Unit cell dimensions	$a = 8.9025(4)$ Å
	$b = 19.9339(9)$ Å
	$c = 9.8991(5)$ Å
	$\alpha = 90°$
	$\beta = 116.4691(11)°$
	$\gamma = 90°$
Unit cell volume	1572.56(13) $Å^3$
Z	2
Cell measurement refections used	9240
θ range for cell measurement	2.52° to 33.43°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	2.043° to 33.581°
Completeness to $\theta = 25.242°$ (to θ_{max})	100.0% (99.2%)
Index ranges	$-13\le h\le 13$
	$-30\le k\le 30$
	$-15\le l\le 15$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$0.991\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.67
R_{merg} before/after correction	0.0523/0.0327
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	57529
Independent reflections	6296 ($R_{int} = 0.0207$)
Reflections with $I > 2\sigma(I)$	5891
Data / retraints / parameter	6296 / 60 / 224
Goodness-of-fit on F^2	1.074
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0450P)^2 + 0.7876P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0305$
	$wR2 = 0.0840$
R indices [all data]	$R1 = 0.0332$
	$wR2 = 0.0858$
Largest diff. peak and hole	2.838 and -0.623 $Å^{-3}$

Comments

The electron desity near H1 is indecisive. The found sum formula and composition should be confirmed by other analytical means.

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The coordinates of the Ga–H hydrogen atom were refined freely.

Disorder

The triflate group is disordered over a mirror plane. Its local symmetry was ignored in the refinement (negative `PART`). Solving the strucutre in the corresponding non-centrosymmetric subgroup without the mirror plane did not resolve the disorder thus this model was discarded. The O–S–O bond angles were restrained to be equal (`SADI`) and `RIGU` restraints were applied to the displacement parameters of the triflate's atoms.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_117_1film. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Ga(1)	4784(1)	2500	2187(1)	12(1)
O(1)	6561(2)	2500	1584(1)	29(1)
C(1)	5060(1)	3131(1)	4830(1)	14(1)
N(1)	5291(1)	3221(1)	3593(1)	13(1)
C(2)	4818(2)	2500	5328(2)	15(1)
C(4)	5743(1)	3870(1)	3242(1)	14(1)
C(3)	5051(2)	3731(1)	5749(1)	22(1)
C(5)	7455(1)	4011(1)	3718(1)	17(1)
C(7)	6637(2)	5097(1)	2489(1)	24(1)
C(6)	7872(2)	4636(1)	3338(1)	22(1)
C(9)	4475(1)	4329(1)	2382(1)	17(1)
C(8)	4961(2)	4942(1)	2004(1)	22(1)
C(10)	8811(1)	3503(1)	4616(1)	21(1)
C(11)	9401(2)	3577(1)	6318(2)	31(1)
C(12)	10331(2)	3542(1)	4284(2)	33(1)
C(13)	2627(1)	4178(1)	1845(1)	20(1)
C(14)	1740(2)	4740(1)	2273(2)	29(1)
C(15)	1755(2)	4065(1)	131(2)	31(1)
S(1)	6435(1)	2246(1)	70(1)	37(1)
F(1)	9558(2)	2614(4)	1165(2)	49(2)
C(16)	8105(4)	2761(2)	46(3)	36(1)
F(3)	7810(5)	3408(2)	159(4)	62(1)
O(3)	6953(7)	1577(2)	21(6)	80(2)
F(2)	8190(3)	2665(2)	−1246(2)	63(2)
O(2)	4945(3)	2550(9)	−1129(2)	80(2)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_117_1film.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ga(1)	16(1)	12(1)	8(1)	0	5(1)	0
O(1)	24(1)	55(1)	12(1)	0	12(1)	0
C(1)	13(1)	18(1)	11(1)	−2(1)	5(1)	3(1)
N(1)	15(1)	12(1)	11(1)	0(1)	5(1)	2(1)
C(2)	15(1)	21(1)	11(1)	0	7(1)	0
C(4)	18(1)	11(1)	13(1)	−1(1)	6(1)	2(1)
C(3)	26(1)	22(1)	16(1)	−5(1)	10(1)	6(1)
C(5)	18(1)	13(1)	19(1)	−2(1)	6(1)	0(1)
C(7)	34(1)	13(1)	29(1)	1(1)	18(1)	0(1)
C(6)	25(1)	15(1)	28(1)	−3(1)	13(1)	−3(1)
C(9)	21(1)	14(1)	15(1)	1(1)	7(1)	4(1)
C(8)	30(1)	14(1)	22(1)	3(1)	13(1)	5(1)
C(10)	16(1)	15(1)	25(1)	−2(1)	4(1)	−1(1)
C(11)	24(1)	41(1)	25(1)	9(1)	7(1)	6(1)
C(12)	30(1)	36(1)	38(1)	2(1)	18(1)	11(1)
C(13)	19(1)	19(1)	19(1)	4(1)	6(1)	7(1)
C(14)	29(1)	26(1)	36(1)	6(1)	17(1)	12(1)
C(15)	27(1)	36(1)	21(1)	2(1)	1(1)	9(1)
S(1)	42(1)	61(1)	20(1)	−19(1)	23(1)	−27(1)
F(1)	31(1)	87(5)	33(1)	−4(1)	17(1)	−14(1)
C(16)	35(1)	56(2)	24(1)	4(1)	20(1)	−9(1)
F(3)	87(2)	44(1)	68(2)	15(1)	45(2)	−13(2)
O(3)	140(5)	56(2)	92(3)	−49(2)	96(4)	−43(3)
F(2)	51(1)	122(5)	30(1)	2(1)	31(1)	−21(2)
O(2)	33(1)	194(6)	14(1)	24(4)	11(1)	10(5)

Table 4: Bond lengths [Å] for mw_117_1film.

Ga(1)–N(1)#1	1.9099(8)
Ga(1)–N(1)	1.9099(8)
Ga(1)–O(1)	1.9241(12)
O(1)–S(1)	1.5375(12)
C(1)–N(1)	1.3412(12)
C(1)–C(2)	1.4025(12)
C(1)–C(3)	1.5047(14)
N(1)–C(4)	1.4431(13)
C(4)–C(9)	1.4071(14)
C(4)–C(5)	1.4086(14)
C(5)–C(6)	1.3995(15)
C(5)–C(10)	1.5217(15)
C(7)–C(8)	1.3833(18)
C(7)–C(6)	1.3909(17)
C(9)–C(8)	1.4010(15)
C(9)–C(13)	1.5164(16)
C(10)–C(12)	1.5304(19)
C(10)–C(11)	1.5320(18)
C(13)–C(15)	1.5350(17)
C(13)–C(14)	1.5358(17)
S(1)–O(3)	1.419(5)
S(1)–O(2)	1.460(7)
S(1)–C(16)	1.815(3)
F(1)–C(16)	1.307(4)
C(16)–F(2)	1.329(3)
C(16)–F(3)	1.332(5)

#1 x,-y+1/2,z

Table 5: Bond angles [°] for mw_117_1film.

N(1)#1–Ga(1)–N(1)	97.60(5)
N(1)#1–Ga(1)–O(1)	105.43(4)
N(1)–Ga(1)–O(1)	105.43(4)
S(1)–O(1)–Ga(1)	126.09(8)
N(1)–C(1)–C(2)	123.40(9)
N(1)–C(1)–C(3)	119.34(9)
C(2)–C(1)–C(3)	117.26(9)
C(1)–N(1)–C(4)	120.81(8)
C(1)–N(1)–Ga(1)	118.86(7)
C(4)–N(1)–Ga(1)	120.00(6)
C(1)#1–C(2)–C(1)	127.58(12)
C(9)–C(4)–C(5)	121.99(9)
C(9)–C(4)–N(1)	119.62(9)
C(5)–C(4)–N(1)	118.32(9)
C(6)–C(5)–C(4)	117.69(10)
C(6)–C(5)–C(10)	120.91(10)
C(4)–C(5)–C(10)	121.40(9)
C(8)–C(7)–C(6)	120.18(10)
C(7)–C(6)–C(5)	121.14(11)
C(8)–C(9)–C(4)	117.93(10)
C(8)–C(9)–C(13)	119.70(9)
C(4)–C(9)–C(13)	122.36(9)
C(7)–C(8)–C(9)	121.04(10)
C(5)–C(10)–C(12)	112.80(10)
C(5)–C(10)–C(11)	111.86(10)
C(12)–C(10)–C(11)	109.21(10)
C(9)–C(13)–C(15)	110.61(10)
C(9)–C(13)–C(14)	111.67(10)
C(15)–C(13)–C(14)	110.04(10)
O(3)–S(1)–O(2)	123.6(6)
O(3)–S(1)–O(1)	117.4(2)
O(2)–S(1)–O(1)	107.5(4)
O(3)–S(1)–C(16)	104.5(2)
O(2)–S(1)–C(16)	101.9(5)
O(1)–S(1)–C(16)	97.00(11)
F(1)–C(16)–F(2)	108.9(3)
F(1)–C(16)–F(3)	107.6(4)
F(2)–C(16)–F(3)	108.5(3)
F(1)–C(16)–S(1)	111.7(3)
F(2)–C(16)–S(1)	109.3(2)
F(3)–C(16)–S(1)	110.7(2)

#1 x,-y+1/2,z

Crystal structure of mw_085_1m

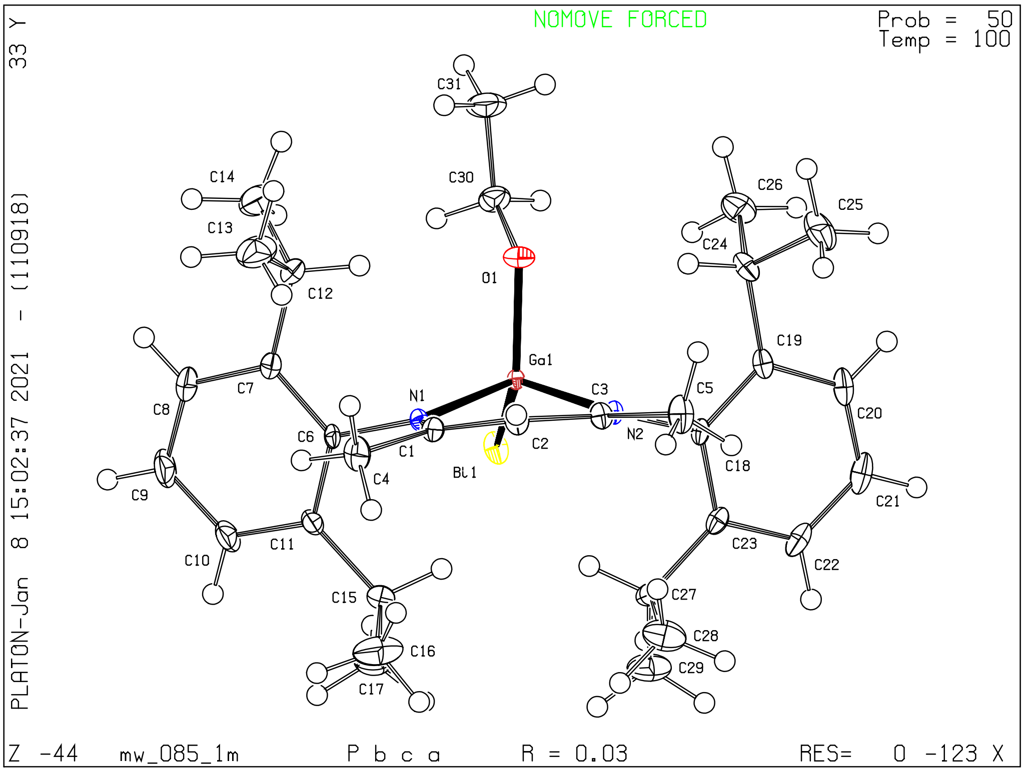

Table 1: Crystal data and structure refinement for mw_085_1m.

Identification code	mw_085_1m
Empirical Formula	$C_{62}\,H_{92}\,Bi_2\,Ga_2\,N_4\,O_2$
Formula weight	1482.79 Da
Density (calculated)	$1.563\,\mathrm{g\cdot cm^{-3}}$
$F(000)$	2944
Temperature	100(2) K
Crystal size	0.357 × 0.288 × 0.180 mm
Crystal appearance	red block
Wavelength (MoK_α)	0.71073 Å
Crystal system	Orthorhombic
Space group	*Pbca*
Unit cell dimensions	$a = 16.0046(5)$ Å
	$b = 18.5086(6)$ Å
	$c = 21.2763(6)$ Å
	$\alpha = 90°$
	$\beta = 90°$
	$\gamma = 90°$
Unit cell volume	6302.5(3) $Å^3$
Z	4
Cell measurement refections used	9752
θ range for cell measurement	2.20° to 34.87°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.914° to 36.428°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.8%)
Index ranges	$-26 \le h \le 26$
	$-30 \le k \le 30$
	$-35 \le l \le 35$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$6.455\,\mathrm{mm^{-1}}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.48
R_{merg} before/after correction	0.1098/0.0571
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	481040
Independent reflections	15367 ($R_{int} = 0.0655$)
Reflections with $I > 2\sigma(I)$	12607
Data / retraints / parameter	15367 / 0 / 336
Goodness-of-fit on F^2	1.159
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0150P)^2 + 8.4138P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0255$
	$wR2 = 0.0483$
R indices [all data]	$R1 = 0.0412$
	$wR2 = 0.0530$
Largest diff. peak and hole	1.634 and -1.438 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_085_1m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Bi(1)	4511(1)	5168(1)	4472(1)	15(1)
Ga(1)	5830(1)	5719(1)	3860(1)	8(1)
O(1)	6575(1)	5088(1)	3501(1)	16(1)
N(1)	5475(1)	6366(1)	3167(1)	10(1)
N(2)	6608(1)	6411(1)	4236(1)	9(1)
C(1)	5940(1)	6921(1)	2987(1)	12(1)
C(2)	6672(1)	7134(1)	3295(1)	14(1)
C(3)	6964(1)	6924(1)	3886(1)	12(1)
C(4)	5701(1)	7379(1)	2426(1)	20(1)
C(5)	7733(1)	7303(1)	4126(1)	20(1)
C(6)	4702(1)	6202(1)	2852(1)	10(1)
C(7)	4704(1)	5724(1)	2339(1)	17(1)
C(8)	3941(1)	5578(1)	2045(1)	24(1)
C(9)	3204(1)	5875(1)	2255(1)	26(1)
C(10)	3211(1)	6323(1)	2775(1)	21(1)
C(11)	3950(1)	6492(1)	3088(1)	14(1)
C(12)	5500(1)	5372(1)	2101(1)	23(1)
C(13)	5875(2)	5771(2)	1541(1)	33(1)
C(14)	5362(2)	4582(1)	1918(1)	34(1)
C(15)	3933(1)	6963(1)	3670(1)	21(1)
C(16)	4058(2)	7756(1)	3523(2)	39(1)
C(17)	3138(2)	6869(1)	4059(1)	31(1)
C(18)	6798(1)	6347(1)	4893(1)	11(1)
C(19)	7442(1)	5897(1)	5105(1)	14(1)
C(20)	7556(1)	5830(1)	5754(1)	21(1)
C(21)	7053(1)	6188(1)	6177(1)	25(1)
C(22)	6416(1)	6628(1)	5958(1)	21(1)
C(23)	6277(1)	6720(1)	5316(1)	14(1)
C(24)	8005(1)	5479(1)	4665(1)	17(1)
C(25)	8927(1)	5657(1)	4777(1)	30(1)
C(26)	7861(1)	4667(1)	4731(1)	26(1)
C(27)	5588(1)	7212(1)	5084(1)	18(1)
C(28)	5911(2)	7980(1)	4976(1)	30(1)
C(29)	4825(1)	7229(1)	5511(1)	30(1)
C(30)	6403(1)	4350(1)	3430(1)	21(1)
C(31)	7056(2)	4018(1)	3005(1)	34(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_085_1m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi(1)	10(1)	21(1)	15(1)	7(1)	0(1)	−5(1)
Ga(1)	8(1)	9(1)	7(1)	1(1)	0(1)	−1(1)
O(1)	16(1)	13(1)	19(1)	0(1)	5(1)	3(1)
N(1)	9(1)	11(1)	8(1)	2(1)	−1(1)	0(1)
N(2)	9(1)	12(1)	8(1)	1(1)	−1(1)	−2(1)
C(1)	14(1)	12(1)	9(1)	3(1)	1(1)	0(1)
C(2)	14(1)	16(1)	13(1)	5(1)	0(1)	−5(1)
C(3)	10(1)	13(1)	13(1)	2(1)	0(1)	−3(1)
C(4)	26(1)	20(1)	14(1)	9(1)	−3(1)	−2(1)
C(5)	16(1)	24(1)	20(1)	5(1)	−3(1)	−12(1)
C(6)	10(1)	14(1)	7(1)	2(1)	−2(1)	0(1)
C(7)	17(1)	23(1)	12(1)	−3(1)	−4(1)	3(1)
C(8)	23(1)	31(1)	19(1)	−6(1)	−9(1)	−1(1)
C(9)	17(1)	38(1)	25(1)	−1(1)	−11(1)	−2(1)
C(10)	11(1)	32(1)	21(1)	1(1)	−4(1)	3(1)
C(11)	11(1)	19(1)	14(1)	1(1)	−2(1)	3(1)
C(12)	22(1)	31(1)	16(1)	−10(1)	−4(1)	8(1)
C(13)	26(1)	41(1)	32(1)	−11(1)	10(1)	0(1)
C(14)	46(1)	29(1)	26(1)	−8(1)	−2(1)	10(1)
C(15)	16(1)	27(1)	21(1)	−6(1)	−1(1)	7(1)
C(16)	40(1)	25(1)	51(2)	−11(1)	13(1)	3(1)
C(17)	28(1)	41(1)	25(1)	−1(1)	8(1)	11(1)
C(18)	11(1)	12(1)	9(1)	1(1)	−2(1)	−4(1)
C(19)	12(1)	16(1)	14(1)	3(1)	−4(1)	−3(1)
C(20)	21(1)	26(1)	16(1)	6(1)	−9(1)	−4(1)
C(21)	32(1)	32(1)	12(1)	2(1)	−7(1)	−9(1)
C(22)	25(1)	26(1)	12(1)	−6(1)	0(1)	−7(1)
C(23)	16(1)	15(1)	12(1)	−3(1)	−1(1)	−5(1)
C(24)	11(1)	21(1)	20(1)	5(1)	−2(1)	2(1)
C(25)	13(1)	43(1)	35(1)	5(1)	−4(1)	1(1)
C(26)	28(1)	20(1)	30(1)	3(1)	−2(1)	6(1)
C(27)	16(1)	18(1)	18(1)	−6(1)	1(1)	1(1)
C(28)	28(1)	21(1)	40(1)	4(1)	8(1)	3(1)
C(29)	23(1)	25(1)	41(1)	−6(1)	13(1)	1(1)
C(30)	29(1)	13(1)	20(1)	−1(1)	0(1)	4(1)
C(31)	46(1)	27(1)	30(1)	−6(1)	2(1)	20(1)

Table 4: Bond lengths [Å] for mw_085_1m.

Bi(1)–Ga(1)	2.68144(18)
Bi(1)–Bi(1)#1	2.80726(14)
Ga(1)–O(1)	1.8349(12)
Ga(1)–N(2)	1.9579(13)
Ga(1)–N(1)	1.9827(13)
O(1)–C(30)	1.402(2)
N(1)–C(1)	1.323(2)
N(1)–C(6)	1.439(2)
N(2)–C(3)	1.334(2)
N(2)–C(18)	1.436(2)
C(1)–C(2)	1.399(2)
C(1)–C(4)	1.515(2)
C(2)–C(3)	1.396(2)
C(3)–C(5)	1.506(2)
C(6)–C(7)	1.405(2)
C(6)–C(11)	1.410(2)
C(7)–C(8)	1.398(3)
C(7)–C(12)	1.519(3)
C(8)–C(9)	1.377(3)
C(9)–C(10)	1.382(3)
C(10)–C(11)	1.394(2)
C(11)–C(15)	1.516(3)
C(12)–C(13)	1.525(3)
C(12)–C(14)	1.528(3)
C(15)–C(16)	1.515(3)
C(15)–C(17)	1.527(3)
C(18)–C(19)	1.401(2)
C(18)–C(23)	1.408(2)
C(19)–C(20)	1.397(3)
C(19)–C(24)	1.513(3)
C(20)–C(21)	1.377(3)
C(21)–C(22)	1.386(3)
C(22)–C(23)	1.394(3)
C(23)–C(27)	1.513(3)
C(24)–C(26)	1.527(3)
C(24)–C(25)	1.531(3)
C(27)–C(29)	1.523(3)
C(27)–C(28)	1.531(3)
C(30)–C(31)	1.513(3)

#1 -x+1,-y+1,-z+1

Table 5: Bond angles [°] for mw_085_1m.

Ga(1)–Bi(1)–Bi(1)#1	92.006(5)
O(1)–Ga(1)–N(2)	99.94(6)
O(1)–Ga(1)–N(1)	105.18(6)
N(2)–Ga(1)–N(1)	95.21(6)
O(1)–Ga(1)–Bi(1)	118.13(4)
N(2)–Ga(1)–Bi(1)	123.42(4)
N(1)–Ga(1)–Bi(1)	111.45(4)
C(30)–O(1)–Ga(1)	122.49(12)
C(1)–N(1)–C(6)	120.93(13)
C(1)–N(1)–Ga(1)	121.42(11)
C(6)–N(1)–Ga(1)	117.63(10)
C(3)–N(2)–C(18)	120.85(13)
C(3)–N(2)–Ga(1)	120.57(11)
C(18)–N(2)–Ga(1)	118.57(10)
N(1)–C(1)–C(2)	123.76(15)
N(1)–C(1)–C(4)	121.30(15)
C(2)–C(1)–C(4)	114.93(15)
C(3)–C(2)–C(1)	128.48(15)
N(2)–C(3)–C(2)	123.92(15)
N(2)–C(3)–C(5)	119.37(15)
C(2)–C(3)–C(5)	116.70(15)
C(7)–C(6)–C(11)	121.17(15)
C(7)–C(6)–N(1)	119.55(14)
C(11)–C(6)–N(1)	119.19(14)
C(8)–C(7)–C(6)	117.92(17)
C(8)–C(7)–C(12)	119.98(17)
C(6)–C(7)–C(12)	122.10(16)
C(9)–C(8)–C(7)	121.69(19)
C(8)–C(9)–C(10)	119.54(18)
C(9)–C(10)–C(11)	121.57(18)
C(10)–C(11)–C(6)	118.01(16)
C(10)–C(11)–C(15)	120.31(16)
C(6)–C(11)–C(15)	121.67(15)
C(7)–C(12)–C(13)	112.48(18)
C(7)–C(12)–C(14)	111.97(19)
C(13)–C(12)–C(14)	108.86(18)
C(16)–C(15)–C(11)	112.69(19)
C(16)–C(15)–C(17)	109.42(18)
C(11)–C(15)–C(17)	113.04(18)
C(19)–C(18)–C(23)	121.43(15)
C(19)–C(18)–N(2)	121.24(15)
C(23)–C(18)–N(2)	117.22(14)
C(20)–C(19)–C(18)	117.84(17)
C(20)–C(19)–C(24)	119.27(16)
C(18)–C(19)–C(24)	122.88(15)
C(21)–C(20)–C(19)	121.79(18)
C(20)–C(21)–C(22)	119.55(18)
C(21)–C(22)–C(23)	121.20(19)
C(22)–C(23)–C(18)	118.18(17)
C(22)–C(23)–C(27)	120.69(17)
C(18)–C(23)–C(27)	121.13(15)
C(19)–C(24)–C(26)	110.91(16)
C(19)–C(24)–C(25)	111.49(17)

Table 5: (continued)

C(26)–C(24)–C(25)	110.01(17)
C(23)–C(27)–C(29)	113.73(17)
C(23)–C(27)–C(28)	111.15(16)
C(29)–C(27)–C(28)	109.90(16)
O(1)–C(30)–C(31)	108.96(18)

#1 -x+1,-y+1,-z+1

Crystal structure of mw_084filfsm

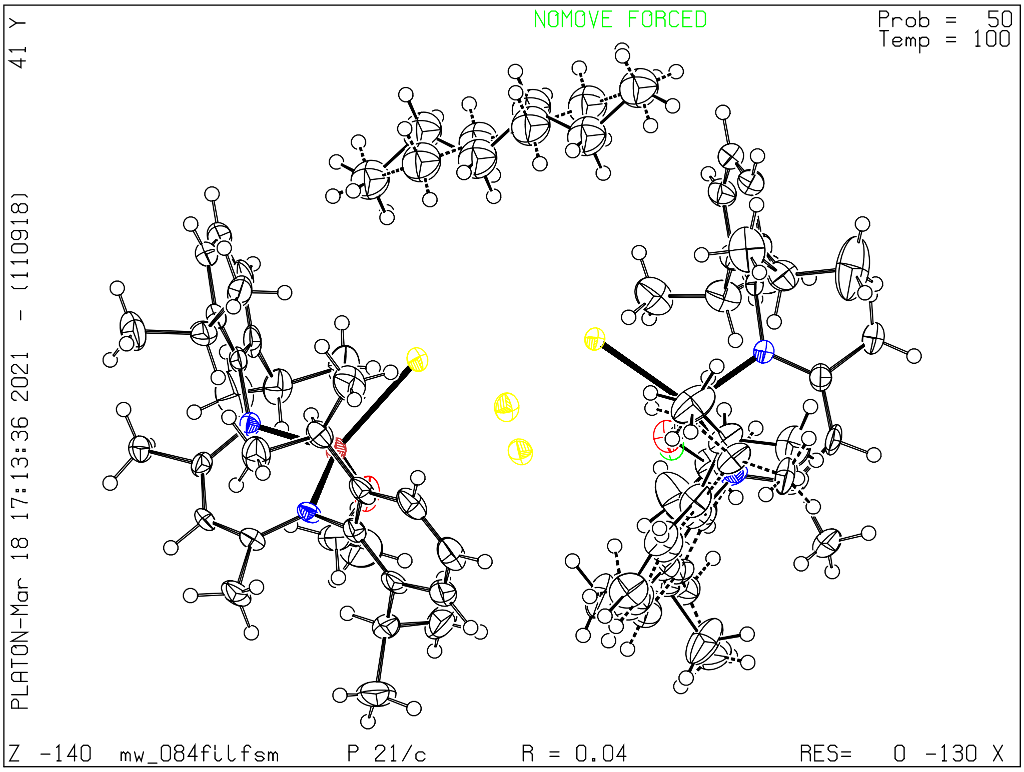

Table 1: Crystal data and structure refinement for mw_084filfsm.

Identification code	mw_084filfsm
Empirical Formula	$C_{64.96}\,H_{98.89}\,Bi_4\,Ga_2\,I_{0.02}\,N_4\,O_{1.98}$
Formula weight	1945.64 Da
Density (calculated)	$1.857\,\mathrm{g\cdot cm^{-3}}$
$F(000)$	3710
Temperature	100(2) K
Crystal size	$0.154 \times 0.056 \times 0.055$ mm
Crystal appearance	dark orange needle
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 20.211(2)$ Å
	$b = 17.2577(19)$ Å
	$c = 20.781(2)$ Å
	$\alpha = 90°$
	$\beta = 106.208(4)°$
	$\gamma = 90°$
Unit cell volume	6960.3(13) $Å^3$
Z	4
Cell measurement refections used	9745
θ range for cell measurement	2.34° to 26.33°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	2.018° to 28.418°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.4%)
Index ranges	$-27 \leq h \leq 27$
	$-23 \leq k \leq 23$
	$-27 \leq l \leq 27$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Numerical
Absorption coefficient	$10.892\,\mathrm{mm^{-1}}$
Absorption correction computing	SADABS
Max./min. transmission	0.17/0.05
R_{merg} before/after correction	0.0776/0.0495
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	135672
Independent reflections	17412 ($R_{int} = 0.0626$)
Reflections with $I > 2\sigma(I)$	13277
Data / retraints / parameter	17412 / 589 / 811
Goodness-of-fit on F^2	1.045
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 54.6383P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0448$
	$wR2 = 0.0894$
R indices [all data]	$R1 = 0.0689$
	$wR2 = 0.0976$
Largest diff. peak and hole	7.197 and -2.935 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

One ethanolate is partially (approx. 3%) replaced by iodine and one dipp group is disordered over two positions. The phenyl rings were contrained to be a regular hexagon with edges 1.39 Å of length (`AFIX 66`). All corresponding bond lengths and angles of the iso-propyl group were restrained to be equal (`SADI`). `RIGU` restraints were applied to the anisotropic displacement parameters of all disordered atoms. Additional `SIMU` restraints were used for the dipp groups. The n-hexane molecule is disordered over a centre of inversion. Its atoms were refined with common displacement parameters (`EADP`).

Absorption

The high residual electron density in the vicinity of the Bi atoms suggests remaining absorption problems. Several methods and parameters were tried but no further improvement could be achieved. Consequently, quantitative results should be carefully accessed.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_084filfsm. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Bi(1)	3649(1)	3549(1)	2872(1)	34(1)
Bi(2)	2757(1)	5246(1)	3440(1)	28(1)
Bi(3)	2253(1)	3623(1)	3105(1)	32(1)
Bi(4)	2538(1)	4593(1)	2050(1)	31(1)
Ga(1)	3228(1)	2330(1)	2066(1)	25(1)
Ga(2)	1456(1)	5670(1)	3271(1)	24(1)
O(1)	2354(3)	2062(3)	2072(3)	44(1)
N(1)	3242(3)	2393(3)	1117(2)	23(1)
N(2)	3790(3)	1388(3)	2259(3)	24(1)
N(3)	1381(3)	6432(3)	3951(3)	28(1)
N(4)	881(3)	6264(3)	2501(3)	31(1)
C(1)	3338(4)	1761(4)	784(3)	27(2)
C(2)	3528(4)	1046(4)	1093(3)	28(2)
C(3)	3784(3)	878(4)	1771(3)	26(1)
C(4)	3241(5)	1795(5)	41(3)	41(2)
C(5)	4067(4)	75(4)	1969(4)	34(2)
C(6)	3107(4)	3138(4)	792(3)	26(1)
C(7)	2427(4)	3342(4)	445(3)	34(2)
C(8)	2307(5)	4105(5)	213(4)	42(2)
C(9)	2837(5)	4631(5)	323(4)	46(2)
C(10)	3499(5)	4420(4)	656(4)	41(2)
C(11)	3648(4)	3666(4)	902(3)	33(2)
C(12)	1836(4)	2780(5)	311(4)	42(2)
C(13)	1496(6)	2704(6)	−445(5)	67(3)
C(14)	1323(5)	3003(6)	688(6)	63(3)
C(15)	4381(4)	3446(4)	1282(4)	32(2)
C(16)	4732(5)	2980(5)	843(4)	48(2)
C(17)	4828(5)	4132(5)	1588(5)	56(3)
C(18)	4241(4)	1259(4)	2933(3)	30(2)
C(19)	3965(5)	990(4)	3450(4)	39(2)
C(20)	4427(6)	918(5)	4091(4)	50(2)
C(21)	5100(6)	1071(5)	4217(4)	54(3)
C(22)	5358(5)	1336(5)	3720(4)	47(2)
C(23)	4934(4)	1444(4)	3066(4)	34(2)
C(24)	3219(5)	805(5)	3325(4)	44(2)
C(25)	3099(6)	−42(6)	3479(6)	69(3)
C(26)	2892(6)	1341(6)	3744(5)	58(3)
C(27)	5238(4)	1765(5)	2540(4)	38(2)
C(28)	5732(5)	1190(6)	2353(5)	57(3)
C(29)	5606(4)	2533(5)	2752(5)	48(2)
C(30)	828(4)	6884(4)	3855(4)	33(2)
C(31)	364(4)	6997(4)	3224(4)	38(2)
C(32)	415(4)	6755(4)	2599(4)	38(2)
C(33)	683(4)	7278(5)	4454(4)	47(2)
C(34)	−112(5)	7096(6)	1995(5)	63(3)
C(35)	1926(4)	6445(4)	4578(3)	29(2)
C(36)	1944(4)	5885(5)	5078(4)	36(2)
C(37)	2496(5)	5905(5)	5653(4)	42(2)
C(38)	3009(4)	6435(5)	5735(4)	47(2)
C(39)	2993(4)	6967(5)	5251(4)	43(2)

Table 2: (continued)

	x	y	z	U_{eq}
C(40)	2461(4)	6983(4)	4647(4)	33(2)
C(41)	1383(5)	5289(5)	5009(4)	48(2)
C(42)	1663(6)	4468(5)	4985(5)	62(3)
C(43)	1030(6)	5351(7)	5572(6)	74(3)
C(44)	2457(5)	7569(5)	4110(5)	45(2)
C(45)	3167(6)	7672(6)	3991(6)	69(3)
C(46)	2185(8)	8340(6)	4245(9)	105(5)
C(47)	1018(5)	6144(6)	1829(4)	28(2)
C(48)	673(5)	5555(5)	1411(4)	32(2)
C(49)	798(6)	5430(5)	795(4)	43(3)
C(50)	1267(6)	5895(7)	595(4)	52(3)
C(51)	1611(6)	6484(6)	1013(5)	47(3)
C(52)	1487(6)	6608(6)	1629(5)	38(3)
C(53)	164(6)	5013(6)	1613(5)	31(3)
C(54)	296(9)	4169(8)	1532(12)	67(5)
C(55)	−560(7)	5197(10)	1230(13)	76(6)
C(56)	1911(7)	7179(7)	2149(7)	47(3)
C(57)	2636(7)	7303(12)	2131(15)	69(6)
C(58)	1557(8)	7935(8)	2115(10)	70(5)
C(47')	841(14)	6083(15)	1933(11)	29(4)
C(48')	439(14)	5526(14)	1518(13)	37(5)
C(49')	523(15)	5386(15)	887(12)	50(6)
C(50')	1009(16)	5803(18)	670(11)	48(6)
C(51')	1411(15)	6359(17)	1084(14)	49(6)
C(52')	1327(14)	6499(15)	1716(14)	36(5)
C(53')	−122(16)	5045(15)	1720(17)	43(6)
C(54')	100(20)	4212(17)	1780(20)	60(11)
C(55')	−840(20)	5090(20)	1250(30)	72(12)
C(56')	1743(16)	7260(13)	1950(20)	47(7)
C(57')	2499(17)	7130(20)	2070(40)	57(11)
C(58')	1571(16)	8050(15)	1644(19)	44(8)
C(59)	2025(4)	1443(6)	1774(4)	52(2)
C(60)	1448(5)	1190(8)	2071(6)	78(4)
O(2)	916(4)	4851(4)	3336(3)	37(1)
C(61)	231(6)	4950(6)	3336(5)	50(2)
C(62)	−121(7)	4179(8)	3248(8)	100(5)
I(1)	640(14)	4622(16)	3432(11)	27(10)
C11	5060(12)	5338(15)	5261(11)	70(2)
C21	4732(9)	6075(11)	4930(11)	70(2)
C31	4854(6)	6741(7)	5424(6)	70(2)
C12	5040(20)	5440(20)	5000(20)	70(2)
C22	4740(16)	5852(19)	5425(18)	70(2)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_084filfsm.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi(1)	35(1)	38(1)	26(1)	−9(1)	5(1)	13(1)
Bi(2)	24(1)	31(1)	26(1)	−5(1)	4(1)	8(1)
Bi(3)	41(1)	27(1)	31(1)	6(1)	14(1)	5(1)
Bi(4)	46(1)	29(1)	19(1)	4(1)	10(1)	8(1)
Ga(1)	30(1)	24(1)	22(1)	3(1)	9(1)	8(1)
Ga(2)	24(1)	22(1)	25(1)	0(1)	3(1)	5(1)
O(1)	46(3)	39(3)	52(3)	4(3)	23(3)	12(3)
N(1)	33(3)	21(3)	15(2)	−1(2)	5(2)	−2(2)
N(2)	28(3)	22(3)	23(3)	1(2)	7(2)	5(2)
N(3)	25(3)	29(3)	28(3)	−5(2)	4(2)	7(2)
N(4)	27(3)	27(3)	31(3)	5(2)	−6(3)	4(2)
C(1)	33(4)	27(4)	21(3)	−5(3)	7(3)	−5(3)
C(2)	35(4)	22(3)	25(3)	−11(3)	4(3)	1(3)
C(3)	25(3)	19(3)	32(3)	3(3)	5(3)	4(3)
C(4)	65(6)	36(4)	18(3)	−5(3)	7(4)	2(4)
C(5)	43(4)	20(3)	35(4)	−1(3)	4(3)	4(3)
C(6)	40(4)	22(3)	15(3)	2(2)	10(3)	3(3)
C(7)	56(5)	29(4)	14(3)	−4(3)	2(3)	6(3)
C(8)	63(6)	37(4)	21(3)	2(3)	3(4)	15(4)
C(9)	85(7)	27(4)	28(4)	5(3)	17(4)	9(4)
C(10)	72(6)	24(4)	29(4)	−1(3)	19(4)	−6(4)
C(11)	59(5)	22(3)	19(3)	−1(3)	14(3)	−1(3)
C(12)	44(5)	36(4)	36(4)	−1(3)	−5(4)	9(4)
C(13)	81(8)	50(6)	46(5)	1(4)	−23(5)	1(5)
C(14)	33(5)	53(6)	92(8)	−1(6)	−2(5)	8(4)
C(15)	37(4)	27(4)	34(4)	−4(3)	13(3)	−7(3)
C(16)	57(6)	48(5)	45(5)	2(4)	25(4)	10(4)
C(17)	49(5)	34(5)	83(7)	−13(5)	14(5)	−14(4)
C(18)	41(4)	27(4)	22(3)	−3(3)	10(3)	15(3)
C(19)	63(6)	27(4)	29(4)	4(3)	17(4)	25(4)
C(20)	90(8)	32(4)	30(4)	6(3)	20(5)	30(5)
C(21)	83(7)	44(5)	24(4)	−4(4)	−6(4)	34(5)
C(22)	51(5)	40(5)	37(4)	−15(4)	−7(4)	20(4)
C(23)	42(4)	27(4)	30(4)	−10(3)	2(3)	11(3)
C(24)	57(5)	35(4)	45(5)	16(4)	22(4)	8(4)
C(25)	100(9)	45(6)	75(7)	18(5)	45(7)	−5(6)
C(26)	80(7)	55(6)	50(5)	20(5)	36(5)	21(5)
C(27)	27(4)	45(5)	40(4)	−13(4)	4(3)	−1(3)
C(28)	47(5)	50(6)	81(7)	−26(5)	31(5)	0(4)
C(29)	32(4)	36(5)	69(6)	−11(4)	4(4)	7(4)
C(30)	28(4)	27(4)	43(4)	−6(3)	9(3)	3(3)
C(31)	27(4)	20(3)	62(5)	−4(3)	5(4)	13(3)
C(32)	33(4)	26(4)	43(4)	3(3)	−11(3)	6(3)
C(33)	39(5)	49(5)	53(5)	−9(4)	10(4)	20(4)
C(34)	58(6)	50(6)	60(6)	−5(5)	−16(5)	25(5)
C(35)	28(4)	29(4)	27(3)	−7(3)	4(3)	12(3)
C(36)	41(4)	35(4)	30(4)	−3(3)	7(3)	3(3)
C(37)	53(5)	44(5)	29(4)	−2(3)	9(4)	9(4)
C(38)	39(5)	50(5)	43(5)	−14(4)	−2(4)	14(4)
C(39)	36(4)	36(4)	49(5)	−13(4)	−1(4)	2(4)
C(40)	26(4)	30(4)	44(4)	−9(3)	9(3)	7(3)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(41)	56(6)	49(5)	41(5)	5(4)	16(4)	−9(4)
C(42)	90(8)	44(5)	53(6)	3(4)	23(6)	−9(5)
C(43)	71(7)	93(9)	67(7)	2(6)	33(6)	−18(7)
C(44)	45(5)	31(4)	56(5)	−2(4)	7(4)	−9(4)
C(45)	76(8)	58(7)	85(8)	5(6)	42(7)	−2(6)
C(46)	111(11)	38(6)	189(16)	32(8)	79(11)	17(7)
C(47)	22(6)	38(4)	25(4)	17(3)	11(4)	5(4)
C(48)	31(6)	44(5)	22(4)	10(4)	11(4)	4(4)
C(49)	41(7)	63(7)	28(5)	12(5)	17(5)	3(6)
C(50)	57(8)	70(7)	38(6)	19(5)	25(6)	−1(6)
C(51)	41(7)	63(7)	42(5)	22(4)	22(5)	10(5)
C(52)	31(6)	49(6)	42(5)	20(4)	24(4)	2(4)
C(53)	32(6)	40(5)	23(5)	−3(4)	9(4)	−8(4)
C(54)	38(8)	45(6)	120(17)	6(8)	24(9)	10(6)
C(55)	31(7)	50(9)	143(16)	24(10)	18(9)	0(7)
C(56)	32(7)	62(6)	44(7)	15(5)	7(5)	6(5)
C(57)	38(7)	73(14)	90(14)	27(11)	11(8)	−11(7)
C(58)	71(10)	59(8)	81(12)	5(8)	23(9)	8(7)
C(47')	23(9)	34(7)	30(8)	10(6)	8(7)	17(6)
C(48')	39(11)	44(9)	24(9)	9(7)	2(8)	11(8)
C(49')	56(13)	60(12)	34(9)	3(8)	12(10)	13(10)
C(50')	49(12)	61(12)	36(10)	10(9)	15(9)	22(10)
C(51')	51(13)	61(12)	42(10)	15(9)	22(9)	10(10)
C(52')	28(10)	42(9)	39(9)	17(8)	13(8)	18(7)
C(53')	40(13)	35(10)	49(14)	1(10)	3(10)	4(9)
C(54')	60(20)	37(11)	70(20)	−1(13)	−11(18)	5(12)
C(55')	48(14)	44(19)	100(30)	−14(18)	−25(18)	0(15)
C(56')	36(12)	54(10)	48(14)	16(9)	6(12)	7(8)
C(57')	41(12)	18(15)	110(30)	11(18)	14(17)	8(10)
C(58')	35(15)	33(10)	70(20)	1(12)	22(14)	15(10)
C(59)	36(5)	81(7)	37(4)	−11(5)	6(4)	3(5)
C(60)	41(6)	114(10)	87(8)	−22(7)	33(6)	−21(6)
O(2)	41(4)	35(3)	42(4)	2(3)	21(3)	−2(3)
C(61)	43(5)	49(5)	66(6)	−13(5)	28(5)	−17(5)
C(62)	108(10)	79(8)	141(13)	−47(9)	82(10)	−56(8)
I(1)	28(17)	35(15)	27(12)	4(9)	22(10)	−3(11)
C11	55(4)	70(5)	85(6)	−3(5)	19(5)	−5(4)
C21	55(4)	70(5)	85(6)	−3(5)	19(5)	−5(4)
C31	55(4)	70(5)	85(6)	−3(5)	19(5)	−5(4)
C12	55(4)	70(5)	85(6)	−3(5)	19(5)	−5(4)
C22	55(4)	70(5)	85(6)	−3(5)	19(5)	−5(4)

Table 4: Bond lengths [Å] for mw_084filfsm.

Bi(1)–Ga(1)	2.6747(8)
Bi(1)–Bi(3)	2.9964(5)
Bi(1)–Bi(4)	3.0125(4)
Bi(2)–Ga(2)	2.6577(8)
Bi(2)–Bi(3)	2.9960(5)
Bi(2)–Bi(4)	3.0165(5)
Bi(3)–Bi(4)	2.9409(4)
Ga(1)–O(1)	1.829(6)
Ga(1)–N(2)	1.960(5)
Ga(1)–N(1)	1.984(5)
Ga(2)–O(2)	1.815(9)
Ga(2)–N(3)	1.966(6)
Ga(2)–N(4)	1.980(5)
Ga(2)–I(1)	2.53(3)
O(1)–C(59)	1.319(11)
N(1)–C(1)	1.334(8)
N(1)–C(6)	1.443(8)
N(2)–C(3)	1.338(8)
N(2)–C(18)	1.459(8)
N(3)–C(30)	1.332(9)
N(3)–C(35)	1.452(9)
N(4)–C(47')	1.20(2)
N(4)–C(32)	1.323(10)
N(4)–C(47)	1.513(10)
C(1)–C(2)	1.395(10)
C(1)–C(4)	1.502(9)
C(2)–C(3)	1.390(9)
C(3)–C(5)	1.512(9)
C(6)–C(11)	1.392(10)
C(6)–C(7)	1.407(10)
C(7)–C(8)	1.401(10)
C(7)–C(12)	1.503(12)
C(8)–C(9)	1.373(13)
C(9)–C(10)	1.373(13)
C(10)–C(11)	1.401(10)
C(11)–C(15)	1.520(11)
C(12)–C(14)	1.513(13)
C(12)–C(13)	1.533(11)
C(15)–C(17)	1.516(10)
C(15)–C(16)	1.531(11)
C(18)–C(23)	1.387(11)
C(18)–C(19)	1.419(11)
C(19)–C(20)	1.402(11)
C(19)–C(24)	1.492(12)
C(20)–C(21)	1.338(14)
C(21)–C(22)	1.360(14)
C(22)–C(23)	1.400(10)
C(23)–C(27)	1.502(12)
C(24)–C(25)	1.530(12)
C(24)–C(26)	1.540(12)
C(27)–C(29)	1.524(11)
C(27)–C(28)	1.532(11)
C(30)–C(31)	1.397(11)

Table 4: (continued)

C(30)–C(33)	1.517(11)
C(31)–C(32)	1.396(12)
C(32)–C(34)	1.520(11)
C(35)–C(40)	1.401(10)
C(35)–C(36)	1.414(11)
C(36)–C(37)	1.388(11)
C(36)–C(41)	1.508(12)
C(37)–C(38)	1.358(12)
C(38)–C(39)	1.356(13)
C(39)–C(40)	1.407(11)
C(40)–C(44)	1.505(12)
C(41)–C(42)	1.532(13)
C(41)–C(43)	1.535(13)
C(44)–C(46)	1.495(14)
C(44)–C(45)	1.532(13)
C(47)–C(48)	1.3900
C(47)–C(52)	1.3900
C(48)–C(49)	1.3900
C(48)–C(53)	1.533(10)
C(49)–C(50)	1.3900
C(50)–C(51)	1.3900
C(51)–C(52)	1.3900
C(52)–C(56)	1.536(12)
C(53)–C(55)	1.491(12)
C(53)–C(54)	1.499(12)
C(56)–C(58)	1.479(13)
C(56)–C(57)	1.493(13)
C(47')–C(48')	1.3900
C(47')–C(52')	1.3900
C(48')–C(49')	1.3900
C(48')–C(53')	1.555(17)
C(49')–C(50')	1.3900
C(50')–C(51')	1.3900
C(51')–C(52')	1.3900
C(52')–C(56')	1.563(17)
C(53')–C(54')	1.498(16)
C(53')–C(55')	1.502(16)
C(56')–C(57')	1.494(16)
C(56')–C(58')	1.503(16)
C(59)–C(60)	1.528(13)
O(2)–C(61)	1.395(14)
C(61)–C(62)	1.496(14)
C11–C21	1.51(3)
C11–C11#1	1.56(5)
C21–C31	1.51(2)
C31–C22	1.55(3)
C12–C22	1.39(6)
C12–C12#1	1.52(8)

#1 -x+1,-y+1,-z+1

Table 5: Bond angles [°] for mw_084filfsm.

Ga(1)–Bi(1)–Bi(3)	89.15(2)
Ga(1)–Bi(1)–Bi(4)	93.368(19)
Bi(3)–Bi(1)–Bi(4)	58.604(11)
Ga(2)–Bi(2)–Bi(3)	88.082(19)
Ga(2)–Bi(2)–Bi(4)	95.754(19)
Bi(3)–Bi(2)–Bi(4)	58.566(9)
Bi(4)–Bi(3)–Bi(2)	61.066(11)
Bi(4)–Bi(3)–Bi(1)	60.972(10)
Bi(2)–Bi(3)–Bi(1)	78.639(11)
Bi(3)–Bi(4)–Bi(1)	60.424(12)
Bi(3)–Bi(4)–Bi(2)	60.368(12)
Bi(1)–Bi(4)–Bi(2)	78.069(11)
O(1)–Ga(1)–N(2)	107.1(2)
O(1)–Ga(1)–N(1)	107.6(2)
N(2)–Ga(1)–N(1)	94.5(2)
O(1)–Ga(1)–Bi(1)	109.52(18)
N(2)–Ga(1)–Bi(1)	117.36(16)
N(1)–Ga(1)–Bi(1)	119.28(16)
O(2)–Ga(2)–N(3)	107.4(3)
O(2)–Ga(2)–N(4)	103.6(3)
N(3)–Ga(2)–N(4)	95.1(2)
N(3)–Ga(2)–I(1)	101.5(5)
N(4)–Ga(2)–I(1)	102.7(6)
O(2)–Ga(2)–Bi(2)	111.7(2)
N(3)–Ga(2)–Bi(2)	111.11(17)
N(4)–Ga(2)–Bi(2)	125.82(19)
I(1)–Ga(2)–Bi(2)	116.3(6)
C(59)–O(1)–Ga(1)	124.2(5)
C(1)–N(1)–C(6)	121.4(5)
C(1)–N(1)–Ga(1)	121.1(4)
C(6)–N(1)–Ga(1)	117.4(4)
C(3)–N(2)–C(18)	119.9(5)
C(3)–N(2)–Ga(1)	120.5(4)
C(18)–N(2)–Ga(1)	119.5(4)
C(30)–N(3)–C(35)	121.2(6)
C(30)–N(3)–Ga(2)	120.9(5)
C(35)–N(3)–Ga(2)	117.7(4)
C(47')–N(4)–C(32)	117.4(14)
C(32)–N(4)–C(47)	123.4(7)
C(47')–N(4)–Ga(2)	121.5(14)
C(32)–N(4)–Ga(2)	119.3(5)
C(47)–N(4)–Ga(2)	117.3(5)
N(1)–C(1)–C(2)	123.1(6)
N(1)–C(1)–C(4)	120.3(6)
C(2)–C(1)–C(4)	116.5(6)
C(3)–C(2)–C(1)	128.8(6)
N(2)–C(3)–C(2)	123.6(6)
N(2)–C(3)–C(5)	118.3(6)
C(2)–C(3)–C(5)	118.1(6)
C(11)–C(6)–C(7)	122.1(6)
C(11)–C(6)–N(1)	117.9(6)
C(7)–C(6)–N(1)	119.6(6)
C(8)–C(7)–C(6)	117.5(8)

Table 5: (continued)

C(8)–C(7)–C(12)	119.4(7)
C(6)–C(7)–C(12)	123.1(7)
C(9)–C(8)–C(7)	120.9(8)
C(10)–C(9)–C(8)	120.9(8)
C(9)–C(10)–C(11)	120.7(8)
C(6)–C(11)–C(10)	118.0(8)
C(6)–C(11)–C(15)	122.0(6)
C(10)–C(11)–C(15)	120.0(7)
C(7)–C(12)–C(14)	111.3(7)
C(7)–C(12)–C(13)	110.5(8)
C(14)–C(12)–C(13)	112.1(8)
C(17)–C(15)–C(11)	113.8(7)
C(17)–C(15)–C(16)	109.9(7)
C(11)–C(15)–C(16)	111.6(6)
C(23)–C(18)–C(19)	120.7(7)
C(23)–C(18)–N(2)	118.8(6)
C(19)–C(18)–N(2)	120.3(7)
C(20)–C(19)–C(18)	116.8(8)
C(20)–C(19)–C(24)	121.2(8)
C(18)–C(19)–C(24)	122.0(7)
C(21)–C(20)–C(19)	122.6(9)
C(20)–C(21)–C(22)	120.1(8)
C(21)–C(22)–C(23)	121.4(9)
C(18)–C(23)–C(22)	118.3(8)
C(18)–C(23)–C(27)	122.3(6)
C(22)–C(23)–C(27)	119.4(8)
C(19)–C(24)–C(25)	112.3(8)
C(19)–C(24)–C(26)	110.3(8)
C(25)–C(24)–C(26)	109.7(8)
C(23)–C(27)–C(29)	112.2(7)
C(23)–C(27)–C(28)	112.0(7)
C(29)–C(27)–C(28)	109.6(7)
N(3)–C(30)–C(31)	122.5(7)
N(3)–C(30)–C(33)	119.1(7)
C(31)–C(30)–C(33)	118.3(7)
C(32)–C(31)–C(30)	128.8(7)
N(4)–C(32)–C(31)	125.1(7)
N(4)–C(32)–C(34)	119.1(8)
C(31)–C(32)–C(34)	115.8(7)
C(40)–C(35)–C(36)	121.1(7)
C(40)–C(35)–N(3)	118.3(7)
C(36)–C(35)–N(3)	120.4(7)
C(37)–C(36)–C(35)	117.7(7)
C(37)–C(36)–C(41)	120.1(8)
C(35)–C(36)–C(41)	122.2(7)
C(38)–C(37)–C(36)	121.9(8)
C(39)–C(38)–C(37)	120.2(8)
C(38)–C(39)–C(40)	122.0(8)
C(35)–C(40)–C(39)	117.1(7)
C(35)–C(40)–C(44)	121.6(7)
C(39)–C(40)–C(44)	121.3(7)
C(36)–C(41)–C(42)	111.0(8)
C(36)–C(41)–C(43)	112.2(8)

Table 5: (continued)

C(42)–C(41)–C(43)	110.2(8)
C(46)–C(44)–C(40)	112.6(9)
C(46)–C(44)–C(45)	109.7(8)
C(40)–C(44)–C(45)	112.7(8)
C(48)–C(47)–C(52)	120.0
C(48)–C(47)–N(4)	119.2(5)
C(52)–C(47)–N(4)	120.8(5)
C(47)–C(48)–C(49)	120.0
C(47)–C(48)–C(53)	122.2(6)
C(49)–C(48)–C(53)	117.8(6)
C(50)–C(49)–C(48)	120.0
C(49)–C(50)–C(51)	120.0
C(52)–C(51)–C(50)	120.0
C(51)–C(52)–C(47)	120.0
C(51)–C(52)–C(56)	122.6(8)
C(47)–C(52)–C(56)	117.0(8)
C(55)–C(53)–C(54)	109.0(10)
C(55)–C(53)–C(48)	111.0(9)
C(54)–C(53)–C(48)	114.0(10)
C(58)–C(56)–C(57)	109.8(11)
C(58)–C(56)–C(52)	111.3(11)
C(57)–C(56)–C(52)	115.6(13)
N(4)–C(47')–C(48')	131.0(17)
N(4)–C(47')–C(52')	108.9(17)
C(48')–C(47')–C(52')	120.0
C(49')–C(48')–C(47')	120.0
C(49')–C(48')–C(53')	116.9(18)
C(47')–C(48')–C(53')	123.1(18)
C(48')–C(49')–C(50')	120.0
C(49')–C(50')–C(51')	120.0
C(52')–C(51')–C(50')	120.0
C(51')–C(52')–C(47')	120.0
C(51')–C(52')–C(56')	104(2)
C(47')–C(52')–C(56')	135(2)
C(54')–C(53')–C(55')	108.2(15)
C(54')–C(53')–C(48')	108(3)
C(55')–C(53')–C(48')	116(3)
C(57')–C(56')–C(58')	108.1(15)
C(57')–C(56')–C(52')	111(3)
C(58')–C(56')–C(52')	126(3)
O(1)–C(59)–C(60)	112.5(8)
C(61)–O(2)–Ga(2)	121.4(6)
O(2)–C(61)–C(62)	109.1(10)
C21–C11–C11#1	110(2)
C11–C21–C31	111.3(17)
C22–C12–C12#1	118(4)
C12–C22–C31	115(3)

#1 -x+1,-y+1,-z+1

Crystal structure of mw_036_1m

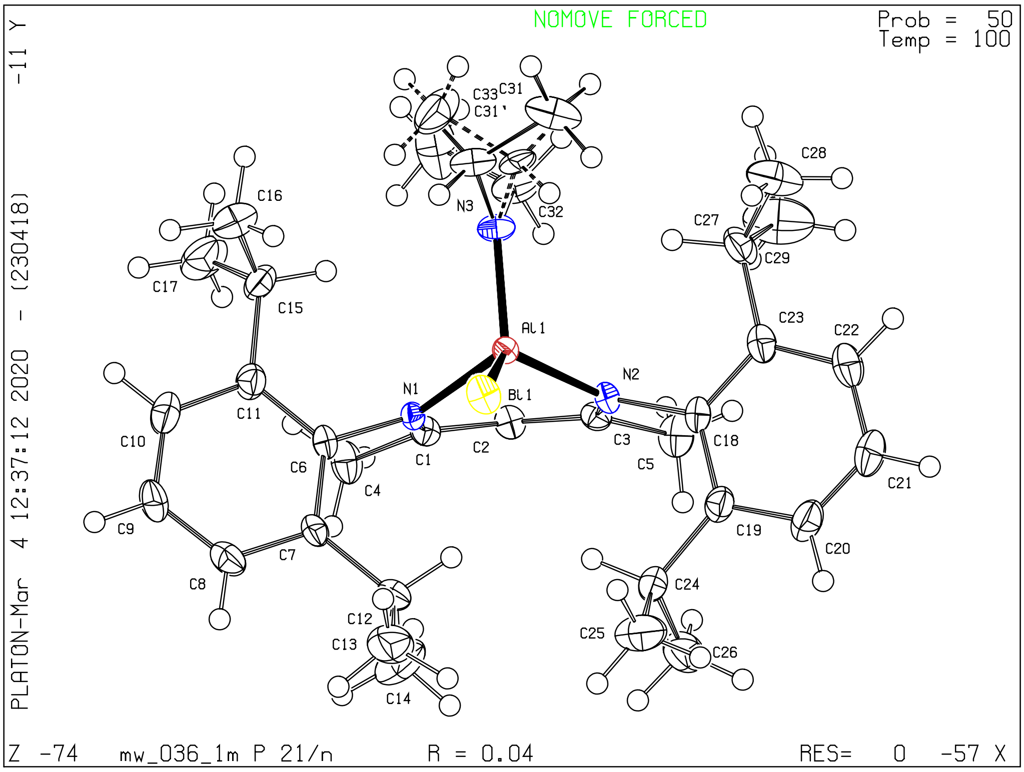

Table 1: Crystal data and structure refinement for mw_036_1m.

Identification code	mw_036_1m
Empirical Formula	$C_{66}\,H_{102}\,Al_2\,Bi_2\,N_6$
Formula weight	1451.45 Da
Density (calculated)	$1.475\,g \cdot cm^{-3}$
$F(000)$	1464
Temperature	100(2) K
Crystal size	0.101 × 0.053 × 0.045 mm
Crystal appearance	red tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	$a = 11.331(4)$ Å
	$b = 13.980(4)$ Å
	$c = 20.635(6)$ Å
	$\alpha = 90°$
	$\beta = 90.306(7)°$
	$\gamma = 90°$
Unit cell volume	3268.9(17) $Å^3$
Z	2
Cell measurement refections used	9975
θ range for cell measurement	2.31° to 25.84°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 2/COSMO
θ range for data collection	2.314° to 33.138°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.9%)
Index ranges	$-17 \leq h \leq 17$
	$-21 \leq k \leq 21$
	$-31 \leq l \leq 31$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$5.445\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.61
R_{merg} before/after correction	0.0808/0.0650
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	78359
Independent reflections	12457 ($R_{int} = 0.0990$)
Reflections with $I > 2\sigma(I)$	8449
Data / retraints / parameter	12457 / 6 / 375
Goodness-of-fit on F^2	1.003
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices [$I > 2\sigma(I)$]	$R1 = 0.0422$
	$wR2 = 0.0826$
R indices [all data]	$R1 = 0.0820$
	$wR2 = 0.0940$
Largest diff. peak and hole	2.336 and -1.379 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

An ethyl group is disordered over two positions. `RIGU` restraints were applied to the anisotropic displacement parameters of the corresponding atoms.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_036_1m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Bi(1)	−448(1)	5187(1)	4376(1)	25(1)
Al(1)	622(1)	3669(1)	3786(1)	15(1)
N(1)	−336(2)	3335(2)	3045(1)	16(1)
N(2)	582(2)	2419(2)	4173(1)	17(1)
N(3)	2125(2)	3926(2)	3536(2)	23(1)
C(1)	−249(3)	2457(2)	2797(2)	19(1)
C(2)	268(3)	1696(2)	3128(2)	20(1)
C(3)	542(3)	1646(2)	3788(2)	19(1)
C(4)	−760(4)	2231(3)	2137(2)	28(1)
C(5)	744(4)	662(3)	4049(2)	29(1)
C(6)	−1063(3)	4017(2)	2695(2)	20(1)
C(7)	−2261(3)	4092(3)	2854(2)	23(1)
C(8)	−2981(3)	4659(3)	2465(2)	30(1)
C(9)	−2528(4)	5162(3)	1950(2)	31(1)
C(10)	−1351(4)	5132(3)	1826(2)	34(1)
C(11)	−592(3)	4570(3)	2195(2)	26(1)
C(12)	−2789(3)	3594(3)	3424(2)	33(1)
C(13)	−3631(4)	4247(4)	3797(2)	48(1)
C(14)	−3386(5)	2686(3)	3234(3)	53(1)
C(15)	711(3)	4613(3)	2056(2)	34(1)
C(16)	1166(4)	5627(4)	2151(3)	48(1)
C(17)	1016(4)	4255(4)	1389(2)	50(1)
C(18)	603(3)	2245(2)	4868(2)	20(1)
C(19)	−472(3)	2076(3)	5177(2)	25(1)
C(20)	−443(4)	1882(3)	5839(2)	33(1)
C(21)	580(4)	1852(3)	6177(2)	36(1)
C(22)	1630(4)	2026(3)	5868(2)	33(1)
C(23)	1669(3)	2238(3)	5215(2)	25(1)
C(24)	−1652(3)	2065(3)	4823(2)	35(1)
C(25)	−2513(4)	2739(3)	5134(3)	48(1)
C(26)	−2181(4)	1062(4)	4795(2)	40(1)
C(27)	2841(3)	2439(3)	4900(2)	32(1)
C(28)	3610(4)	3098(4)	5306(3)	51(1)
C(29)	3517(5)	1540(4)	4757(3)	67(2)
C(30)	2660(6)	4862(5)	3605(4)	32(2)
C(31)	3434(5)	4991(4)	4194(3)	45(2)
C(30’)	2830(20)	4620(20)	3857(12)	35(6)
C(31’)	3060(20)	5518(19)	3478(10)	51(7)
C(32)	2915(4)	3208(3)	3278(2)	34(1)
C(33)	3250(5)	3295(5)	2583(2)	70(2)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_036_1m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi(1)	29(1)	23(1)	23(1)	−6(1)	−1(1)	8(1)
Al(1)	16(1)	16(1)	13(1)	−2(1)	0(1)	1(1)
N(1)	17(1)	17(1)	13(1)	1(1)	−1(1)	1(1)
N(2)	19(1)	17(1)	15(1)	−1(1)	−3(1)	3(1)
N(3)	17(1)	25(2)	27(2)	−3(1)	7(1)	0(1)
C(1)	20(2)	22(2)	16(2)	−4(1)	0(1)	0(1)
C(2)	24(2)	18(2)	20(2)	−4(1)	−1(1)	2(1)
C(3)	18(2)	17(2)	23(2)	−1(1)	−1(1)	0(1)
C(4)	39(2)	27(2)	19(2)	−4(2)	−7(2)	2(2)
C(5)	39(2)	19(2)	30(2)	−2(2)	−1(2)	6(2)
C(6)	23(2)	19(2)	18(2)	3(1)	−4(1)	4(1)
C(7)	20(2)	30(2)	18(2)	1(1)	−6(1)	0(1)
C(8)	20(2)	35(2)	34(2)	2(2)	−5(2)	5(1)
C(9)	32(2)	30(2)	32(2)	8(2)	−8(2)	11(2)
C(10)	42(2)	33(2)	28(2)	13(2)	0(2)	1(2)
C(11)	28(2)	24(2)	25(2)	6(1)	0(2)	3(1)
C(12)	17(2)	50(3)	33(2)	11(2)	−2(2)	2(2)
C(13)	30(2)	74(4)	39(3)	1(2)	7(2)	1(2)
C(14)	59(3)	36(3)	64(3)	14(2)	20(3)	−6(2)
C(15)	27(2)	40(2)	34(2)	19(2)	10(2)	5(2)
C(16)	37(2)	55(3)	54(3)	17(2)	5(2)	−14(2)
C(17)	45(3)	56(3)	47(3)	10(2)	22(2)	6(2)
C(18)	28(2)	17(2)	15(2)	0(1)	−2(1)	2(1)
C(19)	29(2)	24(2)	24(2)	6(1)	1(2)	3(1)
C(20)	40(2)	36(2)	24(2)	9(2)	7(2)	3(2)
C(21)	51(3)	39(2)	18(2)	5(2)	0(2)	0(2)
C(22)	40(2)	38(2)	22(2)	−1(2)	−11(2)	2(2)
C(23)	32(2)	23(2)	21(2)	0(1)	−6(2)	1(1)
C(24)	26(2)	48(3)	31(2)	20(2)	2(2)	3(2)
C(25)	30(2)	33(2)	83(4)	14(2)	9(2)	2(2)
C(26)	34(2)	53(3)	33(2)	−5(2)	−4(2)	0(2)
C(27)	26(2)	46(2)	23(2)	−1(2)	−8(2)	3(2)
C(28)	27(2)	65(3)	60(3)	−14(3)	0(2)	−8(2)
C(29)	47(3)	60(4)	95(5)	−30(3)	18(3)	4(3)
C(30)	22(3)	33(3)	42(4)	−4(3)	8(3)	−8(2)
C(31)	23(3)	49(4)	62(4)	−17(3)	−1(3)	−4(2)
C(30')	19(9)	61(14)	24(11)	11(9)	9(8)	−11(9)
C(31')	67(16)	60(13)	26(10)	3(9)	6(9)	−29(11)
C(32)	27(2)	36(2)	40(2)	−6(2)	16(2)	2(2)
C(33)	65(4)	113(5)	32(3)	8(3)	14(2)	58(4)

Table 4: Bond lengths [Å] for mw_036_1m.

Bi(1)–Al(1)	2.7343(11)
Bi(1)–Bi(1)#1	2.8113(8)
Al(1)–N(3)	1.817(3)
Al(1)–N(2)	1.922(3)
Al(1)–N(1)	1.928(3)
N(1)–C(1)	1.333(4)
N(1)–C(6)	1.450(4)
N(2)–C(3)	1.342(4)
N(2)–C(18)	1.456(4)
N(3)–C(30')	1.42(2)
N(3)–C(30)	1.449(7)
N(3)–C(32)	1.449(5)
C(1)–C(2)	1.392(5)
C(1)–C(4)	1.510(5)
C(2)–C(3)	1.396(5)
C(3)–C(5)	1.495(5)
C(6)–C(11)	1.397(5)
C(6)–C(7)	1.402(5)
C(7)–C(8)	1.389(5)
C(7)–C(12)	1.494(5)
C(8)–C(9)	1.377(6)
C(9)–C(10)	1.361(6)
C(10)–C(11)	1.388(5)
C(11)–C(15)	1.507(5)
C(12)–C(14)	1.490(7)
C(12)–C(13)	1.531(6)
C(15)–C(17)	1.506(6)
C(15)–C(16)	1.522(7)
C(18)–C(19)	1.398(5)
C(18)–C(23)	1.400(5)
C(19)–C(20)	1.393(5)
C(19)–C(24)	1.521(5)
C(20)–C(21)	1.349(6)
C(21)–C(22)	1.375(6)
C(22)–C(23)	1.382(5)
C(23)–C(27)	1.508(6)
C(24)–C(25)	1.503(6)
C(24)–C(26)	1.526(6)
C(27)–C(29)	1.501(7)
C(27)–C(28)	1.518(6)
C(30)–C(31)	1.507(10)
C(30')–C(31')	1.50(4)
C(32)–C(33)	1.491(6)

#1 -x,-y+1,-z+1

Table 5: Bond angles [°] for mw_036_1m.

Al(1)–Bi(1)–Bi(1)#1	96.00(3)
N(3)–Al(1)–N(2)	108.74(13)
N(3)–Al(1)–N(1)	110.39(14)
N(2)–Al(1)–N(1)	95.41(12)
N(3)–Al(1)–Bi(1)	113.04(10)
N(2)–Al(1)–Bi(1)	120.61(9)
N(1)–Al(1)–Bi(1)	107.00(9)
C(1)–N(1)–C(6)	117.2(3)
C(1)–N(1)–Al(1)	119.0(2)
C(6)–N(1)–Al(1)	123.5(2)
C(3)–N(2)–C(18)	116.7(3)
C(3)–N(2)–Al(1)	119.2(2)
C(18)–N(2)–Al(1)	124.1(2)
C(30')–N(3)–C(32)	107.5(11)
C(30)–N(3)–C(32)	113.8(4)
C(30')–N(3)–Al(1)	121.9(9)
C(30)–N(3)–Al(1)	122.9(3)
C(32)–N(3)–Al(1)	123.3(3)
N(1)–C(1)–C(2)	123.1(3)
N(1)–C(1)–C(4)	120.7(3)
C(2)–C(1)–C(4)	116.2(3)
C(1)–C(2)–C(3)	127.4(3)
N(2)–C(3)–C(2)	122.9(3)
N(2)–C(3)–C(5)	121.5(3)
C(2)–C(3)–C(5)	115.5(3)
C(11)–C(6)–C(7)	120.4(3)
C(11)–C(6)–N(1)	120.9(3)
C(7)–C(6)–N(1)	118.7(3)
C(8)–C(7)–C(6)	118.2(3)
C(8)–C(7)–C(12)	119.0(3)
C(6)–C(7)–C(12)	122.8(3)
C(9)–C(8)–C(7)	121.2(4)
C(10)–C(9)–C(8)	119.9(3)
C(9)–C(10)–C(11)	121.3(4)
C(10)–C(11)–C(6)	118.7(3)
C(10)–C(11)–C(15)	118.5(3)
C(6)–C(11)–C(15)	122.8(3)
C(14)–C(12)–C(7)	111.9(4)
C(14)–C(12)–C(13)	110.9(4)
C(7)–C(12)–C(13)	111.8(4)
C(11)–C(15)–C(17)	113.0(4)
C(11)–C(15)–C(16)	110.1(4)
C(17)–C(15)–C(16)	110.4(4)
C(19)–C(18)–C(23)	121.1(3)
C(19)–C(18)–N(2)	117.9(3)
C(23)–C(18)–N(2)	121.0(3)
C(20)–C(19)–C(18)	117.7(3)
C(20)–C(19)–C(24)	119.1(3)
C(18)–C(19)–C(24)	123.3(3)
C(21)–C(20)–C(19)	121.9(4)
C(20)–C(21)–C(22)	119.9(4)
C(21)–C(22)–C(23)	121.5(4)
C(22)–C(23)–C(18)	117.9(4)

Table 5: (continued)

C(22)–C(23)–C(27)	119.6(3)
C(18)–C(23)–C(27)	122.5(3)
C(25)–C(24)–C(19)	111.1(4)
C(25)–C(24)–C(26)	109.6(4)
C(19)–C(24)–C(26)	111.8(3)
C(29)–C(27)–C(23)	112.3(4)
C(29)–C(27)–C(28)	108.9(4)
C(23)–C(27)–C(28)	112.3(4)
N(3)–C(30)–C(31)	115.3(6)
N(3)–C(30')–C(31')	115.4(19)
N(3)–C(32)–C(33)	117.3(4)

#1 -x,-y+1,-z+1

Crystal structure of mw_036_5m

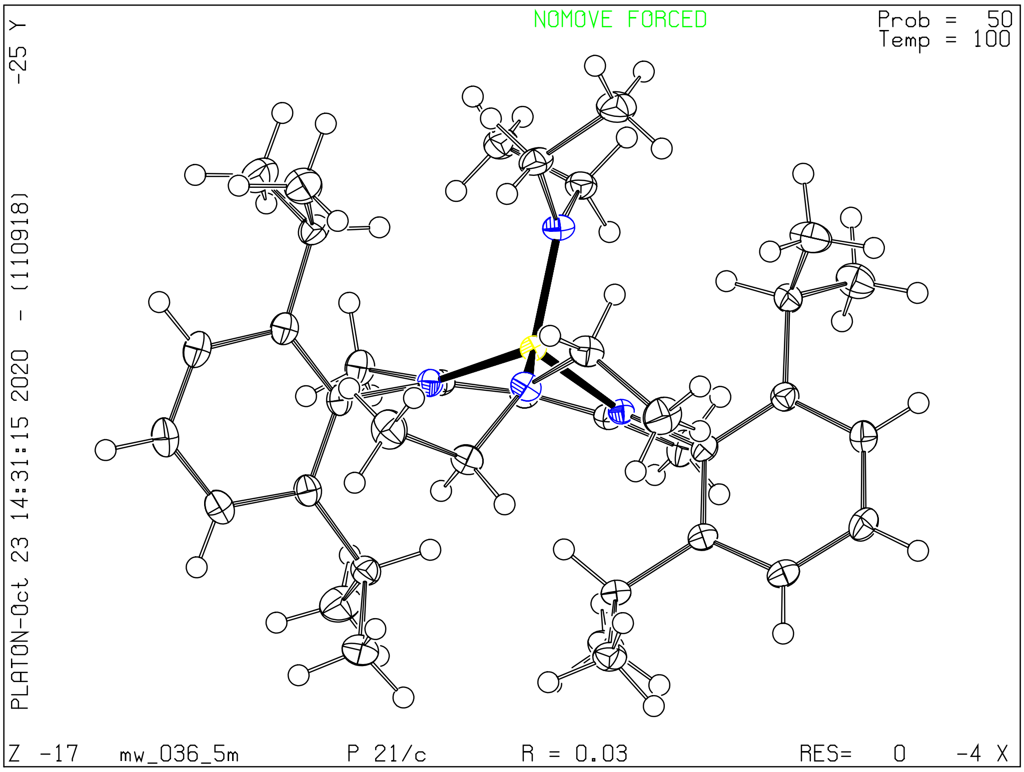

Table 1: Crystal data and structure refinement for mw_036_5m.

Identification code	mw_036_5m
Empirical Formula	$C_{37}H_{61}AlN_4$
Formula weight	588.87 Da
Density (calculated)	$1.101\,g\cdot cm^{-3}$
$F(000)$	1296
Temperature	100(2) K
Crystal size	0.126 × 0.124 × 0.082 mm
Crystal appearance	colourless tablet
Wavelength (CuK_α)	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 19.6396(7)$ Å
	$b = 11.3304(4)$ Å
	$c = 16.2478(6)$ Å
	$\alpha = 90°$
	$\beta = 100.7950(15)°$
	$\gamma = 90°$
Unit cell volume	$3551.6(2)\,Å^3$
Z	4
Cell measurement refections used	9492
θ range for cell measurement	4.53° to 80.69°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	2.290° to 80.903°
Completeness to $\theta = 67.679°$ (to θ_{max})	100.0% (99.5%)
Index ranges	$-24 \leq h \leq 21$
	$-14 \leq k \leq 14$
	$-20 \leq l \leq 20$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$0.707\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.68
R_{merg} before/after correction	0.1069/0.0580
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	120373
Independent reflections	7788 ($R_{int} = 0.0444$)
Reflections with $I > 2\sigma(I)$	7022
Data / retraints / parameter	7788 / 0 / 393
Goodness-of-fit on F^2	1.030
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 1.3241P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0346$
	$wR2 = 0.0885$
R indices [all data]	$R1 = 0.0392$
	$wR2 = 0.0930$
Largest diff. peak and hole	0.279 and $-0.282\,Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_036_5m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Al(1)	2649(1)	5379(1)	2644(1)	14(1)
N(1)	3289(1)	4232(1)	2344(1)	14(1)
N(2)	1981(1)	5228(1)	1625(1)	16(1)
N(3)	2297(1)	5022(1)	3561(1)	18(1)
N(4)	3092(1)	6803(1)	2710(1)	19(1)
C(1)	3357(1)	4138(1)	1544(1)	17(1)
C(2)	2890(1)	4676(1)	887(1)	18(1)
C(3)	2231(1)	5121(1)	910(1)	17(1)
C(4)	3939(1)	3441(1)	1297(1)	23(1)
C(5)	1802(1)	5520(1)	89(1)	22(1)
C(6)	3736(1)	3526(1)	2968(1)	15(1)
C(7)	4407(1)	3911(1)	3327(1)	18(1)
C(8)	4821(1)	3177(1)	3905(1)	22(1)
C(9)	4581(1)	2105(1)	4140(1)	23(1)
C(10)	3911(1)	1752(1)	3802(1)	21(1)
C(11)	3477(1)	2449(1)	3219(1)	17(1)
C(12)	4686(1)	5112(1)	3139(1)	22(1)
C(13)	5348(1)	5042(1)	2775(1)	30(1)
C(14)	4814(1)	5869(1)	3930(1)	32(1)
C(15)	2746(1)	2039(1)	2854(1)	18(1)
C(16)	2738(1)	1327(1)	2051(1)	25(1)
C(17)	2417(1)	1324(1)	3476(1)	23(1)
C(18)	1235(1)	5341(1)	1543(1)	17(1)
C(19)	927(1)	6446(1)	1622(1)	20(1)
C(20)	204(1)	6499(1)	1529(1)	24(1)
C(21)	−200(1)	5502(1)	1362(1)	26(1)
C(22)	108(1)	4421(1)	1283(1)	24(1)
C(23)	827(1)	4311(1)	1381(1)	19(1)
C(24)	1335(1)	7589(1)	1781(1)	22(1)
C(25)	1194(1)	8393(1)	1008(1)	33(1)
C(26)	1167(1)	8253(1)	2542(1)	32(1)
C(27)	1138(1)	3088(1)	1316(1)	21(1)
C(28)	812(1)	2161(1)	1812(1)	28(1)
C(29)	1074(1)	2671(1)	408(1)	32(1)
C(30)	2666(1)	5322(1)	4404(1)	22(1)
C(31)	3019(1)	4287(1)	4913(1)	30(1)
C(32)	1671(1)	4326(1)	3557(1)	20(1)
C(33)	1060(1)	5014(1)	3776(1)	30(1)
C(34)	3503(1)	7184(1)	2093(1)	21(1)
C(35)	3115(1)	7931(1)	1369(1)	25(1)
C(36)	2929(1)	7768(1)	3240(1)	23(1)
C(37)	3539(1)	8218(1)	3893(1)	30(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_036_5m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Al(1)	16(1)	14(1)	13(1)	0(1)	3(1)	0(1)
N(1)	15(1)	14(1)	14(1)	0(1)	3(1)	0(1)
N(2)	15(1)	16(1)	16(1)	0(1)	3(1)	1(1)
N(3)	20(1)	20(1)	15(1)	−1(1)	5(1)	−2(1)
N(4)	23(1)	15(1)	20(1)	−1(1)	5(1)	−1(1)
C(1)	18(1)	16(1)	18(1)	−1(1)	6(1)	−1(1)
C(2)	21(1)	21(1)	14(1)	0(1)	6(1)	0(1)
C(3)	20(1)	15(1)	15(1)	0(1)	2(1)	−1(1)
C(4)	22(1)	28(1)	18(1)	−1(1)	6(1)	6(1)
C(5)	23(1)	28(1)	16(1)	1(1)	3(1)	3(1)
C(6)	17(1)	15(1)	14(1)	0(1)	5(1)	3(1)
C(7)	18(1)	18(1)	19(1)	1(1)	4(1)	1(1)
C(8)	19(1)	24(1)	22(1)	1(1)	1(1)	1(1)
C(9)	25(1)	23(1)	21(1)	4(1)	1(1)	5(1)
C(10)	25(1)	17(1)	20(1)	3(1)	5(1)	1(1)
C(11)	20(1)	16(1)	16(1)	−1(1)	5(1)	1(1)
C(12)	18(1)	20(1)	28(1)	4(1)	2(1)	−2(1)
C(13)	29(1)	32(1)	32(1)	1(1)	12(1)	−6(1)
C(14)	33(1)	24(1)	42(1)	−6(1)	13(1)	−7(1)
C(15)	20(1)	15(1)	19(1)	0(1)	4(1)	−1(1)
C(16)	28(1)	24(1)	25(1)	−7(1)	6(1)	−5(1)
C(17)	24(1)	20(1)	26(1)	4(1)	7(1)	−3(1)
C(18)	15(1)	22(1)	14(1)	1(1)	2(1)	1(1)
C(19)	20(1)	22(1)	17(1)	1(1)	4(1)	2(1)
C(20)	21(1)	27(1)	23(1)	1(1)	4(1)	7(1)
C(21)	17(1)	35(1)	26(1)	1(1)	3(1)	2(1)
C(22)	18(1)	29(1)	24(1)	0(1)	2(1)	−3(1)
C(23)	18(1)	23(1)	16(1)	0(1)	2(1)	0(1)
C(24)	22(1)	19(1)	27(1)	0(1)	6(1)	4(1)
C(25)	35(1)	25(1)	38(1)	8(1)	7(1)	3(1)
C(26)	32(1)	28(1)	36(1)	−10(1)	8(1)	3(1)
C(27)	20(1)	20(1)	21(1)	−1(1)	2(1)	−2(1)
C(28)	28(1)	24(1)	33(1)	2(1)	6(1)	−5(1)
C(29)	45(1)	27(1)	24(1)	−4(1)	4(1)	2(1)
C(30)	27(1)	23(1)	15(1)	−2(1)	5(1)	−2(1)
C(31)	40(1)	30(1)	17(1)	1(1)	0(1)	2(1)
C(32)	22(1)	22(1)	19(1)	0(1)	6(1)	−2(1)
C(33)	25(1)	36(1)	34(1)	1(1)	13(1)	1(1)
C(34)	22(1)	18(1)	22(1)	2(1)	4(1)	−3(1)
C(35)	28(1)	22(1)	24(1)	5(1)	4(1)	−2(1)
C(36)	29(1)	16(1)	23(1)	−2(1)	4(1)	1(1)
C(37)	38(1)	22(1)	28(1)	−7(1)	2(1)	−4(1)

Table 4: Bond lengths [Å] for mw_036_5m.

Al(1)–N(3)	1.8017(9)
Al(1)–N(4)	1.8259(9)
Al(1)–N(2)	1.9180(9)
Al(1)–N(1)	1.9331(9)
N(1)–C(1)	1.3360(13)
N(1)–C(6)	1.4510(12)
N(2)–C(3)	1.3498(13)
N(2)–C(18)	1.4521(12)
N(3)–C(32)	1.4598(13)
N(3)–C(30)	1.4644(13)
N(4)–C(36)	1.4633(13)
N(4)–C(34)	1.4659(13)
C(1)–C(2)	1.4088(14)
C(1)–C(4)	1.5049(14)
C(2)–C(3)	1.3956(14)
C(3)–C(5)	1.5078(14)
C(6)–C(7)	1.4069(14)
C(6)–C(11)	1.4105(14)
C(7)–C(8)	1.3965(15)
C(7)–C(12)	1.5191(14)
C(8)–C(9)	1.3824(16)
C(9)–C(10)	1.3872(15)
C(10)–C(11)	1.3947(14)
C(11)–C(15)	1.5186(14)
C(12)–C(14)	1.5264(17)
C(12)–C(13)	1.5273(15)
C(15)–C(17)	1.5306(14)
C(15)–C(16)	1.5317(14)
C(18)–C(19)	1.4066(14)
C(18)–C(23)	1.4118(14)
C(19)–C(20)	1.4001(14)
C(19)–C(24)	1.5198(15)
C(20)–C(21)	1.3791(17)
C(21)–C(22)	1.3834(17)
C(22)–C(23)	1.3971(14)
C(23)–C(27)	1.5261(15)
C(24)–C(25)	1.5343(16)
C(24)–C(26)	1.5344(16)
C(27)–C(29)	1.5322(15)
C(27)–C(28)	1.5340(15)
C(30)–C(31)	1.5244(16)
C(32)–C(33)	1.5280(15)
C(34)–C(35)	1.5309(15)
C(36)–C(37)	1.5301(16)

Table 5: Bond angles [°] for mw_036_5m.

N(3)–Al(1)–N(4)	113.71(4)
N(3)–Al(1)–N(2)	112.77(4)
N(4)–Al(1)–N(2)	111.81(4)
N(3)–Al(1)–N(1)	115.17(4)
N(4)–Al(1)–N(1)	106.50(4)
N(2)–Al(1)–N(1)	95.40(4)
C(1)–N(1)–C(6)	118.61(8)
C(1)–N(1)–Al(1)	119.17(7)
C(6)–N(1)–Al(1)	122.07(6)
C(3)–N(2)–C(18)	116.91(8)
C(3)–N(2)–Al(1)	116.79(7)
C(18)–N(2)–Al(1)	125.97(6)
C(32)–N(3)–C(30)	113.48(8)
C(32)–N(3)–Al(1)	124.81(7)
C(30)–N(3)–Al(1)	121.46(7)
C(36)–N(4)–C(34)	113.07(8)
C(36)–N(4)–Al(1)	122.71(7)
C(34)–N(4)–Al(1)	122.48(7)
N(1)–C(1)–C(2)	122.20(9)
N(1)–C(1)–C(4)	121.42(9)
C(2)–C(1)–C(4)	116.38(9)
C(3)–C(2)–C(1)	127.72(9)
N(2)–C(3)–C(2)	122.96(9)
N(2)–C(3)–C(5)	120.15(9)
C(2)–C(3)–C(5)	116.87(9)
C(7)–C(6)–C(11)	120.63(9)
C(7)–C(6)–N(1)	120.96(9)
C(11)–C(6)–N(1)	118.40(8)
C(8)–C(7)–C(6)	118.42(9)
C(8)–C(7)–C(12)	118.84(9)
C(6)–C(7)–C(12)	122.69(9)
C(9)–C(8)–C(7)	121.59(10)
C(8)–C(9)–C(10)	119.40(10)
C(9)–C(10)–C(11)	121.31(10)
C(10)–C(11)–C(6)	118.58(9)
C(10)–C(11)–C(15)	120.29(9)
C(6)–C(11)–C(15)	121.12(9)
C(7)–C(12)–C(14)	110.04(9)
C(7)–C(12)–C(13)	113.31(9)
C(14)–C(12)–C(13)	109.65(9)
C(11)–C(15)–C(17)	112.93(9)
C(11)–C(15)–C(16)	110.59(8)
C(17)–C(15)–C(16)	110.22(9)
C(19)–C(18)–C(23)	120.98(9)
C(19)–C(18)–N(2)	120.90(9)
C(23)–C(18)–N(2)	118.12(9)
C(20)–C(19)–C(18)	118.22(10)
C(20)–C(19)–C(24)	118.24(10)
C(18)–C(19)–C(24)	123.52(9)
C(21)–C(20)–C(19)	121.40(10)
C(20)–C(21)–C(22)	119.86(10)
C(21)–C(22)–C(23)	121.29(10)
C(22)–C(23)–C(18)	118.24(10)

Table 5: (continued)

C(22)–C(23)–C(27)	118.84(10)
C(18)–C(23)–C(27)	122.91(9)
C(19)–C(24)–C(25)	110.99(10)
C(19)–C(24)–C(26)	111.63(9)
C(25)–C(24)–C(26)	109.53(10)
C(23)–C(27)–C(29)	112.55(9)
C(23)–C(27)–C(28)	111.92(9)
C(29)–C(27)–C(28)	109.14(9)
N(3)–C(30)–C(31)	115.06(9)
N(3)–C(32)–C(33)	114.92(9)
N(4)–C(34)–C(35)	115.47(9)
N(4)–C(36)–C(37)	115.36(9)

Crystal structure of mw_053m

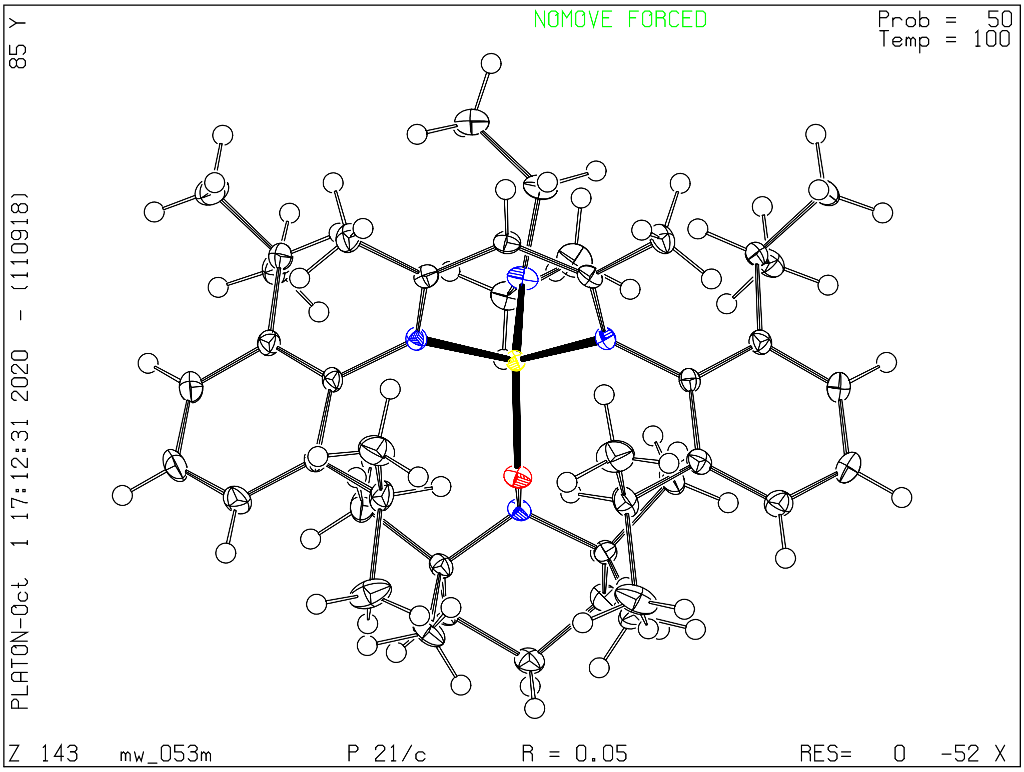

Table 1: Crystal data and structure refinement for mw_053m.

Identification code	mw_053m
Empirical Formula	$C_{42}\,H_{69}\,Ga\,N_4\,O$
Formula weight	715.73 Da
Density (calculated)	$1.213\,\mathrm{g\cdot cm^{-3}}$
$F(000)$	1552
Temperature	100(2) K
Crystal size	0.414 × 0.293 × 0.211 mm
Crystal appearance	colourless block
Wavelength (CuK_α)	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 10.1779(5)$ Å
	$b = 20.8197(9)$ Å
	$c = 19.0447(9)$ Å
	$\alpha = 90°$
	$\beta = 103.7956(14)°$
	$\gamma = 90°$
Unit cell volume	$3919.2(3)\,\text{Å}^3$
Z	4
Cell measurement refections used	9782
θ range for cell measurement	3.20° to 80.47°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	3.196° to 81.033°
Completeness to $\theta = 67.679°$ (to θ_{max})	100.0% (99.4%)
Index ranges	$-13 \leq h \leq 13$
	$-26 \leq k \leq 26$
	$-24 \leq l \leq 24$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.225\,\mathrm{mm^{-1}}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.61
R_{merg} before/after correction	0.1136/0.0643
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	165262
Independent reflections	8587 ($R_{int} = 0.0425$)
Reflections with $I > 2\sigma(I)$	8359
Data / retraints / parameter	8587 / 0 / 449
Goodness-of-fit on F^2	1.055
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0798P)^2 + 3.4801P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0472$
	$wR2 = 0.1273$
R indices [all data]	$R1 = 0.0478$
	$wR2 = 0.1280$
Largest diff. peak and hole	3.278 and $-0.563\,\text{Å}^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Residual electron density

The residual density shows a faint inverted image (pseudo centre of inversion at 1.005035 0.613207 0.750999) of the molecule, suggesting a full body disorder. However since the maximum corresponding to the gallium atom is only 3.28 electrons it is not possible to refine or completely identify the second orientation. The most disagreeing reflections all show higher F_{obs} than F_{calc} thus twinning was considered, however neither signs of non-merohedral twinning could be found in the diffraction pattern nor twin-laws for pseudo-merohedral twinning could be identified.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_053m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Ga(1)	7116(1)	6385(1)	7817(1)	10(1)
O(1)	6452(1)	6410(1)	6840(1)	14(1)
N(1)	8466(1)	7092(1)	8060(1)	12(1)
N(2)	8524(1)	5689(1)	8021(1)	12(1)
N(3)	4992(1)	6381(1)	6522(1)	12(1)
N(4)	6019(2)	6377(1)	8465(1)	16(1)
C(1)	9555(2)	6995(1)	8601(1)	13(1)
C(2)	9984(2)	6387(1)	8879(1)	15(1)
C(3)	9596(2)	5782(1)	8572(1)	14(1)
C(4)	10419(2)	7552(1)	8951(1)	18(1)
C(5)	10493(2)	5226(1)	8900(1)	19(1)
C(6)	8238(2)	7721(1)	7723(1)	12(1)
C(7)	8625(2)	7827(1)	7065(1)	15(1)
C(8)	8353(2)	8420(1)	6726(1)	20(1)
C(9)	7713(2)	8904(1)	7019(1)	21(1)
C(10)	7362(2)	8800(1)	7668(1)	18(1)
C(11)	7624(2)	8215(1)	8033(1)	14(1)
C(12)	9371(2)	7316(1)	6743(1)	21(1)
C(13)	10850(2)	7279(1)	7160(1)	31(1)
C(14)	9323(2)	7421(1)	5937(1)	32(1)
C(15)	7218(2)	8149(1)	8746(1)	16(1)
C(16)	7900(2)	8660(1)	9292(1)	21(1)
C(17)	5678(2)	8196(1)	8627(1)	20(1)
C(18)	8344(2)	5071(1)	7662(1)	14(1)
C(19)	8802(2)	4988(1)	7024(1)	17(1)
C(20)	8548(2)	4404(1)	6657(1)	22(1)
C(21)	7863(2)	3910(1)	6909(1)	23(1)
C(22)	7452(2)	3993(1)	7545(1)	20(1)
C(23)	7687(2)	4567(1)	7934(1)	15(1)
C(24)	9599(2)	5510(1)	6748(1)	22(1)
C(25)	9559(2)	5452(1)	5940(1)	30(1)
C(26)	11083(2)	5510(1)	7169(1)	29(1)
C(27)	7220(2)	4615(1)	8634(1)	18(1)
C(28)	5680(2)	4534(1)	8490(1)	23(1)
C(29)	7911(2)	4109(1)	9186(1)	28(1)
C(30)	4587(2)	7019(1)	6178(1)	15(1)
C(31)	3099(2)	6971(1)	5757(1)	20(1)
C(32)	2830(2)	6424(1)	5213(1)	19(1)
C(33)	3281(2)	5801(1)	5617(1)	17(1)
C(34)	4768(2)	5808(1)	6038(1)	14(1)
C(35)	5468(2)	7279(1)	5693(1)	24(1)
C(36)	4660(2)	7496(1)	6796(1)	22(1)
C(37)	5718(2)	5768(1)	5519(1)	22(1)
C(38)	4988(2)	5218(1)	6528(1)	23(1)
C(39)	4580(2)	6217(1)	8274(1)	20(1)
C(40)	3655(2)	6677(1)	8551(1)	26(1)
C(41)	6582(2)	6502(1)	9237(1)	20(1)
C(42)	6399(2)	5970(1)	9756(1)	31(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_053m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ga(1)	9(1)	10(1)	10(1)	−1(1)	2(1)	0(1)
O(1)	9(1)	20(1)	13(1)	−2(1)	0(1)	1(1)
N(1)	12(1)	11(1)	13(1)	−2(1)	3(1)	−1(1)
N(2)	12(1)	11(1)	13(1)	0(1)	3(1)	2(1)
N(3)	8(1)	14(1)	11(1)	−2(1)	0(1)	2(1)
N(4)	12(1)	24(1)	14(1)	−2(1)	4(1)	−2(1)
C(1)	11(1)	16(1)	13(1)	−3(1)	4(1)	−2(1)
C(2)	11(1)	19(1)	12(1)	−1(1)	0(1)	0(1)
C(3)	12(1)	16(1)	14(1)	2(1)	4(1)	2(1)
C(4)	15(1)	16(1)	21(1)	−5(1)	0(1)	−2(1)
C(5)	16(1)	17(1)	21(1)	1(1)	−1(1)	3(1)
C(6)	12(1)	11(1)	14(1)	−1(1)	2(1)	−3(1)
C(7)	15(1)	15(1)	16(1)	−2(1)	4(1)	−5(1)
C(8)	23(1)	20(1)	18(1)	1(1)	6(1)	−4(1)
C(9)	24(1)	16(1)	24(1)	6(1)	6(1)	0(1)
C(10)	19(1)	14(1)	23(1)	1(1)	6(1)	1(1)
C(11)	14(1)	13(1)	15(1)	−1(1)	3(1)	−2(1)
C(12)	28(1)	16(1)	25(1)	−5(1)	16(1)	−7(1)
C(13)	31(1)	39(1)	26(1)	3(1)	15(1)	15(1)
C(14)	29(1)	46(1)	23(1)	−11(1)	12(1)	−6(1)
C(15)	20(1)	13(1)	15(1)	−1(1)	6(1)	2(1)
C(16)	22(1)	23(1)	18(1)	−6(1)	3(1)	2(1)
C(17)	20(1)	22(1)	20(1)	−4(1)	8(1)	−2(1)
C(18)	13(1)	11(1)	15(1)	−1(1)	0(1)	4(1)
C(19)	17(1)	16(1)	18(1)	2(1)	4(1)	6(1)
C(20)	25(1)	21(1)	20(1)	−4(1)	7(1)	7(1)
C(21)	27(1)	16(1)	25(1)	−8(1)	4(1)	3(1)
C(22)	20(1)	14(1)	24(1)	−1(1)	3(1)	0(1)
C(23)	16(1)	13(1)	16(1)	0(1)	1(1)	2(1)
C(24)	28(1)	16(1)	25(1)	4(1)	14(1)	8(1)
C(25)	24(1)	46(1)	23(1)	11(1)	11(1)	10(1)
C(26)	34(1)	32(1)	23(1)	−4(1)	11(1)	−13(1)
C(27)	24(1)	14(1)	18(1)	0(1)	6(1)	−3(1)
C(28)	24(1)	20(1)	27(1)	2(1)	10(1)	−2(1)
C(29)	32(1)	28(1)	21(1)	5(1)	0(1)	−4(1)
C(30)	16(1)	14(1)	14(1)	0(1)	1(1)	2(1)
C(31)	18(1)	21(1)	19(1)	−2(1)	−2(1)	7(1)
C(32)	16(1)	23(1)	16(1)	−2(1)	−1(1)	2(1)
C(33)	12(1)	18(1)	19(1)	−4(1)	2(1)	−2(1)
C(34)	12(1)	14(1)	14(1)	−3(1)	1(1)	1(1)
C(35)	29(1)	23(1)	20(1)	6(1)	4(1)	−6(1)
C(36)	23(1)	17(1)	23(1)	−6(1)	−1(1)	5(1)
C(37)	16(1)	27(1)	22(1)	−10(1)	5(1)	2(1)
C(38)	22(1)	15(1)	27(1)	1(1)	−4(1)	−1(1)
C(39)	14(1)	26(1)	20(1)	−2(1)	5(1)	−2(1)
C(40)	18(1)	32(1)	29(1)	−3(1)	9(1)	−1(1)
C(41)	17(1)	29(1)	15(1)	−3(1)	5(1)	−2(1)
C(42)	45(1)	30(1)	17(1)	1(1)	7(1)	0(1)

Table 4: Bond lengths [Å] for mw_053m.

Ga(1)–O(1)	1.8235(12)
Ga(1)–N(4)	1.8520(15)
Ga(1)–N(1)	1.9926(13)
Ga(1)–N(2)	2.0090(13)
O(1)–N(3)	1.4657(17)
N(1)–C(1)	1.336(2)
N(1)–C(6)	1.452(2)
N(2)–C(3)	1.334(2)
N(2)–C(18)	1.450(2)
N(3)–C(34)	1.4929(19)
N(3)–C(30)	1.494(2)
N(4)–C(39)	1.461(2)
N(4)–C(41)	1.468(2)
C(1)–C(2)	1.403(2)
C(1)–C(4)	1.511(2)
C(2)–C(3)	1.404(2)
C(3)–C(5)	1.515(2)
C(6)–C(11)	1.404(2)
C(6)–C(7)	1.416(2)
C(7)–C(8)	1.389(2)
C(7)–C(12)	1.519(2)
C(8)–C(9)	1.388(3)
C(9)–C(10)	1.384(3)
C(10)–C(11)	1.396(2)
C(11)–C(15)	1.517(2)
C(12)–C(13)	1.527(3)
C(12)–C(14)	1.539(3)
C(15)–C(17)	1.533(2)
C(15)–C(16)	1.534(2)
C(18)–C(23)	1.408(2)
C(18)–C(19)	1.412(2)
C(19)–C(20)	1.393(2)
C(19)–C(24)	1.524(2)
C(20)–C(21)	1.390(3)
C(21)–C(22)	1.384(3)
C(22)–C(23)	1.396(2)
C(23)–C(27)	1.521(2)
C(24)–C(26)	1.531(3)
C(24)–C(25)	1.535(3)
C(27)–C(29)	1.535(3)
C(27)–C(28)	1.535(2)
C(30)–C(36)	1.528(2)
C(30)–C(35)	1.531(2)
C(30)–C(31)	1.539(2)
C(31)–C(32)	1.520(2)
C(32)–C(33)	1.521(2)
C(33)–C(34)	1.534(2)
C(34)–C(38)	1.526(2)
C(34)–C(37)	1.541(2)
C(39)–C(40)	1.524(3)
C(41)–C(42)	1.526(3)

Table 5: Bond angles [°] for mw_053m.

O(1)–Ga(1)–N(4)	122.99(6)
O(1)–Ga(1)–N(1)	106.41(5)
N(4)–Ga(1)–N(1)	110.12(6)
O(1)–Ga(1)–N(2)	107.02(5)
N(4)–Ga(1)–N(2)	112.39(6)
N(1)–Ga(1)–N(2)	93.89(6)
N(3)–O(1)–Ga(1)	120.87(9)
C(1)–N(1)–C(6)	119.53(13)
C(1)–N(1)–Ga(1)	117.77(11)
C(6)–N(1)–Ga(1)	122.40(10)
C(3)–N(2)–C(18)	119.26(13)
C(3)–N(2)–Ga(1)	117.29(11)
C(18)–N(2)–Ga(1)	122.99(10)
O(1)–N(3)–C(34)	106.17(11)
O(1)–N(3)–C(30)	106.89(11)
C(34)–N(3)–C(30)	117.01(13)
C(39)–N(4)–C(41)	114.82(14)
C(39)–N(4)–Ga(1)	124.30(12)
C(41)–N(4)–Ga(1)	120.80(12)
N(1)–C(1)–C(2)	123.66(15)
N(1)–C(1)–C(4)	120.88(15)
C(2)–C(1)–C(4)	115.47(14)
C(1)–C(2)–C(3)	128.38(16)
N(2)–C(3)–C(2)	123.64(15)
N(2)–C(3)–C(5)	120.78(15)
C(2)–C(3)–C(5)	115.57(14)
C(11)–C(6)–C(7)	120.20(15)
C(11)–C(6)–N(1)	120.96(14)
C(7)–C(6)–N(1)	118.83(14)
C(8)–C(7)–C(6)	118.84(15)
C(8)–C(7)–C(12)	119.85(15)
C(6)–C(7)–C(12)	121.28(15)
C(9)–C(8)–C(7)	121.33(17)
C(10)–C(9)–C(8)	119.40(16)
C(9)–C(10)–C(11)	121.43(17)
C(10)–C(11)–C(6)	118.76(15)
C(10)–C(11)–C(15)	117.65(15)
C(6)–C(11)–C(15)	123.59(15)
C(7)–C(12)–C(13)	110.55(15)
C(7)–C(12)–C(14)	113.83(17)
C(13)–C(12)–C(14)	108.60(15)
C(11)–C(15)–C(17)	110.45(14)
C(11)–C(15)–C(16)	111.57(14)
C(17)–C(15)–C(16)	109.71(14)
C(23)–C(18)–C(19)	120.61(15)
C(23)–C(18)–N(2)	120.39(14)
C(19)–C(18)–N(2)	118.98(15)
C(20)–C(19)–C(18)	118.49(16)
C(20)–C(19)–C(24)	120.07(16)
C(18)–C(19)–C(24)	121.40(15)
C(21)–C(20)–C(19)	121.39(17)
C(22)–C(21)–C(20)	119.42(16)
C(21)–C(22)–C(23)	121.41(17)

Table 5: (continued)

C(22)–C(23)–C(18)	118.62(16)
C(22)–C(23)–C(27)	118.11(15)
C(18)–C(23)–C(27)	123.27(15)
C(19)–C(24)–C(26)	111.05(15)
C(19)–C(24)–C(25)	113.55(17)
C(26)–C(24)–C(25)	108.19(15)
C(23)–C(27)–C(29)	111.55(15)
C(23)–C(27)–C(28)	110.78(14)
C(29)–C(27)–C(28)	109.21(15)
N(3)–C(30)–C(36)	106.35(13)
N(3)–C(30)–C(35)	116.06(14)
C(36)–C(30)–C(35)	107.88(15)
N(3)–C(30)–C(31)	107.77(13)
C(36)–C(30)–C(31)	107.66(14)
C(35)–C(30)–C(31)	110.74(14)
C(32)–C(31)–C(30)	113.44(14)
C(31)–C(32)–C(33)	108.10(15)
C(32)–C(33)–C(34)	113.44(14)
N(3)–C(34)–C(38)	106.73(13)
N(3)–C(34)–C(33)	108.42(13)
C(38)–C(34)–C(33)	107.18(14)
N(3)–C(34)–C(37)	114.35(13)
C(38)–C(34)–C(37)	108.98(14)
C(33)–C(34)–C(37)	110.87(13)
N(4)–C(39)–C(40)	115.78(16)
N(4)–C(41)–C(42)	116.15(16)

Crystal structure of mw_073_0m

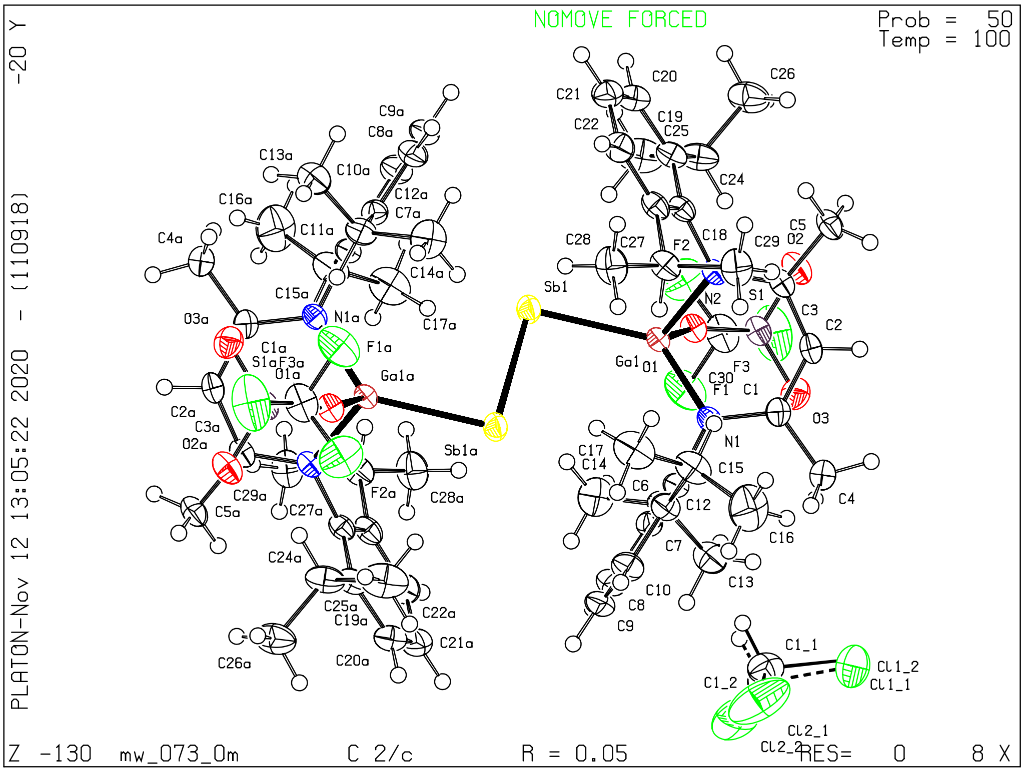

Table 1: Crystal data and structure refinement for mw_073_0m.

Identification code	mw_073_0m
Empirical Formula	$C_{62}H_{86}Cl_4F_6Ga_2N_4O_6S_2Sb_2$
Formula weight	1686.20 Da
Density (calculated)	$1.513\,g\cdot cm^{-3}$
$F(000)$	3408
Temperature	100(2) K
Crystal size	$0.467 \times 0.378 \times 0.348$ mm
Crystal appearance	blue prism
Wavelength (CuK_α)	1.54178 Å
Crystal system	Monoclinic
Space group	$C2/c$
Unit cell dimensions	$a = 27.5361(13)$ Å
	$b = 15.2489(7)$ Å
	$c = 21.8879(11)$ Å
	$\alpha = 90°$
	$\beta = 126.3345(10)°$
	$\gamma = 90°$
Unit cell volume	$7403.7(6)$ Å^3
Z	4
Cell measurement refections used	9964
θ range for cell measurement	3.52° to 80.29°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	3.517° to 80.918°
Completeness to $\theta = 67.679°$ (to θ_{max})	100.0% (99.6%)
Index ranges	$-35 \leq h \leq 34$
	$-19 \leq k \leq 19$
	$-27 \leq l \leq 28$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Numerical
Absorption coefficient	$8.937\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.06/0.01
R_{merg} before/after correction	0.1506/0.1061
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	139400
Independent reflections	8118 ($R_{int} = 0.0699$)
Reflections with $I > 2\sigma(I)$	8113
Data / retraints / parameter	8118 / 25 / 435
Goodness-of-fit on F^2	1.064
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0941P)^2 + 20.0383P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0523$
	$wR2 = 0.1362$
R indices [all data]	$R1 = 0.0523$
	$wR2 = 0.1362$
Largest diff. peak and hole	3.275 and -1.739 Å^{-3}

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

The dichloromethane molecule is disordered over two positions. The bond lengths and angles of the alternate positions were restrained to be equal (`SADI`) and `RIGU` restraints were applied to the anisotropic displacement parameters.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_073_0m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	5174(1)	4392(1)	4738(1)	31(1)
Ga(1)	4221(1)	3461(1)	4219(1)	21(1)
S(1)	3335(1)	2704(1)	2467(1)	27(1)
F(1)	3187(1)	4055(2)	1637(1)	55(1)
F(2)	3844(1)	3131(2)	1807(2)	59(1)
F(3)	2904(2)	2827(2)	1046(1)	69(1)
O(1)	3838(1)	3208(1)	3119(1)	26(1)
O(2)	3480(1)	1808(2)	2461(1)	37(1)
O(3)	2758(1)	2893(2)	2293(1)	36(1)
N(1)	3508(1)	3631(2)	4166(1)	23(1)
N(2)	4396(1)	2280(2)	4602(1)	23(1)
C(1)	3152(1)	2925(2)	3980(2)	26(1)
C(2)	3345(1)	2063(2)	4030(2)	27(1)
C(3)	3937(1)	1747(2)	4380(2)	25(1)
C(4)	2508(2)	3061(2)	3684(2)	37(1)
C(5)	4034(2)	772(2)	4476(2)	33(1)
C(6)	3350(1)	4484(2)	4297(2)	25(1)
C(7)	3145(1)	5159(2)	3754(2)	27(1)
C(8)	3062(2)	5993(2)	3936(2)	32(1)
C(9)	3169(2)	6162(2)	4626(2)	34(1)
C(10)	3355(2)	5490(2)	5145(2)	35(1)
C(11)	3453(2)	4645(2)	4997(2)	30(1)
C(12)	2994(2)	5000(2)	2976(2)	31(1)
C(13)	2314(2)	5085(3)	2360(2)	40(1)
C(14)	3339(2)	5625(3)	2812(2)	46(1)
C(15)	3673(2)	3944(2)	5603(2)	39(1)
C(16)	3200(3)	3712(4)	5732(3)	64(1)
C(17)	4252(2)	4246(3)	6359(2)	49(1)
C(18)	5017(1)	1992(2)	5060(2)	25(1)
C(19)	5284(2)	1707(2)	4714(2)	30(1)
C(20)	5900(2)	1528(2)	5174(2)	35(1)
C(21)	6245(2)	1617(2)	5952(2)	38(1)
C(22)	5970(2)	1889(2)	6283(2)	35(1)
C(23)	5363(2)	2092(2)	5858(2)	28(1)
C(24)	4927(2)	1602(3)	3858(2)	38(1)
C(25)	5158(3)	2226(3)	3536(3)	56(1)
C(26)	4947(2)	654(3)	3644(2)	50(1)
C(27)	5075(2)	2427(2)	6232(2)	31(1)
C(28)	5537(2)	2821(3)	7017(2)	43(1)
C(29)	4716(2)	1729(3)	6304(2)	42(1)
C(30)	3320(2)	3210(3)	1697(2)	40(1)
Cl11	1243(3)	4386(5)	3237(7)	68(2)
Cl21	1819(4)	5404(15)	4617(3)	98(3)
C11	1768(8)	5210(12)	3799(8)	43(3)
C12	1668(12)	5363(13)	3669(13)	45(5)
Cl12	1233(5)	4409(8)	3379(9)	82(3)
Cl22	1811(6)	5793(13)	4493(11)	87(4)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_073_0m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	32(1)	28(1)	39(1)	−11(1)	25(1)	−8(1)
Ga(1)	26(1)	18(1)	20(1)	0(1)	14(1)	−1(1)
S(1)	33(1)	24(1)	20(1)	−1(1)	14(1)	−3(1)
F(1)	86(2)	41(1)	45(1)	16(1)	42(1)	7(1)
F(2)	70(2)	80(2)	50(1)	7(1)	48(1)	2(1)
F(3)	92(2)	76(2)	22(1)	−9(1)	24(1)	−29(2)
O(1)	32(1)	26(1)	21(1)	−1(1)	16(1)	−2(1)
O(2)	47(1)	26(1)	33(1)	−4(1)	22(1)	−3(1)
O(3)	29(1)	41(1)	30(1)	1(1)	13(1)	−2(1)
N(1)	29(1)	20(1)	22(1)	1(1)	16(1)	0(1)
N(2)	30(1)	19(1)	20(1)	0(1)	14(1)	0(1)
C(1)	29(1)	27(2)	23(1)	1(1)	16(1)	−3(1)
C(2)	33(2)	23(1)	26(1)	−2(1)	18(1)	−8(1)
C(3)	34(2)	21(1)	20(1)	0(1)	15(1)	−2(1)
C(4)	32(2)	32(2)	46(2)	−3(1)	23(2)	−5(1)
C(5)	39(2)	21(1)	32(2)	1(1)	17(1)	−1(1)
C(6)	28(1)	22(1)	27(1)	0(1)	18(1)	2(1)
C(7)	25(1)	27(1)	26(1)	1(1)	14(1)	2(1)
C(8)	36(2)	25(2)	33(2)	3(1)	19(1)	5(1)
C(9)	36(2)	27(2)	41(2)	−5(1)	23(2)	4(1)
C(10)	43(2)	35(2)	33(2)	−4(1)	26(2)	2(1)
C(11)	37(2)	29(2)	32(2)	1(1)	25(1)	1(1)
C(12)	38(2)	28(2)	27(1)	6(1)	19(1)	6(1)
C(13)	42(2)	35(2)	30(2)	0(1)	15(2)	4(2)
C(14)	55(2)	54(3)	36(2)	7(2)	30(2)	−2(2)
C(15)	62(2)	34(2)	34(2)	5(1)	36(2)	5(2)
C(16)	83(4)	69(3)	65(3)	7(2)	56(3)	−11(3)
C(17)	69(3)	50(2)	31(2)	8(2)	31(2)	8(2)
C(18)	31(1)	19(1)	20(1)	2(1)	13(1)	2(1)
C(19)	39(2)	25(1)	27(2)	3(1)	21(1)	6(1)
C(20)	38(2)	32(2)	38(2)	4(1)	24(2)	9(1)
C(21)	32(2)	35(2)	38(2)	1(1)	17(2)	5(1)
C(22)	33(2)	35(2)	25(1)	−3(1)	11(1)	1(1)
C(23)	38(2)	22(1)	21(1)	−1(1)	15(1)	0(1)
C(24)	49(2)	42(2)	28(2)	3(1)	25(2)	15(2)
C(25)	81(3)	63(3)	47(2)	16(2)	50(2)	23(2)
C(26)	55(3)	51(2)	37(2)	−9(2)	24(2)	11(2)
C(27)	41(2)	30(2)	22(1)	−1(1)	19(1)	1(1)
C(28)	54(2)	47(2)	31(2)	−12(2)	26(2)	−11(2)
C(29)	53(2)	46(2)	36(2)	−7(2)	31(2)	−10(2)
C(30)	55(2)	42(2)	23(1)	0(1)	24(2)	−6(2)
Cl11	35(2)	51(2)	99(4)	−4(2)	29(2)	−1(1)
Cl21	67(2)	182(9)	64(2)	−1(3)	49(2)	22(4)
C11	44(6)	44(6)	43(6)	16(5)	26(5)	11(5)
C12	49(10)	42(8)	36(6)	21(6)	20(7)	1(8)
Cl12	74(5)	60(4)	138(8)	1(3)	77(6)	−14(3)
Cl22	74(3)	125(8)	94(5)	−32(5)	68(4)	−5(4)

Table 4: Bond lengths [Å] for mw_073_0m.

Sb(1)–Ga(1)	2.5800(4)
Sb(1)–Sb(1)#1	2.6395(4)
Ga(1)–N(1)	1.913(3)
Ga(1)–N(2)	1.924(2)
Ga(1)–O(1)	2.012(2)
S(1)–O(2)	1.426(3)
S(1)–O(3)	1.426(3)
S(1)–O(1)	1.485(2)
S(1)–C(30)	1.830(4)
F(1)–C(30)	1.324(5)
F(2)–C(30)	1.320(5)
F(3)–C(30)	1.322(4)
N(1)–C(1)	1.347(4)
N(1)–C(6)	1.455(4)
N(2)–C(3)	1.330(4)
N(2)–C(18)	1.446(4)
C(1)–C(2)	1.397(4)
C(1)–C(4)	1.499(4)
C(2)–C(3)	1.412(5)
C(3)–C(5)	1.504(4)
C(6)–C(11)	1.404(4)
C(6)–C(7)	1.412(4)
C(7)–C(8)	1.392(5)
C(7)–C(12)	1.512(4)
C(8)–C(9)	1.382(5)
C(9)–C(10)	1.383(5)
C(10)–C(11)	1.393(5)
C(11)–C(15)	1.523(5)
C(12)–C(14)	1.532(5)
C(12)–C(13)	1.532(5)
C(15)–C(16)	1.526(6)
C(15)–C(17)	1.539(6)
C(18)–C(19)	1.400(4)
C(18)–C(23)	1.417(4)
C(19)–C(20)	1.394(5)
C(19)–C(24)	1.523(4)
C(20)–C(21)	1.380(5)
C(21)–C(22)	1.386(5)
C(22)–C(23)	1.383(5)
C(23)–C(27)	1.526(5)
C(24)–C(25)	1.529(6)
C(24)–C(26)	1.530(5)
C(27)–C(29)	1.524(5)
C(27)–C(28)	1.530(5)
Cl11–C11	1.752(10)
Cl21–C11	1.736(10)
C12–Cl22	1.730(13)
C12–Cl12	1.747(13)

#1 -x+1,-y+1,-z+1

Table 5: Bond angles [°] for mw_073_0m.

Ga(1)–Sb(1)–Sb(1)#1	92.444(13)
N(1)–Ga(1)–N(2)	97.88(11)
N(1)–Ga(1)–O(1)	99.34(10)
N(2)–Ga(1)–O(1)	99.25(9)
N(1)–Ga(1)–Sb(1)	133.68(8)
N(2)–Ga(1)–Sb(1)	113.31(8)
O(1)–Ga(1)–Sb(1)	107.90(6)
O(2)–S(1)–O(3)	117.64(16)
O(2)–S(1)–O(1)	113.45(14)
O(3)–S(1)–O(1)	114.18(14)
O(2)–S(1)–C(30)	104.51(17)
O(3)–S(1)–C(30)	104.72(17)
O(1)–S(1)–C(30)	99.58(15)
S(1)–O(1)–Ga(1)	141.10(14)
C(1)–N(1)–C(6)	121.6(3)
C(1)–N(1)–Ga(1)	116.6(2)
C(6)–N(1)–Ga(1)	121.8(2)
C(3)–N(2)–C(18)	123.1(2)
C(3)–N(2)–Ga(1)	118.2(2)
C(18)–N(2)–Ga(1)	118.37(19)
N(1)–C(1)–C(2)	123.6(3)
N(1)–C(1)–C(4)	118.9(3)
C(2)–C(1)–C(4)	117.5(3)
C(1)–C(2)–C(3)	128.8(3)
N(2)–C(3)–C(2)	122.2(3)
N(2)–C(3)–C(5)	120.0(3)
C(2)–C(3)–C(5)	117.8(3)
C(11)–C(6)–C(7)	120.9(3)
C(11)–C(6)–N(1)	118.8(3)
C(7)–C(6)–N(1)	120.1(3)
C(8)–C(7)–C(6)	118.4(3)
C(8)–C(7)–C(12)	119.1(3)
C(6)–C(7)–C(12)	122.5(3)
C(9)–C(8)–C(7)	121.2(3)
C(8)–C(9)–C(10)	119.7(3)
C(9)–C(10)–C(11)	121.5(3)
C(10)–C(11)–C(6)	118.3(3)
C(10)–C(11)–C(15)	118.6(3)
C(6)–C(11)–C(15)	123.2(3)
C(7)–C(12)–C(14)	111.7(3)
C(7)–C(12)–C(13)	110.9(3)
C(14)–C(12)–C(13)	110.2(3)
C(11)–C(15)–C(16)	112.4(4)
C(11)–C(15)–C(17)	110.5(3)
C(16)–C(15)–C(17)	109.0(3)
C(19)–C(18)–C(23)	121.0(3)
C(19)–C(18)–N(2)	120.2(3)
C(23)–C(18)–N(2)	118.4(3)
C(20)–C(19)–C(18)	118.3(3)
C(20)–C(19)–C(24)	119.3(3)
C(18)–C(19)–C(24)	122.4(3)
C(21)–C(20)–C(19)	121.6(3)
C(20)–C(21)–C(22)	119.0(3)

Table 5: (continued)

C(23)–C(22)–C(21)	122.2(3)
C(22)–C(23)–C(18)	117.8(3)
C(22)–C(23)–C(27)	121.2(3)
C(18)–C(23)–C(27)	121.0(3)
C(19)–C(24)–C(25)	111.1(4)
C(19)–C(24)–C(26)	111.3(3)
C(25)–C(24)–C(26)	110.3(3)
C(29)–C(27)–C(23)	113.4(3)
C(29)–C(27)–C(28)	108.5(3)
C(23)–C(27)–C(28)	112.5(3)
F(2)–C(30)–F(3)	108.1(3)
F(2)–C(30)–F(1)	108.4(3)
F(3)–C(30)–F(1)	108.1(3)
F(2)–C(30)–S(1)	111.5(3)
F(3)–C(30)–S(1)	109.8(3)
F(1)–C(30)–S(1)	110.8(3)
Cl21–C11–Cl11	112.0(8)
Cl22–C12–Cl12	112.2(10)

#1 -x+1,-y+1,-z+1

Crystal structure of mw_076_2m

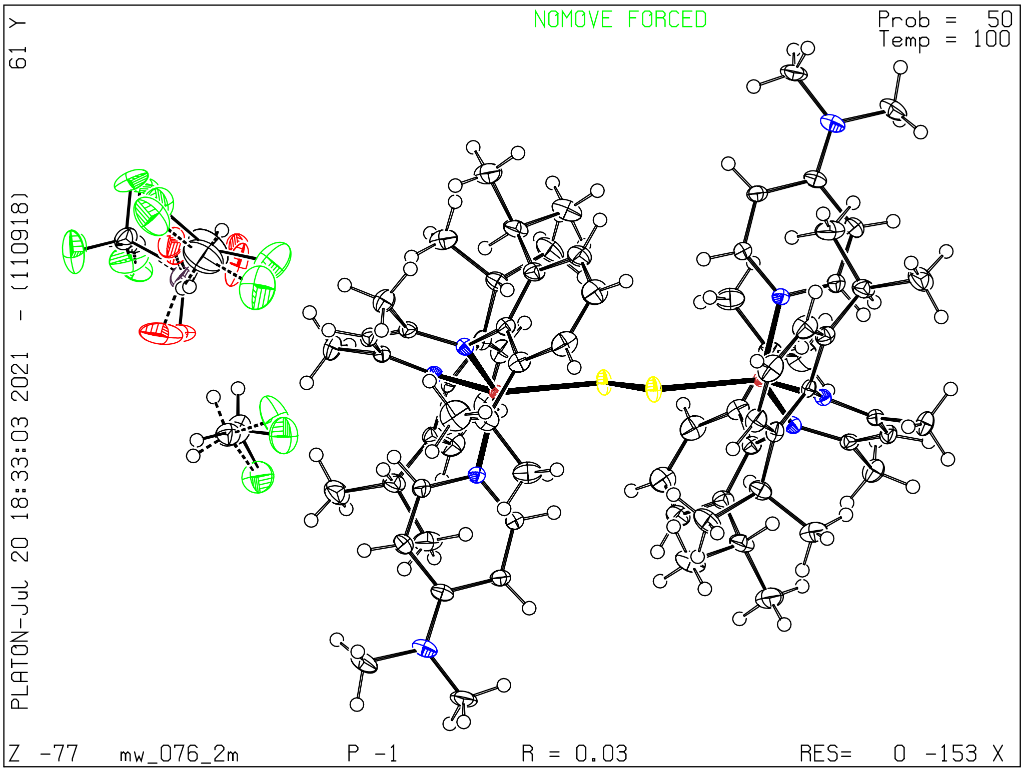

Table 1: Crystal data and structure refinement for mw_076_2m.

Identification code	mw_076_2m
Empirical Formula	$C_{78}\,H_{110}\,Cl_8\,F_6\,Ga_2\,N_8\,O_6\,S_2\,Sb_2$
Formula weight	2100.39 Da
Density (calculated)	$1.507\,\mathrm{g\cdot cm^{-3}}$
$F(000)$	1068
Temperature	100(2) K
Crystal size	0.459 × 0.329 × 0.144 mm
Crystal appearance	yellow tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 12.454(2)$ Å
	$b = 13.829(3)$ Å
	$c = 14.985(3)$ Å
	$\alpha = 103.273(7)°$
	$\beta = 93.858(7)°$
	$\gamma = 110.942(7)°$
Unit cell volume	2314.1(7) $Å^3$
Z	1
Cell measurement refections used	9525
θ range for cell measurement	2.27° to 33.13°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.639° to 33.430°
Completeness to $\theta = 25.242°$ (to θ_{max})	100.0% (98.9%)
Index ranges	$-19 \le h \le 19$
	$-21 \le k \le 21$
	$-23 \le l \le 23$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.493\,\mathrm{mm^{-1}}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.59
R_{merg} before/after correction	0.0980/0.0788
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	132365
Independent reflections	17862 ($R_{int} = 0.0598$)
Reflections with $I > 2\sigma(I)$	14414
Data / retraints / parameter	17862 / 299 / 646
Goodness-of-fit on F^2	1.036
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 1.0015P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0300$
	$wR2 = 0.0723$
R indices [all data]	$R1 = 0.0430$
	$wR2 = 0.0777$
Largest diff. peak and hole	1.091 and −1.352 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

Both solvent molecules and the anion are disordered over two positions. All corresponding bond length and angles of the disordered moieties were restrained to be equal (`SADI`) and `RIGU` restraints were applied to the anisotropic displacement parameters. For the displacement parameters of the solvent molecules additional `SIMU` restraints were required.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_076_2m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb11	3943(1)	9469(1)	5149(1)	22(1)
Ga11	3533(1)	7816(1)	3730(1)	12(1)
N11	4580(1)	7075(1)	3461(1)	15(1)
N21	2156(1)	6552(1)	3696(1)	14(1)
N31	3165(1)	8099(1)	2526(1)	16(1)
N41	2097(1)	8503(1)	−18(1)	25(1)
C11	4175(1)	6008(1)	3081(1)	17(1)
C21	3003(1)	5330(1)	2942(1)	18(1)
C31	2072(1)	5561(1)	3283(1)	16(1)
C41	5024(1)	5500(1)	2778(1)	26(1)
C51	942(1)	4618(1)	3164(1)	24(1)
C61	5813(1)	7694(1)	3770(1)	17(1)
C71	6490(1)	8257(1)	3203(1)	21(1)
C81	7642(1)	8945(1)	3575(1)	29(1)
C91	8110(1)	9073(2)	4471(2)	32(1)
C101	7450(1)	8484(1)	5015(1)	27(1)
C111	6297(1)	7772(1)	4673(1)	21(1)
C121	6020(2)	8131(1)	2204(1)	26(1)
C131	6722(2)	7689(2)	1533(2)	44(1)
C141	6018(2)	9185(2)	2054(1)	33(1)
C151	5638(1)	7078(1)	5265(1)	26(1)
C161	6198(2)	6280(2)	5379(2)	38(1)
C171	5600(2)	7739(2)	6222(1)	35(1)
C181	1244(1)	6748(1)	4152(1)	14(1)
C191	277(1)	6792(1)	3641(1)	20(1)
C201	−526(1)	7090(1)	4137(1)	28(1)
C211	−387(2)	7327(1)	5089(1)	30(1)
C221	546(1)	7256(1)	5582(1)	24(1)
C231	1374(1)	6960(1)	5131(1)	18(1)
C241	63(1)	6531(1)	2591(1)	24(1)
C251	−1101(2)	5579(2)	2172(2)	36(1)
C261	84(2)	7508(2)	2271(2)	34(1)
C271	2365(1)	6843(1)	5684(1)	22(1)
C281	2140(2)	5658(2)	5604(1)	32(1)
C291	2617(2)	7464(2)	6710(1)	37(1)
C301	2872(1)	7303(1)	1721(1)	21(1)
C311	2543(1)	7411(1)	878(1)	23(1)
C321	2472(1)	8389(1)	798(1)	20(1)
C331	2809(1)	9226(1)	1639(1)	20(1)
C341	3131(1)	9047(1)	2454(1)	18(1)
C351	1706(2)	7613(2)	−862(1)	33(1)
C361	2025(2)	9497(2)	−123(1)	31(1)
S12	1344(2)	1751(3)	2011(2)	19(1)
F12	75(11)	−293(8)	1269(6)	62(2)
F22	−685(6)	549(8)	2258(6)	53(2)
F32	720(9)	138(7)	2723(6)	57(2)
O12	794(8)	2076(6)	1336(4)	42(1)
O22	2342(8)	1530(11)	1765(7)	39(2)
O32	1544(6)	2417(5)	2953(3)	37(1)
C12	300(5)	453(6)	2060(6)	28(1)

Table 2: (continued)

	x	y	z	U_{eq}
Cl13	3377(4)	4779(3)	330(4)	54(1)
Cl23	1003(4)	4525(5)	493(6)	46(1)
C13	1982(8)	3867(9)	366(12)	59(3)
Cl14	5181(4)	1220(3)	899(6)	65(1)
Cl24	5934(5)	3534(3)	1385(7)	70(1)
C14	4774(9)	2305(7)	1182(10)	62(2)
Cl15	5129(6)	1203(5)	687(6)	65(1)
Cl25	5690(5)	3476(3)	952(8)	73(2)
C15	4698(14)	2278(9)	1039(16)	72(4)
Cl16	3400(5)	4536(16)	432(7)	78(2)
Cl26	1016(6)	4444(7)	418(8)	51(1)
C16	1932(7)	3743(10)	186(11)	32(2)
C17	273(12)	598(13)	2109(10)	36(2)
O27	2354(17)	1420(20)	1771(14)	45(4)
S17	1408(7)	1749(6)	1893(10)	38(1)
F17	−69(18)	−292(13)	1394(11)	46(2)
O37	1520(14)	2532(12)	2719(18)	70(4)
F37	593(15)	302(16)	2854(11)	53(3)
F27	−732(11)	730(15)	2248(8)	45(2)
O17	795(14)	1790(20)	1081(17)	71(5)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_076_2m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb11	22(1)	18(1)	19(1)	−3(1)	6(1)	3(1)
Ga11	12(1)	12(1)	11(1)	3(1)	2(1)	5(1)
N11	14(1)	17(1)	15(1)	4(1)	2(1)	7(1)
N21	14(1)	15(1)	13(1)	4(1)	3(1)	5(1)
N31	19(1)	16(1)	14(1)	5(1)	2(1)	7(1)
N41	27(1)	36(1)	16(1)	10(1)	2(1)	15(1)
C11	21(1)	19(1)	14(1)	5(1)	4(1)	11(1)
C21	23(1)	15(1)	17(1)	3(1)	4(1)	9(1)
C31	19(1)	15(1)	14(1)	5(1)	2(1)	6(1)
C41	27(1)	24(1)	30(1)	5(1)	9(1)	16(1)
C51	22(1)	15(1)	31(1)	5(1)	6(1)	3(1)
C61	14(1)	19(1)	20(1)	6(1)	4(1)	9(1)
C71	19(1)	24(1)	25(1)	10(1)	9(1)	11(1)
C81	19(1)	30(1)	42(1)	16(1)	11(1)	8(1)
C91	15(1)	34(1)	46(1)	13(1)	1(1)	6(1)
C101	18(1)	32(1)	32(1)	9(1)	−3(1)	10(1)
C111	16(1)	24(1)	24(1)	8(1)	1(1)	9(1)
C121	26(1)	32(1)	22(1)	11(1)	11(1)	10(1)
C131	54(1)	53(1)	33(1)	13(1)	26(1)	27(1)
C141	34(1)	40(1)	31(1)	21(1)	12(1)	16(1)
C151	20(1)	34(1)	24(1)	13(1)	−2(1)	8(1)
C161	42(1)	35(1)	40(1)	20(1)	1(1)	15(1)
C171	32(1)	52(1)	24(1)	15(1)	4(1)	18(1)
C181	15(1)	10(1)	16(1)	4(1)	4(1)	3(1)
C191	17(1)	18(1)	24(1)	8(1)	4(1)	6(1)
C201	20(1)	30(1)	40(1)	11(1)	7(1)	14(1)
C211	26(1)	31(1)	40(1)	10(1)	16(1)	16(1)
C221	27(1)	24(1)	24(1)	7(1)	12(1)	11(1)
C231	19(1)	16(1)	18(1)	5(1)	7(1)	5(1)
C241	19(1)	27(1)	25(1)	11(1)	−1(1)	6(1)
C251	28(1)	37(1)	33(1)	12(1)	−6(1)	1(1)
C261	24(1)	40(1)	43(1)	25(1)	2(1)	10(1)
C271	23(1)	29(1)	16(1)	8(1)	6(1)	10(1)
C281	39(1)	36(1)	31(1)	17(1)	10(1)	21(1)
C291	41(1)	51(1)	17(1)	5(1)	4(1)	18(1)
C301	28(1)	18(1)	17(1)	4(1)	3(1)	10(1)
C311	30(1)	24(1)	15(1)	3(1)	2(1)	11(1)
C321	19(1)	28(1)	16(1)	10(1)	4(1)	10(1)
C331	24(1)	21(1)	19(1)	9(1)	3(1)	11(1)
C341	21(1)	17(1)	18(1)	5(1)	2(1)	8(1)
C351	36(1)	48(1)	16(1)	6(1)	−1(1)	20(1)
C361	36(1)	39(1)	22(1)	16(1)	−2(1)	16(1)
S12	16(1)	23(1)	22(1)	10(1)	2(1)	9(1)
F12	58(3)	40(2)	52(2)	−10(2)	11(2)	−10(2)
F22	31(2)	64(3)	80(3)	47(2)	27(2)	16(2)
F32	77(3)	42(2)	65(3)	36(2)	7(2)	26(2)
O12	36(2)	47(2)	48(2)	33(2)	−4(2)	11(2)
O22	23(2)	35(3)	55(4)	3(2)	11(2)	12(2)
O32	48(2)	35(2)	27(2)	0(1)	3(1)	20(2)
C12	26(2)	22(2)	36(2)	13(2)	5(2)	5(1)
Cl13	51(1)	48(1)	53(1)	4(1)	14(1)	14(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl23	55(2)	35(1)	39(1)	7(1)	3(1)	9(1)
C13	91(5)	33(3)	47(6)	8(3)	1(3)	21(3)
Cl14	43(1)	47(1)	88(3)	21(1)	−6(1)	−1(1)
Cl24	66(1)	58(1)	107(3)	27(1)	41(2)	42(1)
C14	34(3)	108(5)	39(4)	14(3)	21(3)	23(3)
Cl15	37(1)	86(3)	54(2)	13(1)	5(1)	7(1)
Cl25	56(2)	70(1)	93(4)	9(2)	26(2)	30(1)
C15	45(5)	98(7)	71(10)	21(6)	−8(5)	30(5)
Cl16	58(1)	97(5)	49(2)	−22(3)	−1(1)	21(2)
Cl26	61(3)	56(3)	46(2)	12(2)	18(2)	32(2)
C16	36(3)	31(4)	29(4)	11(3)	6(2)	13(2)
C17	52(5)	34(4)	25(4)	8(3)	−4(3)	23(4)
O27	30(5)	35(5)	71(8)	5(4)	−2(4)	20(4)
S17	32(2)	24(1)	57(3)	15(2)	4(2)	10(1)
F17	46(4)	26(3)	50(4)	2(3)	4(4)	0(3)
O37	86(6)	23(3)	87(8)	−5(5)	19(6)	17(3)
F37	54(4)	67(7)	42(4)	36(4)	−8(3)	17(4)
F27	35(3)	63(6)	39(4)	18(3)	8(2)	20(3)
O17	33(4)	87(11)	87(8)	67(8)	−15(6)	−4(5)

Table 4: Bond lengths [Å] for mw_076_2m.

Sb11–Ga11	2.6067(4)
Sb11–Sb11#1	2.6433(5)
Ga11–N11	1.9366(11)
Ga11–N21	1.9502(12)
Ga11–N31	1.9909(13)
N11–C11	1.3416(18)
N11–C61	1.4450(17)
N21–C31	1.3316(17)
N21–C181	1.4386(17)
N31–C341	1.3539(18)
N31–C301	1.3581(19)
N41–C321	1.343(2)
N41–C361	1.451(2)
N41–C351	1.458(2)
C11–C21	1.395(2)
C11–C41	1.505(2)
C21–C31	1.406(2)
C31–C51	1.503(2)
C61–C71	1.404(2)
C61–C111	1.408(2)
C71–C81	1.395(2)
C71–C121	1.517(2)
C81–C91	1.374(3)
C91–C101	1.385(3)
C101–C111	1.397(2)
C111–C151	1.519(2)
C121–C141	1.526(3)
C121–C131	1.539(3)
C151–C171	1.528(3)
C151–C161	1.535(3)
C181–C191	1.411(2)
C181–C231	1.415(2)
C191–C201	1.406(2)
C191–C241	1.513(2)
C201–C211	1.373(3)
C211–C221	1.381(3)
C221–C231	1.398(2)
C231–C271	1.518(2)
C241–C261	1.527(2)
C241–C251	1.537(2)
C271–C291	1.527(2)
C271–C281	1.536(2)
C301–C311	1.359(2)
C311–C321	1.418(2)
C321–C331	1.420(2)
C331–C341	1.362(2)
S12–O12	1.425(5)
S12–O22	1.433(5)
S12–O32	1.448(4)
S12–C12	1.823(5)
F12–C12	1.317(7)
F22–C12	1.326(6)
F32–C12	1.320(7)

Table 4: (continued)

Cl13–C13	1.757(9)
Cl23–C13	1.759(9)
Cl14–C14	1.723(8)
Cl24–C14	1.737(8)
Cl15–C15	1.738(11)
Cl25–C15	1.716(11)
Cl16–C16	1.724(9)
Cl26–C16	1.747(9)
C17–F17	1.343(11)
C17–F27	1.351(11)
C17–F37	1.357(11)
C17–S17	1.823(12)
O27–S17	1.418(10)
S17–O37	1.406(9)
S17–O17	1.417(9)

#1 -x+1,-y+2,-z+1

Table 5: Bond angles [°] for mw_076_2m.

Ga11–Sb11–Sb11#1	94.060(12)
N11–Ga11–N21	96.92(5)
N11–Ga11–N31	102.93(5)
N21–Ga11–N31	101.62(5)
N11–Ga11–Sb11	124.69(4)
N21–Ga11–Sb11	114.82(4)
N31–Ga11–Sb11	112.55(4)
C11–N11–C61	120.85(11)
C11–N11–Ga11	121.37(9)
C61–N11–Ga11	117.49(9)
C31–N21–C181	121.88(11)
C31–N21–Ga11	121.72(9)
C181–N21–Ga11	116.39(8)
C341–N31–C301	116.30(13)
C341–N31–Ga11	123.58(10)
C301–N31–Ga11	120.04(10)
C321–N41–C361	123.15(15)
C321–N41–C351	121.47(15)
C361–N41–C351	115.37(14)
N11–C11–C21	123.90(12)
N11–C11–C41	118.80(13)
C21–C11–C41	117.30(13)
C11–C21–C31	128.66(13)
N21–C31–C21	123.28(13)
N21–C31–C51	120.15(13)
C21–C31–C51	116.56(12)
C71–C61–C111	121.15(13)
C71–C61–N11	120.45(13)
C111–C61–N11	118.28(13)
C81–C71–C61	118.24(15)
C81–C71–C121	119.29(15)
C61–C71–C121	122.46(14)
C91–C81–C71	121.33(16)
C81–C91–C101	120.02(15)
C91–C101–C111	121.01(16)
C101–C111–C61	118.09(15)
C101–C111–C151	119.07(15)
C61–C111–C151	122.77(13)
C71–C121–C141	112.13(15)
C71–C121–C131	110.72(16)
C141–C121–C131	110.03(15)
C111–C151–C171	112.78(15)
C111–C151–C161	109.67(14)
C171–C151–C161	109.54(15)
C191–C181–C231	120.74(13)
C191–C181–N21	120.76(13)
C231–C181–N21	118.40(12)
C201–C191–C181	117.96(15)
C201–C191–C241	118.77(14)
C181–C191–C241	123.27(13)
C211–C201–C191	121.59(15)
C201–C211–C221	120.07(15)
C211–C221–C231	121.20(16)

Table 5: (continued)

C221–C231–C181	118.39(14)
C221–C231–C271	120.21(14)
C181–C231–C271	121.38(12)
C191–C241–C261	111.13(15)
C191–C241–C251	111.30(14)
C261–C241–C251	109.92(14)
C231–C271–C291	113.17(14)
C231–C271–C281	111.63(13)
C291–C271–C281	109.33(15)
N31–C301–C311	123.72(14)
C301–C311–C321	120.45(14)
N41–C321–C311	121.84(15)
N41–C321–C331	122.76(15)
C311–C321–C331	115.39(13)
C341–C331–C321	120.12(14)
N31–C341–C331	123.97(14)
O12–S12–O22	114.8(5)
O12–S12–O32	114.3(3)
O22–S12–O32	112.9(4)
O12–S12–C12	106.3(5)
O22–S12–C12	103.9(6)
O32–S12–C12	103.0(4)
F12–C12–F32	108.3(6)
F12–C12–F22	109.1(6)
F32–C12–F22	108.3(6)
F12–C12–S12	111.9(7)
F32–C12–S12	109.6(6)
F22–C12–S12	109.5(6)
Cl13–C13–Cl23	110.2(6)
Cl14–C14–Cl24	113.2(5)
Cl25–C15–Cl15	113.5(8)
Cl16–C16–Cl26	114.8(8)
F17–C17–F27	103.4(10)
F17–C17–F37	105.1(10)
F27–C17–F37	105.4(10)
F17–C17–S17	113.0(12)
F27–C17–S17	114.9(11)
F37–C17–S17	114.0(12)
O37–S17–O17	116.7(7)
O37–S17–O27	117.3(9)
O17–S17–O27	116.3(9)
O37–S17–C17	99.2(9)
O17–S17–C17	98.0(10)
O27–S17–C17	104.2(13)

#1 -x+1,-y+2,-z+1

Crystal structure of mw_132_2m

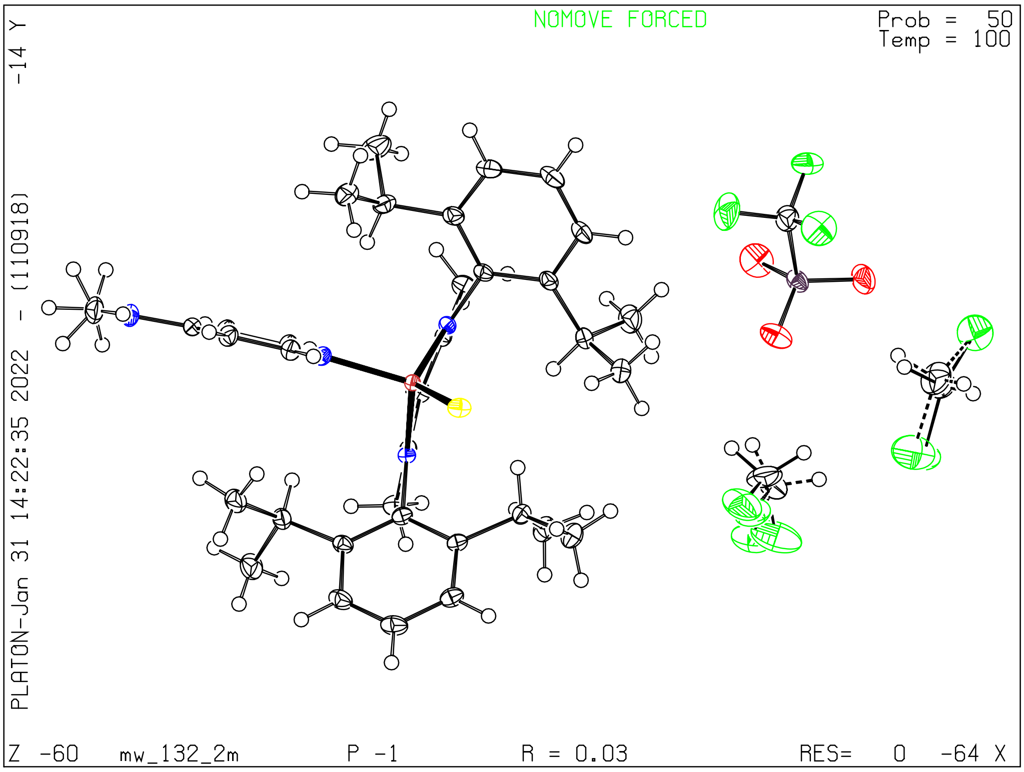

Table 1: Crystal data and structure refinement for mw_132_2m.

Identification code	mw_132_2m
Empirical Formula	$C_{78}H_{110}Bi_2Cl_8F_6Ga_2N_8O_6S_2$
Formula weight	2274.85 Da
Density (calculated)	1.630 g · cm^{-3}
$F(000)$	1132
Temperature	100(2) K
Crystal size	0.217 × 0.079 × 0.064 mm
Crystal appearance	red needle
Wavelength (MoK$_\alpha$)	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 12.4333(11)$ Å
	$b = 13.8507(12)$ Å
	$c = 14.9370(13)$ Å
	$\alpha = 102.794(4)°$
	$\beta = 93.662(4)°$
	$\gamma = 110.684(4)°$
Unit cell volume	2318.1(4) Å^3
Z	1
Cell measurement refections used	9734
θ range for cell measurement	2.83° to 31.30°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	2.089° to 33.630°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (98.7%)
Index ranges	$-19 \leq h \leq 19$
	$-21 \leq k \leq 21$
	$-23 \leq l \leq 23$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	4.698 mm^{-1}
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.50
R_{merg} before/after correction	0.0972/0.0547
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	190248
Independent reflections	18151 ($R_{int} = 0.0588$)
Reflections with $I > 2\sigma(I)$	15564
Data / retraints / parameter	18151 / 70 / 573
Goodness-of-fit on F^2	1.088
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 1.3944P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0291$
	$wR2 = 0.0603$
R indices [all data]	$R1 = 0.0406$
	$wR2 = 0.0632$
Largest diff. peak and hole	1.550 and −1.050 Å^{-3}

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

The dichloromethane molecules are disordered over two positions each. Their bond lengths and angles were restrained to be equal (`SADI`) and `RIGU` restraints were applied to their displacement parameters.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_132_2m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Bi(1)	3847(1)	9481(1)	5135(1)	19(1)
Ga(1)	3507(1)	7785(1)	3705(1)	12(1)
N(1)	2142(1)	6513(1)	3670(1)	13(1)
N(2)	4568(1)	7049(1)	3439(1)	14(1)
C(1)	949(2)	4589(2)	3147(2)	21(1)
C(2)	2072(2)	5532(2)	3261(1)	15(1)
C(3)	3013(2)	5312(2)	2920(1)	17(1)
C(4)	4177(2)	5989(2)	3059(1)	16(1)
C(5)	5041(2)	5492(2)	2759(2)	23(1)
C(6)	1215(2)	6700(2)	4128(1)	16(1)
C(7)	1354(2)	6927(2)	5102(1)	16(1)
C(8)	529(2)	7228(2)	5550(2)	20(1)
C(9)	−407(2)	7295(2)	5056(2)	25(1)
C(10)	−547(2)	7053(2)	4101(2)	23(1)
C(11)	258(2)	6752(2)	3611(2)	17(1)
C(12)	2349(2)	6810(2)	5659(1)	20(1)
C(13)	2128(2)	5633(2)	5594(2)	27(1)
C(14)	2591(2)	7425(2)	6686(2)	30(1)
C(15)	40(2)	6483(2)	2553(2)	21(1)
C(16)	−1120(2)	5539(2)	2151(2)	31(1)
C(17)	56(2)	7454(2)	2217(2)	28(1)
C(18)	5798(2)	7664(2)	3747(1)	16(1)
C(19)	6478(2)	8234(2)	3177(2)	19(1)
C(20)	7628(2)	8903(2)	3543(2)	24(1)
C(21)	8096(2)	9014(2)	4440(2)	26(1)
C(22)	7429(2)	8427(2)	4986(2)	23(1)
C(23)	6280(2)	7729(2)	4650(2)	18(1)
C(24)	6006(2)	8128(2)	2182(2)	23(1)
C(25)	6708(3)	7706(2)	1497(2)	38(1)
C(26)	5991(2)	9188(2)	2051(2)	30(1)
C(27)	5616(2)	7036(2)	5251(2)	22(1)
C(28)	6187(2)	6243(2)	5376(2)	32(1)
C(29)	5568(2)	7695(2)	6202(2)	30(1)
N11	3136(2)	8065(1)	2485(1)	15(1)
N21	2074(2)	8501(2)	−57(1)	23(1)
C11	3099(2)	9010(2)	2412(1)	17(1)
C21	2780(2)	9202(2)	1600(1)	19(1)
C31	2447(2)	8379(2)	760(1)	18(1)
C41	2520(2)	7397(2)	835(2)	21(1)
C51	2849(2)	7281(2)	1682(1)	19(1)
C61	2000(2)	9500(2)	−157(2)	28(1)
C71	1692(2)	7627(2)	−900(2)	29(1)
S12	8632(1)	8264(1)	7987(1)	22(1)
F12	10690(2)	9406(2)	7696(1)	48(1)
F22	9968(2)	10297(1)	8661(1)	50(1)
F32	9308(2)	9848(2)	7207(1)	51(1)
O12	7652(2)	8530(2)	8223(2)	36(1)
O22	8454(2)	7593(2)	7063(2)	44(1)
O32	9211(2)	7989(2)	8693(2)	47(1)
C12	9697(2)	9519(2)	7888(2)	30(1)

Table 2: (continued)

	x	y	z	U_{eq}
Cl13	6603(5)	5229(5)	9672(5)	42(1)
Cl23	8986(4)	5499(3)	9529(2)	29(1)
C13	8009(8)	6165(8)	9760(15)	29(2)
Cl14	4851(5)	8848(4)	9149(5)	63(1)
Cl24	4287(6)	6573(3)	8930(8)	72(1)
C14	5289(10)	7784(7)	8816(11)	55(3)
Cl15	6614(7)	5440(20)	9595(10)	73(3)
Cl25	8999(7)	5526(6)	9534(5)	59(3)
C15	8073(13)	6234(15)	9650(20)	48(5)
Cl16	4009(9)	6438(7)	8578(9)	50(2)
Cl26	4806(9)	8730(8)	9288(6)	53(2)
C16	5209(15)	7640(13)	8930(20)	53(5)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_132_2m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi(1)	19(1)	15(1)	18(1)	−1(1)	5(1)	5(1)
Ga(1)	12(1)	11(1)	12(1)	3(1)	2(1)	5(1)
N(1)	13(1)	12(1)	14(1)	3(1)	3(1)	5(1)
N(2)	14(1)	15(1)	16(1)	5(1)	3(1)	9(1)
C(1)	22(1)	13(1)	27(1)	5(1)	6(1)	4(1)
C(2)	18(1)	13(1)	15(1)	4(1)	3(1)	6(1)
C(3)	21(1)	13(1)	17(1)	3(1)	3(1)	8(1)
C(4)	20(1)	17(1)	14(1)	5(1)	4(1)	11(1)
C(5)	23(1)	22(1)	28(1)	4(1)	7(1)	15(1)
C(6)	18(1)	14(1)	17(1)	4(1)	5(1)	6(1)
C(7)	17(1)	14(1)	17(1)	4(1)	6(1)	6(1)
C(8)	24(1)	18(1)	21(1)	5(1)	9(1)	9(1)
C(9)	23(1)	25(1)	34(1)	8(1)	12(1)	14(1)
C(10)	18(1)	25(1)	32(1)	10(1)	6(1)	12(1)
C(11)	15(1)	16(1)	23(1)	7(1)	4(1)	6(1)
C(12)	21(1)	24(1)	16(1)	7(1)	4(1)	10(1)
C(13)	35(1)	30(1)	26(1)	14(1)	8(1)	19(1)
C(14)	32(1)	40(1)	16(1)	4(1)	4(1)	13(1)
C(15)	18(1)	23(1)	22(1)	10(1)	0(1)	6(1)
C(16)	24(1)	29(1)	29(1)	8(1)	−5(1)	1(1)
C(17)	22(1)	31(1)	36(1)	18(1)	2(1)	10(1)
C(18)	14(1)	16(1)	20(1)	5(1)	4(1)	9(1)
C(19)	18(1)	21(1)	24(1)	7(1)	6(1)	11(1)
C(20)	18(1)	23(1)	34(1)	12(1)	10(1)	9(1)
C(21)	14(1)	25(1)	38(1)	10(1)	1(1)	7(1)
C(22)	16(1)	25(1)	30(1)	7(1)	−1(1)	10(1)
C(23)	15(1)	21(1)	22(1)	7(1)	2(1)	10(1)
C(24)	23(1)	28(1)	21(1)	10(1)	10(1)	10(1)
C(25)	46(2)	45(2)	30(1)	10(1)	21(1)	22(1)
C(26)	29(1)	36(1)	31(1)	18(1)	9(1)	13(1)
C(27)	17(1)	30(1)	22(1)	11(1)	0(1)	8(1)
C(28)	33(1)	28(1)	37(1)	16(1)	0(1)	11(1)
C(29)	28(1)	45(1)	23(1)	14(1)	4(1)	17(1)
N11	18(1)	14(1)	15(1)	5(1)	3(1)	7(1)
N21	24(1)	33(1)	16(1)	9(1)	3(1)	15(1)
C11	20(1)	15(1)	18(1)	4(1)	3(1)	8(1)
C21	22(1)	19(1)	20(1)	8(1)	4(1)	10(1)
C31	16(1)	25(1)	17(1)	8(1)	4(1)	10(1)
C41	26(1)	21(1)	16(1)	4(1)	3(1)	11(1)
C51	24(1)	17(1)	17(1)	5(1)	3(1)	10(1)
C61	31(1)	32(1)	24(1)	14(1)	−1(1)	12(1)
C71	33(1)	41(1)	17(1)	6(1)	1(1)	20(1)
S12	19(1)	19(1)	31(1)	9(1)	1(1)	9(1)
F12	28(1)	64(1)	57(1)	33(1)	18(1)	13(1)
F22	50(1)	26(1)	50(1)	−2(1)	−1(1)	−3(1)
F32	62(1)	44(1)	53(1)	33(1)	−2(1)	15(1)
O12	24(1)	33(1)	49(1)	4(1)	6(1)	13(1)
O22	50(1)	32(1)	44(1)	−5(1)	4(1)	19(1)
O32	31(1)	56(1)	61(1)	42(1)	−2(1)	9(1)
C12	29(1)	28(1)	31(1)	13(1)	2(1)	8(1)
Cl13	37(2)	37(2)	44(1)	2(1)	11(1)	8(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl23	38(2)	25(2)	22(2)	6(1)	5(1)	11(1)
C13	37(4)	25(4)	33(4)	16(3)	12(3)	16(3)
Cl14	34(1)	49(1)	105(3)	40(2)	7(2)	1(1)
Cl24	48(2)	53(1)	113(4)	1(2)	27(2)	25(1)
C14	38(4)	84(5)	37(4)	14(4)	23(3)	15(3)
Cl15	52(2)	83(6)	50(3)	−20(3)	7(2)	8(3)
Cl25	61(4)	56(4)	59(4)	12(3)	10(3)	25(3)
C15	52(6)	39(6)	48(9)	23(5)	6(5)	7(4)
Cl16	42(3)	41(2)	80(4)	16(2)	24(2)	28(2)
Cl26	41(2)	50(3)	49(2)	11(2)	9(1)	−7(2)
C16	29(7)	87(8)	51(11)	27(7)	7(7)	25(5)

Table 4: Bond lengths [Å] for mw_132_2m.

Bi(1)–Ga(1)	2.6873(3)
Bi(1)–Bi(1)#1	2.8193(3)
Ga(1)–N(2)	1.9418(16)
Ga(1)–N(1)	1.9546(16)
Ga(1)–N11	2.0039(17)
N(1)–C(2)	1.329(2)
N(1)–C(6)	1.448(3)
N(2)–C(4)	1.344(2)
N(2)–C(18)	1.447(3)
C(1)–C(2)	1.506(3)
C(2)–C(3)	1.408(3)
C(3)–C(4)	1.392(3)
C(4)–C(5)	1.509(3)
C(6)–C(7)	1.405(3)
C(6)–C(11)	1.410(3)
C(7)–C(8)	1.393(3)
C(7)–C(12)	1.523(3)
C(8)–C(9)	1.380(3)
C(9)–C(10)	1.376(3)
C(10)–C(11)	1.402(3)
C(11)–C(15)	1.523(3)
C(12)–C(14)	1.532(3)
C(12)–C(13)	1.533(3)
C(15)–C(17)	1.531(3)
C(15)–C(16)	1.535(3)
C(18)–C(19)	1.407(3)
C(18)–C(23)	1.412(3)
C(19)–C(20)	1.394(3)
C(19)–C(24)	1.518(3)
C(20)–C(21)	1.380(3)
C(21)–C(22)	1.385(3)
C(22)–C(23)	1.395(3)
C(23)–C(27)	1.524(3)
C(24)–C(26)	1.530(3)
C(24)–C(25)	1.536(3)
C(27)–C(29)	1.526(3)
C(27)–C(28)	1.540(3)
N11–C11	1.353(2)
N11–C51	1.357(3)
N21–C31	1.345(3)
N21–C71	1.456(3)
N21–C61	1.458(3)
C11–C21	1.362(3)
C21–C31	1.419(3)
C31–C41	1.422(3)
C41–C51	1.364(3)
S12–O32	1.432(2)
S12–O12	1.4355(19)
S12–O22	1.437(2)
S12–C12	1.819(3)
F12–C12	1.339(3)
F22–C12	1.323(3)
F32–C12	1.332(3)

Table 4: (continued)

Cl13–C13	1.746(9)
Cl23–C13	1.774(7)
Cl14–C14	1.729(9)
Cl24–C14	1.752(9)
Cl15–C15	1.742(11)
Cl25–C15	1.751(12)
Cl16–C16	1.741(13)
Cl26–C16	1.739(12)

#1 -x+1,-y+2,-z+1

Table 5: Bond angles [°] for mw_132_2m.

Ga(1)–Bi(1)–Bi(1)#1	92.122(8)
N(2)–Ga(1)–N(1)	96.32(7)
N(2)–Ga(1)–N11	102.79(7)
N(1)–Ga(1)–N11	101.23(7)
N(2)–Ga(1)–Bi(1)	126.56(5)
N(1)–Ga(1)–Bi(1)	114.79(5)
N11–Ga(1)–Bi(1)	111.51(5)
C(2)–N(1)–C(6)	121.74(16)
C(2)–N(1)–Ga(1)	122.21(13)
C(6)–N(1)–Ga(1)	116.04(12)
C(4)–N(2)–C(18)	120.53(16)
C(4)–N(2)–Ga(1)	121.65(14)
C(18)–N(2)–Ga(1)	117.55(12)
N(1)–C(2)–C(3)	123.16(18)
N(1)–C(2)–C(1)	120.23(18)
C(3)–C(2)–C(1)	116.61(17)
C(4)–C(3)–C(2)	128.59(18)
N(2)–C(4)–C(3)	123.85(18)
N(2)–C(4)–C(5)	118.79(18)
C(3)–C(4)–C(5)	117.36(17)
C(7)–C(6)–C(11)	121.32(18)
C(7)–C(6)–N(1)	118.13(18)
C(11)–C(6)–N(1)	120.27(17)
C(8)–C(7)–C(6)	118.17(19)
C(8)–C(7)–C(12)	120.34(18)
C(6)–C(7)–C(12)	121.45(18)
C(9)–C(8)–C(7)	121.3(2)
C(10)–C(9)–C(8)	120.1(2)
C(9)–C(10)–C(11)	121.3(2)
C(10)–C(11)–C(6)	117.81(19)
C(10)–C(11)–C(15)	118.38(19)
C(6)–C(11)–C(15)	123.80(18)
C(7)–C(12)–C(14)	113.10(18)
C(7)–C(12)–C(13)	111.62(18)
C(14)–C(12)–C(13)	108.99(19)
C(11)–C(15)–C(17)	111.13(19)
C(11)–C(15)–C(16)	111.28(18)
C(17)–C(15)–C(16)	109.96(19)
C(19)–C(18)–C(23)	121.06(19)
C(19)–C(18)–N(2)	120.41(18)
C(23)–C(18)–N(2)	118.42(17)
C(20)–C(19)–C(18)	118.2(2)
C(20)–C(19)–C(24)	119.49(19)
C(18)–C(19)–C(24)	122.31(19)
C(21)–C(20)–C(19)	121.4(2)
C(20)–C(21)–C(22)	119.9(2)
C(21)–C(22)–C(23)	121.1(2)
C(22)–C(23)–C(18)	118.17(19)
C(22)–C(23)–C(27)	119.01(19)
C(18)–C(23)–C(27)	122.77(18)
C(19)–C(24)–C(26)	111.68(19)
C(19)–C(24)–C(25)	111.0(2)
C(26)–C(24)–C(25)	110.2(2)

Table 5: (continued)

C(23)–C(27)–C(29)	112.59(19)
C(23)–C(27)–C(28)	109.52(19)
C(29)–C(27)–C(28)	109.55(19)
C11–N11–C51	116.18(17)
C11–N11–Ga(1)	123.00(14)
C51–N11–Ga(1)	120.75(13)
C31–N21–C71	121.66(19)
C31–N21–C61	122.72(19)
C71–N21–C61	115.60(18)
N11–C11–C21	124.29(19)
C11–C21–C31	119.99(18)
N21–C31–C21	122.96(19)
N21–C31–C41	121.48(19)
C21–C31–C41	115.55(18)
C51–C41–C31	120.12(19)
N11–C51–C41	123.82(18)
O32–S12–O12	115.77(14)
O32–S12–O22	115.18(14)
O12–S12–O22	114.26(13)
O32–S12–C12	103.98(12)
O12–S12–C12	103.62(12)
O22–S12–C12	101.47(13)
F22–C12–F32	107.6(2)
F22–C12–F12	106.7(2)
F32–C12–F12	107.5(2)
F22–C12–S12	112.84(18)
F32–C12–S12	111.14(18)
F12–C12–S12	110.75(18)
Cl13–C13–Cl23	109.8(6)
Cl14–C14–Cl24	113.5(6)
Cl15–C15–Cl25	114.3(10)
Cl26–C16–Cl16	112.2(9)

#1 -x+1,-y+2,-z+1

Crystal structure of mw_155_3m

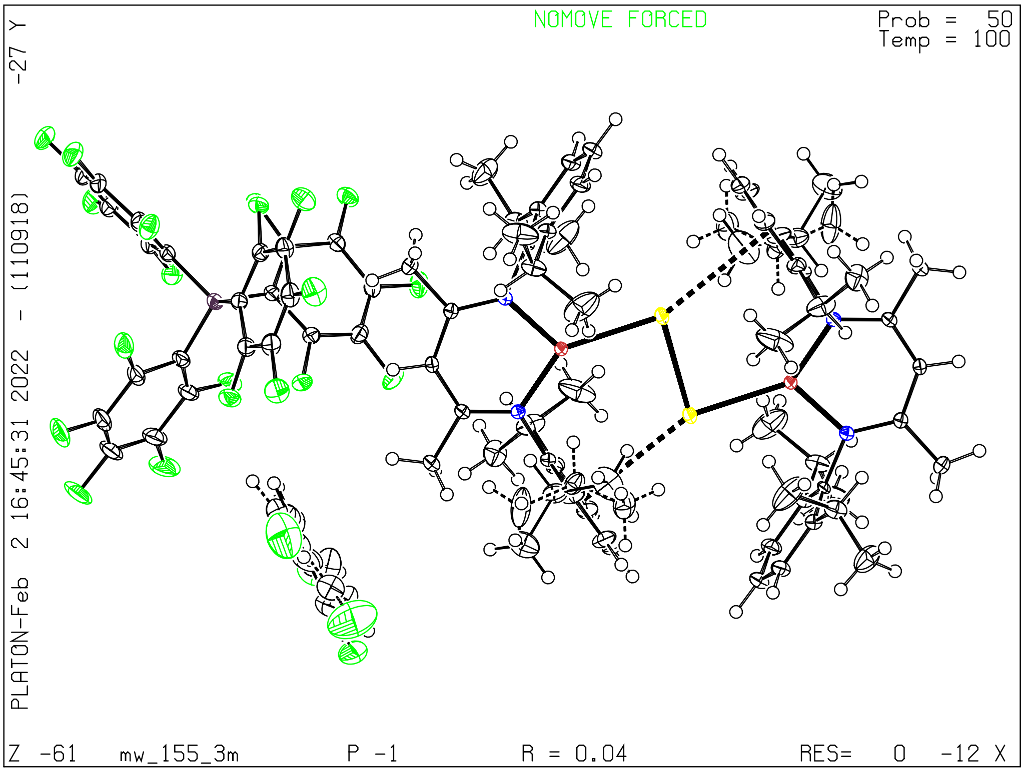

Table 1: Crystal data and structure refinement for mw_155_3m.

Identification code	mw_155_3m
Empirical Formula	$C_{118}\,H_{90}\,B_2\,F_{44}\,Ga_2\,N_4\,Sb_2$
Formula weight	2804.49 Da
Density (calculated)	$1.630\,\mathrm{g\cdot cm^{-3}}$
$F(000)$	1396
Temperature	100(2) K
Crystal size	$0.591 \times 0.366 \times 0.232$ mm
Crystal appearance	red tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 14.5284(17)$ Å
	$b = 14.8141(16)$ Å
	$c = 15.7805(18)$ Å
	$\alpha = 66.932(5)^\circ$
	$\beta = 67.280(5)^\circ$
	$\gamma = 74.700(5)^\circ$
Unit cell volume	2856.9(6) $\mathrm{Å^3}$
Z	1
Cell measurement refections used	9772
θ range for cell measurement	2.72° to 36.24°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.734° to 36.403°
Completeness to $\theta = 25.242^\circ$ (to θ_{max})	99.9% (99.8%)
Index ranges	$-24 \le h \le 24$
	$-24 \le k \le 24$
	$-26 \le l \le 26$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Numerical
Absorption coefficient	$1.057\,\mathrm{mm^{-1}}$
Absorption correction computing	SADABS
Max./min. transmission	0.27/0.19
R_{merg} before/after correction	0.0860/0.0454
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	296022
Independent reflections	27796 ($R_{int} = 0.0320$)
Reflections with $I > 2\sigma(I)$	22251
Data / retraints / parameter	27796 / 240 / 888
Goodness-of-fit on F^2	1.102
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2 + 3.1341P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0354$
	$wR2 = 0.0807$
R indices [all data]	$R1 = 0.0534$
	$wR2 = 0.0967$
Largest diff. peak and hole	3.022 and $-0.954\,\mathrm{Å^{-3}}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

An isopropyl group and the solvent molecule are disordered over two positions. The bond lengths and angles of the solvent's phenyl ring were restrained to be equal (`SADI`) and `RIGU` restraints were applied to all displacement parameters of the solvent molecule.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_155_3m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	5058(1)	569(1)	5445(1)	25(1)
Ga(1)	3893(1)	1929(1)	4600(1)	17(1)
N(1)	3652(1)	3190(1)	4706(1)	17(1)
N(2)	3144(1)	2157(1)	3790(1)	16(1)
C(1)	3071(1)	3954(1)	4274(1)	18(1)
C(2)	2585(1)	3868(1)	3703(1)	18(1)
C(3)	2630(1)	3046(1)	3450(1)	17(1)
C(4)	2953(1)	4935(1)	4402(1)	26(1)
C(5)	2109(1)	3168(1)	2750(1)	22(1)
C(6)	4182(1)	3224(1)	5300(1)	16(1)
C(7)	5199(1)	3408(1)	4835(1)	18(1)
C(8)	5772(1)	3224(1)	5435(1)	21(1)
C(9)	5360(1)	2877(1)	6437(1)	23(1)
C(10)	4357(1)	2732(1)	6867(1)	23(1)
C(11)	3745(1)	2917(1)	6301(1)	19(1)
C(12)	5679(1)	3768(1)	3741(1)	26(1)
C(13)	6465(2)	2969(2)	3388(2)	54(1)
C(14)	6174(2)	4693(2)	3406(2)	41(1)
C(15)	2645(1)	2756(1)	6784(1)	26(1)
C(16)	2527(2)	1664(2)	7118(2)	58(1)
C(17)	2131(2)	3136(2)	7646(2)	47(1)
C(18)	3245(1)	1345(1)	3454(1)	16(1)
C(19)	4021(1)	1291(1)	2603(1)	21(1)
C(20)	4153(1)	467(1)	2322(1)	25(1)
C(21)	3531(1)	−261(1)	2874(1)	25(1)
C(22)	2781(1)	−200(1)	3714(1)	29(1)
C(23)	2616(1)	606(1)	4030(1)	26(1)
C(24)	4727(2)	2071(2)	2009(1)	33(1)
C(25)	5787(2)	1638(2)	2087(1)	52(1)
C(26)	4763(2)	2501(2)	945(1)	34(1)
C(27)	1673(4)	793(4)	4846(4)	27(1)
C(28)	1752(4)	−37(7)	5777(4)	51(2)
C(29)	683(3)	853(5)	4685(4)	42(1)
C(27')	1895(4)	554(4)	5066(4)	26(1)
C(28')	1690(4)	−466(4)	5800(4)	37(1)
C(29')	903(4)	1187(4)	4939(5)	53(2)
F121	121(1)	6787(1)	2636(1)	29(1)
F131	−736(1)	5909(1)	4495(1)	35(1)
F141	−80(1)	6002(1)	5861(1)	37(1)
F151	1507(1)	6999(1)	5277(1)	32(1)
F161	2421(1)	7851(1)	3401(1)	22(1)
F221	2124(1)	5915(1)	1801(1)	26(1)
F231	3769(1)	4602(1)	1509(1)	32(1)
F241	5580(1)	5012(1)	1291(1)	33(1)
F251	5717(1)	6821(1)	1273(1)	26(1)
F261	4124(1)	8167(1)	1480(1)	19(1)
F321	−37(1)	8922(1)	1847(1)	36(1)
F331	−1033(1)	9319(1)	602(1)	56(1)
F341	−147(2)	8735(1)	−1004(1)	69(1)
F351	1717(1)	7676(1)	−1285(1)	55(1)

Table 2: (continued)

	x	y	z	U_{eq}
F361	2697(1)	7233(1)	−50(1)	31(1)
F421	3286(1)	9006(1)	−48(1)	27(1)
F431	3648(1)	10860(1)	−638(1)	39(1)
F441	2700(1)	11998(1)	548(1)	40(1)
F451	1345(1)	11228(1)	2306(1)	37(1)
F461	967(1)	9392(1)	2912(1)	30(1)
C111	1307(1)	7411(1)	2901(1)	19(1)
C121	501(1)	6882(1)	3248(1)	23(1)
C131	34(1)	6412(1)	4224(1)	26(1)
C141	359(1)	6451(1)	4918(1)	26(1)
C151	1162(1)	6960(1)	4618(1)	23(1)
C161	1615(1)	7406(1)	3638(1)	20(1)
C211	3020(1)	7134(1)	1627(1)	17(1)
C221	3004(1)	6180(1)	1663(1)	20(1)
C231	3837(1)	5477(1)	1537(1)	22(1)
C241	4762(1)	5685(1)	1415(1)	23(1)
C251	4827(1)	6598(1)	1410(1)	19(1)
C261	3970(1)	7295(1)	1510(1)	16(1)
C311	1380(1)	8042(1)	985(1)	24(1)
C321	423(1)	8582(1)	1084(2)	31(1)
C331	−106(2)	8803(1)	447(2)	42(1)
C341	331(2)	8507(2)	−358(2)	48(1)
C351	1278(2)	7976(2)	−503(2)	40(1)
C361	1775(1)	7756(1)	165(1)	29(1)
C411	2146(1)	9068(1)	1482(1)	20(1)
C421	2797(1)	9525(1)	574(1)	22(1)
C431	2992(1)	10490(1)	248(1)	27(1)
C441	2514(1)	11065(1)	839(1)	28(1)
C451	1835(1)	10671(1)	1732(1)	26(1)
C461	1660(1)	9697(1)	2030(1)	23(1)
B11	1963(1)	7915(1)	1752(1)	19(1)
C12	807(2)	3763(2)	408(2)	35(1)
F12	924(2)	3128(1)	−56(2)	50(1)
C22	1453(2)	4459(2)	6(3)	41(1)
F22	2177(2)	4477(2)	−832(2)	68(1)
C32	1348(6)	5124(5)	468(5)	50(1)
C42	578(5)	5079(4)	1332(4)	54(1)
C52	−75(3)	4393(4)	1720(3)	51(1)
C62	45(3)	3717(3)	1266(3)	44(1)
C13	−235(13)	4630(11)	1976(14)	73(4)
F13	−1092(11)	4803(11)	2834(12)	116(5)
C23	−195(12)	3780(10)	1818(15)	82(4)
F23	−866(14)	3112(12)	2458(15)	149(7)
C33	551(15)	3547(10)	1042(16)	84(5)
C43	1263(15)	4174(12)	441(15)	92(6)
C53	1200(30)	5050(20)	570(20)	83(7)
C63	448(18)	5286(13)	1346(19)	74(5)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_155_3m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	36(1)	16(1)	34(1)	−11(1)	−27(1)	8(1)
Ga(1)	24(1)	12(1)	23(1)	−8(1)	−17(1)	3(1)
N(1)	21(1)	14(1)	22(1)	−8(1)	−13(1)	1(1)
N(2)	21(1)	13(1)	21(1)	−7(1)	−13(1)	1(1)
C(1)	21(1)	14(1)	23(1)	−8(1)	−12(1)	2(1)
C(2)	22(1)	13(1)	24(1)	−7(1)	−14(1)	4(1)
C(3)	19(1)	16(1)	20(1)	−6(1)	−12(1)	0(1)
C(4)	33(1)	16(1)	38(1)	−13(1)	−21(1)	4(1)
C(5)	26(1)	21(1)	27(1)	−8(1)	−18(1)	1(1)
C(6)	19(1)	14(1)	23(1)	−11(1)	−16(1)	6(1)
C(7)	21(1)	17(1)	22(1)	−8(1)	−11(1)	−1(1)
C(8)	20(1)	23(1)	26(1)	−10(1)	−11(1)	−2(1)
C(9)	24(1)	26(1)	26(1)	−9(1)	−16(1)	−2(1)
C(10)	26(1)	26(1)	22(1)	−8(1)	−13(1)	−5(1)
C(11)	21(1)	21(1)	22(1)	−9(1)	−10(1)	−3(1)
C(12)	26(1)	32(1)	23(1)	−9(1)	−8(1)	−7(1)
C(13)	71(2)	36(1)	39(1)	−21(1)	14(1)	−18(1)
C(14)	61(1)	26(1)	32(1)	−3(1)	−9(1)	−15(1)
C(15)	22(1)	38(1)	26(1)	−14(1)	−8(1)	−8(1)
C(16)	42(1)	48(1)	78(2)	−28(1)	9(1)	−25(1)
C(17)	26(1)	81(2)	49(1)	−43(1)	−2(1)	−12(1)
C(18)	20(1)	15(1)	20(1)	−8(1)	−12(1)	0(1)
C(19)	28(1)	20(1)	17(1)	−7(1)	−10(1)	−4(1)
C(20)	31(1)	26(1)	23(1)	−14(1)	−11(1)	−1(1)
C(21)	30(1)	21(1)	34(1)	−15(1)	−17(1)	2(1)
C(22)	31(1)	24(1)	39(1)	−16(1)	−10(1)	−8(1)
C(23)	22(1)	27(1)	34(1)	−18(1)	−4(1)	−8(1)
C(24)	50(1)	37(1)	16(1)	−8(1)	−2(1)	−22(1)
C(25)	54(1)	86(2)	20(1)	4(1)	−14(1)	−45(1)
C(26)	42(1)	33(1)	19(1)	−5(1)	−6(1)	−5(1)
C(27)	22(2)	32(2)	30(2)	−15(2)	−3(1)	−8(2)
C(28)	37(2)	73(5)	32(2)	−13(3)	−4(2)	−5(3)
C(29)	21(2)	60(3)	46(2)	−20(2)	−5(1)	−7(2)
C(27')	22(2)	20(2)	31(2)	−8(2)	−2(1)	−5(1)
C(28')	35(2)	29(2)	35(2)	1(2)	−7(2)	−8(2)
C(29')	27(2)	29(2)	61(3)	4(2)	4(2)	4(2)
F121	27(1)	29(1)	35(1)	−2(1)	−16(1)	−13(1)
F131	25(1)	34(1)	40(1)	0(1)	−6(1)	−16(1)
F141	31(1)	41(1)	26(1)	0(1)	−2(1)	−10(1)
F151	29(1)	41(1)	24(1)	−10(1)	−9(1)	−5(1)
F161	19(1)	25(1)	27(1)	−7(1)	−9(1)	−6(1)
F221	30(1)	20(1)	33(1)	−4(1)	−15(1)	−10(1)
F231	45(1)	16(1)	34(1)	−9(1)	−12(1)	−5(1)
F241	31(1)	26(1)	38(1)	−14(1)	−11(1)	9(1)
F251	17(1)	32(1)	31(1)	−13(1)	−10(1)	−1(1)
F261	20(1)	18(1)	24(1)	−8(1)	−10(1)	−3(1)
F321	22(1)	27(1)	54(1)	−2(1)	−17(1)	−2(1)
F331	38(1)	37(1)	90(1)	14(1)	−48(1)	−10(1)
F341	89(1)	56(1)	86(1)	12(1)	−80(1)	−24(1)
F351	84(1)	58(1)	45(1)	−7(1)	−45(1)	−23(1)
F361	39(1)	36(1)	25(1)	−6(1)	−17(1)	−10(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F421	31(1)	24(1)	23(1)	−3(1)	−9(1)	−8(1)
F431	44(1)	29(1)	34(1)	6(1)	−9(1)	−18(1)
F441	45(1)	16(1)	59(1)	−2(1)	−25(1)	−10(1)
F451	37(1)	22(1)	55(1)	−18(1)	−18(1)	4(1)
F461	24(1)	22(1)	37(1)	−10(1)	−4(1)	−1(1)
C111	16(1)	16(1)	25(1)	−4(1)	−8(1)	−3(1)
C121	19(1)	19(1)	29(1)	−3(1)	−10(1)	−5(1)
C131	18(1)	22(1)	31(1)	−2(1)	−6(1)	−6(1)
C141	21(1)	24(1)	26(1)	−2(1)	−4(1)	−2(1)
C151	20(1)	23(1)	24(1)	−6(1)	−8(1)	0(1)
C161	16(1)	17(1)	25(1)	−6(1)	−7(1)	−1(1)
C211	19(1)	15(1)	17(1)	−3(1)	−9(1)	−4(1)
C221	24(1)	17(1)	21(1)	−4(1)	−11(1)	−5(1)
C231	31(1)	16(1)	21(1)	−5(1)	−10(1)	−3(1)
C241	25(1)	20(1)	21(1)	−7(1)	−8(1)	3(1)
C251	18(1)	22(1)	18(1)	−7(1)	−8(1)	−1(1)
C261	18(1)	17(1)	16(1)	−5(1)	−8(1)	−2(1)
C311	24(1)	20(1)	31(1)	2(1)	−18(1)	−9(1)
C321	26(1)	22(1)	44(1)	6(1)	−23(1)	−9(1)
C331	37(1)	26(1)	64(1)	12(1)	−39(1)	−13(1)
C341	61(1)	36(1)	61(1)	12(1)	−53(1)	−21(1)
C351	59(1)	35(1)	42(1)	4(1)	−38(1)	−20(1)
C361	36(1)	27(1)	31(1)	2(1)	−24(1)	−12(1)
C411	17(1)	16(1)	27(1)	−3(1)	−12(1)	−2(1)
C421	22(1)	18(1)	24(1)	−1(1)	−11(1)	−4(1)
C431	26(1)	20(1)	31(1)	2(1)	−14(1)	−9(1)
C441	29(1)	15(1)	43(1)	0(1)	−22(1)	−5(1)
C451	24(1)	17(1)	42(1)	−8(1)	−19(1)	2(1)
C461	18(1)	16(1)	33(1)	−5(1)	−11(1)	0(1)
B11	18(1)	16(1)	24(1)	−2(1)	−12(1)	−4(1)
C12	42(1)	31(1)	44(1)	−16(1)	−24(1)	2(1)
F12	60(1)	45(1)	65(1)	−33(1)	−28(1)	0(1)
C22	42(1)	38(2)	49(2)	−12(1)	−22(1)	−4(1)
F22	52(1)	85(2)	61(1)	−27(1)	−6(1)	−15(1)
C32	59(2)	34(2)	77(3)	−20(2)	−42(2)	−3(2)
C42	67(2)	47(2)	79(2)	−35(2)	−57(2)	18(2)
C52	48(2)	75(3)	50(2)	−37(2)	−25(1)	5(2)
C62	42(2)	53(2)	46(2)	−20(1)	−21(1)	−6(1)
C13	84(9)	52(7)	119(12)	−28(7)	−81(7)	10(6)
F13	102(9)	102(10)	141(11)	−32(8)	−63(7)	16(7)
C23	95(10)	49(7)	139(13)	−25(7)	−89(8)	1(6)
F23	156(13)	106(10)	211(17)	−31(10)	−74(11)	−66(10)
C33	110(12)	34(6)	151(15)	−38(8)	−94(10)	16(6)
C43	121(13)	45(8)	128(16)	−22(9)	−79(10)	9(7)
C53	84(15)	43(11)	144(17)	−22(11)	−77(10)	5(8)
C63	84(10)	34(7)	141(13)	−23(7)	−90(8)	11(7)

Table 4: Bond lengths [Å] for mw_155_3m.

Sb(1)–Ga(1)	2.5578(3)
Sb(1)–Sb(1)#1	2.6530(3)
Ga(1)–N(2)	1.8646(11)
Ga(1)–N(1)	1.8690(11)
N(1)–C(1)	1.3390(17)
N(1)–C(6)	1.4454(15)
N(2)–C(3)	1.3471(16)
N(2)–C(18)	1.4480(16)
C(1)–C(2)	1.3994(18)
C(1)–C(4)	1.5010(19)
C(2)–C(3)	1.4014(18)
C(3)–C(5)	1.4976(18)
C(6)–C(11)	1.386(2)
C(6)–C(7)	1.419(2)
C(7)–C(8)	1.3967(19)
C(7)–C(12)	1.516(2)
C(8)–C(9)	1.384(2)
C(9)–C(10)	1.384(2)
C(10)–C(11)	1.3977(19)
C(11)–C(15)	1.519(2)
C(12)–C(13)	1.526(3)
C(12)–C(14)	1.526(3)
C(15)–C(17)	1.522(3)
C(15)–C(16)	1.528(3)
C(18)–C(19)	1.395(2)
C(18)–C(23)	1.402(2)
C(19)–C(20)	1.399(2)
C(19)–C(24)	1.517(2)
C(20)–C(21)	1.382(2)
C(21)–C(22)	1.371(3)
C(22)–C(23)	1.398(2)
C(23)–C(27)	1.526(5)
C(23)–C(27')	1.548(5)
C(24)–C(26)	1.529(2)
C(24)–C(25)	1.536(4)
C(27)–C(28)	1.524(8)
C(27)–C(29)	1.530(6)
C(27')–C(28')	1.521(6)
C(27')–C(29')	1.535(7)
F121–C121	1.3481(18)
F131–C131	1.3451(18)
F141–C141	1.3338(19)
F151–C151	1.3420(19)
F161–C161	1.3503(16)
F221–C221	1.3490(17)
F231–C231	1.3442(17)
F241–C241	1.3385(18)
F251–C251	1.3349(17)
F261–C261	1.3484(15)
F321–C321	1.351(3)
F331–C331	1.344(3)
F341–C341	1.337(2)
F351–C351	1.341(3)

Table 4: (continued)

F361–C361	1.348(2)
F421–C421	1.3497(19)
F431–C431	1.346(2)
F441–C441	1.3410(18)
F451–C451	1.336(2)
F461–C461	1.3492(19)
C111–C121	1.3913(19)
C111–C161	1.394(2)
C111–B11	1.654(2)
C121–C131	1.386(2)
C131–C141	1.376(3)
C141–C151	1.382(2)
C151–C161	1.380(2)
C211–C261	1.3926(18)
C211–C221	1.3979(19)
C211–B11	1.656(2)
C221–C231	1.379(2)
C231–C241	1.382(2)
C241–C251	1.378(2)
C251–C261	1.3913(19)
C311–C361	1.383(3)
C311–C321	1.393(2)
C311–B11	1.657(2)
C321–C331	1.384(2)
C331–C341	1.370(4)
C341–C351	1.374(4)
C351–C361	1.390(2)
C411–C461	1.388(2)
C411–C421	1.392(2)
C411–B11	1.659(2)
C421–C431	1.384(2)
C431–C441	1.373(3)
C441–C451	1.373(3)
C451–C461	1.392(2)
C12–F12	1.347(3)
C12–C62	1.369(4)
C12–C22	1.372(4)
C22–F22	1.331(4)
C22–C32	1.386(5)
C32–C42	1.380(6)
C42–C52	1.371(6)
C52–C62	1.386(5)
C13–C23	1.359(11)
C13–C63	1.381(12)
C13–F13	1.50(2)
C23–C33	1.380(12)
C23–F23	1.38(2)
C33–C43	1.375(12)
C43–C53	1.371(12)
C53–C63	1.378(12)

#1 -x+1,-y,-z+1

Table 5: Bond angles [°] for mw_155_3m.

Ga(1)–Sb(1)–Sb(1)#1	88.266(10)
N(2)–Ga(1)–N(1)	99.59(5)
N(2)–Ga(1)–Sb(1)	141.07(3)
N(1)–Ga(1)–Sb(1)	119.29(3)
C(1)–N(1)–C(6)	125.31(11)
C(1)–N(1)–Ga(1)	123.70(9)
C(6)–N(1)–Ga(1)	110.99(8)
C(3)–N(2)–C(18)	121.53(10)
C(3)–N(2)–Ga(1)	122.80(9)
C(18)–N(2)–Ga(1)	115.29(8)
N(1)–C(1)–C(2)	122.15(11)
N(1)–C(1)–C(4)	118.50(12)
C(2)–C(1)–C(4)	119.34(12)
C(1)–C(2)–C(3)	128.81(12)
N(2)–C(3)–C(2)	122.87(11)
N(2)–C(3)–C(5)	118.51(11)
C(2)–C(3)–C(5)	118.60(11)
C(11)–C(6)–C(7)	122.71(11)
C(11)–C(6)–N(1)	119.03(12)
C(7)–C(6)–N(1)	117.35(12)
C(8)–C(7)–C(6)	116.99(13)
C(8)–C(7)–C(12)	119.71(13)
C(6)–C(7)–C(12)	123.28(12)
C(9)–C(8)–C(7)	121.03(13)
C(8)–C(9)–C(10)	120.47(13)
C(9)–C(10)–C(11)	120.86(14)
C(6)–C(11)–C(10)	117.84(13)
C(6)–C(11)–C(15)	121.91(12)
C(10)–C(11)–C(15)	120.24(13)
C(7)–C(12)–C(13)	111.38(15)
C(7)–C(12)–C(14)	111.29(14)
C(13)–C(12)–C(14)	109.04(17)
C(11)–C(15)–C(17)	112.57(13)
C(11)–C(15)–C(16)	111.38(16)
C(17)–C(15)–C(16)	109.1(2)
C(19)–C(18)–C(23)	122.52(12)
C(19)–C(18)–N(2)	118.24(12)
C(23)–C(18)–N(2)	119.04(12)
C(18)–C(19)–C(20)	117.66(14)
C(18)–C(19)–C(24)	122.13(13)
C(20)–C(19)–C(24)	120.19(14)
C(21)–C(20)–C(19)	120.57(15)
C(22)–C(21)–C(20)	120.82(14)
C(21)–C(22)–C(23)	121.03(15)
C(22)–C(23)–C(18)	117.38(15)
C(22)–C(23)–C(27)	121.8(2)
C(18)–C(23)–C(27)	119.7(2)
C(22)–C(23)–C(27')	118.9(2)
C(18)–C(23)–C(27')	122.8(2)
C(19)–C(24)–C(26)	112.13(15)
C(19)–C(24)–C(25)	110.14(17)
C(26)–C(24)–C(25)	110.60(16)
C(28)–C(27)–C(23)	106.7(4)

Table 5: (continued)

C(28)–C(27)–C(29)	111.0(4)
C(23)–C(27)–C(29)	114.5(3)
C(28')–C(27')–C(29')	109.9(4)
C(28')–C(27')–C(23)	117.5(4)
C(29')–C(27')–C(23)	106.1(4)
C121–C111–C161	113.10(13)
C121–C111–B11	126.91(13)
C161–C111–B11	119.66(12)
F121–C121–C131	114.78(13)
F121–C121–C111	121.26(14)
C131–C121–C111	123.96(15)
F131–C131–C141	119.74(15)
F131–C131–C121	120.06(15)
C141–C131–C121	120.20(14)
F141–C141–C131	121.10(15)
F141–C141–C151	120.38(16)
C131–C141–C151	118.51(15)
F151–C151–C161	120.66(14)
F151–C151–C141	119.97(14)
C161–C151–C141	119.35(15)
F161–C161–C151	115.79(13)
F161–C161–C111	119.37(13)
C151–C161–C111	124.83(13)
C261–C211–C221	112.88(12)
C261–C211–B11	127.60(12)
C221–C211–B11	119.50(12)
F221–C221–C231	115.96(12)
F221–C221–C211	119.15(13)
C231–C221–C211	124.86(13)
F231–C231–C221	121.15(14)
F231–C231–C241	119.43(14)
C221–C231–C241	119.41(13)
F241–C241–C251	120.85(14)
F241–C241–C231	120.33(14)
C251–C241–C231	118.82(13)
F251–C251–C241	119.77(13)
F251–C251–C261	120.51(13)
C241–C251–C261	119.67(13)
F261–C261–C251	114.61(11)
F261–C261–C211	121.13(12)
C251–C261–C211	124.26(12)
C361–C311–C321	113.38(15)
C361–C311–B11	127.15(14)
C321–C311–B11	119.11(16)
F321–C321–C331	116.51(18)
F321–C321–C311	119.09(15)
C331–C321–C311	124.4(2)
F331–C331–C341	119.97(18)
F331–C331–C321	120.6(2)
C341–C331–C321	119.4(2)
F341–C341–C331	120.9(2)
F341–C341–C351	120.0(3)
C331–C341–C351	119.17(16)

Table 5: (continued)

F351–C351–C341	120.12(17)
F351–C351–C361	120.3(2)
C341–C351–C361	119.5(2)
F361–C361–C311	121.48(13)
F361–C361–C351	114.40(19)
C311–C361–C351	124.11(19)
C461–C411–C421	113.07(13)
C461–C411–B11	127.81(13)
C421–C411–B11	118.91(13)
F421–C421–C431	116.22(14)
F421–C421–C411	119.09(13)
C431–C421–C411	124.69(15)
F431–C431–C441	120.34(14)
F431–C431–C421	120.22(16)
C441–C431–C421	119.44(16)
F441–C441–C451	120.43(17)
F441–C441–C431	120.70(17)
C451–C441–C431	118.87(14)
F451–C451–C441	119.63(14)
F451–C451–C461	120.61(16)
C441–C451–C461	119.75(16)
F461–C461–C411	121.22(13)
F461–C461–C451	114.69(15)
C411–C461–C451	124.09(15)
C111–B11–C211	102.36(10)
C111–B11–C311	112.94(11)
C211–B11–C311	112.86(12)
C111–B11–C411	113.64(12)
C211–B11–C411	113.27(11)
C311–B11–C411	102.23(11)
F12–C12–C62	120.0(3)
F12–C12–C22	119.3(3)
C62–C12–C22	120.7(3)
F22–C22–C12	118.3(3)
F22–C22–C32	121.2(3)
C12–C22–C32	120.5(3)
C42–C32–C22	118.7(4)
C52–C42–C32	120.5(4)
C42–C52–C62	120.5(3)
C12–C62–C52	119.0(3)
C23–C13–C63	120.6(10)
C23–C13–F13	114.9(14)
C63–C13–F13	124.4(13)
C13–C23–C33	120.2(9)
C13–C23–F23	120.8(16)
C33–C23–F23	118.9(15)
C43–C33–C23	119.4(9)
C53–C43–C33	120.4(10)
C43–C53–C63	120.0(10)
C53–C63–C13	119.2(9)

#1 -x+1,-y,-z+1

Crystal structure of mw_154_3bm

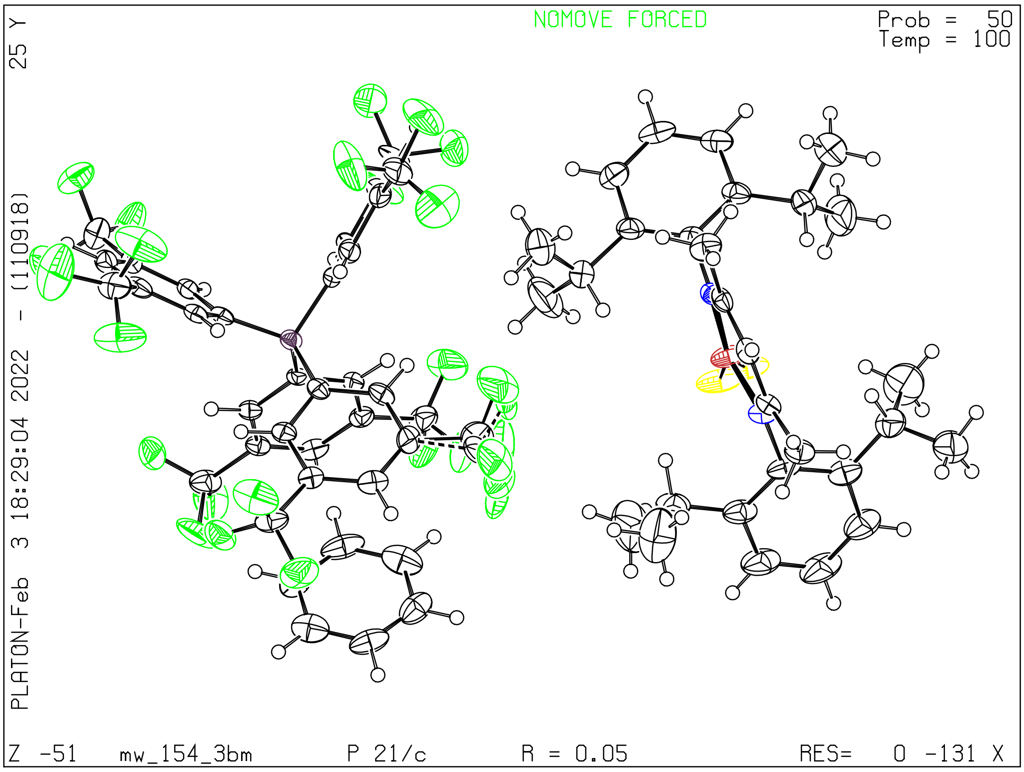

Table 1: Crystal data and structure refinement for mw_154_3bm.

Identification code	mw_154_3bm
Empirical Formula	$C_{134} H_{118} B_2 Bi_2 F_{48} Ga_2 N_4$
Formula weight	3275.34 Da
Density (calculated)	$1.608\,g \cdot cm^{-3}$
$F(000)$	3240
Temperature	100(2) K
Crystal size	0.138 × 0.117 × 0.075 mm
Crystal appearance	purpleish red tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 13.615(2)$ Å
	$b = 19.075(3)$ Å
	$c = 26.067(4)$ Å
	$\alpha = 90°$
	$\beta = 91.714(3)°$
	$\gamma = 90°$
Unit cell volume	6766.3(19) $Å^3$
Z	2
Cell measurement refections used	9942
θ range for cell measurement	2.38° to 27.22°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	2.384° to 27.238°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.6%)
Index ranges	$-17 \le h \le 17$
	$-24 \le k \le 24$
	$-33 \le l \le 33$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$3.103\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.69
R_{merg} before/after correction	0.0853/0.0675
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	164613
Independent reflections	15092 ($R_{int} = 0.1579$)
Reflections with $I > 2\sigma(I)$	8798
Data / retraints / parameter	15092 / 66 / 916
Goodness-of-fit on F^2	1.010
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0381P)^2 + 6.7515P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0527$
	$wR2 = 0.0864$
R indices [all data]	$R1 = 0.1174$
	$wR2 = 0.1017$
Largest diff. peak and hole	0.978 and −0.896 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

The displacement ellipsoids of the CF_3 groups suggest minor disorder. In one case two alternate positions could be identified and refined. The corresponding bond lengths and angles were restrained to be equal (`SADI`) and RIGU restraints were applied to the displacement parameters of these atoms. The bismuth atom is disordered over two positions. The displacement of the alternate positions was refined with common parameters (`EADP`).

Formation of ice

During the course of the measurement ice formed on the crystal. The resulting diffraction hampered the integration of the frames and lead to a rather high R_{int}.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_154_3bm. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Bi(1)	4460(1)	5586(1)	5174(1)	52(1)
Bi(1')	4853(8)	5572(2)	5320(3)	52(1)
Ga(1)	5587(1)	6371(1)	4589(1)	36(1)
N(1)	5625(3)	7346(2)	4673(1)	28(1)
N(2)	6491(2)	6278(2)	4068(1)	25(1)
C(1)	6170(3)	7776(2)	4394(2)	27(1)
C(2)	6754(3)	7521(2)	4001(2)	28(1)
C(3)	6917(3)	6836(2)	3850(2)	27(1)
C(4)	6186(3)	8544(2)	4509(2)	36(1)
C(5)	7612(4)	6706(3)	3423(2)	40(1)
C(6)	5020(4)	7596(2)	5082(2)	35(1)
C(7)	3997(4)	7641(2)	4981(2)	43(1)
C(8)	3424(4)	7838(3)	5386(3)	60(2)
C(9)	3830(5)	7973(3)	5861(2)	66(2)
C(10)	4823(4)	7912(3)	5952(2)	56(2)
C(11)	5453(4)	7717(2)	5562(2)	40(1)
C(12)	3536(4)	7479(3)	4460(2)	52(1)
C(13)	2555(5)	7088(4)	4490(3)	106(3)
C(14)	3422(7)	8119(4)	4139(3)	103(3)
C(15)	6537(4)	7616(3)	5672(2)	45(1)
C(16)	6734(6)	6920(3)	5949(3)	84(2)
C(17)	7017(4)	8216(3)	5978(2)	64(2)
C(18)	6772(3)	5570(2)	3944(2)	25(1)
C(19)	6184(3)	5182(2)	3599(2)	36(1)
C(20)	6428(4)	4485(3)	3524(2)	45(1)
C(21)	7225(4)	4187(3)	3780(2)	45(1)
C(22)	7799(4)	4581(2)	4106(2)	39(1)
C(23)	7601(3)	5284(2)	4199(2)	33(1)
C(24)	5324(4)	5502(3)	3299(2)	50(1)
C(25)	5546(5)	5532(3)	2732(2)	70(2)
C(26)	4361(4)	5117(4)	3388(3)	87(2)
C(27)	8238(4)	5717(3)	4575(2)	45(1)
C(28)	9316(4)	5679(3)	4459(2)	61(2)
C(29)	8072(5)	5481(4)	5127(2)	81(2)
F111	2832(11)	6810(6)	3005(3)	102(5)
F121	3045(12)	7766(5)	2607(6)	80(4)
F131	3974(7)	6897(6)	2476(8)	117(6)
C171	3056(11)	7074(7)	2558(6)	63(5)
F11'1	2404(7)	7357(11)	2963(4)	94(7)
F12'1	3364(14)	7782(7)	2421(9)	74(5)
F13'1	3642(12)	6773(6)	2738(5)	67(5)
C17'1	2940(12)	7196(8)	2568(6)	40(5)
F141	−299(2)	7161(1)	975(1)	49(1)
F151	1002(2)	7652(2)	709(1)	69(1)
F161	304(3)	8051(1)	1361(1)	66(1)
F211	2572(2)	5124(2)	−463(1)	81(1)
F221	1233(3)	4787(2)	−794(1)	97(1)
F231	1296(3)	5724(2)	−367(1)	75(1)
F241	1149(2)	2510(1)	148(1)	59(1)
F251	−287(3)	2838(2)	308(2)	83(1)

Table 2: (continued)

	x	y	z	U_{eq}
F261	714(3)	2535(2)	917(1)	65(1)
F311	1281(2)	5278(2)	3645(1)	60(1)
F321	1819(3)	4246(2)	3561(1)	94(1)
F331	384(2)	4415(2)	3825(1)	59(1)
F341	−2154(2)	5036(2)	2099(2)	86(1)
F351	−2214(2)	4102(2)	2545(1)	74(1)
F361	−1868(2)	4056(2)	1760(1)	56(1)
F411	5631(3)	5624(2)	1507(1)	81(1)
F421	5309(2)	5082(2)	813(1)	84(1)
F431	6300(2)	4652(2)	1370(1)	76(1)
F441	3324(3)	2821(2)	2571(2)	100(1)
F451	4514(3)	2557(2)	2110(1)	85(1)
F461	4761(3)	3181(2)	2770(1)	64(1)
C111	1811(3)	5817(2)	1640(2)	23(1)
C121	2399(3)	6130(2)	2022(2)	29(1)
C131	2369(3)	6841(2)	2129(2)	34(1)
C141	1744(3)	7278(2)	1844(2)	33(1)
C151	1170(3)	6987(2)	1463(2)	26(1)
C161	1187(3)	6268(2)	1366(2)	26(1)
C181	542(4)	7454(2)	1131(2)	39(1)
C211	1473(3)	4640(2)	1036(2)	23(1)
C221	1621(3)	4989(2)	576(2)	24(1)
C231	1437(3)	4674(2)	101(2)	30(1)
C241	1106(3)	3991(2)	64(2)	31(1)
C251	972(3)	3624(2)	516(2)	28(1)
C261	1140(3)	3942(2)	991(2)	24(1)
C271	1632(4)	5083(3)	−375(2)	44(1)
C281	632(4)	2888(3)	479(2)	42(1)
C311	1009(3)	4746(2)	2043(2)	21(1)
C321	1289(3)	4744(2)	2561(2)	24(1)
C331	641(3)	4626(2)	2950(2)	27(1)
C341	−346(3)	4511(2)	2835(2)	28(1)
C351	−650(3)	4515(2)	2328(2)	24(1)
C361	12(3)	4634(2)	1940(2)	23(1)
C371	1031(4)	4639(2)	3487(2)	38(1)
C381	−1709(3)	4428(2)	2185(2)	39(1)
C411	2879(3)	4629(2)	1719(2)	24(1)
C421	3692(3)	4926(2)	1500(2)	31(1)
C431	4631(3)	4635(2)	1558(2)	34(1)
C441	4772(3)	4031(3)	1846(2)	37(1)
C451	3977(3)	3725(2)	2062(2)	35(1)
C461	3051(3)	4009(2)	1998(2)	27(1)
C471	5462(4)	4996(3)	1311(2)	47(1)
C481	4132(4)	3070(3)	2380(2)	49(1)
B11	1776(3)	4957(2)	1598(2)	22(1)
C12	−294(5)	6410(3)	2579(2)	54(2)
C22	−966(4)	6688(3)	2241(2)	51(2)
C32	−1117(4)	7404(3)	2248(2)	49(1)
C42	−617(4)	7816(2)	2589(2)	47(1)
C52	53(4)	7543(3)	2927(2)	49(1)
C62	211(4)	6824(3)	2925(2)	56(2)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_154_3bm.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi(1)	60(1)	29(1)	72(1)	8(1)	48(1)	4(1)
Bi(1')	60(1)	29(1)	72(1)	8(1)	48(1)	4(1)
Ga(1)	43(1)	25(1)	40(1)	2(1)	24(1)	2(1)
N(1)	29(2)	24(2)	31(2)	5(2)	10(2)	6(2)
N(2)	22(2)	33(2)	21(2)	2(2)	2(2)	4(2)
C(1)	20(2)	28(2)	31(2)	6(2)	1(2)	4(2)
C(2)	24(3)	38(2)	22(2)	6(2)	2(2)	−3(2)
C(3)	19(2)	41(3)	19(2)	6(2)	−1(2)	0(2)
C(4)	34(3)	30(2)	44(3)	4(2)	6(2)	2(2)
C(5)	45(3)	46(3)	30(3)	4(2)	15(2)	1(2)
C(6)	41(3)	21(2)	45(3)	−1(2)	21(2)	0(2)
C(7)	33(3)	32(3)	64(4)	−7(2)	17(3)	−3(2)
C(8)	39(3)	56(3)	88(5)	−21(3)	28(3)	−5(3)
C(9)	58(4)	73(4)	71(4)	−25(3)	44(3)	−10(3)
C(10)	61(4)	61(4)	47(3)	−11(3)	25(3)	−1(3)
C(11)	50(3)	35(3)	37(3)	4(2)	17(2)	3(2)
C(12)	30(3)	57(3)	71(4)	−15(3)	11(3)	8(3)
C(13)	65(5)	131(7)	123(7)	−9(6)	−9(5)	−41(5)
C(14)	141(8)	83(5)	85(5)	7(4)	−29(5)	−26(5)
C(15)	57(4)	54(3)	25(3)	3(2)	3(2)	13(3)
C(16)	118(6)	61(4)	73(5)	11(3)	−15(4)	15(4)
C(17)	51(4)	80(4)	60(4)	−8(3)	6(3)	7(3)
C(18)	26(2)	29(2)	22(2)	3(2)	8(2)	4(2)
C(19)	31(3)	43(3)	33(3)	−3(2)	6(2)	11(2)
C(20)	47(3)	45(3)	44(3)	−13(2)	5(3)	3(3)
C(21)	57(4)	33(3)	47(3)	−4(2)	21(3)	13(3)
C(22)	45(3)	42(3)	30(3)	8(2)	10(2)	19(2)
C(23)	33(3)	41(3)	27(3)	6(2)	7(2)	13(2)
C(24)	44(3)	55(3)	48(3)	−19(3)	−13(3)	11(3)
C(25)	72(5)	89(5)	48(4)	−6(3)	−21(3)	18(4)
C(26)	41(4)	123(6)	96(5)	−2(5)	−20(4)	6(4)
C(27)	46(3)	53(3)	35(3)	−4(2)	−13(2)	19(3)
C(28)	47(4)	69(4)	68(4)	−5(3)	−5(3)	3(3)
C(29)	68(4)	139(7)	38(3)	−14(4)	−3(3)	9(4)
F111	139(11)	92(8)	70(5)	−6(5)	−56(5)	−33(8)
F121	90(12)	34(5)	113(11)	−32(4)	−38(7)	−1(5)
F131	44(5)	74(7)	229(17)	−62(8)	−38(6)	−4(4)
C171	57(9)	28(6)	101(10)	−16(7)	−17(10)	−2(6)
F11'1	49(6)	167(16)	66(6)	−71(8)	3(4)	−30(7)
F12'1	53(9)	44(6)	122(15)	−1(6)	−23(6)	−24(5)
F13'1	68(10)	37(5)	94(10)	−18(5)	−55(7)	4(6)
C17'1	20(8)	43(9)	57(10)	−3(7)	−3(7)	−5(6)
F141	43(2)	45(2)	57(2)	9(1)	−10(2)	9(2)
F151	68(2)	85(2)	55(2)	40(2)	22(2)	20(2)
F161	95(3)	37(2)	65(2)	0(2)	−6(2)	25(2)
F211	58(2)	116(3)	71(2)	55(2)	38(2)	27(2)
F221	163(4)	101(3)	27(2)	21(2)	−11(2)	−24(3)
F231	104(3)	64(2)	60(2)	36(2)	38(2)	43(2)
F241	86(2)	37(2)	55(2)	−12(1)	9(2)	6(2)
F251	47(2)	53(2)	147(4)	−18(2)	−27(2)	−11(2)
F261	117(3)	40(2)	38(2)	−1(1)	2(2)	−28(2)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F311	90(3)	57(2)	32(2)	0(1)	−9(2)	−28(2)
F321	108(3)	141(3)	31(2)	2(2)	−13(2)	82(3)
F331	92(2)	60(2)	23(1)	2(1)	9(2)	−24(2)
F341	23(2)	52(2)	181(4)	−12(2)	−20(2)	9(2)
F351	42(2)	119(3)	61(2)	6(2)	16(2)	−39(2)
F361	29(2)	77(2)	60(2)	−19(2)	−3(1)	−9(2)
F411	73(3)	77(2)	95(3)	−8(2)	33(2)	−34(2)
F421	34(2)	181(4)	38(2)	21(2)	5(2)	−22(2)
F431	22(2)	119(3)	88(3)	12(2)	12(2)	3(2)
F441	46(2)	79(3)	174(4)	68(3)	−1(2)	15(2)
F451	105(3)	56(2)	90(3)	−22(2)	−46(2)	41(2)
F461	76(2)	65(2)	50(2)	−2(2)	−26(2)	13(2)
C111	14(2)	29(2)	27(2)	2(2)	5(2)	−2(2)
C121	15(2)	34(2)	39(3)	4(2)	3(2)	−1(2)
C131	24(3)	35(3)	42(3)	−7(2)	2(2)	−12(2)
C141	31(3)	23(2)	45(3)	1(2)	13(2)	−4(2)
C151	27(3)	23(2)	29(2)	1(2)	6(2)	0(2)
C161	20(2)	30(2)	27(2)	1(2)	7(2)	1(2)
C181	50(4)	31(2)	37(3)	6(2)	12(3)	11(2)
C211	13(2)	28(2)	28(2)	2(2)	3(2)	5(2)
C221	16(2)	29(2)	27(2)	5(2)	3(2)	6(2)
C231	23(3)	45(3)	22(2)	10(2)	4(2)	13(2)
C241	26(3)	44(3)	23(2)	−2(2)	−1(2)	7(2)
C251	22(3)	35(2)	28(2)	−3(2)	−4(2)	3(2)
C261	18(2)	30(2)	24(2)	2(2)	0(2)	5(2)
C271	51(4)	54(3)	28(3)	10(2)	10(2)	15(3)
C281	51(4)	41(3)	34(3)	−4(2)	−2(3)	−5(3)
C311	21(2)	16(2)	25(2)	1(2)	0(2)	5(2)
C321	22(2)	22(2)	27(2)	−1(2)	−2(2)	4(2)
C331	35(3)	21(2)	24(2)	1(2)	2(2)	6(2)
C341	37(3)	19(2)	30(3)	3(2)	16(2)	2(2)
C351	22(2)	19(2)	31(3)	2(2)	4(2)	1(2)
C361	25(3)	18(2)	26(2)	3(2)	2(2)	4(2)
C371	52(3)	40(3)	24(3)	0(2)	4(2)	9(3)
C381	28(3)	35(2)	55(3)	−3(3)	13(2)	−2(2)
C411	19(2)	32(2)	22(2)	−10(2)	−1(2)	1(2)
C421	21(3)	42(3)	28(2)	−8(2)	2(2)	−2(2)
C431	22(3)	49(3)	31(3)	−16(2)	4(2)	−3(2)
C441	21(3)	49(3)	39(3)	−18(2)	−6(2)	12(2)
C451	26(3)	38(3)	42(3)	−13(2)	−9(2)	9(2)
C461	19(3)	35(2)	28(2)	−4(2)	−3(2)	2(2)
C471	21(3)	69(4)	52(4)	−8(3)	7(2)	1(3)
C481	28(3)	57(3)	61(4)	−1(3)	−9(3)	26(3)
B11	17(3)	24(2)	26(3)	0(2)	2(2)	0(2)
C12	68(4)	21(2)	75(4)	−3(3)	36(3)	1(3)
C22	58(4)	47(3)	50(3)	−9(3)	17(3)	−15(3)
C32	48(4)	51(3)	49(3)	15(3)	18(3)	7(3)
C42	62(4)	24(2)	56(3)	0(3)	28(3)	2(3)
C52	53(4)	46(3)	48(3)	−13(3)	19(3)	−15(3)
C62	45(4)	58(4)	65(4)	23(3)	16(3)	10(3)

Table 4: Bond lengths [Å] for mw_154_3bm.

Bi(1)–Ga(1)	2.6580(6)
Bi(1)–Bi(1)#1	2.8386(11)
Bi(1')–Ga(1)	2.659(4)
Bi(1')–Bi(1')#1	2.786(9)
Ga(1)–N(2)	1.869(3)
Ga(1)–N(1)	1.874(3)
N(1)–C(1)	1.336(5)
N(1)–C(6)	1.448(5)
N(2)–C(3)	1.346(5)
N(2)–C(18)	1.442(5)
C(1)–C(2)	1.403(5)
C(1)–C(4)	1.496(6)
C(2)–C(3)	1.384(6)
C(3)–C(5)	1.503(6)
C(6)–C(11)	1.386(7)
C(6)–C(7)	1.413(7)
C(7)–C(8)	1.384(7)
C(7)–C(12)	1.510(7)
C(8)–C(9)	1.364(8)
C(9)–C(10)	1.370(8)
C(10)–C(11)	1.400(6)
C(11)–C(15)	1.508(7)
C(12)–C(14)	1.486(8)
C(12)–C(13)	1.534(8)
C(15)–C(16)	1.530(7)
C(15)–C(17)	1.531(7)
C(18)–C(19)	1.400(6)
C(18)–C(23)	1.402(6)
C(19)–C(20)	1.386(6)
C(19)–C(24)	1.516(7)
C(20)–C(21)	1.379(7)
C(21)–C(22)	1.363(7)
C(22)–C(23)	1.390(6)
C(23)–C(27)	1.531(7)
C(24)–C(25)	1.518(8)
C(24)–C(26)	1.526(8)
C(27)–C(28)	1.509(7)
C(27)–C(29)	1.531(7)
F111–C171	1.314(12)
F121–C171	1.326(11)
F131–C171	1.318(12)
C171–C131	1.503(19)
F11'1–C17'1	1.316(12)
F12'1–C17'1	1.321(12)
F13'1–C17'1	1.318(12)
C17'1–C131	1.52(2)
F141–C181	1.328(6)
F151–C181	1.337(5)
F161–C181	1.332(5)
F211–C271	1.309(6)
F221–C271	1.330(6)
F231–C271	1.305(6)
F241–C281	1.340(5)

Table 4: (continued)

F251–C281	1.318(6)
F261–C281	1.329(5)
F311–C371	1.327(5)
F321–C371	1.318(6)
F331–C371	1.336(5)
F341–C381	1.325(5)
F351–C381	1.333(5)
F361–C381	1.328(5)
F411–C471	1.321(6)
F421–C471	1.321(6)
F431–C471	1.321(6)
F441–C481	1.309(6)
F451–C481	1.323(6)
F461–C481	1.326(6)
C111–C161	1.392(6)
C111–C121	1.392(6)
C111–B11	1.645(6)
C121–C131	1.385(6)
C131–C141	1.389(6)
C141–C151	1.364(6)
C151–C161	1.394(6)
C151–C181	1.492(6)
C211–C221	1.393(5)
C211–C261	1.409(6)
C211–B11	1.627(6)
C221–C231	1.391(6)
C231–C241	1.382(6)
C231–C271	1.497(6)
C241–C251	1.387(6)
C251–C261	1.392(6)
C251–C281	1.481(6)
C311–C361	1.392(6)
C311–C321	1.392(6)
C311–B11	1.633(6)
C321–C331	1.384(5)
C331–C341	1.385(6)
C331–C371	1.482(6)
C341–C351	1.374(6)
C351–C361	1.395(5)
C351–C381	1.487(6)
C411–C421	1.382(6)
C411–C461	1.404(6)
C411–B11	1.648(6)
C421–C431	1.398(6)
C431–C441	1.385(7)
C431–C471	1.486(7)
C441–C451	1.366(7)
C451–C461	1.378(6)
C451–C481	1.511(7)
C12–C22	1.360(8)
C12–C62	1.368(8)
C22–C32	1.380(7)
C32–C42	1.355(7)

Table 4: (continued)

C42–C52	1.354(7)
C52–C62	1.388(7)

#1 -x+1,-y+1,-z+1

Table 5: Bond angles [°] for mw_154_3bm.

Ga(1)–Bi(1)–Bi(1)#1	86.95(3)
Ga(1)–Bi(1')–Bi(1')#1	87.4(2)
N(2)–Ga(1)–N(1)	99.36(14)
N(2)–Ga(1)–Bi(1)	140.15(11)
N(1)–Ga(1)–Bi(1)	120.47(10)
N(2)–Ga(1)–Bi(1')	137.45(15)
N(1)–Ga(1)–Bi(1')	119.66(14)
C(1)–N(1)–C(6)	122.5(3)
C(1)–N(1)–Ga(1)	124.0(3)
C(6)–N(1)–Ga(1)	113.5(2)
C(3)–N(2)–C(18)	121.7(3)
C(3)–N(2)–Ga(1)	122.2(3)
C(18)–N(2)–Ga(1)	115.9(2)
N(1)–C(1)–C(2)	121.4(4)
N(1)–C(1)–C(4)	119.8(4)
C(2)–C(1)–C(4)	118.8(4)
C(3)–C(2)–C(1)	129.4(4)
N(2)–C(3)–C(2)	123.5(4)
N(2)–C(3)–C(5)	118.1(4)
C(2)–C(3)–C(5)	118.5(4)
C(11)–C(6)–C(7)	123.4(4)
C(11)–C(6)–N(1)	118.9(4)
C(7)–C(6)–N(1)	117.5(4)
C(8)–C(7)–C(6)	116.6(5)
C(8)–C(7)–C(12)	121.0(5)
C(6)–C(7)–C(12)	122.4(4)
C(9)–C(8)–C(7)	121.5(5)
C(8)–C(9)–C(10)	120.8(5)
C(9)–C(10)–C(11)	121.3(5)
C(6)–C(11)–C(10)	116.4(5)
C(6)–C(11)–C(15)	122.7(4)
C(10)–C(11)–C(15)	120.8(5)
C(14)–C(12)–C(7)	111.8(5)
C(14)–C(12)–C(13)	110.6(6)
C(7)–C(12)–C(13)	113.1(5)
C(11)–C(15)–C(16)	110.9(5)
C(11)–C(15)–C(17)	113.8(4)
C(16)–C(15)–C(17)	109.8(5)
C(19)–C(18)–C(23)	122.3(4)
C(19)–C(18)–N(2)	119.2(4)
C(23)–C(18)–N(2)	118.3(4)
C(20)–C(19)–C(18)	117.6(4)
C(20)–C(19)–C(24)	119.9(5)
C(18)–C(19)–C(24)	122.5(4)
C(21)–C(20)–C(19)	121.0(5)
C(22)–C(21)–C(20)	120.2(4)
C(21)–C(22)–C(23)	121.9(5)
C(22)–C(23)–C(18)	116.8(5)
C(22)–C(23)–C(27)	121.5(4)
C(18)–C(23)–C(27)	121.7(4)
C(19)–C(24)–C(25)	110.1(4)
C(19)–C(24)–C(26)	112.5(5)
C(25)–C(24)–C(26)	111.2(5)

Table 5: (continued)

C(28)–C(27)–C(29)	110.2(4)
C(28)–C(27)–C(23)	112.5(4)
C(29)–C(27)–C(23)	110.3(5)
F111–C171–F131	106.9(12)
F111–C171–F121	107.0(12)
F131–C171–F121	106.5(11)
F111–C171–C131	113.0(11)
F131–C171–C131	112.1(12)
F121–C171–C131	111.0(12)
F11'1–C17'1–F13'1	107.1(12)
F11'1–C17'1–F12'1	106.8(12)
F13'1–C17'1–F12'1	107.2(12)
F11'1–C17'1–C131	114.2(12)
F13'1–C17'1–C131	109.2(12)
F12'1–C17'1–C131	112.0(14)
C161–C111–C121	115.4(4)
C161–C111–B11	124.5(4)
C121–C111–B11	119.4(4)
C131–C121–C111	123.0(4)
C121–C131–C141	120.0(4)
C121–C131–C171	114.7(6)
C141–C131–C171	125.3(6)
C121–C131–C17'1	124.7(7)
C141–C131–C17'1	115.2(7)
C151–C141–C131	118.3(4)
C141–C151–C161	121.3(4)
C141–C151–C181	119.0(4)
C161–C151–C181	119.6(4)
C111–C161–C151	121.9(4)
F141–C181–F161	106.2(4)
F141–C181–F151	106.8(4)
F161–C181–F151	104.8(4)
F141–C181–C151	113.6(4)
F161–C181–C151	113.1(4)
F151–C181–C151	111.8(4)
C221–C211–C261	115.8(4)
C221–C211–B11	124.0(4)
C261–C211–B11	119.9(3)
C231–C221–C211	122.2(4)
C241–C231–C221	121.2(4)
C241–C231–C271	119.9(4)
C221–C231–C271	118.8(4)
C231–C241–C251	117.9(4)
C241–C251–C261	120.8(4)
C241–C251–C281	118.1(4)
C261–C251–C281	121.0(4)
C251–C261–C211	122.0(4)
F231–C271–F211	106.9(5)
F231–C271–F221	106.1(4)
F211–C271–F221	105.0(4)
F231–C271–C231	113.8(4)
F211–C271–C231	111.9(4)
F221–C271–C231	112.5(4)

Table 5: (continued)

F251–C281–F261	108.0(4)
F251–C281–F241	104.8(4)
F261–C281–F241	104.4(4)
F251–C281–C251	112.5(4)
F261–C281–C251	113.9(4)
F241–C281–C251	112.5(4)
C361–C311–C321	115.1(4)
C361–C311–B11	122.8(4)
C321–C311–B11	121.7(4)
C331–C321–C311	123.3(4)
C321–C331–C341	120.2(4)
C321–C331–C371	118.1(4)
C341–C331–C371	121.7(4)
C351–C341–C331	118.0(4)
C341–C351–C361	121.1(4)
C341–C351–C381	120.1(4)
C361–C351–C381	118.7(4)
C311–C361–C351	122.2(4)
F321–C371–F311	106.1(5)
F321–C371–F331	105.7(4)
F311–C371–F331	104.9(4)
F321–C371–C331	113.3(4)
F311–C371–C331	112.9(4)
F331–C371–C331	113.1(4)
F341–C381–F361	105.2(4)
F341–C381–F351	106.5(4)
F361–C381–F351	105.3(4)
F341–C381–C351	112.3(4)
F361–C381–C351	113.7(4)
F351–C381–C351	113.1(4)
C421–C411–C461	115.8(4)
C421–C411–B11	120.1(4)
C461–C411–B11	123.7(4)
C411–C421–C431	122.3(4)
C441–C431–C421	120.0(4)
C441–C431–C471	121.6(4)
C421–C431–C471	118.4(5)
C451–C441–C431	118.7(4)
C441–C451–C461	121.0(4)
C441–C451–C481	118.8(4)
C461–C451–C481	120.2(4)
C451–C461–C411	122.1(4)
F411–C471–F421	106.8(5)
F411–C471–F431	105.4(4)
F421–C471–F431	106.5(4)
F411–C471–C431	112.3(4)
F421–C471–C431	112.6(4)
F431–C471–C431	112.7(5)
F441–C481–F451	106.4(5)
F441–C481–F461	107.4(5)
F451–C481–F461	105.7(4)
F441–C481–C451	113.8(4)
F451–C481–C451	111.7(4)

Table 5: (continued)

F461–C481–C451	111.3(5)
C211–B11–C311	113.4(3)
C211–B11–C111	115.9(3)
C311–B11–C111	102.5(3)
C211–B11–C411	103.7(3)
C311–B11–C411	111.7(3)
C111–B11–C411	110.0(3)
C22–C12–C62	121.2(5)
C12–C22–C32	118.3(5)
C42–C32–C22	120.8(5)
C52–C42–C32	121.2(5)
C42–C52–C62	118.6(5)
C12–C62–C52	119.9(6)

#1 -x+1,-y+1,-z+1

Crystal structure of mw_154bm

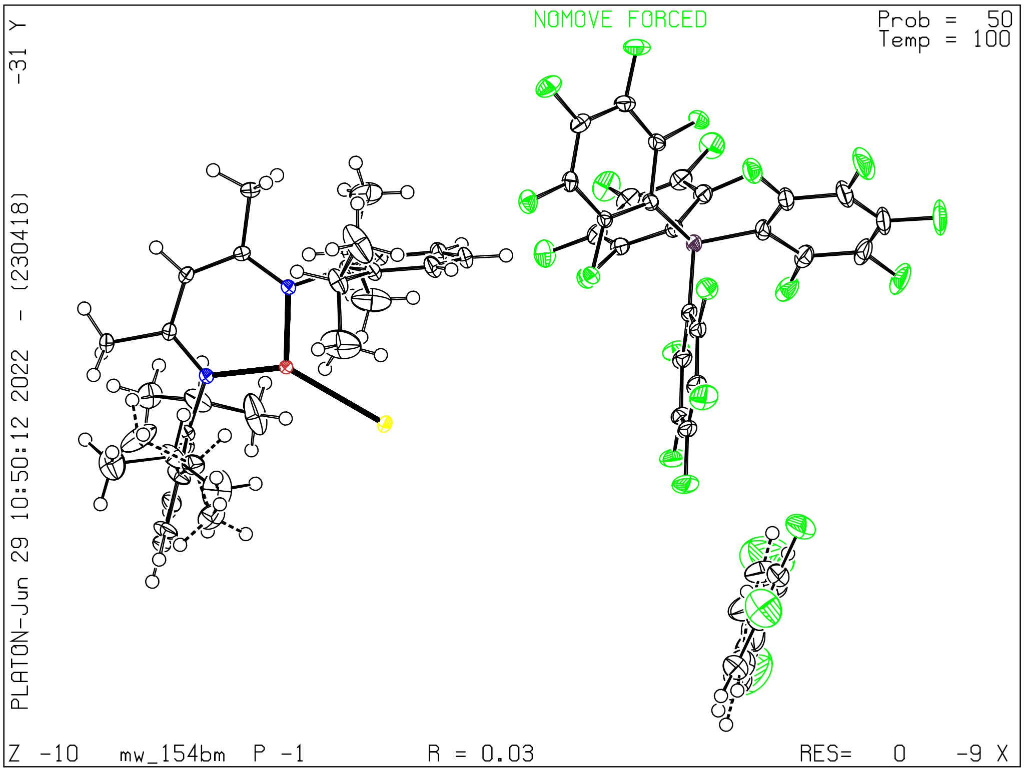

Table 1: Crystal data and structure refinement for mw_154bm.

Identification code	mw_154bm
Empirical Formula	$C_{118}\,H_{90}\,B_2\,Bi_2\,F_{44}\,Ga_2\,N_4$
Formula weight	2978.95 Da
Density (calculated)	$1.723\,g\cdot cm^{-3}$
$F(000)$	1460
Temperature	100(2) K
Crystal size	0.235 × 0.198 × 0.160 mm
Crystal appearance	purple tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 14.5343(6)$ Å
	$b = 14.8399(5)$ Å
	$c = 15.7735(6)$ Å
	$\alpha = 67.1304(16)°$
	$\beta = 67.4082(17)°$
	$\gamma = 75.0320(16)°$
Unit cell volume	$2870.33(19)\,Å^3$
Z	1
Cell measurement refections used	9988
θ range for cell measurement	2.72° to 33.21°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.756° to 33.265°
Completeness to $\theta = 25.242°$ (to θ_{max})	100.0% (99.8%)
Index ranges	$-22 \leq h \leq 22$
	$-22 \leq k \leq 22$
	$-24 \leq l \leq 24$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$3.643\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.56
R_{merg} before/after correction	0.0930/0.0394
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	121681
Independent reflections	22058 ($R_{int} = 0.0280$)
Reflections with $I > 2\sigma(I)$	18670
Data / retraints / parameter	22058 / 370 / 888
Goodness-of-fit on F^2	1.037
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0319P)^2 + 2.4797P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0288$
	$wR2 = 0.0654$
R indices [all data]	$R1 = 0.0390$
	$wR2 = 0.0688$
Largest diff. peak and hole	1.631 and $-0.895\,Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

The solvent molecule is disordered over two positions. All corresponding bond lengths and angles were restrained to be equal (`SADI`) and `RIGU` and `SIMU` restraints were applied to the displacement parameters of the solvent molecule's atoms. An isopropyl group is disordered over two positions.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_154bm. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Bi11	5066(1)	5571(1)	511(1)	25(1)
Ga11	3863(1)	6941(1)	−385(1)	17(1)
N11	3629(1)	8209(1)	−290(1)	16(1)
N21	3115(1)	7180(1)	−1206(1)	15(1)
C11	3058(1)	8969(1)	−725(1)	17(1)
C21	2570(1)	8888(1)	−1296(1)	18(1)
C31	2611(1)	8067(1)	−1548(1)	16(1)
C41	2949(2)	9947(1)	−599(2)	25(1)
C51	2093(2)	8191(1)	−2253(1)	21(1)
C61	4177(1)	8250(1)	286(1)	14(1)
C71	3727(1)	7933(1)	1306(1)	19(1)
C81	4336(2)	7732(2)	1871(1)	22(1)
C91	5347(2)	7854(2)	1445(1)	22(1)
C101	5763(1)	8201(1)	443(1)	20(1)
C111	5188(1)	8400(1)	−155(1)	17(1)
C121	2622(2)	7790(2)	1787(2)	27(1)
C131	2482(2)	6703(3)	2148(3)	61(1)
C141	2122(2)	8188(3)	2632(2)	55(1)
C151	5671(2)	8759(2)	−1252(1)	24(1)
C161	6494(2)	7983(2)	−1601(2)	49(1)
C171	6123(2)	9709(2)	−1583(2)	42(1)
C181	3218(1)	6377(1)	−1552(1)	16(1)
C191	2604(1)	5623(2)	−976(2)	24(1)
C201	2780(2)	4823(2)	−1298(2)	28(1)
C211	3534(2)	4768(1)	−2146(2)	23(1)
C221	4137(2)	5506(2)	−2690(1)	23(1)
C231	3999(2)	6330(1)	−2407(1)	20(1)
C241	1667(6)	5793(7)	−149(6)	30(2)
C251	1738(6)	4956(10)	763(5)	57(2)
C261	669(4)	5887(6)	−322(5)	43(2)
C24'1	1879(6)	5561(6)	62(7)	24(1)
C25'1	1667(6)	4544(6)	789(7)	35(2)
C26'1	893(5)	6179(5)	−81(6)	46(3)
C271	4689(2)	7119(2)	−2992(1)	32(1)
C281	5745(2)	6710(3)	−2901(2)	54(1)
C291	4745(2)	7531(2)	−4061(1)	32(1)
F112	7289(1)	7767(1)	5065(1)	31(1)
F122	8260(2)	7335(1)	6303(1)	56(1)
F132	10112(2)	6282(2)	6036(2)	71(1)
F142	11003(1)	5691(1)	4430(2)	57(1)
F152	10018(1)	6082(1)	3177(1)	36(1)
F212	7875(1)	9076(1)	3212(1)	26(1)
F222	6236(1)	10383(1)	3495(1)	31(1)
F232	4428(1)	9977(1)	3702(1)	32(1)
F242	4284(1)	8173(1)	3722(1)	25(1)
F252	5868(1)	6828(1)	3527(1)	18(1)
F312	6693(1)	5999(1)	5062(1)	26(1)
F322	6333(1)	4150(1)	5653(1)	38(1)
F332	7290(1)	3006(1)	4477(1)	39(1)
F342	8646(1)	3772(1)	2720(1)	36(1)

Table 2: (continued)

	x	y	z	U_{eq}
F352	9020(1)	5602(1)	2110(1)	29(1)
F412	9867(1)	8210(1)	2378(1)	29(1)
F422	10721(1)	9090(1)	518(1)	35(1)
F432	10064(1)	8987(1)	−847(1)	37(1)
F442	8481(1)	7981(1)	−260(1)	31(1)
F452	7573(1)	7131(1)	1616(1)	21(1)
C102	8607(2)	6961(1)	4031(2)	24(1)
C112	8209(2)	7246(2)	4851(2)	28(1)
C122	8698(2)	7035(2)	5525(2)	41(1)
C132	9639(2)	6508(2)	5387(2)	47(1)
C142	10077(2)	6210(2)	4584(2)	44(1)
C152	9556(2)	6426(2)	3938(2)	31(1)
C202	6971(1)	7859(1)	3384(1)	16(1)
C212	6991(1)	8811(1)	3347(1)	18(1)
C222	6164(2)	9511(1)	3465(1)	21(1)
C232	5243(2)	9307(1)	3582(1)	21(1)
C242	5175(1)	8394(1)	3590(1)	18(1)
C252	6028(1)	7700(1)	3492(1)	15(1)
C302	7843(1)	5934(1)	3532(1)	18(1)
C312	7190(1)	5477(1)	4444(1)	21(1)
C322	6994(2)	4516(2)	4771(2)	26(1)
C332	7475(2)	3939(1)	4182(2)	28(1)
C342	8151(2)	4329(1)	3296(2)	26(1)
C352	8327(1)	5300(1)	2994(2)	22(1)
C402	8683(1)	7582(1)	2113(1)	18(1)
C412	9491(1)	8111(1)	1766(2)	22(1)
C422	9951(1)	8582(2)	790(2)	26(1)
C432	9628(2)	8537(2)	98(2)	26(1)
C442	8823(1)	8023(2)	401(1)	22(1)
C452	8377(1)	7583(1)	1377(1)	18(1)
B12	8027(2)	7080(2)	3263(2)	17(1)
F13	9075(2)	1876(2)	5055(2)	52(1)
F23	7818(2)	532(2)	5834(2)	69(1)
C13	9190(3)	1237(3)	4594(3)	35(1)
C23	8543(3)	543(3)	4997(3)	41(1)
C33	8631(6)	−118(5)	4546(5)	50(1)
C43	9410(5)	−93(5)	3696(4)	54(1)
C53	10062(4)	594(4)	3301(3)	53(1)
C63	9956(3)	1274(3)	3739(3)	46(1)
F14	10867(13)	1910(12)	2542(16)	161(8)
F24	11060(11)	205(13)	2221(13)	138(7)
C14	10205(13)	1264(11)	3149(14)	89(5)
C24	10281(13)	403(11)	2979(14)	77(5)
C34	9600(20)	−243(16)	3580(20)	82(7)
C44	8870(20)	−60(20)	4390(20)	79(7)
C54	8765(16)	818(14)	4534(17)	99(7)
C64	9471(15)	1453(12)	3946(15)	87(6)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_154bm.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi11	39(1)	16(1)	35(1)	−11(1)	−30(1)	8(1)
Ga11	25(1)	11(1)	23(1)	−8(1)	−17(1)	3(1)
N11	18(1)	14(1)	21(1)	−8(1)	−11(1)	1(1)
N21	19(1)	14(1)	18(1)	−7(1)	−11(1)	1(1)
C11	18(1)	13(1)	21(1)	−8(1)	−9(1)	2(1)
C21	20(1)	15(1)	22(1)	−6(1)	−12(1)	4(1)
C31	16(1)	17(1)	18(1)	−6(1)	−10(1)	1(1)
C41	31(1)	16(1)	37(1)	−14(1)	−20(1)	5(1)
C51	25(1)	21(1)	25(1)	−9(1)	−17(1)	2(1)
C61	19(1)	13(1)	14(1)	−5(1)	−8(1)	−2(1)
C71	19(1)	21(1)	21(1)	−8(1)	−9(1)	−4(1)
C81	25(1)	27(1)	18(1)	−7(1)	−10(1)	−8(1)
C91	23(1)	26(1)	24(1)	−9(1)	−14(1)	−3(1)
C101	16(1)	22(1)	25(1)	−11(1)	−9(1)	−2(1)
C111	19(1)	16(1)	20(1)	−7(1)	−9(1)	−2(1)
C121	21(1)	41(1)	25(1)	−14(1)	−6(1)	−10(1)
C131	40(2)	52(2)	79(2)	−22(2)	7(2)	−27(1)
C141	26(1)	104(3)	54(2)	−55(2)	2(1)	−15(1)
C151	23(1)	32(1)	20(1)	−9(1)	−7(1)	−7(1)
C161	58(2)	39(1)	37(1)	−22(1)	13(1)	−16(1)
C171	60(2)	26(1)	30(1)	−2(1)	−6(1)	−13(1)
C181	18(1)	15(1)	19(1)	−8(1)	−11(1)	1(1)
C191	19(1)	29(1)	31(1)	−18(1)	−3(1)	−9(1)
C201	30(1)	24(1)	37(1)	−14(1)	−10(1)	−11(1)
C211	27(1)	19(1)	32(1)	−14(1)	−16(1)	3(1)
C221	27(1)	26(1)	21(1)	−14(1)	−10(1)	0(1)
C231	27(1)	19(1)	14(1)	−5(1)	−9(1)	−4(1)
C241	21(3)	43(4)	34(3)	−25(3)	−1(2)	−11(3)
C251	37(3)	91(8)	28(3)	−11(4)	0(2)	−11(4)
C261	20(2)	62(4)	48(3)	−22(3)	−5(2)	−7(2)
C24'1	18(3)	23(3)	29(4)	−7(2)	−3(2)	−8(2)
C25'1	30(3)	28(3)	34(3)	4(3)	−6(2)	−10(2)
C26'1	20(3)	27(3)	50(4)	4(3)	10(3)	3(2)
C271	48(1)	33(1)	14(1)	−6(1)	−2(1)	−22(1)
C281	55(2)	90(2)	20(1)	9(1)	−14(1)	−50(2)
C291	41(1)	33(1)	14(1)	−2(1)	−4(1)	−8(1)
F112	38(1)	36(1)	25(1)	−7(1)	−17(1)	−9(1)
F122	87(1)	59(1)	45(1)	−8(1)	−47(1)	−23(1)
F132	92(2)	57(1)	92(2)	11(1)	−84(1)	−23(1)
F142	38(1)	36(1)	94(1)	12(1)	−50(1)	−9(1)
F152	19(1)	25(1)	56(1)	−1(1)	−17(1)	−3(1)
F212	28(1)	19(1)	34(1)	−4(1)	−14(1)	−10(1)
F222	44(1)	16(1)	33(1)	−9(1)	−11(1)	−6(1)
F232	30(1)	24(1)	36(1)	−13(1)	−10(1)	9(1)
F242	15(1)	32(1)	29(1)	−13(1)	−8(1)	−1(1)
F252	17(1)	17(1)	22(1)	−7(1)	−8(1)	−4(1)
F312	30(1)	24(1)	22(1)	−2(1)	−8(1)	−8(1)
F322	43(1)	27(1)	32(1)	7(1)	−9(1)	−17(1)
F332	44(1)	15(1)	58(1)	−1(1)	−24(1)	−11(1)
F342	36(1)	20(1)	54(1)	−17(1)	−16(1)	3(1)
F352	21(1)	21(1)	36(1)	−9(1)	−1(1)	−1(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F412	24(1)	28(1)	36(1)	−2(1)	−15(1)	−14(1)
F422	24(1)	33(1)	40(1)	2(1)	−6(1)	−18(1)
F432	30(1)	42(1)	24(1)	1(1)	1(1)	−11(1)
F442	28(1)	41(1)	22(1)	−10(1)	−7(1)	−6(1)
F452	16(1)	23(1)	26(1)	−7(1)	−7(1)	−6(1)
C102	24(1)	19(1)	31(1)	4(1)	−18(1)	−11(1)
C112	36(1)	25(1)	30(1)	3(1)	−23(1)	−13(1)
C122	62(2)	37(1)	42(1)	2(1)	−39(1)	−20(1)
C132	63(2)	35(1)	61(2)	10(1)	−54(2)	−21(1)
C142	36(1)	24(1)	72(2)	14(1)	−41(1)	−14(1)
C152	24(1)	21(1)	45(1)	4(1)	−21(1)	−9(1)
C202	18(1)	15(1)	15(1)	−2(1)	−7(1)	−5(1)
C212	23(1)	16(1)	18(1)	−2(1)	−10(1)	−6(1)
C222	30(1)	14(1)	19(1)	−4(1)	−7(1)	−4(1)
C232	24(1)	18(1)	17(1)	−6(1)	−6(1)	3(1)
C242	17(1)	22(1)	14(1)	−6(1)	−6(1)	−1(1)
C252	18(1)	16(1)	13(1)	−4(1)	−7(1)	−3(1)
C302	14(1)	15(1)	26(1)	−2(1)	−11(1)	−3(1)
C312	20(1)	18(1)	26(1)	−2(1)	−12(1)	−5(1)
C322	25(1)	19(1)	30(1)	3(1)	−13(1)	−9(1)
C332	28(1)	14(1)	45(1)	−1(1)	−22(1)	−5(1)
C342	22(1)	16(1)	42(1)	−9(1)	−18(1)	2(1)
C352	15(1)	18(1)	32(1)	−5(1)	−9(1)	−1(1)
C402	13(1)	15(1)	26(1)	−4(1)	−8(1)	−2(1)
C412	17(1)	19(1)	30(1)	−3(1)	−10(1)	−4(1)
C422	16(1)	21(1)	34(1)	−1(1)	−6(1)	−7(1)
C432	18(1)	24(1)	25(1)	−1(1)	−2(1)	−3(1)
C442	18(1)	22(1)	23(1)	−7(1)	−6(1)	1(1)
C452	13(1)	16(1)	25(1)	−6(1)	−5(1)	−2(1)
B12	14(1)	16(1)	23(1)	−3(1)	−9(1)	−4(1)
F13	60(1)	46(1)	68(2)	−35(1)	−28(1)	1(1)
F23	54(2)	87(2)	66(2)	−31(2)	−7(1)	−17(1)
C13	40(2)	34(2)	44(2)	−19(1)	−23(1)	1(1)
C23	43(2)	39(2)	49(2)	−14(2)	−21(2)	−5(2)
C33	57(4)	36(2)	76(3)	−18(2)	−41(2)	−5(2)
C43	64(3)	51(3)	81(3)	−40(2)	−56(2)	20(2)
C53	46(2)	78(3)	54(2)	−40(2)	−27(2)	11(2)
C63	42(2)	55(2)	49(2)	−23(2)	−21(2)	−2(2)
F14	124(13)	111(12)	260(20)	−48(13)	−68(13)	−47(10)
F24	92(10)	128(14)	173(15)	−51(11)	−41(9)	22(9)
C14	97(12)	54(9)	144(15)	−25(9)	−85(10)	8(7)
C24	74(10)	59(8)	123(14)	−30(8)	−75(8)	18(7)
C34	69(11)	42(9)	154(17)	−34(9)	−74(9)	26(7)
C44	65(14)	51(11)	147(17)	−35(12)	−71(10)	12(8)
C54	105(14)	42(9)	160(19)	−37(11)	−65(12)	17(8)
C64	112(14)	30(7)	153(16)	−34(9)	−89(11)	16(8)

Table 4: Bond lengths [Å] for mw_154bm.

Bi11–Ga11	2.6492(2)
Bi11–Bi11#1	2.83467(15)
Ga11–N21	1.8742(14)
Ga11–N11	1.8772(14)
N11–C11	1.335(2)
N11–C61	1.446(2)
N21–C31	1.347(2)
N21–C181	1.446(2)
C11–C21	1.396(2)
C11–C41	1.501(2)
C21–C31	1.402(2)
C31–C51	1.500(2)
C61–C111	1.398(2)
C61–C71	1.414(2)
C71–C81	1.389(3)
C71–C121	1.522(3)
C81–C91	1.389(3)
C91–C101	1.386(3)
C101–C111	1.391(2)
C111–C151	1.521(3)
C121–C141	1.517(3)
C121–C131	1.528(4)
C151–C171	1.528(3)
C151–C161	1.529(3)
C181–C231	1.403(3)
C181–C191	1.405(3)
C191–C201	1.394(3)
C191–C241	1.527(8)
C191–C24'1	1.552(9)
C201–C211	1.382(3)
C211–C221	1.376(3)
C221–C231	1.400(3)
C231–C271	1.512(3)
C241–C251	1.510(11)
C241–C261	1.540(8)
C24'1–C25'1	1.521(10)
C24'1–C26'1	1.535(9)
C271–C291	1.530(3)
C271–C281	1.538(4)
F112–C112	1.349(3)
F122–C122	1.337(4)
F132–C132	1.337(3)
F142–C142	1.350(3)
F152–C152	1.353(3)
F212–C212	1.355(2)
F222–C222	1.345(2)
F232–C232	1.340(2)
F242–C242	1.336(2)
F252–C252	1.3488(19)
F312–C312	1.352(2)
F322–C322	1.346(2)
F332–C332	1.343(2)
F342–C342	1.342(3)

Table 4: (continued)

F352–C352	1.352(2)
F412–C412	1.345(2)
F422–C422	1.349(2)
F432–C432	1.338(2)
F442–C442	1.343(2)
F452–C452	1.351(2)
C102–C112	1.382(3)
C102–C152	1.387(3)
C102–B12	1.659(3)
C112–C122	1.393(3)
C122–C132	1.371(4)
C132–C142	1.370(5)
C142–C152	1.390(3)
C202–C252	1.387(2)
C202–C212	1.399(2)
C202–B12	1.660(3)
C212–C222	1.376(3)
C222–C232	1.377(3)
C232–C242	1.379(3)
C242–C252	1.392(2)
C302–C352	1.386(3)
C302–C312	1.397(3)
C302–B12	1.653(3)
C312–C322	1.381(3)
C322–C332	1.376(3)
C332–C342	1.366(3)
C342–C352	1.389(3)
C402–C412	1.393(2)
C402–C452	1.395(3)
C402–B12	1.656(3)
C412–C422	1.386(3)
C422–C432	1.371(3)
C432–C442	1.388(3)
C442–C452	1.374(3)
F13–C13	1.347(4)
F23–C23	1.333(5)
C13–C23	1.371(5)
C13–C63	1.372(5)
C23–C33	1.376(5)
C33–C43	1.378(7)
C43–C53	1.370(6)
C53–C63	1.379(6)
F14–C14	1.348(12)
F24–C24	1.364(12)
C14–C24	1.374(11)
C14–C64	1.374(11)
C24–C34	1.362(11)
C34–C44	1.383(12)
C44–C54	1.375(12)
C54–C64	1.375(12)

#1 -x+1,-y+1,-z

Table 5: Bond angles [°] for mw_154bm.

Ga11–Bi11–Bi11#1	84.838(6)
N21–Ga11–N11	98.76(6)
N21–Ga11–Bi11	142.94(4)
N11–Ga11–Bi11	118.23(4)
C11–N11–C61	125.21(14)
C11–N11–Ga11	124.15(12)
C61–N11–Ga11	110.61(11)
C31–N21–C181	121.42(14)
C31–N21–Ga11	123.03(12)
C181–N21–Ga11	115.11(11)
N11–C11–C21	122.42(15)
N11–C11–C41	118.43(16)
C21–C11–C41	119.15(16)
C11–C21–C31	128.44(16)
N21–C31–C21	123.11(15)
N21–C31–C51	118.49(15)
C21–C31–C51	118.37(15)
C111–C61–C71	122.14(16)
C111–C61–N11	119.15(15)
C71–C61–N11	117.35(15)
C81–C71–C61	117.62(17)
C81–C71–C121	120.10(17)
C61–C71–C121	122.26(16)
C91–C81–C71	120.94(18)
C101–C91–C81	120.34(17)
C91–C101–C111	120.91(17)
C101–C111–C61	117.98(16)
C101–C111–C151	119.70(16)
C61–C111–C151	122.32(16)
C141–C121–C71	112.34(17)
C141–C121–C131	108.7(2)
C71–C121–C131	111.4(2)
C111–C151–C171	110.93(17)
C111–C151–C161	111.43(19)
C171–C151–C161	108.9(2)
C231–C181–C191	122.23(16)
C231–C181–N21	118.22(15)
C191–C181–N21	119.22(16)
C201–C191–C181	117.46(18)
C201–C191–C241	122.2(3)
C181–C191–C241	119.3(4)
C201–C191–C24'1	118.9(3)
C181–C191–C24'1	122.8(3)
C211–C201–C191	121.38(19)
C221–C211–C201	120.17(17)
C211–C221–C231	121.24(18)
C221–C231–C181	117.49(17)
C221–C231–C271	120.72(18)
C181–C231–C271	121.77(17)
C251–C241–C191	107.1(6)
C251–C241–C261	111.4(6)
C191–C241–C261	114.4(5)
C25'1–C24'1–C26'1	109.5(6)

Table 5: (continued)

C25'1–C24'1–C191	117.7(7)
C26'1–C24'1–C191	105.1(5)
C231–C271–C291	112.15(18)
C231–C271–C281	110.1(2)
C291–C271–C281	110.29(19)
C112–C102–C152	113.35(19)
C112–C102–B12	127.11(18)
C152–C102–B12	119.1(2)
F112–C112–C102	121.64(17)
F112–C112–C122	113.9(2)
C102–C112–C122	124.5(2)
F122–C122–C132	119.9(2)
F122–C122–C112	120.9(3)
C132–C122–C112	119.3(3)
F132–C132–C142	120.9(3)
F132–C132–C122	120.1(3)
C142–C132–C122	119.0(2)
F142–C142–C132	120.3(2)
F142–C142–C152	120.0(3)
C132–C142–C152	119.7(2)
F152–C152–C102	119.18(19)
F152–C152–C142	116.7(2)
C102–C152–C142	124.1(3)
C252–C202–C212	112.90(16)
C252–C202–B12	127.65(15)
C212–C202–B12	119.41(15)
F212–C212–C222	116.10(16)
F212–C212–C202	119.04(16)
C222–C212–C202	124.84(17)
F222–C222–C212	120.97(18)
F222–C222–C232	119.45(17)
C212–C222–C232	119.56(17)
F232–C232–C222	120.47(17)
F232–C232–C242	120.86(18)
C222–C232–C242	118.65(17)
F242–C242–C232	119.61(16)
F242–C242–C252	120.60(16)
C232–C242–C252	119.76(17)
F252–C252–C202	121.24(15)
F252–C252–C242	114.57(15)
C202–C252–C242	124.18(16)
C352–C302–C312	112.67(17)
C352–C302–B12	128.17(16)
C312–C302–B12	118.91(17)
F312–C312–C322	116.07(17)
F312–C312–C302	119.15(16)
C322–C312–C302	124.78(19)
F322–C322–C332	120.33(18)
F322–C322–C312	120.3(2)
C332–C322–C312	119.33(19)
F332–C332–C342	120.5(2)
F332–C332–C322	120.6(2)
C342–C332–C322	118.85(18)

Table 5: (continued)

F342–C342–C332	119.81(18)
F342–C342–C352	120.2(2)
C332–C342–C352	120.0(2)
F352–C352–C302	120.92(17)
F352–C352–C342	114.78(18)
C302–C352–C342	124.30(19)
C412–C402–C452	113.09(17)
C412–C402–B12	126.94(17)
C452–C402–B12	119.68(15)
F412–C412–C422	115.23(16)
F412–C412–C402	121.12(18)
C422–C412–C402	123.64(19)
F422–C422–C432	119.76(18)
F422–C422–C412	119.74(19)
C432–C422–C412	120.51(18)
F432–C432–C422	121.24(19)
F432–C432–C442	120.3(2)
C422–C432–C442	118.47(18)
F442–C442–C452	121.12(17)
F442–C442–C432	119.75(18)
C452–C442–C432	119.12(19)
F452–C452–C442	115.69(17)
F452–C452–C402	119.16(16)
C442–C452–C402	125.15(17)
C302–B12–C402	113.70(15)
C302–B12–C102	102.28(14)
C402–B12–C102	113.01(14)
C302–B12–C202	113.31(14)
C402–B12–C202	102.22(14)
C102–B12–C202	112.76(16)
F13–C13–C23	119.2(3)
F13–C13–C63	120.2(3)
C23–C13–C63	120.6(3)
F23–C23–C13	118.2(3)
F23–C23–C33	120.8(4)
C13–C23–C33	121.0(4)
C23–C33–C43	118.5(4)
C53–C43–C33	120.3(4)
C43–C53–C63	121.2(4)
C13–C63–C53	118.4(4)
F14–C14–C24	119.7(10)
F14–C14–C64	120.2(10)
C24–C14–C64	120.0(9)
C34–C24–F24	121.4(10)
C34–C24–C14	120.0(9)
F24–C24–C14	118.6(10)
C24–C34–C44	120.1(10)
C54–C44–C34	119.8(10)
C44–C54–C64	119.4(10)
C14–C64–C54	120.1(10)

#1 -x+1,-y+1,-z

Crystal structure of mw_071_7m

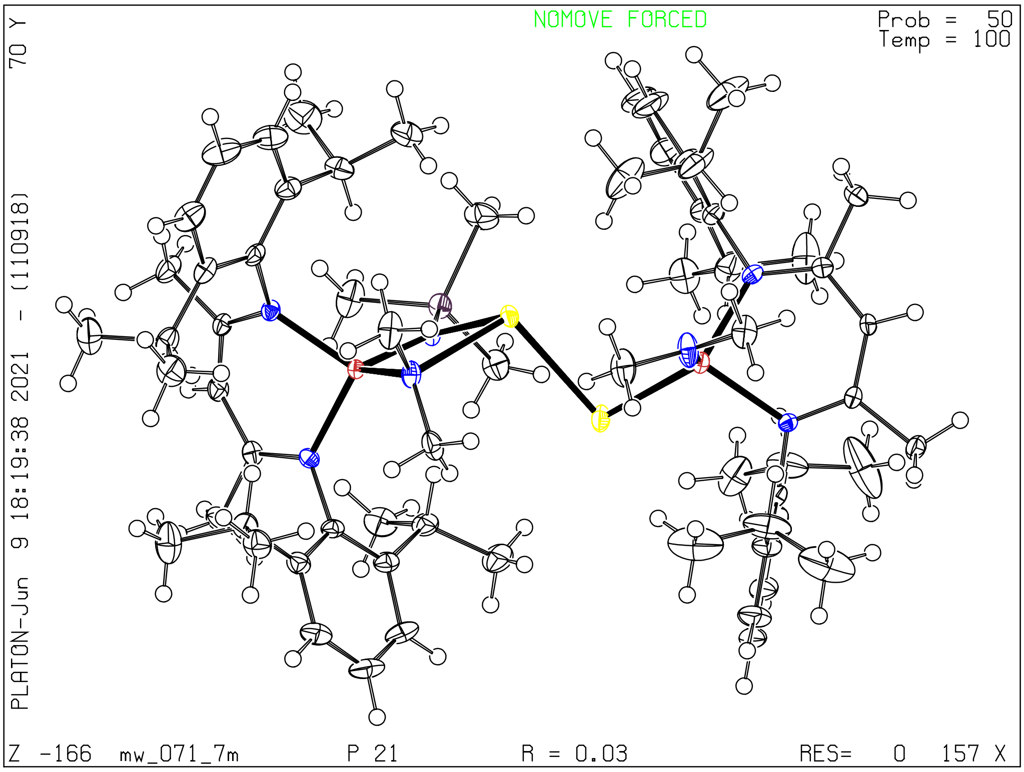

Table 1: Crystal data and structure refinement for mw_071_7m.

Identification code	mw_071_7m
Empirical Formula	$C_{65} H_{103} Ga_2 N_7 Sb_2 Si$
Formula weight	1393.57 Da
Density (calculated)	$1.346\,g \cdot cm^{-3}$
$F(000)$	1440
Temperature	100(2) K
Crystal size	0.271 × 0.263 × 0.131 mm
Crystal appearance	red tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	$a = 10.7967(17)$ Å
	$b = 21.163(3)$ Å
	$c = 15.164(2)$ Å
	$\alpha = 90°$
	$\beta = 96.979(3)°$
	$\gamma = 90°$
Unit cell volume	3439.2(9) $Å^3$
Z	2
Cell measurement refections used	9808
θ range for cell measurement	2.19° to 30.26°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.925° to 33.208°
Completeness to $\theta = 25.242°$ (to θ_{max})	100.0% (99.7%)
Index ranges	$-16 \leq h \leq 16$
	$-32 \leq k \leq 32$
	$-23 \leq l \leq 23$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.611\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.64
R_{merg} before/after correction	0.0679/0.0545
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	108278
Independent reflections	26282 ($R_{int} = 0.0441$)
Reflections with $I > 2\sigma(I)$	23400
Data / retraints / parameter	26282 / 1 / 722
Goodness-of-fit on F^2	1.036
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 0.2629P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0323$
	$wR2 = 0.0658$
R indices [all data]	$R1 = 0.0413$
	$wR2 = 0.0689$
Absolute structure parameter	0.131(7)
Largest diff. peak and hole	1.095 and -0.509 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Twinning

The model was refined as a 2-component inversion twin.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_071_7m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	7578(1)	5488(1)	3905(1)	17(1)
Sb(2)	6244(1)	4531(1)	3167(1)	21(1)
Ga(1)	8356(1)	5216(1)	5898(1)	12(1)
Ga(2)	6715(1)	4823(1)	1587(1)	14(1)
Si(1)	5576(1)	5843(1)	5338(1)	19(1)
N(1)	9074(2)	5826(1)	6784(2)	14(1)
N(2)	8168(2)	4521(1)	6736(2)	14(1)
N(3)	5724(2)	4221(1)	748(2)	14(1)
N(4)	5938(3)	5574(1)	925(2)	18(1)
N(5)	6964(2)	5503(1)	5159(2)	15(1)
N(6)	9290(2)	5010(1)	4919(2)	18(1)
N(7)	8367(2)	4833(2)	1327(2)	26(1)
C(1)	8638(3)	5813(2)	7578(2)	17(1)
C(2)	8033(3)	5295(2)	7896(2)	19(1)
C(3)	7948(3)	4677(2)	7557(2)	17(1)
C(4)	8785(4)	6382(2)	8183(2)	26(1)
C(5)	7623(3)	4170(2)	8198(2)	25(1)
C(6)	10059(3)	6271(2)	6659(2)	18(1)
C(7)	11276(3)	6125(2)	7057(2)	21(1)
C(8)	12234(3)	6556(2)	6939(3)	30(1)
C(9)	12019(4)	7093(2)	6449(3)	38(1)
C(10)	10821(4)	7228(2)	6055(3)	32(1)
C(11)	9821(3)	6822(2)	6152(2)	22(1)
C(12)	11588(3)	5541(2)	7618(2)	24(1)
C(13)	11839(4)	5696(2)	8608(3)	40(1)
C(14)	12713(3)	5187(2)	7330(3)	33(1)
C(15)	8519(3)	7012(2)	5742(3)	26(1)
C(16)	8034(5)	7560(2)	6276(3)	44(1)
C(17)	8502(4)	7204(2)	4768(3)	37(1)
C(18)	8214(3)	3855(1)	6524(2)	17(1)
C(19)	9338(3)	3523(2)	6766(2)	20(1)
C(20)	9326(4)	2868(2)	6650(3)	27(1)
C(21)	8253(4)	2557(2)	6286(3)	33(1)
C(22)	7190(4)	2894(2)	6011(3)	30(1)
C(23)	7137(3)	3549(2)	6117(2)	20(1)
C(24)	10560(3)	3852(2)	7124(2)	24(1)
C(25)	10829(4)	3810(3)	8135(3)	41(1)
C(26)	11674(3)	3588(2)	6711(3)	29(1)
C(27)	5931(3)	3907(2)	5823(2)	24(1)
C(28)	5193(3)	4057(2)	6611(3)	32(1)
C(29)	5072(4)	3551(2)	5106(3)	37(1)
C(30)	5342(3)	4364(1)	−90(2)	14(1)
C(31)	5376(3)	4981(2)	−429(2)	18(1)
C(32)	5567(3)	5547(2)	53(2)	18(1)
C(33)	4834(3)	3853(2)	−736(2)	21(1)
C(34)	5311(4)	6150(2)	−468(2)	28(1)
C(35)	5457(3)	3604(2)	1079(2)	16(1)
C(36)	6332(3)	3119(2)	1093(2)	24(1)
C(37)	6056(4)	2536(2)	1451(3)	31(1)
C(38)	4936(4)	2433(2)	1791(2)	28(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(39)	4083(3)	2914(2)	1771(3)	26(1)
C(40)	4310(3)	3509(2)	1423(2)	21(1)
C(41)	7594(4)	3199(2)	738(4)	44(1)
C(42)	7717(6)	2753(3)	−40(4)	69(2)
C(43)	8651(4)	3086(3)	1481(5)	62(2)
C(44)	3335(4)	4023(2)	1425(3)	36(1)
C(45)	2293(5)	3952(4)	661(3)	74(2)
C(46)	2761(4)	4055(2)	2302(3)	42(1)
C(47)	5878(4)	6179(2)	1371(2)	23(1)
C(48)	6861(4)	6615(2)	1398(3)	32(1)
C(49)	6741(5)	7186(2)	1835(3)	46(1)
C(50)	5709(5)	7328(2)	2237(3)	45(1)
C(51)	4738(5)	6894(2)	2207(3)	36(1)
C(52)	4800(4)	6311(2)	1788(2)	26(1)
C(53)	8051(5)	6496(2)	982(3)	44(1)
C(54)	8340(7)	7041(2)	358(4)	63(2)
C(55)	9146(5)	6400(3)	1699(4)	54(1)
C(56)	3734(4)	5839(2)	1789(3)	33(1)
C(57)	2820(5)	5861(3)	951(3)	56(2)
C(58)	3022(4)	5894(2)	2590(3)	41(1)
C(59)	5614(3)	6054(2)	6543(3)	33(1)
C(60)	4175(3)	5332(2)	5025(3)	28(1)
C(61)	5256(4)	6592(2)	4697(3)	35(1)
C(62)	9424(3)	4335(2)	4713(2)	25(1)
C(63)	10468(3)	5347(2)	4835(2)	30(1)
C(64)	9445(3)	4703(2)	1972(3)	33(1)
C(65)	8707(3)	4876(2)	441(2)	28(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_071_7m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	20(1)	18(1)	11(1)	1(1)	0(1)	1(1)
Sb(2)	23(1)	28(1)	13(1)	−2(1)	0(1)	−5(1)
Ga(1)	12(1)	13(1)	10(1)	−1(1)	1(1)	0(1)
Ga(2)	14(1)	16(1)	12(1)	−2(1)	−1(1)	0(1)
Si(1)	15(1)	22(1)	21(1)	−2(1)	0(1)	5(1)
N(1)	14(1)	16(1)	13(1)	−1(1)	2(1)	−2(1)
N(2)	14(1)	15(1)	14(1)	2(1)	3(1)	0(1)
N(3)	15(1)	12(1)	14(1)	−1(1)	1(1)	0(1)
N(4)	24(1)	12(1)	17(1)	−4(1)	1(1)	0(1)
N(5)	14(1)	18(1)	13(1)	−1(1)	0(1)	2(1)
N(6)	15(1)	26(1)	12(1)	−3(1)	4(1)	2(1)
N(7)	14(1)	46(2)	17(1)	1(1)	−1(1)	−2(1)
C(1)	19(1)	17(1)	13(1)	−3(1)	2(1)	0(1)
C(2)	22(1)	22(2)	13(1)	−2(1)	6(1)	1(1)
C(3)	14(1)	22(2)	14(1)	1(1)	3(1)	0(1)
C(4)	32(2)	26(2)	21(2)	−9(1)	9(1)	−6(1)
C(5)	31(2)	25(2)	21(2)	6(1)	10(1)	0(1)
C(6)	22(1)	17(1)	14(1)	−6(1)	5(1)	−2(1)
C(7)	19(1)	23(2)	21(2)	−7(1)	3(1)	−4(1)
C(8)	16(2)	32(2)	42(2)	−7(2)	4(1)	−6(1)
C(9)	28(2)	29(2)	58(3)	−2(2)	13(2)	−15(2)
C(10)	32(2)	24(2)	43(2)	4(2)	11(2)	−8(2)
C(11)	23(2)	20(2)	24(2)	−1(1)	7(1)	−4(1)
C(12)	19(1)	27(2)	25(2)	−5(1)	−2(1)	−3(1)
C(13)	42(2)	50(3)	25(2)	−3(2)	−2(2)	4(2)
C(14)	25(2)	35(2)	37(2)	−2(2)	−2(1)	7(2)
C(15)	27(2)	21(2)	30(2)	7(1)	4(1)	0(1)
C(16)	41(2)	40(2)	51(3)	0(2)	10(2)	14(2)
C(17)	46(2)	29(2)	36(2)	11(2)	2(2)	−6(2)
C(18)	21(1)	13(1)	17(1)	1(1)	7(1)	−1(1)
C(19)	23(2)	18(1)	19(1)	1(1)	4(1)	4(1)
C(20)	31(2)	18(2)	34(2)	5(1)	9(2)	6(1)
C(21)	43(2)	13(2)	44(2)	−2(2)	14(2)	−2(2)
C(22)	31(2)	17(2)	43(2)	−6(2)	10(2)	−10(1)
C(23)	22(1)	16(1)	23(2)	1(1)	6(1)	−3(1)
C(24)	21(2)	23(2)	27(2)	−2(1)	−1(1)	7(1)
C(25)	30(2)	63(3)	29(2)	−7(2)	−2(2)	10(2)
C(26)	23(2)	31(2)	32(2)	2(2)	0(1)	6(1)
C(27)	20(2)	20(2)	30(2)	2(1)	0(1)	−6(1)
C(28)	24(2)	34(2)	39(2)	6(2)	11(2)	−2(2)
C(29)	31(2)	31(2)	47(2)	0(2)	−9(2)	−12(2)
C(30)	12(1)	17(1)	13(1)	−3(1)	1(1)	−1(1)
C(31)	25(2)	17(1)	10(1)	0(1)	−1(1)	0(1)
C(32)	22(1)	15(1)	17(1)	0(1)	1(1)	1(1)
C(33)	27(2)	22(2)	15(1)	−4(1)	3(1)	−6(1)
C(34)	45(2)	19(2)	19(2)	3(1)	0(1)	2(2)
C(35)	18(1)	16(1)	14(1)	−5(1)	1(1)	−2(1)
C(36)	28(2)	17(2)	29(2)	1(1)	10(1)	4(1)
C(37)	40(2)	17(2)	37(2)	5(2)	11(2)	6(2)
C(38)	43(2)	16(2)	25(2)	2(1)	6(2)	−7(1)
C(39)	28(2)	22(2)	29(2)	1(1)	7(1)	−9(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(40)	19(1)	21(2)	23(2)	2(1)	3(1)	−4(1)
C(41)	40(2)	25(2)	73(3)	13(2)	32(2)	16(2)
C(42)	90(4)	49(3)	80(4)	18(3)	63(4)	34(3)
C(43)	31(2)	44(3)	115(5)	14(3)	25(3)	8(2)
C(44)	22(2)	28(2)	61(3)	13(2)	16(2)	2(2)
C(45)	40(3)	146(7)	38(3)	28(3)	13(2)	49(3)
C(46)	24(2)	51(3)	52(3)	−19(2)	0(2)	7(2)
C(47)	38(2)	15(1)	17(1)	−4(1)	2(1)	−1(1)
C(48)	53(2)	22(2)	23(2)	−10(1)	9(2)	−10(2)
C(49)	76(3)	22(2)	42(2)	−16(2)	18(2)	−17(2)
C(50)	75(3)	19(2)	41(2)	−14(2)	13(2)	−3(2)
C(51)	53(3)	24(2)	32(2)	−8(2)	6(2)	12(2)
C(52)	35(2)	19(2)	24(2)	−4(1)	−3(1)	7(1)
C(53)	62(3)	33(2)	40(2)	−20(2)	22(2)	−27(2)
C(54)	106(5)	43(3)	47(3)	−22(2)	39(3)	−43(3)
C(55)	48(3)	59(3)	57(3)	−28(3)	17(2)	−27(2)
C(56)	29(2)	31(2)	37(2)	−13(2)	−1(2)	11(2)
C(57)	38(2)	99(5)	31(2)	−8(3)	0(2)	−5(3)
C(58)	41(2)	47(3)	35(2)	0(2)	2(2)	2(2)
C(59)	20(2)	48(2)	31(2)	−14(2)	7(1)	7(2)
C(60)	17(1)	35(2)	31(2)	1(1)	1(1)	2(1)
C(61)	25(2)	27(2)	51(3)	8(2)	−3(2)	8(2)
C(62)	31(2)	30(2)	15(1)	0(1)	2(1)	12(1)
C(63)	17(1)	54(3)	21(2)	−4(2)	7(1)	−7(2)
C(64)	14(1)	55(3)	29(2)	−1(2)	−4(1)	−2(2)
C(65)	20(2)	42(2)	23(2)	−3(2)	6(1)	−5(2)

Table 4: Bond lengths [Å] for mw_071_7m.

Sb(1)–N(5)	2.089(2)
Sb(1)–N(6)	2.472(3)
Sb(1)–Sb(2)	2.6541(4)
Sb(1)–Ga(1)	3.0897(6)
Sb(2)–Ga(2)	2.5836(5)
Ga(1)–N(5)	1.863(2)
Ga(1)–N(6)	1.943(2)
Ga(1)–N(1)	1.954(3)
Ga(1)–N(2)	1.971(3)
Ga(2)–N(7)	1.873(3)
Ga(2)–N(4)	2.008(3)
Ga(2)–N(3)	2.014(3)
Si(1)–N(5)	1.713(3)
Si(1)–C(61)	1.870(4)
Si(1)–C(60)	1.873(4)
Si(1)–C(59)	1.877(4)
N(1)–C(1)	1.346(4)
N(1)–C(6)	1.450(4)
N(2)–C(3)	1.336(4)
N(2)–C(18)	1.447(4)
N(3)–C(30)	1.323(4)
N(3)–C(35)	1.439(4)
N(4)–C(32)	1.335(4)
N(4)–C(47)	1.453(4)
N(6)–C(62)	1.473(5)
N(6)–C(63)	1.477(4)
N(7)–C(65)	1.439(4)
N(7)–C(64)	1.453(4)
C(1)–C(2)	1.392(4)
C(1)–C(4)	1.511(4)
C(2)–C(3)	1.405(4)
C(3)–C(5)	1.518(4)
C(6)–C(11)	1.404(5)
C(6)–C(7)	1.412(5)
C(7)–C(8)	1.407(5)
C(7)–C(12)	1.515(5)
C(8)–C(9)	1.362(6)
C(9)–C(10)	1.387(6)
C(10)–C(11)	1.401(5)
C(11)–C(15)	1.520(5)
C(12)–C(13)	1.529(5)
C(12)–C(14)	1.536(5)
C(15)–C(17)	1.529(6)
C(15)–C(16)	1.543(6)
C(18)–C(23)	1.407(5)
C(18)–C(19)	1.412(5)
C(19)–C(20)	1.396(5)
C(19)–C(24)	1.532(5)
C(20)–C(21)	1.388(6)
C(21)–C(22)	1.373(6)
C(22)–C(23)	1.397(5)
C(23)–C(27)	1.526(5)
C(24)–C(25)	1.527(5)

Table 4: (continued)

C(24)–C(26)	1.528(5)
C(27)–C(29)	1.538(5)
C(27)–C(28)	1.547(5)
C(30)–C(31)	1.405(4)
C(30)–C(33)	1.516(4)
C(31)–C(32)	1.406(4)
C(32)–C(34)	1.508(5)
C(35)–C(36)	1.395(5)
C(35)–C(40)	1.415(4)
C(36)–C(37)	1.394(5)
C(36)–C(41)	1.535(5)
C(37)–C(38)	1.388(5)
C(38)–C(39)	1.370(6)
C(39)–C(40)	1.398(5)
C(40)–C(44)	1.515(5)
C(41)–C(43)	1.523(8)
C(41)–C(42)	1.529(8)
C(44)–C(45)	1.521(7)
C(44)–C(46)	1.536(6)
C(47)–C(48)	1.403(5)
C(47)–C(52)	1.419(5)
C(48)–C(49)	1.392(5)
C(48)–C(53)	1.519(6)
C(49)–C(50)	1.367(7)
C(50)–C(51)	1.392(7)
C(51)–C(52)	1.393(5)
C(52)–C(56)	1.524(6)
C(53)–C(55)	1.520(8)
C(53)–C(54)	1.547(7)
C(56)–C(57)	1.512(6)
C(56)–C(58)	1.519(6)

Table 5: Bond angles [°] for mw_071_7m.

N(5)–Sb(1)–N(6)	74.71(9)
N(5)–Sb(1)–Sb(2)	100.33(8)
N(6)–Sb(1)–Sb(2)	106.04(7)
N(5)–Sb(1)–Ga(1)	36.02(7)
N(6)–Sb(1)–Ga(1)	38.94(6)
Sb(2)–Sb(1)–Ga(1)	109.846(12)
Ga(2)–Sb(2)–Sb(1)	92.905(13)
N(5)–Ga(1)–N(6)	94.00(11)
N(5)–Ga(1)–N(1)	115.01(12)
N(6)–Ga(1)–N(1)	118.29(11)
N(5)–Ga(1)–N(2)	119.47(11)
N(6)–Ga(1)–N(2)	115.36(11)
N(1)–Ga(1)–N(2)	96.47(11)
N(5)–Ga(1)–Sb(1)	41.25(7)
N(6)–Ga(1)–Sb(1)	53.10(8)
N(1)–Ga(1)–Sb(1)	125.99(8)
N(2)–Ga(1)–Sb(1)	137.10(8)
N(7)–Ga(2)–N(4)	103.67(13)
N(7)–Ga(2)–N(3)	108.69(12)
N(4)–Ga(2)–N(3)	91.57(11)
N(7)–Ga(2)–Sb(2)	119.84(9)
N(4)–Ga(2)–Sb(2)	122.39(8)
N(3)–Ga(2)–Sb(2)	106.56(7)
N(5)–Si(1)–C(61)	112.58(16)
N(5)–Si(1)–C(60)	114.33(15)
C(61)–Si(1)–C(60)	105.38(18)
N(5)–Si(1)–C(59)	109.77(15)
C(61)–Si(1)–C(59)	106.5(2)
C(60)–Si(1)–C(59)	107.81(18)
C(1)–N(1)–C(6)	118.1(3)
C(1)–N(1)–Ga(1)	116.7(2)
C(6)–N(1)–Ga(1)	125.14(19)
C(3)–N(2)–C(18)	117.5(3)
C(3)–N(2)–Ga(1)	117.4(2)
C(18)–N(2)–Ga(1)	125.09(19)
C(30)–N(3)–C(35)	119.4(3)
C(30)–N(3)–Ga(2)	122.8(2)
C(35)–N(3)–Ga(2)	117.77(19)
C(32)–N(4)–C(47)	118.3(3)
C(32)–N(4)–Ga(2)	121.2(2)
C(47)–N(4)–Ga(2)	120.3(2)
Si(1)–N(5)–Ga(1)	134.30(14)
Si(1)–N(5)–Sb(1)	122.07(13)
Ga(1)–N(5)–Sb(1)	102.73(11)
C(62)–N(6)–C(63)	110.0(3)
C(62)–N(6)–Ga(1)	116.9(2)
C(63)–N(6)–Ga(1)	119.3(2)
C(62)–N(6)–Sb(1)	110.5(2)
C(63)–N(6)–Sb(1)	109.6(2)
Ga(1)–N(6)–Sb(1)	87.96(10)
C(65)–N(7)–C(64)	111.5(3)
C(65)–N(7)–Ga(2)	123.7(2)
C(64)–N(7)–Ga(2)	124.2(2)

Table 5: (continued)

N(1)–C(1)–C(2)	123.7(3)
N(1)–C(1)–C(4)	120.4(3)
C(2)–C(1)–C(4)	115.9(3)
C(1)–C(2)–C(3)	128.3(3)
N(2)–C(3)–C(2)	124.0(3)
N(2)–C(3)–C(5)	120.3(3)
C(2)–C(3)–C(5)	115.7(3)
C(11)–C(6)–C(7)	121.0(3)
C(11)–C(6)–N(1)	121.6(3)
C(7)–C(6)–N(1)	117.4(3)
C(8)–C(7)–C(6)	117.6(3)
C(8)–C(7)–C(12)	118.9(3)
C(6)–C(7)–C(12)	123.4(3)
C(9)–C(8)–C(7)	122.0(4)
C(8)–C(9)–C(10)	119.7(3)
C(9)–C(10)–C(11)	121.3(4)
C(10)–C(11)–C(6)	118.3(3)
C(10)–C(11)–C(15)	118.8(3)
C(6)–C(11)–C(15)	122.8(3)
C(7)–C(12)–C(13)	112.2(3)
C(7)–C(12)–C(14)	111.6(3)
C(13)–C(12)–C(14)	109.4(3)
C(11)–C(15)–C(17)	111.5(3)
C(11)–C(15)–C(16)	109.8(3)
C(17)–C(15)–C(16)	110.0(3)
C(23)–C(18)–C(19)	121.5(3)
C(23)–C(18)–N(2)	119.8(3)
C(19)–C(18)–N(2)	118.7(3)
C(20)–C(19)–C(18)	117.9(3)
C(20)–C(19)–C(24)	119.3(3)
C(18)–C(19)–C(24)	122.8(3)
C(21)–C(20)–C(19)	121.0(3)
C(22)–C(21)–C(20)	120.1(3)
C(21)–C(22)–C(23)	121.7(4)
C(22)–C(23)–C(18)	117.7(3)
C(22)–C(23)–C(27)	120.2(3)
C(18)–C(23)–C(27)	122.0(3)
C(25)–C(24)–C(26)	109.1(3)
C(25)–C(24)–C(19)	112.4(3)
C(26)–C(24)–C(19)	112.0(3)
C(23)–C(27)–C(29)	112.6(3)
C(23)–C(27)–C(28)	112.2(3)
C(29)–C(27)–C(28)	108.9(3)
N(3)–C(30)–C(31)	123.0(3)
N(3)–C(30)–C(33)	120.2(3)
C(31)–C(30)–C(33)	116.8(3)
C(30)–C(31)–C(32)	127.6(3)
N(4)–C(32)–C(31)	124.0(3)
N(4)–C(32)–C(34)	119.8(3)
C(31)–C(32)–C(34)	116.2(3)
C(36)–C(35)–C(40)	120.7(3)
C(36)–C(35)–N(3)	120.6(3)
C(40)–C(35)–N(3)	118.6(3)

Table 5: (continued)

C(37)–C(36)–C(35)	118.8(3)
C(37)–C(36)–C(41)	118.4(3)
C(35)–C(36)–C(41)	122.8(3)
C(38)–C(37)–C(36)	121.3(3)
C(39)–C(38)–C(37)	119.3(3)
C(38)–C(39)–C(40)	121.9(3)
C(39)–C(40)–C(35)	118.0(3)
C(39)–C(40)–C(44)	119.5(3)
C(35)–C(40)–C(44)	122.5(3)
C(43)–C(41)–C(42)	110.3(4)
C(43)–C(41)–C(36)	109.9(4)
C(42)–C(41)–C(36)	111.5(4)
C(40)–C(44)–C(45)	112.2(4)
C(40)–C(44)–C(46)	112.7(4)
C(45)–C(44)–C(46)	109.0(3)
C(48)–C(47)–C(52)	121.0(3)
C(48)–C(47)–N(4)	121.1(3)
C(52)–C(47)–N(4)	117.8(3)
C(49)–C(48)–C(47)	118.1(4)
C(49)–C(48)–C(53)	118.3(4)
C(47)–C(48)–C(53)	123.6(3)
C(50)–C(49)–C(48)	122.2(4)
C(49)–C(50)–C(51)	119.4(4)
C(50)–C(51)–C(52)	121.5(4)
C(51)–C(52)–C(47)	117.8(4)
C(51)–C(52)–C(56)	120.1(4)
C(47)–C(52)–C(56)	122.1(3)
C(48)–C(53)–C(55)	110.4(4)
C(48)–C(53)–C(54)	112.0(5)
C(55)–C(53)–C(54)	109.8(4)
C(57)–C(56)–C(58)	109.1(4)
C(57)–C(56)–C(52)	113.2(4)
C(58)–C(56)–C(52)	113.9(3)

Crystal structure of mw_071_8m_sq

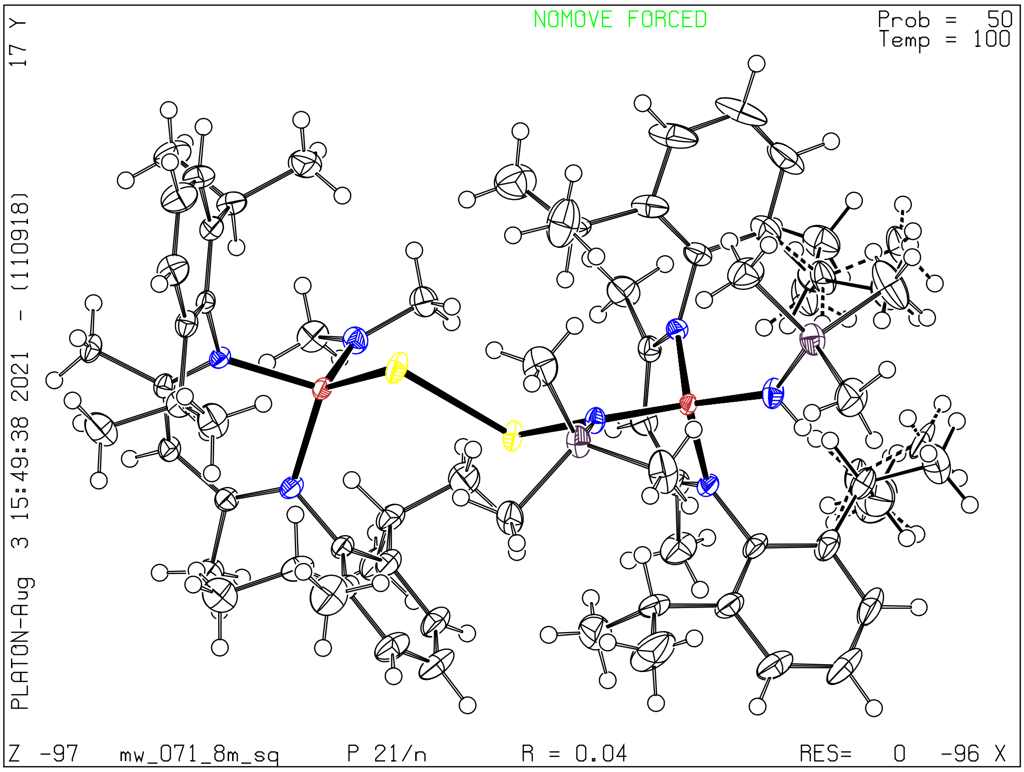

Table 1: Crystal data and structure refinement for mw_071_8m_sq.

Identification code	mw_071_8m_sq
Empirical Formula	$C_{68}\,H_{110}\,Ga_2\,N_8\,Sb_2\,Si_2$
Formula weight	1478.75 Da
Density (calculated)	$1.350\,g \cdot cm^{-3}$
$F(000)$	3064
Temperature	100(2) K
Crystal size	0.483 × 0.182 × 0.144 mm
Crystal appearance	dark orange block
Wavelength (MoK_{α})	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	$a = 11.889(2)$ Å
	$b = 18.460(4)$ Å
	$c = 33.366(7)$ Å
	$\alpha = 90°$
	$\beta = 96.360(11)°$
	$\gamma = 90°$
Unit cell volume	7278(2) $Å^3$
Z	4
Cell measurement refections used	9177
θ range for cell measurement	2.29° to 28.93°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	2.046° to 31.059°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (97.7%)
Index ranges	$-17 \leq h \leq 17$
	$-26 \leq k \leq 26$
	$-39 \leq l \leq 47$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.543\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.58
R_{merg} before/after correction	0.0854/0.0509
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	119071
Independent reflections	22799 ($R_{int} = 0.0518$)
Reflections with $I > 2\sigma(I)$	17644
Data / retraints / parameter	22799 / 118 / 804
Goodness-of-fit on F^2	1.041
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0273P)^2 + 10.7567P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0404$
	$wR2 = 0.0794$
R indices [all data]	$R1 = 0.0615$
	$wR2 = 0.0866$
Largest diff. peak and hole	2.358 and −1.236 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The NH hydrogen atom was refined freely.

Disorder

Two iso propyl groups are disordered over two positions. Their corresponding bond lengths and angles were restrained to be equal (SADI) and RIGU and SIMU restraints applied to the anisotropic displacement parameters of the respective atoms.

SQUEEZE

The structure contains a highly disordered acetonitril molecule. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run. (For details see: A. L. Spek, *Acta Cryst. A46* **(1990)**, 194–201). The molecule was included in the sum formula for completeness.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_071_8m_sq. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	5410(1)	3239(1)	5879(1)	27(1)
Sb(2)	4153(1)	3100(1)	6484(1)	21(1)
Ga(1)	4600(1)	2052(1)	5523(1)	16(1)
Ga(2)	4733(1)	3560(1)	7451(1)	15(1)
Si(1)	4756(1)	4780(1)	6743(1)	25(1)
Si(2)	6187(1)	4676(1)	8118(1)	26(1)
N(1)	2985(2)	1964(1)	5290(1)	20(1)
N(2)	5156(2)	1989(1)	4981(1)	16(1)
N(3)	3222(2)	3154(1)	7530(1)	19(1)
N(4)	5541(2)	2626(1)	7499(1)	18(1)
N(5)	4972(2)	1188(1)	5794(1)	24(1)
N(6)	4690(2)	3888(1)	6904(1)	18(1)
N(7)	5110(2)	4155(1)	7894(1)	25(1)
C(1)	2687(2)	1618(1)	4943(1)	20(1)
C(2)	3456(2)	1409(1)	4673(1)	20(1)
C(3)	4583(2)	1632(1)	4674(1)	18(1)
C(4)	1449(2)	1444(2)	4813(1)	27(1)
C(5)	5164(2)	1448(1)	4305(1)	23(1)
C(6)	2097(2)	2234(1)	5515(1)	22(1)
C(7)	1603(2)	1780(2)	5786(1)	26(1)
C(8)	732(2)	2069(2)	5988(1)	32(1)
C(9)	358(3)	2768(2)	5922(1)	38(1)
C(10)	871(2)	3212(2)	5660(1)	35(1)
C(11)	1760(2)	2960(2)	5456(1)	27(1)
C(12)	1988(2)	1011(2)	5876(1)	29(1)
C(13)	1006(3)	466(2)	5795(1)	36(1)
C(14)	2533(3)	942(2)	6316(1)	39(1)
C(15)	2329(2)	3463(2)	5175(1)	30(1)
C(16)	1911(3)	3353(2)	4732(1)	39(1)
C(17)	2230(3)	4263(2)	5282(1)	46(1)
C(18)	6221(2)	2326(1)	4920(1)	17(1)
C(19)	7250(2)	1968(1)	5026(1)	22(1)
C(20)	8257(2)	2326(2)	4969(1)	31(1)
C(21)	8239(3)	3013(2)	4804(1)	38(1)
C(22)	7224(2)	3360(2)	4698(1)	31(1)
C(23)	6193(2)	3031(1)	4756(1)	21(1)
C(24)	7302(2)	1209(2)	5201(1)	27(1)
C(25)	7903(3)	685(2)	4937(1)	39(1)
C(26)	7886(3)	1207(2)	5635(1)	38(1)
C(27)	5084(2)	3428(1)	4640(1)	24(1)
C(28)	4705(3)	3370(2)	4187(1)	38(1)
C(29)	5132(3)	4218(2)	4762(1)	36(1)
C(30)	2986(2)	2479(1)	7405(1)	23(1)
C(31)	3795(2)	1993(1)	7290(1)	25(1)
C(32)	4978(2)	2028(1)	7370(1)	21(1)
C(33)	1787(2)	2185(2)	7382(1)	39(1)
C(34)	5624(3)	1341(2)	7306(1)	34(1)
C(35)	2371(2)	3543(2)	7726(1)	24(1)
C(36)	1659(2)	4057(2)	7510(1)	30(1)
C(37)	787(3)	4364(2)	7702(1)	40(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(38)	641(3)	4196(2)	8097(1)	47(1)
C(39)	1380(3)	3730(2)	8312(1)	42(1)
C(40)	2260(2)	3392(2)	8136(1)	31(1)
C(41)	1810(3)	4284(2)	7080(1)	38(1)
C(42)	1205(3)	3774(3)	6763(1)	67(1)
C(43)	1421(4)	5065(3)	6993(1)	79(2)
C(44')	3080(30)	2745(17)	8382(7)	29(4)
C(45')	2390(40)	2100(20)	8517(15)	58(8)
C(46')	3750(20)	3089(16)	8754(5)	39(4)
C(44)	3039(10)	2947(9)	8404(3)	33(2)
C(45)	2500(16)	2226(9)	8505(5)	54(3)
C(46)	3473(11)	3341(9)	8800(3)	53(3)
C(47)	6716(2)	2562(1)	7670(1)	24(1)
C(48)	7591(2)	2702(2)	7430(1)	32(1)
C(49)	8703(3)	2667(2)	7612(1)	52(1)
C(50)	8956(3)	2479(2)	8015(1)	57(1)
C(51)	8090(3)	2312(2)	8240(1)	48(1)
C(52)	6956(3)	2348(2)	8078(1)	38(1)
C(53)	7377(2)	2868(2)	6978(1)	37(1)
C(54)	7796(4)	3605(2)	6881(1)	57(1)
C(55)	7919(3)	2305(2)	6723(1)	55(1)
C(56)	5991(6)	1997(4)	8325(2)	30(2)
C(57)	6204(5)	1204(3)	8447(2)	42(2)
C(58)	5915(7)	2454(3)	8702(2)	43(2)
C(56')	6125(8)	2315(5)	8365(2)	32(2)
C(57')	5523(7)	1572(4)	8303(2)	41(2)
C(58')	6588(9)	2350(5)	8813(2)	47(2)
C(59)	4759(3)	494(1)	5602(1)	30(1)
C(60)	5512(2)	1113(2)	6205(1)	30(1)
C(61)	6134(3)	5058(2)	6566(1)	42(1)
C(62)	3657(3)	4960(2)	6298(1)	32(1)
C(63)	4495(3)	5433(2)	7152(1)	43(1)
C(64)	7344(3)	4758(2)	7789(1)	41(1)
C(65)	6842(4)	4305(2)	8613(1)	54(1)
C(66)	5623(3)	5588(2)	8237(1)	42(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_071_8m_sq.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	28(1)	33(1)	22(1)	−13(1)	11(1)	−12(1)
Sb(2)	30(1)	20(1)	15(1)	−2(1)	7(1)	−6(1)
Ga(1)	16(1)	19(1)	15(1)	−3(1)	4(1)	−1(1)
Ga(2)	15(1)	17(1)	12(1)	−1(1)	3(1)	−1(1)
Si(1)	38(1)	16(1)	20(1)	3(1)	3(1)	1(1)
Si(2)	32(1)	24(1)	22(1)	−2(1)	2(1)	−8(1)
N(1)	16(1)	23(1)	22(1)	−6(1)	6(1)	−2(1)
N(2)	15(1)	17(1)	17(1)	−2(1)	5(1)	−2(1)
N(3)	17(1)	23(1)	18(1)	−1(1)	5(1)	−1(1)
N(4)	16(1)	21(1)	16(1)	3(1)	2(1)	2(1)
N(5)	27(1)	24(1)	21(1)	3(1)	3(1)	1(1)
N(6)	25(1)	14(1)	15(1)	−1(1)	4(1)	0(1)
N(7)	30(1)	26(1)	18(1)	−6(1)	5(1)	−6(1)
C(1)	18(1)	21(1)	22(1)	−3(1)	3(1)	−2(1)
C(2)	21(1)	18(1)	19(1)	−6(1)	2(1)	−3(1)
C(3)	21(1)	16(1)	17(1)	−1(1)	4(1)	1(1)
C(4)	20(1)	34(1)	27(1)	−9(1)	2(1)	−5(1)
C(5)	25(1)	24(1)	20(1)	−8(1)	7(1)	−5(1)
C(6)	16(1)	31(1)	22(1)	−11(1)	4(1)	−3(1)
C(7)	21(1)	30(1)	28(1)	−11(1)	8(1)	−5(1)
C(8)	26(1)	37(2)	36(2)	−11(1)	15(1)	−7(1)
C(9)	30(2)	36(2)	53(2)	−15(1)	23(1)	−2(1)
C(10)	28(1)	28(1)	49(2)	−14(1)	14(1)	−2(1)
C(11)	19(1)	30(1)	32(1)	−10(1)	6(1)	−4(1)
C(12)	23(1)	33(1)	32(1)	−2(1)	12(1)	−3(1)
C(13)	35(2)	33(2)	41(2)	−6(1)	13(1)	−5(1)
C(14)	32(2)	53(2)	34(2)	5(1)	8(1)	−7(1)
C(15)	22(1)	28(1)	41(2)	−4(1)	8(1)	1(1)
C(16)	43(2)	31(2)	43(2)	0(1)	0(1)	−1(1)
C(17)	53(2)	31(2)	55(2)	−10(2)	12(2)	−11(2)
C(18)	17(1)	20(1)	14(1)	−4(1)	3(1)	−1(1)
C(19)	20(1)	27(1)	21(1)	−2(1)	5(1)	1(1)
C(20)	16(1)	41(2)	37(2)	1(1)	4(1)	−1(1)
C(21)	25(1)	42(2)	49(2)	3(1)	13(1)	−11(1)
C(22)	31(1)	28(1)	36(2)	5(1)	9(1)	−7(1)
C(23)	24(1)	20(1)	19(1)	−1(1)	6(1)	−4(1)
C(24)	20(1)	28(1)	32(1)	2(1)	5(1)	4(1)
C(25)	31(2)	33(2)	53(2)	−7(1)	9(1)	8(1)
C(26)	32(2)	47(2)	36(2)	10(1)	2(1)	10(1)
C(27)	26(1)	20(1)	27(1)	3(1)	6(1)	−1(1)
C(28)	44(2)	32(2)	36(2)	−3(1)	−10(1)	5(1)
C(29)	49(2)	24(1)	34(2)	−4(1)	−1(1)	5(1)
C(30)	21(1)	29(1)	20(1)	−4(1)	3(1)	−5(1)
C(31)	27(1)	20(1)	27(1)	−3(1)	1(1)	−6(1)
C(32)	27(1)	18(1)	18(1)	1(1)	2(1)	3(1)
C(33)	27(2)	41(2)	52(2)	−13(2)	10(1)	−16(1)
C(34)	40(2)	22(1)	38(2)	−4(1)	−3(1)	7(1)
C(35)	18(1)	31(1)	26(1)	−9(1)	10(1)	−5(1)
C(36)	24(1)	35(2)	33(2)	−8(1)	9(1)	4(1)
C(37)	30(2)	41(2)	53(2)	−11(2)	17(1)	6(1)
C(38)	41(2)	49(2)	56(2)	−19(2)	33(2)	−3(2)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(39)	42(2)	55(2)	32(2)	−14(1)	24(1)	−12(2)
C(40)	27(1)	41(2)	28(1)	−7(1)	14(1)	−10(1)
C(41)	26(2)	55(2)	35(2)	3(1)	9(1)	19(1)
C(42)	36(2)	125(4)	40(2)	−13(2)	2(2)	−5(2)
C(43)	88(3)	86(3)	71(3)	34(2)	40(3)	64(3)
C(44')	39(8)	32(10)	19(6)	1(6)	12(5)	−2(7)
C(45')	70(14)	42(11)	68(16)	3(10)	30(11)	−19(9)
C(46')	42(8)	48(10)	32(6)	−17(6)	26(6)	−2(6)
C(44)	32(3)	46(6)	25(3)	4(3)	17(2)	−2(4)
C(45)	57(6)	54(6)	51(5)	20(4)	9(4)	−4(4)
C(46)	55(5)	76(6)	26(3)	1(4)	0(3)	−1(5)
C(47)	21(1)	22(1)	27(1)	1(1)	−4(1)	4(1)
C(48)	19(1)	31(1)	46(2)	12(1)	0(1)	3(1)
C(49)	19(1)	59(2)	77(3)	25(2)	−5(2)	−3(1)
C(50)	28(2)	53(2)	82(3)	17(2)	−28(2)	−2(2)
C(51)	43(2)	53(2)	41(2)	4(2)	−21(2)	10(2)
C(52)	37(2)	44(2)	29(2)	4(1)	−7(1)	12(1)
C(53)	16(1)	53(2)	44(2)	12(2)	9(1)	4(1)
C(54)	86(3)	46(2)	42(2)	4(2)	25(2)	−3(2)
C(55)	44(2)	53(2)	66(3)	−14(2)	3(2)	−1(2)
C(56)	30(3)	29(4)	29(3)	4(3)	−2(2)	1(3)
C(57)	42(3)	39(3)	43(4)	16(3)	−1(3)	−1(3)
C(58)	49(4)	43(3)	36(4)	4(3)	−2(3)	0(3)
C(56')	45(5)	29(4)	20(3)	7(3)	−3(3)	5(4)
C(57')	55(5)	41(5)	26(3)	10(3)	4(3)	−12(4)
C(58')	63(6)	51(5)	23(4)	5(3)	−8(4)	6(4)
C(59)	35(2)	21(1)	36(2)	2(1)	8(1)	0(1)
C(60)	34(2)	31(1)	26(1)	8(1)	4(1)	1(1)
C(61)	51(2)	36(2)	40(2)	10(1)	7(2)	−11(1)
C(62)	47(2)	24(1)	23(1)	7(1)	4(1)	9(1)
C(63)	78(3)	21(1)	29(2)	−2(1)	0(2)	11(2)
C(64)	30(2)	45(2)	50(2)	−7(2)	9(1)	−8(1)
C(65)	78(3)	41(2)	38(2)	6(2)	−22(2)	−22(2)
C(66)	50(2)	36(2)	42(2)	−17(1)	6(2)	−6(2)

Table 4: Bond lengths [Å] for mw_071_8m_sq.

Sb(1)–Ga(1)	2.6241(5)
Sb(1)–Sb(2)	2.6534(5)
Sb(2)–N(6)	2.071(2)
Ga(1)–N(5)	1.861(2)
Ga(1)–N(1)	1.996(2)
Ga(1)–N(2)	1.9964(19)
Ga(2)–N(7)	1.857(2)
Ga(2)–N(6)	1.917(2)
Ga(2)–N(4)	1.973(2)
Ga(2)–N(3)	1.991(2)
Si(1)–N(6)	1.736(2)
Si(1)–C(63)	1.871(3)
Si(1)–C(61)	1.874(3)
Si(1)–C(62)	1.894(3)
Si(2)–N(7)	1.706(2)
Si(2)–C(64)	1.859(3)
Si(2)–C(66)	1.872(3)
Si(2)–C(65)	1.873(3)
N(1)–C(1)	1.337(3)
N(1)–C(6)	1.449(3)
N(2)–C(3)	1.339(3)
N(2)–C(18)	1.444(3)
N(3)–C(30)	1.332(3)
N(3)–C(35)	1.456(3)
N(4)–C(32)	1.337(3)
N(4)–C(47)	1.454(3)
N(5)–C(59)	1.441(3)
N(5)–C(60)	1.456(3)
C(1)–C(2)	1.407(3)
C(1)–C(4)	1.522(3)
C(2)–C(3)	1.401(3)
C(3)–C(5)	1.516(3)
C(6)–C(11)	1.407(4)
C(6)–C(7)	1.409(4)
C(7)–C(8)	1.401(3)
C(7)–C(12)	1.512(4)
C(8)–C(9)	1.374(4)
C(9)–C(10)	1.387(4)
C(10)–C(11)	1.400(4)
C(11)–C(15)	1.530(4)
C(12)–C(13)	1.542(4)
C(12)–C(14)	1.542(4)
C(15)–C(16)	1.518(4)
C(15)–C(17)	1.527(4)
C(18)–C(19)	1.400(3)
C(18)–C(23)	1.411(3)
C(19)–C(20)	1.399(4)
C(19)–C(24)	1.518(4)
C(20)–C(21)	1.381(4)
C(21)–C(22)	1.378(4)
C(22)–C(23)	1.401(4)
C(23)–C(27)	1.521(4)
C(24)–C(26)	1.535(4)

Table 4: (continued)

C(24)–C(25)	1.536(4)
C(27)–C(29)	1.515(4)
C(27)–C(28)	1.533(4)
C(30)–C(31)	1.400(4)
C(30)–C(33)	1.519(4)
C(31)–C(32)	1.404(4)
C(32)–C(34)	1.509(4)
C(35)–C(36)	1.415(4)
C(35)–C(40)	1.415(4)
C(36)–C(37)	1.399(4)
C(36)–C(41)	1.524(4)
C(37)–C(38)	1.385(5)
C(38)–C(39)	1.372(5)
C(39)–C(40)	1.400(4)
C(40)–C(44)	1.466(12)
C(40)–C(44')	1.70(3)
C(41)–C(43)	1.531(5)
C(41)–C(42)	1.532(5)
C(44')–C(46')	1.535(13)
C(44')–C(45')	1.537(14)
C(44)–C(45)	1.531(8)
C(44)–C(46)	1.548(7)
C(47)–C(48)	1.403(4)
C(47)–C(52)	1.416(4)
C(48)–C(49)	1.393(4)
C(48)–C(53)	1.533(4)
C(49)–C(50)	1.390(6)
C(50)–C(51)	1.374(6)
C(51)–C(52)	1.397(4)
C(52)–C(56')	1.451(10)
C(52)–C(56)	1.621(8)
C(53)–C(54)	1.495(5)
C(53)–C(55)	1.529(5)
C(56)–C(58)	1.524(8)
C(56)–C(57)	1.534(8)
C(56')–C(58')	1.539(9)
C(56')–C(57')	1.550(9)

Table 5: Bond angles [°] for mw_071_8m_sq.

Ga(1)–Sb(1)–Sb(2)	93.112(12)
N(6)–Sb(2)–Sb(1)	106.81(5)
N(5)–Ga(1)–N(1)	106.58(9)
N(5)–Ga(1)–N(2)	107.75(9)
N(1)–Ga(1)–N(2)	92.48(8)
N(5)–Ga(1)–Sb(1)	116.14(7)
N(1)–Ga(1)–Sb(1)	122.20(6)
N(2)–Ga(1)–Sb(1)	108.47(6)
N(7)–Ga(2)–N(6)	123.37(9)
N(7)–Ga(2)–N(4)	112.31(10)
N(6)–Ga(2)–N(4)	108.38(8)
N(7)–Ga(2)–N(3)	105.03(9)
N(6)–Ga(2)–N(3)	108.39(9)
N(4)–Ga(2)–N(3)	95.60(8)
N(6)–Si(1)–C(63)	111.66(12)
N(6)–Si(1)–C(61)	115.38(13)
C(63)–Si(1)–C(61)	105.90(17)
N(6)–Si(1)–C(62)	110.98(12)
C(63)–Si(1)–C(62)	107.55(14)
C(61)–Si(1)–C(62)	104.83(14)
N(7)–Si(2)–C(64)	110.81(13)
N(7)–Si(2)–C(66)	109.28(14)
C(64)–Si(2)–C(66)	110.92(16)
N(7)–Si(2)–C(65)	113.56(14)
C(64)–Si(2)–C(65)	106.67(19)
C(66)–Si(2)–C(65)	105.48(17)
C(1)–N(1)–C(6)	118.3(2)
C(1)–N(1)–Ga(1)	121.84(16)
C(6)–N(1)–Ga(1)	119.66(16)
C(3)–N(2)–C(18)	118.88(18)
C(3)–N(2)–Ga(1)	122.01(15)
C(18)–N(2)–Ga(1)	119.09(14)
C(30)–N(3)–C(35)	118.0(2)
C(30)–N(3)–Ga(2)	118.24(16)
C(35)–N(3)–Ga(2)	123.75(16)
C(32)–N(4)–C(47)	119.0(2)
C(32)–N(4)–Ga(2)	118.25(16)
C(47)–N(4)–Ga(2)	122.75(16)
C(59)–N(5)–C(60)	111.7(2)
C(59)–N(5)–Ga(1)	121.78(18)
C(60)–N(5)–Ga(1)	126.50(18)
Si(1)–N(6)–Ga(2)	126.59(11)
Si(1)–N(6)–Sb(2)	118.56(11)
Ga(2)–N(6)–Sb(2)	113.32(9)
Si(2)–N(7)–Ga(2)	141.79(14)
N(1)–C(1)–C(2)	123.9(2)
N(1)–C(1)–C(4)	120.2(2)
C(2)–C(1)–C(4)	115.9(2)
C(3)–C(2)–C(1)	127.3(2)
N(2)–C(3)–C(2)	123.5(2)
N(2)–C(3)–C(5)	119.6(2)
C(2)–C(3)–C(5)	116.9(2)
C(11)–C(6)–C(7)	121.6(2)

Table 5: (continued)

C(11)–C(6)–N(1)	117.9(2)
C(7)–C(6)–N(1)	120.5(2)
C(8)–C(7)–C(6)	117.7(3)
C(8)–C(7)–C(12)	119.1(2)
C(6)–C(7)–C(12)	123.2(2)
C(9)–C(8)–C(7)	121.6(3)
C(8)–C(9)–C(10)	119.9(3)
C(9)–C(10)–C(11)	121.2(3)
C(10)–C(11)–C(6)	117.9(3)
C(10)–C(11)–C(15)	120.4(3)
C(6)–C(11)–C(15)	121.7(2)
C(7)–C(12)–C(13)	111.8(2)
C(7)–C(12)–C(14)	110.6(2)
C(13)–C(12)–C(14)	110.1(2)
C(16)–C(15)–C(17)	109.4(3)
C(16)–C(15)–C(11)	113.3(2)
C(17)–C(15)–C(11)	113.1(2)
C(19)–C(18)–C(23)	120.9(2)
C(19)–C(18)–N(2)	121.2(2)
C(23)–C(18)–N(2)	117.9(2)
C(20)–C(19)–C(18)	118.8(2)
C(20)–C(19)–C(24)	119.3(2)
C(18)–C(19)–C(24)	121.9(2)
C(21)–C(20)–C(19)	120.8(3)
C(22)–C(21)–C(20)	120.3(3)
C(21)–C(22)–C(23)	121.1(3)
C(22)–C(23)–C(18)	118.1(2)
C(22)–C(23)–C(27)	120.2(2)
C(18)–C(23)–C(27)	121.7(2)
C(19)–C(24)–C(26)	111.1(2)
C(19)–C(24)–C(25)	111.2(2)
C(26)–C(24)–C(25)	110.4(2)
C(29)–C(27)–C(23)	113.0(2)
C(29)–C(27)–C(28)	109.2(2)
C(23)–C(27)–C(28)	111.6(2)
N(3)–C(30)–C(31)	123.8(2)
N(3)–C(30)–C(33)	121.0(2)
C(31)–C(30)–C(33)	115.2(2)
C(30)–C(31)–C(32)	128.6(2)
N(4)–C(32)–C(31)	123.6(2)
N(4)–C(32)–C(34)	119.6(2)
C(31)–C(32)–C(34)	116.7(2)
C(36)–C(35)–C(40)	120.8(2)
C(36)–C(35)–N(3)	120.4(2)
C(40)–C(35)–N(3)	118.8(2)
C(37)–C(36)–C(35)	118.0(3)
C(37)–C(36)–C(41)	119.3(3)
C(35)–C(36)–C(41)	122.7(2)
C(38)–C(37)–C(36)	121.5(3)
C(39)–C(38)–C(37)	119.8(3)
C(38)–C(39)–C(40)	121.7(3)
C(39)–C(40)–C(35)	118.0(3)
C(39)–C(40)–C(44)	116.5(6)

Table 5: (continued)

C(35)–C(40)–C(44)	125.4(5)
C(39)–C(40)–C(44')	121.9(11)
C(35)–C(40)–C(44')	119.7(11)
C(36)–C(41)–C(43)	111.9(3)
C(36)–C(41)–C(42)	112.6(3)
C(43)–C(41)–C(42)	109.8(4)
C(46')–C(44')–C(45')	108.9(13)
C(46')–C(44')–C(40)	108.5(15)
C(45')–C(44')–C(40)	113(3)
C(40)–C(44)–C(45)	111.8(10)
C(40)–C(44)–C(46)	112.6(7)
C(45)–C(44)–C(46)	109.1(6)
C(48)–C(47)–C(52)	121.0(3)
C(48)–C(47)–N(4)	120.2(2)
C(52)–C(47)–N(4)	118.8(2)
C(49)–C(48)–C(47)	118.1(3)
C(49)–C(48)–C(53)	118.9(3)
C(47)–C(48)–C(53)	123.0(2)
C(50)–C(49)–C(48)	121.7(3)
C(51)–C(50)–C(49)	119.3(3)
C(50)–C(51)–C(52)	121.8(3)
C(51)–C(52)–C(47)	117.9(3)
C(51)–C(52)–C(56')	116.2(4)
C(47)–C(52)–C(56')	124.5(4)
C(51)–C(52)–C(56)	119.4(4)
C(47)–C(52)–C(56)	121.5(3)
C(54)–C(53)–C(55)	109.0(3)
C(54)–C(53)–C(48)	111.8(3)
C(55)–C(53)–C(48)	112.2(3)
C(58)–C(56)–C(57)	109.4(5)
C(58)–C(56)–C(52)	108.0(5)
C(57)–C(56)–C(52)	114.3(5)
C(52)–C(56')–C(58')	116.4(7)
C(52)–C(56')–C(57')	106.7(6)
C(58')–C(56')–C(57')	106.1(6)

Crystal structure of mw_071m

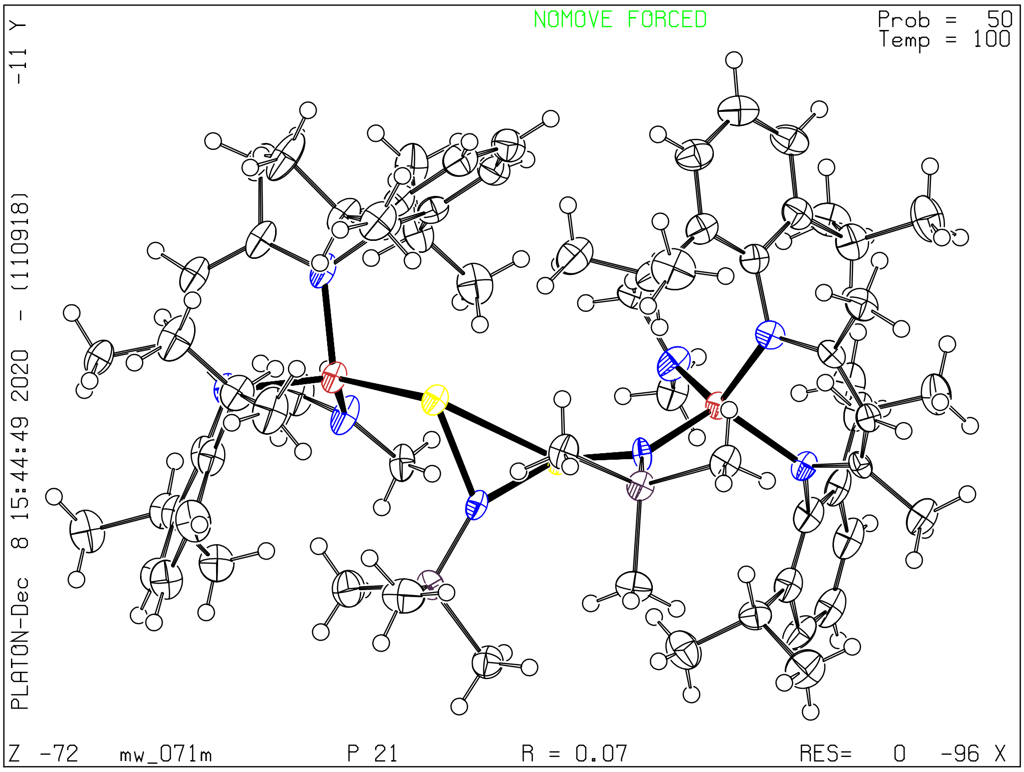

Table 1: Crystal data and structure refinement for mw_071m.

Identification code	mw_071m
Empirical Formula	$C_{68} H_{112} Ga_2 N_8 Sb_2 Si_2$
Formula weight	1480.77 Da
Density (calculated)	$1.344\,g \cdot cm^{-3}$
$F(000)$	1536
Temperature	100(2) K
Crystal size	0.151 × 0.113 × 0.113 mm
Crystal appearance	orange tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	$a = 12.700(3)$ Å
	$b = 17.555(5)$ Å
	$c = 16.953(4)$ Å
	$\alpha = 90°$
	$\beta = 104.569(7)°$
	$\gamma = 90°$
Unit cell volume	3658.4(17) $Å^3$
Z	2
Cell measurement refections used	9931
θ range for cell measurement	2.32° to 26.18°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	2.307° to 26.638°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.8% (98.4%)
Index ranges	$-15 \leq h \leq 16$
	$-22 \leq k \leq 21$
	$-21 \leq l \leq 21$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.534\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.52
R_{merg} before/after correction	0.1202/0.0950
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	99252
Independent reflections	15095 ($R_{int} = 0.1111$)
Reflections with $I > 2\sigma(I)$	12420
Data / retraints / parameter	15095 / 676 / 769
Goodness-of-fit on F^2	1.155
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0998P)^2 + 13.868P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0733$
	$wR2 = 0.1735$
R indices [all data]	$R1 = 0.0979$
	$wR2 = 0.1929$
Absolute structure parameter	0.024(10)
Largest diff. peak and hole	5.212 and -1.533 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Satellite crystals

The crystal was covered with several satellite crystals that could not be removed. Their reflections are clearly visiable in the frames, however they were to weak to be successfully integrated. Thus the obtained intensity data is likely distorted by the contribution of overlapps. Consequently, quantitative results should be considered unreliable and carefully accessed.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_071m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	5254(1)	4557(1)	4067(1)	25(1)
Sb(2)	4787(1)	5165(1)	2460(1)	26(1)
Ga(1)	4577(1)	3984(1)	1419(1)	24(1)
Ga(2)	7139(1)	5138(1)	5550(1)	21(1)
Si(1)	5082(3)	6309(2)	4864(2)	25(1)
Si(2)	2459(3)	4838(2)	3104(2)	29(1)
N(1)	5848(11)	4031(7)	917(7)	28(2)
N(2)	3498(10)	4021(6)	310(7)	28(2)
N(3)	8254(10)	5937(6)	5778(7)	25(2)
N(4)	7154(10)	4944(6)	6720(7)	24(2)
N(5)	4488(12)	2990(6)	1782(7)	32(3)
N(6)	7560(12)	4297(7)	5017(8)	34(3)
N(7)	5768(9)	5444(6)	4866(7)	23(2)
N(8)	3851(10)	4952(6)	3308(6)	24(2)
C(1)	5797(14)	3768(7)	162(8)	31(3)
C(2)	4817(14)	3619(8)	−414(9)	34(3)
C(3)	3764(14)	3794(8)	−377(8)	33(3)
C(4)	6835(15)	3636(9)	−102(10)	39(3)
C(5)	2908(14)	3706(9)	−1167(9)	34(3)
C(6)	6862(12)	4326(8)	1409(9)	27(3)
C(7)	7064(12)	5115(9)	1369(8)	31(3)
C(8)	8027(14)	5410(9)	1858(10)	38(3)
C(9)	8770(14)	4939(9)	2380(11)	40(3)
C(10)	8563(13)	4169(9)	2396(10)	36(3)
C(11)	7627(12)	3851(8)	1914(9)	28(3)
C(12)	6243(15)	5630(8)	772(9)	35(3)
C(13)	6217(16)	6446(9)	1064(11)	42(4)
C(14)	6510(20)	5634(9)	−71(10)	54(5)
C(15)	7477(14)	2982(8)	1932(10)	37(3)
C(16)	7379(16)	2704(9)	2758(11)	45(4)
C(17)	8400(16)	2582(9)	1667(11)	45(4)
C(18)	2387(13)	4262(8)	245(9)	30(3)
C(19)	2165(13)	5049(8)	255(8)	31(3)
C(20)	1125(15)	5267(10)	257(11)	44(4)
C(21)	296(15)	4752(9)	230(10)	41(3)
C(22)	514(14)	3976(10)	205(10)	38(3)
C(23)	1559(13)	3711(8)	213(9)	31(3)
C(24)	3046(14)	5628(8)	240(10)	35(3)
C(25)	3199(19)	5728(9)	−626(10)	50(5)
C(26)	2857(18)	6418(9)	571(11)	48(5)
C(27)	1755(14)	2848(8)	186(9)	34(3)
C(28)	939(16)	2481(9)	−544(11)	44(4)
C(29)	1637(15)	2467(9)	972(10)	39(4)
C(30)	8398(11)	6369(7)	6461(8)	23(2)
C(31)	7945(11)	6189(7)	7106(8)	23(3)
C(32)	7479(11)	5506(7)	7263(8)	22(2)
C(33)	9074(13)	7087(8)	6533(10)	34(3)
C(34)	7363(15)	5409(8)	8126(9)	34(3)
C(35)	9074(12)	6028(8)	5327(9)	28(2)
C(36)	10121(13)	5718(8)	5666(9)	32(3)

Table 2: (continued)

	x	y	z	U_{eq}
C(37)	10954(13)	5880(9)	5304(11)	39(3)
C(38)	10762(15)	6319(11)	4597(12)	49(4)
C(39)	9731(15)	6589(9)	4245(11)	41(3)
C(40)	8881(13)	6462(8)	4604(9)	31(3)
C(41)	10376(13)	5209(10)	6417(9)	37(3)
C(42)	11220(17)	5541(11)	7116(12)	53(5)
C(43)	10718(14)	4415(9)	6188(12)	43(4)
C(44)	7754(14)	6797(8)	4205(10)	34(3)
C(45)	7751(17)	7660(9)	4306(13)	51(5)
C(46)	7398(18)	6607(12)	3304(11)	52(4)
C(47)	6778(14)	4232(7)	7021(9)	29(3)
C(48)	7564(14)	3657(8)	7301(8)	32(3)
C(49)	7184(15)	3022(8)	7671(9)	37(3)
C(50)	6152(15)	2957(8)	7725(9)	36(3)
C(51)	5394(15)	3524(8)	7416(9)	36(3)
C(52)	5713(13)	4179(8)	7054(9)	31(3)
C(53)	8696(14)	3699(8)	7253(9)	35(3)
C(54)	9462(14)	4115(9)	7990(10)	41(4)
C(55)	9215(16)	2920(9)	7137(10)	42(4)
C(56)	4855(13)	4787(8)	6734(10)	32(3)
C(57)	4469(16)	5175(13)	7421(11)	50(4)
C(58)	3900(14)	4442(11)	6119(11)	47(4)
C(59)	4420(14)	2795(8)	2592(8)	32(3)
C(60)	4564(15)	2326(8)	1288(9)	37(4)
C(61)	7446(15)	3499(8)	5191(10)	35(3)
C(62)	8070(12)	4388(8)	4347(10)	34(3)
C(63)	3751(14)	6212(9)	5160(11)	38(3)
C(64)	5899(13)	7010(8)	5620(9)	31(3)
C(65)	4716(14)	6808(8)	3854(9)	31(3)
C(66)	2057(13)	4482(10)	4034(9)	36(3)
C(67)	1935(16)	4096(11)	2309(11)	47(4)
C(68)	1798(16)	5780(11)	2745(12)	48(4)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_071m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	32(1)	16(1)	24(1)	−3(1)	4(1)	−1(1)
Sb(2)	39(1)	15(1)	24(1)	−3(1)	9(1)	−3(1)
Ga(1)	38(1)	12(1)	21(1)	0(1)	7(1)	−1(1)
Ga(2)	27(1)	12(1)	23(1)	−2(1)	6(1)	0(1)
Si(1)	32(2)	15(2)	27(2)	−1(1)	7(2)	2(2)
Si(2)	27(2)	28(2)	30(2)	−2(2)	4(2)	−2(2)
N(1)	49(6)	16(5)	19(5)	0(4)	9(4)	3(5)
N(2)	38(6)	15(5)	29(5)	3(4)	4(4)	−2(4)
N(3)	28(6)	16(5)	32(5)	−1(4)	8(5)	2(4)
N(4)	35(6)	16(5)	21(5)	3(3)	8(4)	−1(4)
N(5)	67(9)	6(4)	22(5)	0(4)	12(5)	−4(5)
N(6)	53(8)	16(5)	36(6)	−10(5)	18(6)	−2(5)
N(7)	27(6)	16(4)	19(5)	−3(4)	−6(4)	1(4)
N(8)	34(5)	21(6)	15(5)	1(4)	5(4)	0(4)
C(1)	62(7)	10(6)	24(5)	3(4)	15(5)	5(6)
C(2)	60(7)	18(6)	25(6)	−1(5)	14(5)	−4(6)
C(3)	56(7)	18(6)	23(5)	5(5)	9(5)	−3(6)
C(4)	61(9)	27(8)	33(8)	−5(6)	17(7)	1(7)
C(5)	51(9)	27(7)	25(6)	5(6)	10(6)	5(7)
C(6)	35(6)	23(6)	28(6)	1(4)	15(5)	1(4)
C(7)	46(7)	20(5)	31(6)	−2(5)	16(5)	−3(5)
C(8)	49(8)	25(7)	43(8)	−6(5)	18(6)	−9(5)
C(9)	39(8)	36(7)	45(8)	−11(6)	12(6)	−5(6)
C(10)	33(8)	34(6)	40(8)	−6(6)	11(6)	−1(6)
C(11)	34(7)	22(6)	32(7)	−2(5)	15(5)	1(5)
C(12)	61(9)	16(6)	31(7)	2(5)	19(6)	−1(6)
C(13)	67(12)	20(6)	42(9)	1(6)	20(8)	0(7)
C(14)	117(18)	21(8)	31(8)	5(6)	32(9)	0(9)
C(15)	42(9)	21(6)	42(8)	−4(6)	−2(7)	1(6)
C(16)	57(11)	23(8)	50(9)	4(6)	5(8)	−4(7)
C(17)	62(11)	26(8)	42(9)	−6(7)	3(8)	13(7)
C(18)	42(6)	19(5)	23(7)	6(5)	−1(5)	0(5)
C(19)	48(7)	17(6)	25(6)	−1(5)	5(6)	−1(5)
C(20)	51(7)	27(7)	49(9)	3(7)	2(7)	7(6)
C(21)	46(8)	31(7)	41(8)	−4(6)	4(7)	7(5)
C(22)	45(8)	29(7)	40(8)	2(7)	11(7)	0(6)
C(23)	45(7)	20(5)	27(7)	4(5)	6(6)	1(5)
C(24)	51(9)	15(6)	39(7)	1(5)	13(7)	−2(6)
C(25)	94(15)	19(7)	39(8)	5(6)	21(9)	−4(8)
C(26)	82(14)	17(6)	44(9)	−3(6)	11(9)	1(7)
C(27)	47(9)	20(6)	33(7)	3(5)	8(6)	1(6)
C(28)	56(11)	20(7)	50(9)	−3(6)	3(8)	0(7)
C(29)	52(10)	21(7)	44(8)	5(6)	9(7)	−8(7)
C(30)	21(6)	13(5)	32(6)	−1(4)	3(5)	2(4)
C(31)	26(7)	17(5)	25(6)	−3(5)	4(5)	−1(5)
C(32)	16(6)	20(5)	25(6)	−4(4)	0(5)	5(4)
C(33)	38(9)	22(6)	43(9)	−6(6)	9(7)	−8(6)
C(34)	57(10)	18(6)	30(7)	−3(5)	15(7)	5(6)
C(35)	34(6)	17(6)	33(6)	−10(4)	11(5)	−5(5)
C(36)	34(6)	24(6)	39(7)	−10(5)	8(5)	−2(5)
C(37)	29(7)	33(8)	57(9)	−4(6)	14(6)	6(6)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(38)	42(8)	52(10)	58(10)	1(7)	24(7)	−1(7)
C(39)	47(7)	33(8)	49(9)	1(6)	21(7)	−5(6)
C(40)	41(7)	18(6)	36(7)	−5(5)	15(5)	−2(5)
C(41)	44(8)	25(7)	43(7)	−5(6)	8(6)	1(6)
C(42)	57(11)	37(9)	54(10)	−3(7)	−7(8)	−6(8)
C(43)	40(9)	25(7)	64(11)	3(6)	17(8)	4(6)
C(44)	44(8)	21(6)	40(7)	3(5)	17(6)	−1(6)
C(45)	62(12)	21(7)	71(12)	8(7)	17(10)	2(7)
C(46)	62(12)	58(11)	41(8)	0(8)	20(8)	−1(9)
C(47)	53(7)	5(5)	31(7)	−7(4)	13(6)	−3(5)
C(48)	58(7)	16(6)	21(6)	−5(5)	9(6)	3(5)
C(49)	67(8)	14(6)	29(7)	−1(5)	11(7)	4(6)
C(50)	69(9)	13(6)	29(7)	−2(5)	15(7)	−6(6)
C(51)	61(9)	21(6)	31(7)	2(5)	21(7)	−5(6)
C(52)	46(7)	18(6)	28(7)	−2(5)	8(6)	−3(5)
C(53)	56(8)	20(6)	27(7)	−1(5)	7(6)	7(6)
C(54)	44(9)	32(8)	39(8)	−3(6)	−3(7)	9(7)
C(55)	60(11)	24(7)	39(8)	1(6)	7(8)	9(7)
C(56)	35(7)	26(7)	37(7)	3(5)	12(6)	−4(5)
C(57)	58(11)	42(9)	54(9)	−2(8)	19(8)	10(9)
C(58)	44(9)	42(10)	52(9)	1(7)	3(7)	−6(7)
C(59)	49(9)	19(7)	23(6)	7(5)	−1(6)	−10(6)
C(60)	67(11)	12(6)	30(7)	−4(5)	7(7)	−2(6)
C(61)	56(10)	15(6)	34(8)	0(5)	8(7)	7(6)
C(62)	23(7)	30(8)	50(8)	−6(6)	13(6)	−3(6)
C(63)	36(8)	31(8)	48(9)	3(7)	14(7)	3(6)
C(64)	44(9)	16(6)	33(7)	−2(5)	11(6)	5(6)
C(65)	43(9)	20(7)	29(7)	8(5)	6(6)	7(6)
C(66)	41(8)	34(8)	34(7)	1(6)	9(6)	−4(7)
C(67)	51(11)	48(10)	42(9)	−15(7)	11(8)	−12(8)
C(68)	45(10)	43(9)	59(11)	22(8)	17(9)	11(8)

Table 4: Bond lengths [Å] for mw_071m.

Sb(1)–N(8)	2.040(11)
Sb(1)–N(7)	2.058(10)
Sb(1)–Sb(2)	2.8463(14)
Sb(2)–N(8)	2.116(11)
Sb(2)–Ga(1)	2.6934(17)
Ga(1)–N(5)	1.863(11)
Ga(1)–N(1)	2.006(13)
Ga(1)–N(2)	2.030(12)
Ga(2)–N(6)	1.878(11)
Ga(2)–N(7)	1.911(11)
Ga(2)–N(3)	1.961(12)
Ga(2)–N(4)	2.008(11)
Si(1)–N(7)	1.751(11)
Si(1)–C(65)	1.875(14)
Si(1)–C(64)	1.887(15)
Si(1)–C(63)	1.888(16)
Si(2)–N(8)	1.725(13)
Si(2)–C(67)	1.873(17)
Si(2)–C(66)	1.881(15)
Si(2)–C(68)	1.886(18)
N(1)–C(1)	1.348(18)
N(1)–C(6)	1.44(2)
N(2)–C(3)	1.351(19)
N(2)–C(18)	1.45(2)
N(3)–C(30)	1.357(17)
N(3)–C(35)	1.447(19)
N(4)–C(32)	1.341(17)
N(4)–C(47)	1.474(17)
N(5)–C(59)	1.438(18)
N(5)–C(60)	1.452(17)
N(6)–C(61)	1.446(18)
N(6)–C(62)	1.45(2)
C(1)–C(2)	1.40(2)
C(1)–C(4)	1.51(2)
C(2)–C(3)	1.39(2)
C(3)–C(5)	1.51(2)
C(6)–C(11)	1.40(2)
C(6)–C(7)	1.41(2)
C(7)–C(8)	1.39(2)
C(7)–C(12)	1.55(2)
C(8)–C(9)	1.39(3)
C(9)–C(10)	1.38(2)
C(10)–C(11)	1.38(2)
C(11)–C(15)	1.54(2)
C(12)–C(13)	1.52(2)
C(12)–C(14)	1.55(2)
C(15)–C(16)	1.52(2)
C(15)–C(17)	1.53(2)
C(18)–C(19)	1.41(2)
C(18)–C(23)	1.42(2)
C(19)–C(20)	1.38(2)
C(19)–C(24)	1.52(2)
C(20)–C(21)	1.38(3)

Table 4: (continued)

C(21)–C(22)	1.39(2)
C(22)–C(23)	1.40(2)
C(23)–C(27)	1.54(2)
C(24)–C(26)	1.54(2)
C(24)–C(25)	1.54(2)
C(27)–C(29)	1.53(2)
C(27)–C(28)	1.54(2)
C(30)–C(31)	1.395(19)
C(30)–C(33)	1.513(19)
C(31)–C(32)	1.391(19)
C(32)–C(34)	1.52(2)
C(35)–C(40)	1.41(2)
C(35)–C(36)	1.42(2)
C(36)–C(37)	1.38(2)
C(36)–C(41)	1.52(2)
C(37)–C(38)	1.39(3)
C(38)–C(39)	1.38(3)
C(39)–C(40)	1.38(2)
C(40)–C(44)	1.54(2)
C(41)–C(42)	1.50(2)
C(41)–C(43)	1.54(2)
C(44)–C(46)	1.52(2)
C(44)–C(45)	1.52(2)
C(47)–C(52)	1.37(2)
C(47)–C(48)	1.42(2)
C(48)–C(49)	1.42(2)
C(48)–C(53)	1.46(3)
C(49)–C(50)	1.34(3)
C(50)–C(51)	1.39(2)
C(51)–C(52)	1.41(2)
C(52)–C(56)	1.52(2)
C(53)–C(55)	1.55(2)
C(53)–C(54)	1.56(2)
C(56)–C(58)	1.51(2)
C(56)–C(57)	1.53(2)

Table 5: Bond angles [°] for mw_071m.

N(8)–Sb(1)–N(7)	103.8(4)
N(8)–Sb(1)–Sb(2)	47.9(3)
N(7)–Sb(1)–Sb(2)	107.5(3)
N(8)–Sb(2)–Ga(1)	109.2(3)
N(8)–Sb(2)–Sb(1)	45.7(3)
Ga(1)–Sb(2)–Sb(1)	107.50(5)
N(5)–Ga(1)–N(1)	107.5(5)
N(5)–Ga(1)–N(2)	104.6(5)
N(1)–Ga(1)–N(2)	91.9(5)
N(5)–Ga(1)–Sb(2)	120.6(3)
N(1)–Ga(1)–Sb(2)	106.8(3)
N(2)–Ga(1)–Sb(2)	121.0(3)
N(6)–Ga(2)–N(7)	104.7(5)
N(6)–Ga(2)–N(3)	112.2(5)
N(7)–Ga(2)–N(3)	114.9(5)
N(6)–Ga(2)–N(4)	114.2(5)
N(7)–Ga(2)–N(4)	115.4(5)
N(3)–Ga(2)–N(4)	95.7(5)
N(7)–Si(1)–C(65)	114.5(6)
N(7)–Si(1)–C(64)	112.1(6)
C(65)–Si(1)–C(64)	106.5(7)
N(7)–Si(1)–C(63)	113.6(7)
C(65)–Si(1)–C(63)	104.6(8)
C(64)–Si(1)–C(63)	104.7(7)
N(8)–Si(2)–C(67)	112.7(7)
N(8)–Si(2)–C(66)	110.6(6)
C(67)–Si(2)–C(66)	104.5(8)
N(8)–Si(2)–C(68)	108.2(7)
C(67)–Si(2)–C(68)	109.2(10)
C(66)–Si(2)–C(68)	111.6(8)
C(1)–N(1)–C(6)	119.7(13)
C(1)–N(1)–Ga(1)	122.5(11)
C(6)–N(1)–Ga(1)	117.7(8)
C(3)–N(2)–C(18)	118.0(12)
C(3)–N(2)–Ga(1)	122.1(11)
C(18)–N(2)–Ga(1)	119.8(9)
C(30)–N(3)–C(35)	115.4(11)
C(30)–N(3)–Ga(2)	120.2(9)
C(35)–N(3)–Ga(2)	123.7(9)
C(32)–N(4)–C(47)	117.2(11)
C(32)–N(4)–Ga(2)	118.5(9)
C(47)–N(4)–Ga(2)	124.2(8)
C(59)–N(5)–C(60)	112.8(11)
C(59)–N(5)–Ga(1)	124.1(9)
C(60)–N(5)–Ga(1)	122.9(9)
C(61)–N(6)–C(62)	110.7(11)
C(61)–N(6)–Ga(2)	127.4(10)
C(62)–N(6)–Ga(2)	121.8(9)
Si(1)–N(7)–Ga(2)	128.4(6)
Si(1)–N(7)–Sb(1)	125.5(6)
Ga(2)–N(7)–Sb(1)	106.1(5)
Si(2)–N(8)–Sb(1)	140.8(6)
Si(2)–N(8)–Sb(2)	127.4(6)

Table 5: (continued)

Sb(1)–N(8)–Sb(2)	86.4(4)
N(1)–C(1)–C(2)	123.2(15)
N(1)–C(1)–C(4)	119.7(15)
C(2)–C(1)–C(4)	117.0(13)
C(3)–C(2)–C(1)	128.7(14)
N(2)–C(3)–C(2)	123.8(14)
N(2)–C(3)–C(5)	121.1(15)
C(2)–C(3)–C(5)	115.1(13)
C(11)–C(6)–C(7)	120.5(14)
C(11)–C(6)–N(1)	121.4(12)
C(7)–C(6)–N(1)	118.1(13)
C(8)–C(7)–C(6)	118.6(15)
C(8)–C(7)–C(12)	121.2(14)
C(6)–C(7)–C(12)	120.2(14)
C(9)–C(8)–C(7)	120.7(15)
C(10)–C(9)–C(8)	119.6(17)
C(9)–C(10)–C(11)	121.7(17)
C(10)–C(11)–C(6)	118.9(14)
C(10)–C(11)–C(15)	118.8(14)
C(6)–C(11)–C(15)	122.2(14)
C(13)–C(12)–C(14)	108.9(12)
C(13)–C(12)–C(7)	113.8(14)
C(14)–C(12)–C(7)	109.8(14)
C(16)–C(15)–C(17)	111.8(14)
C(16)–C(15)–C(11)	112.1(13)
C(17)–C(15)–C(11)	110.0(14)
C(19)–C(18)–C(23)	121.3(15)
C(19)–C(18)–N(2)	118.5(13)
C(23)–C(18)–N(2)	120.1(13)
C(20)–C(19)–C(18)	117.9(15)
C(20)–C(19)–C(24)	121.7(14)
C(18)–C(19)–C(24)	120.4(14)
C(19)–C(20)–C(21)	122.8(15)
C(20)–C(21)–C(22)	119.0(17)
C(21)–C(22)–C(23)	121.3(16)
C(22)–C(23)–C(18)	117.6(14)
C(22)–C(23)–C(27)	119.1(14)
C(18)–C(23)–C(27)	123.3(14)
C(19)–C(24)–C(26)	114.5(14)
C(19)–C(24)–C(25)	111.3(13)
C(26)–C(24)–C(25)	108.3(13)
C(29)–C(27)–C(23)	110.6(13)
C(29)–C(27)–C(28)	108.9(13)
C(23)–C(27)–C(28)	110.8(13)
N(3)–C(30)–C(31)	123.4(12)
N(3)–C(30)–C(33)	119.1(12)
C(31)–C(30)–C(33)	117.5(12)
C(32)–C(31)–C(30)	128.5(12)
N(4)–C(32)–C(31)	125.1(12)
N(4)–C(32)–C(34)	119.4(12)
C(31)–C(32)–C(34)	115.5(12)
C(40)–C(35)–C(36)	119.9(13)
C(40)–C(35)–N(3)	121.9(13)

Table 5: (continued)

C(36)–C(35)–N(3)	118.0(13)
C(37)–C(36)–C(35)	119.1(15)
C(37)–C(36)–C(41)	117.9(14)
C(35)–C(36)–C(41)	123.0(14)
C(36)–C(37)–C(38)	120.6(15)
C(39)–C(38)–C(37)	120.2(16)
C(38)–C(39)–C(40)	121.0(17)
C(39)–C(40)–C(35)	119.0(15)
C(39)–C(40)–C(44)	119.2(14)
C(35)–C(40)–C(44)	121.8(13)
C(42)–C(41)–C(36)	113.0(14)
C(42)–C(41)–C(43)	111.1(15)
C(36)–C(41)–C(43)	109.6(13)
C(46)–C(44)–C(45)	108.8(15)
C(46)–C(44)–C(40)	111.5(14)
C(45)–C(44)–C(40)	111.1(14)
C(52)–C(47)–C(48)	123.9(13)
C(52)–C(47)–N(4)	118.7(13)
C(48)–C(47)–N(4)	117.3(14)
C(47)–C(48)–C(49)	114.7(15)
C(47)–C(48)–C(53)	124.4(14)
C(49)–C(48)–C(53)	120.9(14)
C(50)–C(49)–C(48)	122.9(15)
C(49)–C(50)–C(51)	120.5(14)
C(50)–C(51)–C(52)	120.0(16)
C(47)–C(52)–C(51)	117.9(14)
C(47)–C(52)–C(56)	124.2(13)
C(51)–C(52)–C(56)	117.9(14)
C(48)–C(53)–C(55)	114.6(14)
C(48)–C(53)–C(54)	113.8(13)
C(55)–C(53)–C(54)	108.4(13)
C(58)–C(56)–C(52)	110.0(13)
C(58)–C(56)–C(57)	110.3(15)
C(52)–C(56)–C(57)	112.2(13)

Crystal structure of mw_124_1m_sq

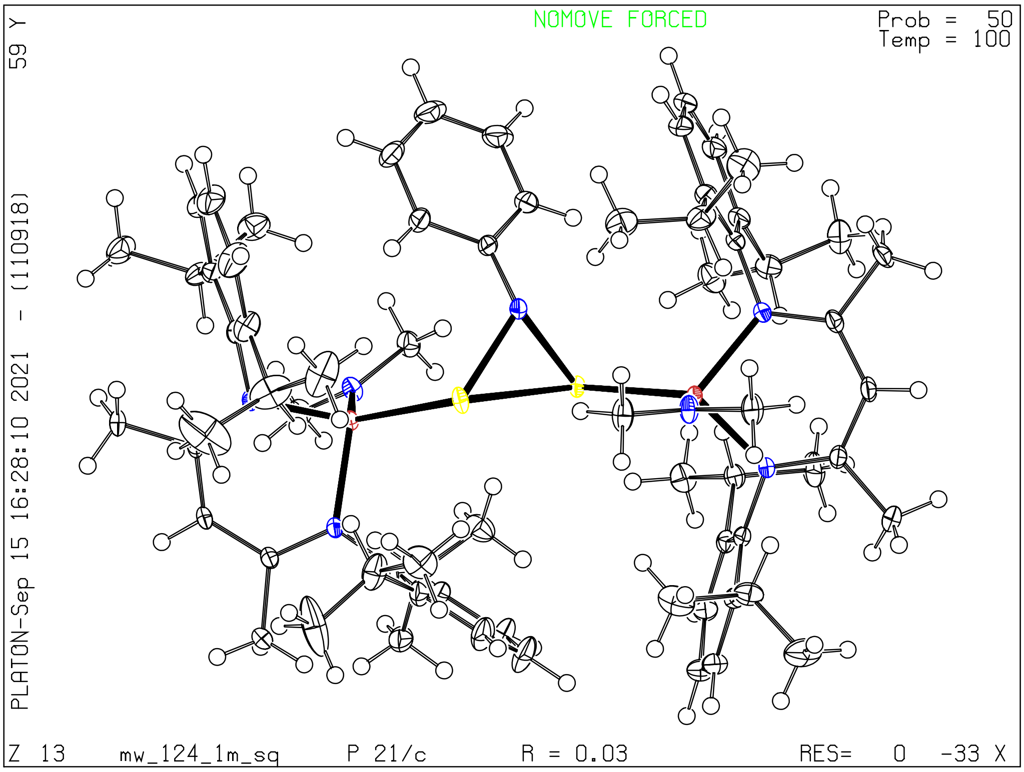

Table 1: Crystal data and structure refinement for mw_124_1m_sq.

Identification code	mw_124_1m_sq
Empirical Formula	$C_{71.50}\,H_{103}\,Ga_2\,N_7\,Sb_2$
Formula weight	1443.54 Da
Density (calculated)	$1.372\,g \cdot cm^{-3}$
$F(000)$	2980
Temperature	100(2) K
Crystal size	$0.276 \times 0.203 \times 0.134$ mm
Crystal appearance	dark red tablet
Wavelength (MoK_{α})	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 19.9634(10)$ Å
	$b = 12.5667(7)$ Å
	$c = 29.4717(15)$ Å
	$\alpha = 90°$
	$\beta = 109.0277(16)°$
	$\gamma = 90°$
Unit cell volume	$6989.7(6)$ Å^3
Z	4
Cell measurement refections used	9867
θ range for cell measurement	2.18° to 36.28°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.947° to 36.384°
Completeness to $\theta = 25.242°$ (to θ_{max})	100.0% (99.8%)
Index ranges	$-33 \leq h \leq 33$
	$-20 \leq k \leq 20$
	$-49 \leq l \leq 49$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.572\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.67
R_{merg} before/after correction	0.0578/0.0472
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	369240
Independent reflections	33974 ($R_{int} = 0.0450$)
Reflections with $I > 2\sigma(I)$	27533
Data / retraints / parameter	33974 / 0 / 736
Goodness-of-fit on F^2	1.084
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0260P)^2 + 4.6571P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0283$
	$wR2 = 0.0630$
R indices [all data]	$R1 = 0.0431$
	$wR2 = 0.0687$
Largest diff. peak and hole	1.133 and -0.634 Å^{-3}

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

SQUEEZE

The structure contains a toluene molecule highly disordered over a centre of inversion. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run. (For details see: A. L. Spek, *Acta Cryst. A46* **(1990)**, 194–201). The molecule was included in the sum formula for completeness.

Table 2: Atom coordinates ($\times10^4$) and equivalent isotropic displacement parameters ($\times10^3$) for mw_124_1m_sq. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	2118(1)	4417(1)	8168(1)	12(1)
Sb(2)	2811(1)	5086(1)	9106(1)	16(1)
Ga(1)	3144(1)	4180(1)	7789(1)	10(1)
Ga(2)	1783(1)	4869(1)	9488(1)	11(1)
N(1)	3090(1)	2764(1)	7466(1)	13(1)
N(2)	2927(1)	4954(1)	7168(1)	14(1)
N(3)	2055(1)	3517(1)	9857(1)	14(1)
N(4)	1890(1)	5690(1)	10090(1)	13(1)
N(5)	4090(1)	4419(1)	8136(1)	17(1)
N(6)	827(1)	4894(1)	9133(1)	16(1)
N(7)	2398(1)	5946(1)	8470(1)	15(1)
C(1)	3284(1)	2661(1)	7076(1)	16(1)
C(2)	3372(1)	3529(1)	6800(1)	18(1)
C(3)	3155(1)	4581(1)	6820(1)	16(1)
C(4)	3420(1)	1570(1)	6905(1)	24(1)
C(5)	3175(1)	5312(1)	6416(1)	23(1)
C(6)	2929(1)	1816(1)	7688(1)	14(1)
C(7)	3478(1)	1209(1)	8004(1)	17(1)
C(8)	3297(1)	271(1)	8189(1)	21(1)
C(9)	2599(1)	−56(1)	8076(1)	23(1)
C(10)	2063(1)	564(1)	7774(1)	20(1)
C(11)	2213(1)	1507(1)	7576(1)	16(1)
C(12)	4249(1)	1537(1)	8151(1)	22(1)
C(13)	4725(1)	639(2)	8074(1)	38(1)
C(14)	4502(1)	1898(2)	8675(1)	34(1)
C(15)	1618(1)	2147(1)	7227(1)	18(1)
C(16)	1521(1)	1822(2)	6709(1)	29(1)
C(17)	912(1)	2063(1)	7324(1)	24(1)
C(18)	2544(1)	5949(1)	7087(1)	17(1)
C(19)	2885(1)	6899(1)	7287(1)	21(1)
C(20)	2489(1)	7842(1)	7196(1)	26(1)
C(21)	1784(1)	7845(1)	6914(1)	28(1)
C(22)	1457(1)	6906(1)	6720(1)	25(1)
C(23)	1821(1)	5939(1)	6805(1)	20(1)
C(24)	3660(1)	6936(1)	7594(1)	26(1)
C(25)	4091(1)	7671(2)	7378(1)	40(1)
C(26)	3740(1)	7283(1)	8106(1)	32(1)
C(27)	1428(1)	4923(1)	6595(1)	22(1)
C(28)	1196(1)	4917(2)	6044(1)	30(1)
C(29)	784(1)	4753(2)	6760(1)	28(1)
C(30)	1907(1)	3331(1)	10259(1)	15(1)
C(31)	1722(1)	4138(1)	10523(1)	17(1)
C(32)	1777(1)	5239(1)	10468(1)	15(1)
C(33)	1934(1)	2212(1)	10453(1)	22(1)
C(34)	1707(1)	5922(1)	10873(1)	22(1)
C(35)	2367(1)	2697(1)	9649(1)	16(1)
C(36)	1930(1)	2017(1)	9298(1)	18(1)
C(37)	2254(1)	1262(1)	9089(1)	28(1)
C(38)	2982(1)	1186(2)	9224(1)	36(1)
C(39)	3406(1)	1866(2)	9566(1)	30(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(40)	3113(1)	2636(1)	9785(1)	21(1)
C(41)	1128(1)	2066(1)	9143(1)	19(1)
C(42)	818(1)	1047(1)	9280(1)	25(1)
C(43)	804(1)	2264(1)	8604(1)	27(1)
C(44)	3596(1)	3367(2)	10165(1)	30(1)
C(45)	3739(1)	2934(3)	10668(1)	62(1)
C(46)	4304(1)	3598(2)	10089(1)	34(1)
C(47)	2034(1)	6816(1)	10101(1)	15(1)
C(48)	1480(1)	7561(1)	9968(1)	17(1)
C(49)	1653(1)	8639(1)	9977(1)	24(1)
C(50)	2350(1)	8974(1)	10112(1)	30(1)
C(51)	2889(1)	8232(1)	10246(1)	32(1)
C(52)	2749(1)	7148(1)	10241(1)	24(1)
C(53)	706(1)	7242(1)	9818(1)	21(1)
C(54)	315(1)	7790(1)	10125(1)	30(1)
C(55)	334(1)	7495(1)	9289(1)	30(1)
C(56)	3353(1)	6352(2)	10399(1)	39(1)
C(57)	3582(1)	6175(3)	10936(1)	64(1)
C(58)	3989(1)	6644(2)	10251(1)	44(1)
C(59)	4646(1)	4359(1)	7923(1)	24(1)
C(60)	4362(1)	4778(1)	8626(1)	24(1)
C(61)	283(1)	4572(1)	9328(1)	21(1)
C(62)	540(1)	5149(1)	8627(1)	21(1)
C(63)	1931(1)	6804(1)	8400(1)	18(1)
C(64)	1961(1)	7510(1)	8775(1)	26(1)
C(65)	1524(1)	8402(1)	8693(1)	36(1)
C(66)	1051(1)	8615(1)	8244(1)	36(1)
C(67)	1015(1)	7923(1)	7869(1)	31(1)
C(68)	1450(1)	7031(1)	7944(1)	23(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_124_1m_sq.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	13(1)	15(1)	12(1)	−2(1)	6(1)	−1(1)
Sb(2)	13(1)	26(1)	10(1)	0(1)	5(1)	0(1)
Ga(1)	11(1)	12(1)	9(1)	−1(1)	5(1)	0(1)
Ga(2)	11(1)	14(1)	8(1)	0(1)	4(1)	1(1)
N(1)	16(1)	14(1)	10(1)	−1(1)	6(1)	1(1)
N(2)	17(1)	15(1)	13(1)	2(1)	7(1)	1(1)
N(3)	16(1)	16(1)	11(1)	1(1)	7(1)	3(1)
N(4)	15(1)	16(1)	10(1)	−1(1)	5(1)	1(1)
N(5)	12(1)	26(1)	14(1)	−4(1)	5(1)	−2(1)
N(6)	13(1)	23(1)	13(1)	2(1)	4(1)	0(1)
N(7)	22(1)	14(1)	13(1)	−1(1)	9(1)	0(1)
C(1)	18(1)	18(1)	13(1)	−2(1)	7(1)	2(1)
C(2)	21(1)	23(1)	13(1)	−1(1)	10(1)	2(1)
C(3)	16(1)	21(1)	13(1)	2(1)	8(1)	1(1)
C(4)	35(1)	21(1)	21(1)	−4(1)	15(1)	4(1)
C(5)	27(1)	29(1)	18(1)	8(1)	14(1)	3(1)
C(6)	18(1)	13(1)	12(1)	−2(1)	6(1)	0(1)
C(7)	18(1)	15(1)	18(1)	−1(1)	6(1)	1(1)
C(8)	25(1)	16(1)	22(1)	2(1)	7(1)	2(1)
C(9)	28(1)	15(1)	26(1)	2(1)	10(1)	−2(1)
C(10)	22(1)	17(1)	22(1)	−1(1)	8(1)	−4(1)
C(11)	17(1)	16(1)	14(1)	−4(1)	6(1)	−2(1)
C(12)	17(1)	22(1)	26(1)	5(1)	4(1)	1(1)
C(13)	26(1)	34(1)	59(1)	12(1)	20(1)	11(1)
C(14)	30(1)	35(1)	28(1)	4(1)	−5(1)	−7(1)
C(15)	17(1)	21(1)	14(1)	−2(1)	4(1)	−2(1)
C(16)	26(1)	44(1)	14(1)	−6(1)	3(1)	0(1)
C(17)	17(1)	31(1)	25(1)	0(1)	7(1)	−1(1)
C(18)	22(1)	15(1)	15(1)	4(1)	10(1)	3(1)
C(19)	27(1)	16(1)	24(1)	3(1)	16(1)	0(1)
C(20)	40(1)	16(1)	30(1)	6(1)	21(1)	4(1)
C(21)	43(1)	21(1)	25(1)	10(1)	20(1)	14(1)
C(22)	30(1)	27(1)	20(1)	9(1)	10(1)	13(1)
C(23)	24(1)	21(1)	16(1)	6(1)	8(1)	7(1)
C(24)	25(1)	17(1)	38(1)	−1(1)	15(1)	−5(1)
C(25)	42(1)	32(1)	55(1)	−4(1)	30(1)	−15(1)
C(26)	31(1)	27(1)	36(1)	−2(1)	10(1)	−4(1)
C(27)	19(1)	26(1)	19(1)	3(1)	2(1)	6(1)
C(28)	25(1)	43(1)	22(1)	−4(1)	8(1)	4(1)
C(29)	24(1)	36(1)	21(1)	5(1)	5(1)	1(1)
C(30)	18(1)	18(1)	12(1)	2(1)	7(1)	2(1)
C(31)	23(1)	20(1)	12(1)	2(1)	10(1)	2(1)
C(32)	17(1)	20(1)	10(1)	−1(1)	6(1)	2(1)
C(33)	32(1)	19(1)	18(1)	5(1)	13(1)	4(1)
C(34)	32(1)	24(1)	14(1)	−3(1)	13(1)	3(1)
C(35)	19(1)	17(1)	13(1)	2(1)	9(1)	4(1)
C(36)	23(1)	16(1)	19(1)	−1(1)	11(1)	2(1)
C(37)	31(1)	26(1)	29(1)	−11(1)	13(1)	2(1)
C(38)	35(1)	40(1)	37(1)	−14(1)	18(1)	11(1)
C(39)	24(1)	40(1)	28(1)	−6(1)	11(1)	11(1)
C(40)	20(1)	28(1)	16(1)	0(1)	8(1)	6(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(41)	22(1)	14(1)	22(1)	−2(1)	10(1)	−2(1)
C(42)	35(1)	18(1)	28(1)	−3(1)	18(1)	−4(1)
C(43)	28(1)	27(1)	24(1)	3(1)	6(1)	−7(1)
C(44)	17(1)	45(1)	27(1)	−11(1)	5(1)	5(1)
C(45)	32(1)	135(3)	19(1)	−9(1)	8(1)	−17(1)
C(46)	21(1)	44(1)	35(1)	5(1)	5(1)	2(1)
C(47)	16(1)	17(1)	13(1)	−4(1)	5(1)	−1(1)
C(48)	20(1)	17(1)	17(1)	−3(1)	8(1)	−1(1)
C(49)	32(1)	16(1)	28(1)	−2(1)	14(1)	−1(1)
C(50)	37(1)	20(1)	38(1)	−10(1)	18(1)	−11(1)
C(51)	26(1)	29(1)	43(1)	−16(1)	12(1)	−12(1)
C(52)	18(1)	25(1)	26(1)	−10(1)	4(1)	−5(1)
C(53)	17(1)	17(1)	29(1)	−1(1)	8(1)	2(1)
C(54)	29(1)	24(1)	44(1)	−1(1)	22(1)	4(1)
C(55)	25(1)	28(1)	31(1)	0(1)	1(1)	6(1)
C(56)	16(1)	34(1)	55(1)	−8(1)	−3(1)	−2(1)
C(57)	21(1)	98(2)	65(2)	37(2)	2(1)	0(1)
C(58)	19(1)	62(1)	45(1)	−25(1)	2(1)	0(1)
C(59)	15(1)	36(1)	22(1)	−4(1)	10(1)	−2(1)
C(60)	15(1)	40(1)	18(1)	−10(1)	4(1)	−3(1)
C(61)	16(1)	24(1)	23(1)	0(1)	8(1)	−2(1)
C(62)	18(1)	27(1)	14(1)	1(1)	2(1)	3(1)
C(63)	25(1)	13(1)	22(1)	1(1)	16(1)	0(1)
C(64)	42(1)	16(1)	29(1)	−2(1)	23(1)	−1(1)
C(65)	57(1)	16(1)	50(1)	−2(1)	40(1)	4(1)
C(66)	45(1)	19(1)	61(1)	10(1)	39(1)	11(1)
C(67)	31(1)	26(1)	42(1)	14(1)	21(1)	11(1)
C(68)	29(1)	21(1)	25(1)	6(1)	15(1)	7(1)

Table 4: Bond lengths [Å] for mw_124_1m_sq.

Sb(1)–N(7)	2.1141(11)
Sb(1)–Ga(1)	2.65203(18)
Sb(1)–Sb(2)	2.78824(16)
Sb(2)–N(7)	2.0874(11)
Sb(2)–Ga(2)	2.65640(18)
Ga(1)–N(5)	1.8558(11)
Ga(1)–N(2)	1.9904(11)
Ga(1)–N(1)	2.0041(11)
Ga(2)–N(6)	1.8534(11)
Ga(2)–N(3)	1.9946(11)
Ga(2)–N(4)	2.0028(10)
N(1)–C(1)	1.3333(15)
N(1)–C(6)	1.4445(16)
N(2)–C(3)	1.3377(16)
N(2)–C(18)	1.4439(17)
N(3)–C(30)	1.3322(16)
N(3)–C(35)	1.4397(16)
N(4)–C(32)	1.3329(16)
N(4)–C(47)	1.4422(17)
N(5)–C(60)	1.4412(18)
N(5)–C(59)	1.4421(17)
N(6)–C(61)	1.4442(17)
N(6)–C(62)	1.4472(17)
N(7)–C(63)	1.3952(17)
C(1)–C(2)	1.4057(19)
C(1)–C(4)	1.5159(19)
C(2)–C(3)	1.3982(19)
C(3)–C(5)	1.5155(18)
C(6)–C(7)	1.4089(18)
C(6)–C(11)	1.4118(18)
C(7)–C(8)	1.394(2)
C(7)–C(12)	1.516(2)
C(8)–C(9)	1.386(2)
C(9)–C(10)	1.387(2)
C(10)–C(11)	1.3962(19)
C(11)–C(15)	1.5217(19)
C(12)–C(14)	1.530(2)
C(12)–C(13)	1.538(2)
C(15)–C(17)	1.531(2)
C(15)–C(16)	1.531(2)
C(18)–C(19)	1.405(2)
C(18)–C(23)	1.411(2)
C(19)–C(20)	1.401(2)
C(19)–C(24)	1.517(2)
C(20)–C(21)	1.381(3)
C(21)–C(22)	1.380(3)
C(22)–C(23)	1.397(2)
C(23)–C(27)	1.521(2)
C(24)–C(26)	1.527(3)
C(24)–C(25)	1.536(2)
C(27)–C(29)	1.530(2)
C(27)–C(28)	1.536(2)
C(30)–C(31)	1.4001(18)

Table 4: (continued)

C(30)–C(33)	1.5132(19)
C(31)–C(32)	1.4007(19)
C(32)–C(34)	1.5132(18)
C(35)–C(36)	1.4047(19)
C(35)–C(40)	1.4118(19)
C(36)–C(37)	1.400(2)
C(36)–C(41)	1.516(2)
C(37)–C(38)	1.379(2)
C(38)–C(39)	1.379(3)
C(39)–C(40)	1.394(2)
C(40)–C(44)	1.524(2)
C(41)–C(43)	1.526(2)
C(41)–C(42)	1.533(2)
C(44)–C(45)	1.515(3)
C(44)–C(46)	1.529(2)
C(47)–C(48)	1.4033(19)
C(47)–C(52)	1.4127(19)
C(48)–C(49)	1.397(2)
C(48)–C(53)	1.516(2)
C(49)–C(50)	1.383(2)
C(50)–C(51)	1.381(3)
C(51)–C(52)	1.390(2)
C(52)–C(56)	1.519(2)
C(53)–C(55)	1.526(2)
C(53)–C(54)	1.536(2)
C(56)–C(58)	1.515(3)
C(56)–C(57)	1.515(3)
C(63)–C(68)	1.402(2)
C(63)–C(64)	1.405(2)
C(64)–C(65)	1.392(2)
C(65)–C(66)	1.381(3)
C(66)–C(67)	1.388(3)
C(67)–C(68)	1.392(2)

Table 5: Bond angles [°] for mw_124_1m_sq.

N(7)–Sb(1)–Ga(1)	98.30(3)
N(7)–Sb(1)–Sb(2)	48.01(3)
Ga(1)–Sb(1)–Sb(2)	104.460(6)
N(7)–Sb(2)–Ga(2)	107.45(3)
N(7)–Sb(2)–Sb(1)	48.84(3)
Ga(2)–Sb(2)–Sb(1)	100.733(6)
N(5)–Ga(1)–N(2)	107.77(5)
N(5)–Ga(1)–N(1)	107.02(5)
N(2)–Ga(1)–N(1)	92.06(4)
N(5)–Ga(1)–Sb(1)	122.52(3)
N(2)–Ga(1)–Sb(1)	111.44(3)
N(1)–Ga(1)–Sb(1)	111.70(3)
N(6)–Ga(2)–N(3)	111.66(5)
N(6)–Ga(2)–N(4)	106.50(5)
N(3)–Ga(2)–N(4)	91.43(4)
N(6)–Ga(2)–Sb(2)	123.68(3)
N(3)–Ga(2)–Sb(2)	101.98(3)
N(4)–Ga(2)–Sb(2)	116.65(3)
C(1)–N(1)–C(6)	118.64(11)
C(1)–N(1)–Ga(1)	120.61(9)
C(6)–N(1)–Ga(1)	120.26(7)
C(3)–N(2)–C(18)	118.09(11)
C(3)–N(2)–Ga(1)	120.49(9)
C(18)–N(2)–Ga(1)	121.38(8)
C(30)–N(3)–C(35)	120.33(11)
C(30)–N(3)–Ga(2)	122.27(9)
C(35)–N(3)–Ga(2)	117.19(8)
C(32)–N(4)–C(47)	119.04(10)
C(32)–N(4)–Ga(2)	121.53(9)
C(47)–N(4)–Ga(2)	119.23(8)
C(60)–N(5)–C(59)	111.14(11)
C(60)–N(5)–Ga(1)	125.83(9)
C(59)–N(5)–Ga(1)	122.78(9)
C(61)–N(6)–C(62)	112.08(11)
C(61)–N(6)–Ga(2)	122.73(9)
C(62)–N(6)–Ga(2)	125.03(9)
C(63)–N(7)–Sb(2)	125.58(8)
C(63)–N(7)–Sb(1)	124.61(9)
Sb(2)–N(7)–Sb(1)	83.15(4)
N(1)–C(1)–C(2)	123.40(12)
N(1)–C(1)–C(4)	120.56(12)
C(2)–C(1)–C(4)	116.04(11)
C(3)–C(2)–C(1)	127.62(11)
N(2)–C(3)–C(2)	123.46(11)
N(2)–C(3)–C(5)	119.60(12)
C(2)–C(3)–C(5)	116.93(11)
C(7)–C(6)–C(11)	121.02(12)
C(7)–C(6)–N(1)	120.39(11)
C(11)–C(6)–N(1)	118.59(11)
C(8)–C(7)–C(6)	118.17(12)
C(8)–C(7)–C(12)	119.11(12)
C(6)–C(7)–C(12)	122.72(12)
C(9)–C(8)–C(7)	121.61(13)

Table 5: (continued)

C(8)–C(9)–C(10)	119.56(13)
C(9)–C(10)–C(11)	121.26(13)
C(10)–C(11)–C(6)	118.33(12)
C(10)–C(11)–C(15)	120.29(12)
C(6)–C(11)–C(15)	121.30(12)
C(7)–C(12)–C(14)	109.80(13)
C(7)–C(12)–C(13)	112.16(14)
C(14)–C(12)–C(13)	110.50(15)
C(11)–C(15)–C(17)	113.63(12)
C(11)–C(15)–C(16)	110.50(12)
C(17)–C(15)–C(16)	109.99(12)
C(19)–C(18)–C(23)	121.17(13)
C(19)–C(18)–N(2)	120.56(12)
C(23)–C(18)–N(2)	118.27(12)
C(20)–C(19)–C(18)	118.19(14)
C(20)–C(19)–C(24)	119.37(14)
C(18)–C(19)–C(24)	122.45(13)
C(21)–C(20)–C(19)	121.20(15)
C(22)–C(21)–C(20)	119.93(14)
C(21)–C(22)–C(23)	121.44(15)
C(22)–C(23)–C(18)	118.05(14)
C(22)–C(23)–C(27)	119.20(14)
C(18)–C(23)–C(27)	122.75(12)
C(19)–C(24)–C(26)	110.79(13)
C(19)–C(24)–C(25)	111.84(15)
C(26)–C(24)–C(25)	110.27(14)
C(23)–C(27)–C(29)	111.28(13)
C(23)–C(27)–C(28)	111.86(13)
C(29)–C(27)–C(28)	109.93(13)
N(3)–C(30)–C(31)	122.91(12)
N(3)–C(30)–C(33)	120.57(11)
C(31)–C(30)–C(33)	116.51(11)
C(30)–C(31)–C(32)	127.30(12)
N(4)–C(32)–C(31)	123.93(11)
N(4)–C(32)–C(34)	120.14(12)
C(31)–C(32)–C(34)	115.93(11)
C(36)–C(35)–C(40)	121.34(12)
C(36)–C(35)–N(3)	119.83(11)
C(40)–C(35)–N(3)	118.73(12)
C(37)–C(36)–C(35)	118.14(13)
C(37)–C(36)–C(41)	119.28(13)
C(35)–C(36)–C(41)	122.58(11)
C(38)–C(37)–C(36)	120.95(15)
C(39)–C(38)–C(37)	120.36(15)
C(38)–C(39)–C(40)	121.23(15)
C(39)–C(40)–C(35)	117.96(14)
C(39)–C(40)–C(44)	119.91(14)
C(35)–C(40)–C(44)	122.12(12)
C(36)–C(41)–C(43)	111.58(12)
C(36)–C(41)–C(42)	111.36(12)
C(43)–C(41)–C(42)	109.84(12)
C(45)–C(44)–C(40)	112.01(18)
C(45)–C(44)–C(46)	108.84(15)

Table 5: (continued)

C(40)–C(44)–C(46)	113.60(14)
C(48)–C(47)–C(52)	120.91(13)
C(48)–C(47)–N(4)	120.94(12)
C(52)–C(47)–N(4)	118.14(12)
C(49)–C(48)–C(47)	118.31(13)
C(49)–C(48)–C(53)	118.94(13)
C(47)–C(48)–C(53)	122.75(12)
C(50)–C(49)–C(48)	121.35(15)
C(51)–C(50)–C(49)	119.60(15)
C(50)–C(51)–C(52)	121.55(15)
C(51)–C(52)–C(47)	118.27(15)
C(51)–C(52)–C(56)	120.30(15)
C(47)–C(52)–C(56)	121.41(14)
C(48)–C(53)–C(55)	110.68(13)
C(48)–C(53)–C(54)	111.99(13)
C(55)–C(53)–C(54)	109.65(13)
C(58)–C(56)–C(57)	109.96(16)
C(58)–C(56)–C(52)	114.15(18)
C(57)–C(56)–C(52)	110.74(19)
N(7)–C(63)–C(68)	120.97(12)
N(7)–C(63)–C(64)	121.15(14)
C(68)–C(63)–C(64)	117.74(14)
C(65)–C(64)–C(63)	120.61(17)
C(66)–C(65)–C(64)	121.15(16)
C(65)–C(66)–C(67)	118.86(15)
C(66)–C(67)–C(68)	120.75(18)
C(67)–C(68)–C(63)	120.89(15)

Crystal structure of mw_125_5m

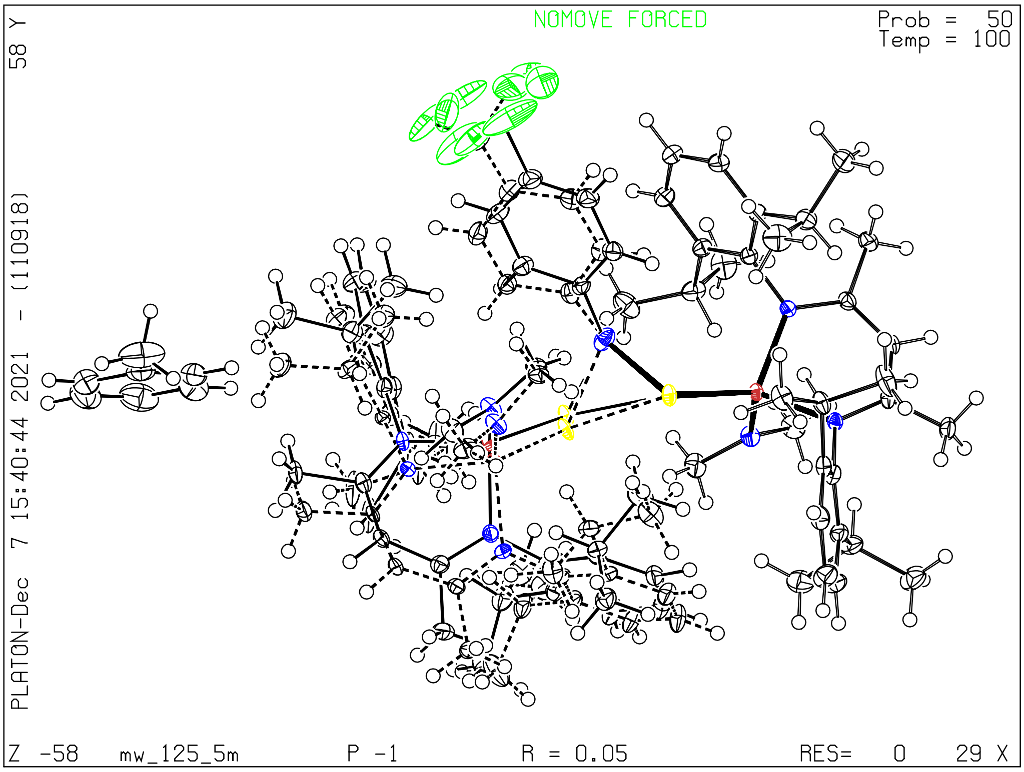

Table 1: Crystal data and structure refinement for mw_125_5m.

Identification code	mw_125_5m
Empirical Formula	$C_{72.50}\,H_{102}\,F_3\,Ga_2\,N_7\,Sb_2$
Formula weight	1511.54 Da
Density (calculated)	$1.396\,g \cdot cm^{-3}$
$F(000)$	1554
Temperature	100(2) K
Crystal size	0.392 × 0.197 × 0.126 mm
Crystal appearance	orange tablet
Wavelength (MoK_α)	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 10.6581(5)$ Å
	$b = 12.7136(6)$ Å
	$c = 27.5744(13)$ Å
	$\alpha = 102.129(2)°$
	$\beta = 92.993(2)°$
	$\gamma = 98.869(3)°$
Unit cell volume	3595.4(3) $Å^3$
Z	2
Cell measurement refections used	9083
θ range for cell measurement	2.49° to 33.43°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	0.758° to 33.683°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.8% (98.5%)
Index ranges	$-16 \le h \le 16$
	$-19 \le k \le 19$
	$-42 \le l \le 42$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.537\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.55
R_{merg} before/after correction	0.0772/0.0492
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	190515
Independent reflections	28194 ($R_{int} = 0.0415$)
Reflections with $I > 2\sigma(I)$	21619
Data / retraints / parameter	28194 / 2926 / 1250
Goodness-of-fit on F^2	1.132
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0400P)^2 + 11.3395P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0457$
	$wR2 = 0.1082$
R indices [all data]	$R1 = 0.0720$
	$wR2 = 0.1266$
Largest diff. peak and hole	2.725 and −1.306 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

One half of the molecule and the –Ph–CF_3 moiety are disordered over two positions. The corresponding bond lengths and angles of the diisopropyl phenyl groups were restrained to be equal (`SADI`) as well as those of the –Ph–CF_3 unit. The displacement parameters of all disordered atoms were refined with `RIGU` restraints. Additional `SIMU` and `ISOR` restraints were required for the fluorine atoms. Their disorder is more diffuse than the one of the remaining moiety and consequently an extra alternate position was used to model the electron density. Still, the displacement ellipsoids suggest further disorder, however no other alternate positions could be identified. Disordered atoms in close proximity to its alternate positions were refined with common displacement parameters (`EADP`). Finally, the Ga2–N6 bond length of both alternate positions were restrained to be equal (`SADI`). The solvent molecule is disordered over a centre of inversion. The local symmetry was ignored in the refinement (negative `PART`). All its corresponding bond lengths and angles were restrained to be equal (`SADI`) and its atoms were restrained to lie on a common plane (`FLAT`). `RIGU` restraints were applied to the atoms' displacement parameters.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_125_5m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	3631(1)	2929(1)	7163(1)	15(1)
Ga(1)	2429(1)	2131(1)	6268(1)	12(1)
N(5)	656(2)	1834(2)	6171(1)	17(1)
N(7)	3312(3)	4557(2)	7260(1)	23(1)
N11	3171(2)	2851(2)	5751(1)	14(1)
N21	2923(2)	695(2)	5968(1)	14(1)
C11	3168(2)	2263(2)	5285(1)	16(1)
C21	2989(3)	1125(2)	5160(1)	17(1)
C31	2994(3)	397(2)	5482(1)	16(1)
C41	3399(3)	2841(2)	4864(1)	21(1)
C51	3090(3)	−764(2)	5237(1)	22(1)
C61	3708(2)	3998(2)	5860(1)	16(1)
C71	2925(3)	4787(2)	5985(1)	19(1)
C81	3481(3)	5887(2)	6098(1)	24(1)
C91	4779(3)	6206(2)	6091(1)	24(1)
C101	5546(3)	5423(2)	5967(1)	22(1)
C111	5038(3)	4312(2)	5852(1)	18(1)
C121	1481(3)	4489(2)	5971(1)	23(1)
C131	849(3)	4607(3)	5479(1)	34(1)
C141	930(3)	5161(3)	6410(1)	32(1)
C151	5953(3)	3502(2)	5734(1)	23(1)
C161	6847(3)	3769(3)	5341(1)	32(1)
C171	6741(3)	3451(3)	6206(1)	34(1)
C181	3002(2)	−66(2)	6284(1)	16(1)
C191	1927(3)	−822(2)	6327(1)	19(1)
C201	2044(3)	−1514(2)	6651(1)	25(1)
C211	3196(3)	−1474(3)	6924(1)	27(1)
C221	4248(3)	−727(2)	6875(1)	22(1)
C231	4175(2)	−13(2)	6557(1)	17(1)
C241	649(3)	−941(2)	6027(1)	22(1)
C251	281(4)	−2092(3)	5689(1)	32(1)
C261	−407(3)	−705(3)	6368(1)	31(1)
C271	5365(2)	750(2)	6484(1)	19(1)
C281	6025(3)	202(3)	6044(1)	34(1)
C291	6324(3)	1147(3)	6942(1)	24(1)
Sb(2)	1924(2)	4117(2)	7652(1)	16(1)
Ga(2)	3005(1)	4463(1)	8574(1)	13(1)
N(6)	4745(9)	4684(10)	8744(6)	18(2)
C(61)	5660(50)	4600(40)	8396(19)	19(3)
C(62)	5256(9)	4731(7)	9251(3)	23(2)
N12	2336(4)	5615(4)	9042(2)	13(1)
C12	2099(5)	5510(5)	9499(2)	17(1)
N22	2106(6)	3271(5)	8862(2)	14(1)
C22	1973(5)	4512(6)	9641(2)	16(1)
C62	2301(5)	6615(4)	8878(2)	17(1)
C52	1423(6)	2514(5)	9580(2)	23(1)
C42	1945(6)	6491(5)	9895(2)	23(1)
C32	1863(5)	3461(6)	9337(2)	16(1)
C292	−1395(7)	2900(7)	8113(3)	31(2)
C282	−1542(15)	1981(15)	8835(6)	34(3)

Table 2: (continued)

	x	y	z	U_{eq}
C272	−631(7)	2606(6)	8539(3)	25(1)
C262	4977(12)	1602(8)	8199(4)	27(2)
C252	4313(6)	613(5)	8860(2)	24(1)
C242	3991(6)	1486(5)	8583(2)	19(1)
C232	384(6)	1944(5)	8343(3)	19(1)
C222	−2(6)	1020(5)	7962(3)	26(1)
C212	875(7)	400(6)	7760(2)	26(1)
C202	2160(6)	700(5)	7926(2)	23(1)
C192	2587(5)	1602(5)	8322(2)	18(1)
C182	1685(6)	2241(5)	8519(2)	15(1)
C172	−915(9)	5771(7)	8103(3)	32(1)
C162	−915(6)	5443(6)	8989(2)	32(1)
C152	−17(7)	5790(6)	8550(3)	32(1)
C142	5750(6)	7444(6)	9003(3)	29(1)
C132	4773(8)	8461(6)	9730(2)	35(2)
C122	4564(6)	7453(5)	9294(2)	25(1)
C112	1194(5)	6687(5)	8588(2)	20(1)
C102	1203(6)	7600(5)	8383(3)	29(1)
C92	2267(6)	8412(5)	8452(3)	30(1)
C82	3330(6)	8346(4)	8745(2)	26(1)
C72	3369(5)	7454(4)	8963(2)	20(1)
Sb(2')	1835(2)	3935(2)	7705(1)	16(1)
N(6')	4642(9)	4404(10)	8773(7)	18(2)
C(61')	5610(60)	4470(40)	8410(20)	19(3)
C(62')	5204(10)	4321(7)	9243(4)	22(2)
Ga(2')	2902(1)	4140(1)	8613(1)	12(1)
C43	1648(6)	5873(5)	9980(2)	18(1)
C33	1860(5)	2946(6)	9337(2)	15(1)
C23	1881(5)	3948(5)	9670(2)	15(1)
N23	2073(6)	2873(5)	8860(2)	13(1)
C13	1919(5)	4970(6)	9560(2)	11(1)
N13	2170(5)	5174(4)	9119(2)	12(1)
C73	3142(5)	7084(4)	9157(2)	16(1)
C63	2109(5)	6223(4)	9011(2)	12(1)
C53	1592(6)	1921(5)	9534(2)	19(1)
C123	4333(5)	7000(5)	9471(2)	19(1)
C133	4520(7)	7830(5)	9975(2)	28(1)
C143	5520(6)	7166(6)	9189(3)	25(1)
C153	−108(8)	5436(6)	8545(3)	32(1)
C163	−768(6)	5992(7)	8993(2)	32(1)
C183	1730(6)	1859(5)	8501(2)	15(1)
C173	−907(10)	5503(7)	8068(3)	32(1)
C193	2641(5)	1208(5)	8348(2)	16(1)
C203	2296(6)	277(6)	7966(2)	22(1)
C243	3987(6)	1884(6)	8526(2)	22(1)
C233	467(6)	1572(6)	8281(3)	20(1)
C223	153(6)	640(6)	7908(3)	22(1)
C213	1050(6)	−11(6)	7752(3)	26(1)
C253	4139(7)	1678(6)	9051(2)	26(1)
C263	4853(12)	1235(8)	8196(4)	29(2)
C273	−560(8)	2249(7)	8450(3)	24(2)
C293	−1427(7)	2391(8)	8013(3)	30(2)

Table 2: (continued)

	x	y	z	U_{eq}
C283	−1378(18)	1751(18)	8814(7)	38(4)
C113	1042(5)	6347(5)	8717(2)	18(1)
C103	1024(5)	7334(5)	8579(2)	21(1)
C93	2049(5)	8201(4)	8727(2)	22(1)
C83	3087(5)	8066(4)	9016(2)	21(1)
C(59)	3(3)	1561(3)	5674(1)	24(1)
C(60)	−183(3)	2190(3)	6543(1)	25(1)
F(1)	7554(12)	8669(9)	7475(4)	89(4)
F(2)	7820(18)	8398(17)	8195(5)	82(5)
F(3)	6477(7)	9315(5)	8032(4)	66(3)
C(63)	4134(11)	5505(8)	7433(6)	18(2)
C(64)	3887(7)	6417(6)	7781(3)	20(1)
C(65)	4775(7)	7365(5)	7907(3)	24(1)
C(66)	5931(7)	7432(5)	7697(3)	21(1)
C(67)	6198(7)	6537(6)	7356(3)	25(2)
C(68)	5295(8)	5587(7)	7223(4)	24(2)
C(69)	6923(8)	8424(7)	7852(3)	32(2)
C44	−1553(9)	9971(8)	9866(4)	53(2)
C14	895(8)	9942(6)	10237(3)	38(2)
C34	−784(9)	9359(8)	9583(3)	51(2)
C64	121(8)	10555(7)	10518(3)	45(2)
C24	426(8)	9346(6)	9772(3)	41(2)
C54	−1092(9)	10560(7)	10335(3)	51(2)
C74	2240(11)	9970(9)	10425(5)	68(3)
F(3’)	8203(15)	8265(13)	7366(6)	101(6)
F(2’)	6938(14)	9188(10)	7745(6)	67(5)
F(1’)	7990(30)	8300(20)	8112(7)	56(4)
C(63’)	4382(10)	5443(7)	7364(6)	18(2)
C(64’)	4144(7)	6456(5)	7625(3)	22(1)
C(65’)	5103(7)	7369(5)	7726(3)	25(1)
C(66’)	6302(7)	7294(5)	7565(3)	26(1)
C(67’)	6557(7)	6301(6)	7310(3)	24(1)
C(68’)	5604(7)	5387(6)	7213(4)	21(2)
C(69’)	7346(9)	8261(6)	7681(4)	37(2)
F(1”)	8357(17)	8112(14)	7818(9)	86(8)
F(2”)	7517(19)	8643(16)	7244(6)	52(4)
F(3”)	7010(20)	9140(20)	7955(9)	92(10)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_125_5m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	15(1)	19(1)	11(1)	−2(1)	−1(1)	5(1)
Ga(1)	10(1)	14(1)	10(1)	0(1)	0(1)	2(1)
N(5)	10(1)	22(1)	18(1)	1(1)	0(1)	2(1)
N(7)	31(1)	17(1)	19(1)	2(1)	−7(1)	2(1)
N11	15(1)	14(1)	12(1)	2(1)	2(1)	1(1)
N21	15(1)	14(1)	10(1)	1(1)	0(1)	2(1)
C11	16(1)	20(1)	12(1)	3(1)	1(1)	1(1)
C21	21(1)	18(1)	10(1)	0(1)	1(1)	3(1)
C31	18(1)	17(1)	12(1)	−2(1)	1(1)	3(1)
C41	27(1)	23(1)	13(1)	5(1)	2(1)	1(1)
C51	31(2)	19(1)	15(1)	−2(1)	1(1)	4(1)
C61	17(1)	15(1)	14(1)	3(1)	1(1)	1(1)
C71	23(1)	15(1)	19(1)	5(1)	3(1)	5(1)
C81	30(1)	16(1)	26(1)	6(1)	7(1)	6(1)
C91	31(2)	16(1)	24(1)	3(1)	5(1)	−1(1)
C101	21(1)	21(1)	22(1)	4(1)	4(1)	−2(1)
C111	18(1)	17(1)	16(1)	2(1)	2(1)	0(1)
C121	19(1)	19(1)	34(2)	10(1)	4(1)	8(1)
C131	26(2)	41(2)	33(2)	4(1)	−2(1)	8(1)
C141	28(2)	45(2)	31(2)	14(1)	10(1)	15(1)
C151	17(1)	23(1)	28(1)	3(1)	5(1)	2(1)
C161	26(2)	31(2)	38(2)	2(1)	16(1)	2(1)
C171	23(1)	39(2)	42(2)	13(2)	1(1)	9(1)
C181	19(1)	13(1)	14(1)	0(1)	−1(1)	4(1)
C191	22(1)	16(1)	16(1)	2(1)	0(1)	2(1)
C201	31(2)	19(1)	23(1)	7(1)	−3(1)	−3(1)
C211	38(2)	21(1)	22(1)	8(1)	−6(1)	3(1)
C221	26(1)	24(1)	16(1)	4(1)	−2(1)	9(1)
C231	19(1)	18(1)	13(1)	0(1)	1(1)	7(1)
C241	22(1)	19(1)	23(1)	6(1)	−2(1)	−2(1)
C251	34(2)	25(2)	32(2)	2(1)	−6(1)	−6(1)
C261	24(1)	34(2)	34(2)	10(1)	3(1)	0(1)
C271	14(1)	27(1)	15(1)	2(1)	2(1)	7(1)
C281	23(1)	54(2)	20(1)	−3(1)	6(1)	10(1)
C291	17(1)	35(2)	20(1)	3(1)	−1(1)	7(1)
Sb(2)	16(1)	24(1)	8(1)	1(1)	0(1)	6(1)
Ga(2)	11(1)	20(1)	8(1)	2(1)	1(1)	4(1)
N(6)	9(2)	29(6)	15(2)	6(4)	0(2)	3(2)
C(61)	14(4)	20(8)	22(3)	6(5)	3(2)	2(6)
C(62)	17(3)	32(4)	17(3)	4(4)	−4(2)	2(4)
N12	15(2)	15(2)	8(2)	−1(2)	2(1)	4(2)
C12	19(2)	21(2)	11(2)	1(2)	1(2)	4(2)
N22	14(2)	15(2)	13(2)	1(2)	2(1)	2(2)
C22	21(2)	18(3)	8(2)	4(2)	1(2)	3(2)
C62	20(2)	15(2)	14(2)	1(2)	1(2)	7(2)
C52	27(3)	22(3)	20(3)	8(2)	4(2)	−2(2)
C42	32(3)	21(3)	12(2)	−3(2)	5(2)	6(2)
C32	15(2)	17(2)	16(2)	3(2)	−1(2)	0(2)
C292	20(3)	29(4)	42(4)	6(3)	−1(3)	7(3)
C282	23(5)	47(7)	26(4)	2(4)	3(3)	−1(5)
C272	14(2)	24(4)	31(4)	−3(3)	−3(2)	0(2)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C262	23(3)	31(5)	34(4)	16(4)	10(3)	13(4)
C252	30(3)	21(2)	19(2)	3(2)	−3(2)	2(2)
C242	20(2)	15(3)	20(3)	4(2)	3(2)	−1(2)
C232	20(2)	19(3)	16(3)	1(2)	0(2)	0(2)
C222	26(3)	18(3)	30(3)	−2(3)	−4(2)	6(2)
C212	38(3)	20(3)	18(3)	−4(2)	−3(2)	9(3)
C202	31(3)	20(3)	20(3)	4(2)	9(2)	9(2)
C192	25(2)	14(3)	14(2)	5(2)	4(2)	3(2)
C182	17(2)	12(3)	17(2)	4(2)	3(2)	1(2)
C172	21(1)	38(2)	27(1)	−20(2)	−4(1)	12(2)
C162	21(1)	38(2)	27(1)	−20(2)	−4(1)	12(2)
C152	21(1)	38(2)	27(1)	−20(2)	−4(1)	12(2)
C142	21(3)	32(3)	31(3)	9(3)	−1(2)	−3(2)
C132	46(4)	28(3)	25(3)	−1(2)	−4(3)	−2(3)
C122	26(3)	24(3)	22(3)	2(2)	1(2)	0(2)
C112	21(2)	19(3)	19(3)	3(2)	0(2)	10(2)
C102	34(3)	24(3)	35(4)	12(3)	5(3)	13(2)
C92	37(3)	22(3)	37(3)	14(3)	7(3)	10(2)
C82	34(3)	17(2)	29(3)	7(2)	5(2)	5(2)
C72	23(2)	16(2)	22(3)	4(2)	2(2)	3(2)
Sb(2')	13(1)	27(1)	6(1)	2(1)	1(1)	5(1)
N(6')	9(2)	29(6)	15(2)	6(4)	0(2)	3(2)
C(61')	14(4)	20(8)	22(3)	6(5)	3(2)	2(6)
C(62')	18(3)	21(4)	26(3)	6(4)	−4(2)	−1(3)
Ga(2')	10(1)	16(1)	9(1)	2(1)	1(1)	2(1)
C43	25(3)	19(2)	12(2)	3(2)	4(2)	8(2)
C33	14(2)	17(2)	11(2)	2(2)	0(2)	−3(2)
C23	19(2)	17(2)	8(2)	2(2)	2(2)	2(2)
N23	13(2)	11(2)	15(2)	2(2)	2(2)	−1(2)
C13	12(2)	17(3)	5(2)	2(2)	1(2)	3(2)
N13	15(2)	12(2)	11(2)	3(2)	3(1)	1(2)
C73	20(2)	13(2)	15(2)	0(2)	1(2)	4(2)
C63	15(2)	12(2)	9(2)	3(2)	1(2)	0(2)
C53	28(3)	14(2)	14(2)	4(2)	1(2)	1(2)
C123	21(2)	13(2)	21(2)	2(2)	−4(2)	−2(2)
C133	36(3)	23(3)	19(3)	−1(2)	−7(2)	−4(2)
C143	18(3)	25(3)	29(3)	2(3)	0(2)	−1(2)
C153	21(1)	38(2)	27(1)	−20(2)	−4(1)	12(2)
C163	21(1)	38(2)	27(1)	−20(2)	−4(1)	12(2)
C183	21(2)	10(3)	12(2)	2(2)	−2(2)	−1(2)
C173	21(1)	38(2)	27(1)	−20(2)	−4(1)	12(2)
C193	18(2)	11(3)	19(3)	4(2)	3(2)	0(2)
C203	24(3)	18(3)	22(3)	−1(2)	0(2)	2(2)
C243	22(3)	17(3)	27(3)	8(2)	7(2)	0(2)
C233	17(2)	17(3)	21(3)	−2(3)	1(2)	−2(2)
C223	23(3)	15(3)	22(3)	−4(2)	−4(2)	1(2)
C213	25(3)	25(3)	21(3)	−9(3)	−3(2)	5(3)
C253	29(3)	29(3)	21(3)	3(2)	3(2)	10(2)
C263	28(4)	38(6)	28(4)	15(4)	7(3)	19(5)
C273	21(3)	21(4)	24(3)	−6(3)	−2(2)	0(3)
C293	19(3)	39(4)	32(4)	7(3)	0(2)	3(3)
C283	25(5)	64(11)	25(5)	7(6)	5(3)	14(5)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C113	20(2)	20(3)	16(3)	5(2)	2(2)	10(2)
C103	22(3)	27(3)	20(3)	10(2)	2(2)	10(2)
C93	25(3)	19(2)	25(3)	10(2)	2(2)	6(2)
C83	23(3)	15(2)	24(3)	4(2)	1(2)	3(2)
C(59)	17(1)	33(2)	21(1)	6(1)	−4(1)	1(1)
C(60)	14(1)	30(2)	29(2)	0(1)	4(1)	4(1)
F(1)	100(8)	68(6)	66(6)	−8(5)	24(5)	−59(5)
F(2)	82(9)	44(7)	103(7)	14(6)	−70(7)	−17(5)
F(3)	48(4)	18(2)	117(8)	−8(3)	−13(4)	1(3)
C(63)	21(4)	22(3)	12(4)	4(2)	−1(3)	4(3)
C(64)	23(3)	18(3)	18(3)	4(2)	2(2)	5(2)
C(65)	30(3)	17(3)	23(3)	1(2)	1(2)	7(2)
C(66)	24(3)	17(2)	20(3)	4(2)	−5(2)	3(2)
C(67)	23(4)	25(3)	26(3)	5(3)	5(3)	1(3)
C(68)	27(4)	20(3)	23(3)	1(3)	3(3)	3(3)
C(69)	30(4)	23(3)	38(4)	1(3)	−7(3)	0(3)
C44	41(5)	62(6)	67(5)	36(4)	11(4)	14(4)
C14	42(4)	25(3)	51(4)	18(3)	19(3)	3(3)
C34	66(5)	48(5)	39(4)	12(4)	12(4)	2(4)
C64	63(5)	30(4)	44(5)	10(3)	19(4)	8(4)
C24	51(4)	28(3)	48(4)	12(3)	26(3)	8(3)
C54	60(5)	45(5)	62(5)	24(4)	33(4)	24(4)
C74	50(5)	62(7)	98(9)	43(7)	7(5)	−6(5)
F(3’)	91(10)	77(9)	88(8)	−35(8)	44(8)	−69(7)
F(2’)	47(7)	23(5)	124(13)	27(7)	−43(7)	−11(4)
F(1’)	61(10)	21(6)	74(7)	7(7)	−39(7)	−7(6)
C(63’)	23(4)	15(3)	13(4)	2(2)	−3(3)	−1(3)
C(64’)	27(3)	17(2)	23(3)	5(2)	2(3)	2(2)
C(65’)	31(3)	14(2)	27(3)	4(2)	−4(3)	−1(2)
C(66’)	29(3)	23(3)	22(3)	6(2)	−2(2)	−5(2)
C(67’)	24(3)	26(3)	21(3)	5(2)	1(3)	−5(2)
C(68’)	22(3)	23(3)	16(3)	4(3)	0(3)	−2(3)
C(69’)	36(4)	25(3)	45(5)	13(3)	−6(3)	−10(3)
F(1”)	50(10)	39(9)	150(20)	31(13)	−56(13)	−28(7)
F(2”)	47(9)	48(9)	64(11)	34(9)	0(8)	−15(7)
F(3”)	81(16)	55(13)	106(17)	−44(12)	55(14)	−26(10)

Table 4: Bond lengths [Å] for mw_125_5m.

Sb(1)–N(7)	2.113(3)
Sb(1)–Ga(1)	2.6434(3)
Sb(1)–Sb(2)	2.766(3)
Sb(1)–Sb(2')	2.789(3)
Ga(1)–N(5)	1.863(2)
Ga(1)–N11	1.985(2)
Ga(1)–N21	2.001(2)
N(5)–C(60)	1.442(4)
N(5)–C(59)	1.452(4)
N(7)–C(63)	1.355(9)
N(7)–C(63')	1.444(8)
N(7)–Sb(2)	1.959(3)
N(7)–Sb(2')	2.200(3)
N11–C11	1.343(3)
N11–C61	1.444(3)
N21–C31	1.322(3)
N21–C181	1.439(3)
C11–C21	1.395(4)
C11–C41	1.511(4)
C21–C31	1.413(4)
C31–C51	1.510(4)
C61–C71	1.401(4)
C61–C111	1.414(4)
C71–C81	1.395(4)
C71–C121	1.524(4)
C81–C91	1.383(4)
C91–C101	1.383(4)
C101–C111	1.396(4)
C111–C151	1.523(4)
C121–C141	1.528(4)
C121–C131	1.530(5)
C151–C171	1.530(5)
C151–C161	1.537(4)
C181–C191	1.405(4)
C181–C231	1.411(4)
C191–C201	1.393(4)
C191–C241	1.526(4)
C201–C211	1.395(4)
C211–C221	1.385(4)
C221–C231	1.396(4)
C231–C271	1.523(4)
C241–C261	1.529(4)
C241–C251	1.542(4)
C271–C291	1.528(4)
C271–C281	1.529(4)
Sb(2)–Ga(2)	2.657(3)
Ga(2)–N(6)	1.852(9)
Ga(2)–N12	1.986(4)
Ga(2)–N22	1.995(6)
N(6)–C(61)	1.40(6)
N(6)–C(62)	1.462(17)
N12–C12	1.328(7)
N12–C62	1.441(8)

Table 4: (continued)

C12–C22	1.394(10)
C12–C42	1.511(8)
N22–C32	1.328(8)
N22–C182	1.437(8)
C22–C32	1.404(9)
C62–C72	1.408(7)
C62–C112	1.415(7)
C52–C32	1.520(9)
C292–C272	1.535(9)
C282–C272	1.536(10)
C272–C232	1.523(8)
C262–C242	1.543(9)
C252–C242	1.544(8)
C242–C192	1.666(8)
C232–C222	1.393(8)
C232–C182	1.412(7)
C222–C212	1.379(8)
C212–C202	1.389(8)
C202–C192	1.404(7)
C192–C182	1.411(7)
C172–C152	1.515(8)
C162–C152	1.670(9)
C152–C112	1.568(8)
C142–C122	1.531(8)
C132–C122	1.542(7)
C122–C72	1.527(7)
C112–C102	1.393(7)
C102–C92	1.387(8)
C92–C82	1.380(8)
C82–C72	1.396(7)
Sb(2')–Ga(2')	2.641(3)
N(6')–C(62')	1.428(18)
N(6')–C(61')	1.48(6)
N(6')–Ga(2')	1.846(9)
Ga(2')–N23	1.980(6)
Ga(2')–N13	1.985(5)
C43–C13	1.523(8)
C33–N23	1.333(8)
C33–C23	1.402(8)
C33–C53	1.507(9)
C23–C13	1.389(10)
N23–C183	1.433(8)
C13–N13	1.330(8)
N13–C63	1.436(7)
C73–C83	1.391(7)
C73–C63	1.403(7)
C73–C123	1.529(7)
C63–C113	1.410(7)
C123–C143	1.528(8)
C123–C133	1.540(7)
C153–C113	1.529(9)
C153–C163	1.548(8)
C153–C173	1.555(9)

Table 4: (continued)

C183–C193	1.396(8)
C183–C233	1.408(8)
C193–C203	1.395(7)
C193–C243	1.552(8)
C203–C213	1.387(8)
C243–C253	1.530(8)
C243–C263	1.538(9)
C233–C223	1.381(8)
C233–C273	1.527(9)
C223–C213	1.387(8)
C273–C283	1.535(11)
C273–C293	1.537(9)
C113–C103	1.389(7)
C103–C93	1.403(7)
C93–C83	1.384(7)
F(1)–C(69)	1.332(10)
F(2)–C(69)	1.319(10)
F(3)–C(69)	1.308(9)
C(63)–C(68)	1.392(9)
C(63)–C(64)	1.410(9)
C(64)–C(65)	1.380(8)
C(65)–C(66)	1.387(8)
C(66)–C(67)	1.391(8)
C(66)–C(69)	1.485(10)
C(67)–C(68)	1.392(9)
C44–C54	1.375(10)
C44–C34	1.376(10)
C14–C24	1.369(9)
C14–C64	1.378(9)
C14–C74	1.491(14)
C34–C24	1.369(10)
C64–C54	1.364(10)
F(3')–C(69')	1.294(11)
F(2')–C(69')	1.299(11)
F(1')–C(69')	1.329(12)
C(63')–C(68')	1.395(9)
C(63')–C(64')	1.403(8)
C(64')–C(65')	1.392(8)
C(65')–C(66')	1.385(8)
C(66')–C(67')	1.384(8)
C(66')–C(69')	1.492(10)
C(67')–C(68')	1.390(8)

Table 5: Bond angles [°] for mw_125_5m.

N(7)–Sb(1)–Ga(1)	98.86(7)
N(7)–Sb(1)–Sb(2)	44.92(9)
Ga(1)–Sb(1)–Sb(2)	102.53(5)
N(7)–Sb(1)–Sb(2')	51.07(9)
Ga(1)–Sb(1)–Sb(2')	103.68(5)
N(5)–Ga(1)–N11	111.26(10)
N(5)–Ga(1)–N21	102.88(10)
N11–Ga(1)–N21	93.46(9)
N(5)–Ga(1)–Sb(1)	121.57(7)
N11–Ga(1)–Sb(1)	113.12(6)
N21–Ga(1)–Sb(1)	110.26(6)
C(60)–N(5)–C(59)	111.3(2)
C(60)–N(5)–Ga(1)	124.46(19)
C(59)–N(5)–Ga(1)	121.06(19)
C(63')–N(7)–Sb(2)	132.6(5)
C(63)–N(7)–Sb(1)	129.7(7)
C(63')–N(7)–Sb(1)	119.8(5)
Sb(2)–N(7)–Sb(1)	85.48(12)
C(63)–N(7)–Sb(2')	122.3(5)
Sb(1)–N(7)–Sb(2')	80.56(11)
C11–N11–C61	118.8(2)
C11–N11–Ga(1)	119.46(18)
C61–N11–Ga(1)	121.74(16)
C31–N21–C181	120.9(2)
C31–N21–Ga(1)	120.75(18)
C181–N21–Ga(1)	117.66(16)
N11–C11–C21	123.9(2)
N11–C11–C41	119.6(2)
C21–C11–C41	116.5(2)
C11–C21–C31	128.1(2)
N21–C31–C21	123.1(2)
N21–C31–C51	121.3(2)
C21–C31–C51	115.6(2)
C71–C61–C111	120.6(2)
C71–C61–N11	120.3(2)
C111–C61–N11	119.1(2)
C81–C71–C61	118.8(3)
C81–C71–C121	118.8(2)
C61–C71–C121	122.3(2)
C91–C81–C71	121.3(3)
C81–C91–C101	119.6(3)
C91–C101–C111	121.3(3)
C101–C111–C61	118.4(2)
C101–C111–C151	118.0(2)
C61–C111–C151	123.6(2)
C71–C121–C141	112.8(3)
C71–C121–C131	110.4(3)
C141–C121–C131	110.3(3)
C111–C151–C171	110.9(3)
C111–C151–C161	112.4(3)
C171–C151–C161	109.7(3)
C191–C181–C231	121.0(2)
C191–C181–N21	120.7(2)

Table 5: (continued)

C231–C181–N21	118.3(2)
C201–C191–C181	118.4(3)
C201–C191–C241	118.4(3)
C181–C191–C241	123.2(2)
C191–C201–C211	121.4(3)
C221–C211–C201	119.5(3)
C211–C221–C231	121.1(3)
C221–C231–C181	118.6(3)
C221–C231–C271	120.1(2)
C181–C231–C271	121.1(2)
C191–C241–C261	111.3(3)
C191–C241–C251	111.1(3)
C261–C241–C251	109.8(3)
C231–C271–C291	114.6(2)
C231–C271–C281	110.1(3)
C291–C271–C281	109.5(2)
N(7)–Sb(2)–Ga(2)	104.81(13)
N(7)–Sb(2)–Sb(1)	49.60(9)
Ga(2)–Sb(2)–Sb(1)	98.42(8)
N(6)–Ga(2)–N12	106.1(6)
N(6)–Ga(2)–N22	110.8(3)
N12–Ga(2)–N22	92.9(2)
N(6)–Ga(2)–Sb(2)	124.8(5)
N12–Ga(2)–Sb(2)	112.36(15)
N22–Ga(2)–Sb(2)	105.31(18)
C(61)–N(6)–C(62)	113(2)
C(61)–N(6)–Ga(2)	124(2)
C(62)–N(6)–Ga(2)	121.2(10)
C12–N12–C62	122.8(5)
C12–N12–Ga(2)	121.1(4)
C62–N12–Ga(2)	115.5(3)
N12–C12–C22	122.9(5)
N12–C12–C42	120.5(6)
C22–C12–C42	116.5(5)
C32–N22–C182	123.3(6)
C32–N22–Ga(2)	120.7(5)
C182–N22–Ga(2)	115.9(4)
C12–C22–C32	128.4(5)
C72–C62–C112	120.8(5)
C72–C62–N12	121.3(4)
C112–C62–N12	117.7(5)
N22–C32–C22	123.5(6)
N22–C32–C52	120.2(6)
C22–C32–C52	116.3(5)
C232–C272–C292	111.3(6)
C232–C272–C282	110.9(8)
C292–C272–C282	109.7(7)
C262–C242–C252	108.0(6)
C262–C242–C192	107.4(6)
C252–C242–C192	128.8(5)
C222–C232–C182	119.2(5)
C222–C232–C272	117.6(5)
C182–C232–C272	123.2(5)

Table 5: (continued)

C212–C222–C232	120.5(6)
C222–C212–C202	120.5(5)
C212–C202–C192	121.0(5)
C202–C192–C182	117.8(5)
C202–C192–C242	110.0(5)
C182–C192–C242	129.3(5)
C192–C182–C232	120.8(5)
C192–C182–N22	119.9(5)
C232–C182–N22	118.9(5)
C172–C152–C112	110.6(7)
C172–C152–C162	107.1(5)
C112–C152–C162	130.8(6)
C72–C122–C142	112.1(5)
C72–C122–C132	109.6(5)
C142–C122–C132	109.8(5)
C102–C112–C62	118.1(5)
C102–C112–C152	123.0(5)
C62–C112–C152	118.7(6)
C92–C102–C112	121.4(5)
C82–C92–C102	119.9(5)
C92–C82–C72	121.1(5)
C82–C72–C62	118.6(5)
C82–C72–C122	118.0(5)
C62–C72–C122	123.3(5)
N(7)–Sb(2')–Ga(2')	107.67(12)
N(7)–Sb(2')–Sb(1)	48.36(8)
Ga(2')–Sb(2')–Sb(1)	99.03(9)
C(62')–N(6')–C(61')	111(2)
C(62')–N(6')–Ga(2')	122.7(10)
C(61')–N(6')–Ga(2')	125(2)
N(6')–Ga(2')–N23	111.1(4)
N(6')–Ga(2')–N13	106.9(6)
N23–Ga(2')–N13	91.8(2)
N(6')–Ga(2')–Sb(2')	123.6(6)
N23–Ga(2')–Sb(2')	106.5(2)
N13–Ga(2')–Sb(2')	112.45(16)
N23–C33–C23	122.6(6)
N23–C33–C53	119.6(6)
C23–C33–C53	117.9(5)
C13–C23–C33	127.8(5)
C33–N23–C183	121.2(6)
C33–N23–Ga(2')	122.1(5)
C183–N23–Ga(2')	116.7(5)
N13–C13–C23	123.4(5)
N13–C13–C43	120.5(6)
C23–C13–C43	116.1(5)
C13–N13–C63	121.4(5)
C13–N13–Ga(2')	122.0(5)
C63–N13–Ga(2')	115.9(4)
C83–C73–C63	119.2(5)
C83–C73–C123	117.9(5)
C63–C73–C123	122.9(5)
C73–C63–C113	120.3(5)

Table 5: (continued)

C73–C63–N13	120.7(4)
C113–C63–N13	118.8(5)
C143–C123–C73	110.8(5)
C143–C123–C133	109.6(5)
C73–C123–C133	111.9(5)
C113–C153–C163	87.6(5)
C113–C153–C173	115.3(7)
C163–C153–C173	106.5(6)
C193–C183–C233	120.7(5)
C193–C183–N23	121.0(6)
C233–C183–N23	118.2(6)
C203–C193–C183	119.4(5)
C203–C193–C243	128.6(5)
C183–C193–C243	108.8(5)
C213–C203–C193	120.0(5)
C253–C243–C263	108.7(6)
C253–C243–C193	99.9(5)
C263–C243–C193	102.7(7)
C223–C233–C183	118.6(5)
C223–C233–C273	119.4(6)
C183–C233–C273	122.0(6)
C233–C223–C213	121.2(5)
C223–C213–C203	120.1(5)
C233–C273–C283	111.1(9)
C233–C273–C293	112.9(6)
C283–C273–C293	109.5(8)
C103–C113–C63	119.1(5)
C103–C113–C153	118.4(6)
C63–C113–C153	122.6(6)
C113–C103–C93	120.9(5)
C83–C93–C103	119.2(5)
C93–C83–C73	121.3(5)
N(7)–C(63)–C(68)	115.8(7)
N(7)–C(63)–C(64)	126.0(7)
C(68)–C(63)–C(64)	118.1(7)
C(65)–C(64)–C(63)	120.7(6)
C(64)–C(65)–C(66)	120.5(6)
C(65)–C(66)–C(67)	119.8(6)
C(65)–C(66)–C(69)	120.9(6)
C(67)–C(66)–C(69)	119.2(7)
C(66)–C(67)–C(68)	119.8(6)
C(67)–C(68)–C(63)	121.2(7)
F(3)–C(69)–F(2)	103.9(9)
F(3)–C(69)–F(1)	103.5(8)
F(2)–C(69)–F(1)	104.6(10)
F(3)–C(69)–C(66)	114.2(7)
F(2)–C(69)–C(66)	116.4(12)
F(1)–C(69)–C(66)	112.9(7)
C54–C44–C34	119.3(7)
C24–C14–C64	118.8(7)
C24–C14–C74	120.6(8)
C64–C14–C74	120.6(8)
C24–C34–C44	119.6(7)

Table 5: (continued)

C54–C64–C14	120.3(7)
C14–C24–C34	121.3(7)
C64–C54–C44	120.7(7)
C(68')–C(63')–C(64')	117.8(6)
C(68')–C(63')–N(7)	125.8(6)
C(64')–C(63')–N(7)	116.3(6)
C(65')–C(64')–C(63')	120.5(6)
C(66')–C(65')–C(64')	120.5(6)
C(67')–C(66')–C(65')	119.8(5)
C(67')–C(66')–C(69')	119.1(7)
C(65')–C(66')–C(69')	121.0(6)
C(66')–C(67')–C(68')	119.7(6)
C(67')–C(68')–C(63')	121.6(6)
F(3')–C(69')–F(2')	108.1(10)
F(3')–C(69')–F(1')	104.5(11)
F(2')–C(69')–F(1')	104.5(11)
F(3')–C(69')–C(66')	115.5(8)
F(2')–C(69')–C(66')	113.5(9)
F(1')–C(69')–C(66')	109.8(16)

Crystal structure of mw_097_3m

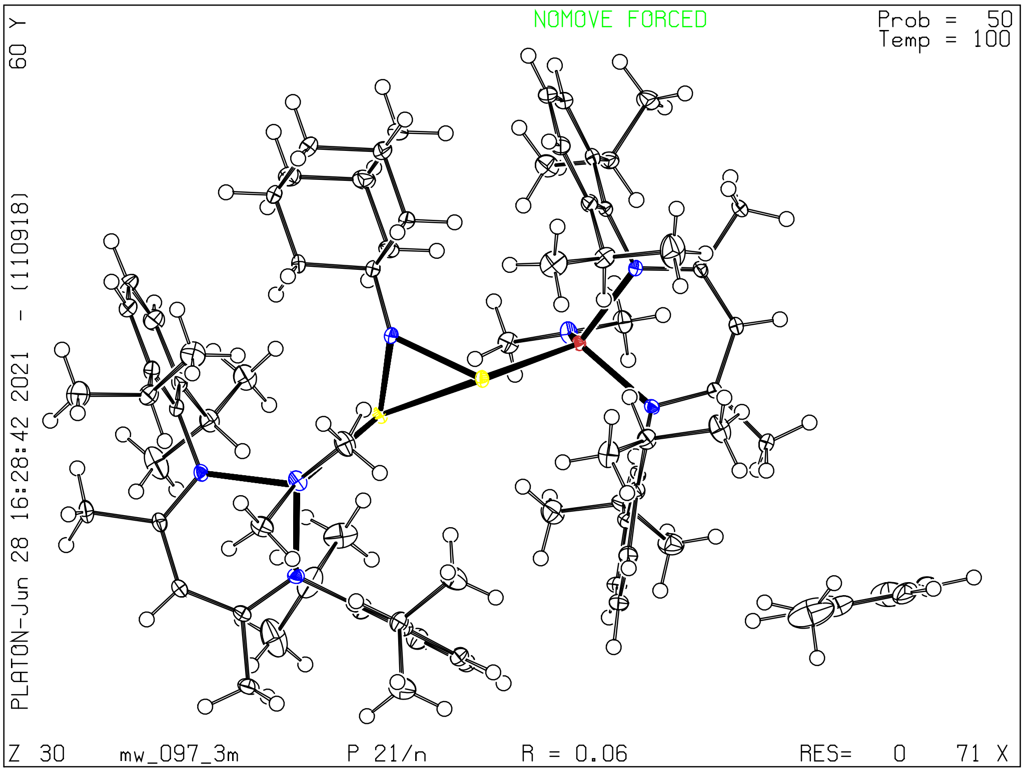

Table 1: Crystal data and structure refinement for mw_097_3m.

Identification code	mw_097_3m
Empirical Formula	$C_{79}\,H_{117}\,Ga_2\,N_7\,Sb_2$
Formula weight	1547.73 Da
Density (calculated)	$1.345\,g \cdot cm^{-3}$
$F(000)$	3216
Temperature	100(2) K
Crystal size	0.409 × 0.235 × 0.160 mm
Crystal appearance	orange block
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	$a = 10.9672(11)$ Å
	$b = 45.894(5)$ Å
	$c = 15.2335(16)$ Å
	$\alpha = 90°$
	$\beta = 94.502(5)°$
	$\gamma = 90°$
Unit cell volume	7643.8(13) $Å^3$
Z	4
Cell measurement refections used	9495
θ range for cell measurement	2.22° to 33.15°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.775° to 33.532°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.1% (97.8%)
Index ranges	$-16 \le h \le 16$
	$-70 \le k \le 70$
	$-23 \le l \le 23$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.442\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.66
R_{merg} before/after correction	0.0903/0.0643
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	368631
Independent reflections	29384 ($R_{int} = 0.0535$)
Reflections with $I > 2\sigma(I)$	26874
Data / retraints / parameter	29384 / 0 / 836
Goodness-of-fit on F^2	1.368
Weighting details	$w = 1/[\sigma^2(F_o^2) + 44.7381P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0646$
	$wR2 = 0.1299$
R indices [all data]	$R1 = 0.0713$
	$wR2 = 0.1323$
Largest diff. peak and hole	1.745 and −3.007 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Overlapping reflections

Due to the long axis the integration of the intensities was hampered by overlap. The 7 most disagreeable refections were ignored in the refinement (`OMIT`). Since the intensities might be disorted due to the overlap quantitative results should be carefully assessed.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_097_3m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	24(1)	3523(1)	7249(1)	10(1)
Sb(2)	2133(1)	3726(1)	8211(1)	10(1)
Ga(1)	702(1)	3092(1)	6239(1)	9(1)
Ga(2)	1490(1)	4254(1)	8794(1)	8(1)
N(1)	436(3)	3211(1)	4984(2)	11(1)
N(2)	−496(3)	2758(1)	6056(2)	11(1)
N(3)	2571(3)	4541(1)	8230(2)	10(1)
N(4)	2192(3)	4372(1)	10004(2)	10(1)
N(5)	2185(3)	2903(1)	6491(2)	13(1)
N(6)	−100(3)	4397(1)	8706(2)	14(1)
N(7)	926(3)	3386(1)	8454(2)	11(1)
C(1)	169(3)	3015(1)	4341(2)	12(1)
C(2)	−254(3)	2733(1)	4498(2)	14(1)
C(3)	−675(3)	2622(1)	5288(2)	13(1)
C(4)	332(4)	3097(1)	3398(2)	18(1)
C(5)	−1362(4)	2336(1)	5198(3)	20(1)
C(6)	576(3)	3512(1)	4736(2)	12(1)
C(7)	1756(3)	3631(1)	4674(2)	13(1)
C(8)	1855(4)	3921(1)	4412(2)	16(1)
C(9)	824(4)	4092(1)	4208(2)	17(1)
C(10)	−328(4)	3974(1)	4283(3)	18(1)
C(11)	−476(3)	3686(1)	4557(2)	16(1)
C(12)	2907(3)	3453(1)	4897(2)	15(1)
C(13)	3709(4)	3431(1)	4119(3)	23(1)
C(14)	3647(4)	3583(1)	5690(3)	26(1)
C(15)	−1765(4)	3569(1)	4636(3)	27(1)
C(16)	−2476(4)	3534(1)	3731(4)	40(1)
C(17)	−2481(4)	3766(1)	5230(3)	32(1)
C(18)	−1081(3)	2647(1)	6802(2)	13(1)
C(19)	−549(4)	2419(1)	7321(2)	16(1)
C(20)	−1171(4)	2319(1)	8033(3)	20(1)
C(21)	−2282(4)	2439(1)	8216(3)	23(1)
C(22)	−2784(4)	2665(1)	7712(3)	21(1)
C(23)	−2187(3)	2777(1)	7005(2)	15(1)
C(24)	653(4)	2273(1)	7146(3)	18(1)
C(25)	496(5)	1943(1)	6992(3)	28(1)
C(26)	1630(4)	2329(1)	7899(3)	27(1)
C(27)	−2735(3)	3034(1)	6478(3)	18(1)
C(28)	−3590(4)	2921(1)	5697(3)	30(1)
C(29)	−3389(4)	3252(1)	7042(3)	24(1)
C(30)	2899(3)	4794(1)	8616(2)	11(1)
C(31)	2837(3)	4846(1)	9514(2)	13(1)
C(32)	2626(3)	4641(1)	10171(2)	11(1)
C(33)	3392(4)	5041(1)	8078(2)	16(1)
C(34)	2932(4)	4737(1)	11108(2)	17(1)
C(35)	2948(3)	4490(1)	7354(2)	11(1)
C(36)	2202(3)	4574(1)	6608(2)	15(1)
C(37)	2646(4)	4532(1)	5785(2)	17(1)
C(38)	3793(4)	4412(1)	5702(2)	18(1)
C(39)	4500(4)	4323(1)	6441(2)	17(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(40)	4093(3)	4354(1)	7277(2)	13(1)
C(41)	930(4)	4702(1)	6667(2)	17(1)
C(42)	781(4)	4999(1)	6193(3)	24(1)
C(43)	−41(4)	4485(1)	6283(3)	24(1)
C(44)	4882(3)	4252(1)	8088(2)	16(1)
C(45)	5710(4)	4498(1)	8479(3)	23(1)
C(46)	5642(4)	3980(1)	7912(3)	22(1)
C(47)	2129(3)	4173(1)	10731(2)	11(1)
C(48)	1134(3)	4185(1)	11268(2)	13(1)
C(49)	1119(4)	3988(1)	11965(2)	16(1)
C(50)	2045(4)	3784(1)	12135(2)	17(1)
C(51)	3009(3)	3773(1)	11603(2)	16(1)
C(52)	3075(3)	3966(1)	10899(2)	13(1)
C(53)	86(3)	4404(1)	11121(2)	15(1)
C(54)	−140(4)	4568(1)	11972(3)	22(1)
C(55)	−1100(4)	4252(1)	10769(3)	21(1)
C(56)	4170(3)	3955(1)	10342(3)	17(1)
C(57)	5199(5)	4155(1)	10702(4)	38(1)
C(58)	4659(4)	3645(1)	10222(3)	26(1)
C(59)	2692(4)	2706(1)	5874(3)	18(1)
C(60)	3072(4)	2988(1)	7194(3)	21(1)
C(61)	−1149(3)	4240(1)	8317(3)	16(1)
C(62)	−409(4)	4694(1)	8920(3)	18(1)
C(63)	259(3)	3314(1)	9226(2)	12(1)
C(64)	−207(4)	2999(1)	9084(2)	18(1)
C(65)	−849(4)	2892(1)	9882(3)	21(1)
C(66)	50(4)	2901(1)	10702(3)	22(1)
C(67)	504(4)	3214(1)	10860(2)	18(1)
C(68)	1146(3)	3321(1)	10058(2)	15(1)
C(69)	−827(3)	3513(1)	9378(2)	16(1)
C(70)	−1491(4)	3405(1)	10173(3)	20(1)
C(71)	−1944(4)	3092(1)	10009(3)	25(1)
C(72)	−596(4)	3413(1)	10996(2)	21(1)
C11	6031(4)	5221(1)	6380(3)	28(1)
C21	4821(5)	5182(1)	6053(3)	28(1)
C31	3994(5)	5413(2)	6063(4)	40(1)
C41	4348(7)	5677(1)	6418(4)	45(2)
C51	5530(7)	5716(1)	6750(3)	43(2)
C61	6365(5)	5496(1)	6728(3)	35(1)
C71	6940(7)	4976(2)	6354(5)	56(2)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_097_3m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	10(1)	10(1)	11(1)	−2(1)	1(1)	0(1)
Sb(2)	9(1)	9(1)	13(1)	−2(1)	2(1)	−1(1)
Ga(1)	8(1)	9(1)	9(1)	−1(1)	0(1)	0(1)
Ga(2)	8(1)	9(1)	9(1)	−1(1)	1(1)	0(1)
N(1)	12(1)	13(1)	10(1)	1(1)	0(1)	0(1)
N(2)	10(1)	12(1)	12(1)	−1(1)	−1(1)	−2(1)
N(3)	10(1)	12(1)	10(1)	−2(1)	2(1)	−1(1)
N(4)	12(1)	8(1)	10(1)	0(1)	1(1)	−1(1)
N(5)	10(1)	14(1)	15(1)	−3(1)	−1(1)	3(1)
N(6)	9(1)	13(1)	21(1)	−4(1)	0(1)	2(1)
N(7)	11(1)	10(1)	11(1)	0(1)	1(1)	−3(1)
C(1)	12(1)	14(1)	10(1)	−1(1)	−1(1)	1(1)
C(2)	16(2)	13(1)	12(1)	−3(1)	0(1)	−2(1)
C(3)	12(1)	11(1)	14(1)	−2(1)	−2(1)	−1(1)
C(4)	24(2)	20(2)	10(1)	−1(1)	1(1)	0(1)
C(5)	25(2)	15(2)	20(2)	−4(1)	−2(1)	−8(1)
C(6)	15(2)	11(1)	9(1)	0(1)	0(1)	1(1)
C(7)	12(1)	15(1)	11(1)	1(1)	1(1)	−1(1)
C(8)	18(2)	14(1)	15(2)	2(1)	1(1)	−1(1)
C(9)	24(2)	13(1)	13(1)	1(1)	0(1)	0(1)
C(10)	20(2)	16(2)	18(2)	2(1)	−1(1)	5(1)
C(11)	14(2)	16(2)	18(2)	2(1)	−1(1)	2(1)
C(12)	13(2)	15(1)	18(2)	1(1)	1(1)	0(1)
C(13)	22(2)	26(2)	22(2)	−1(2)	4(2)	9(2)
C(14)	18(2)	38(2)	22(2)	−4(2)	−5(2)	5(2)
C(15)	14(2)	23(2)	45(3)	9(2)	2(2)	4(1)
C(16)	18(2)	43(3)	57(3)	−21(3)	−4(2)	1(2)
C(17)	18(2)	48(3)	30(2)	8(2)	4(2)	8(2)
C(18)	14(2)	12(1)	13(1)	−1(1)	1(1)	−5(1)
C(19)	20(2)	13(1)	16(2)	0(1)	0(1)	−4(1)
C(20)	28(2)	17(2)	15(2)	2(1)	2(1)	−8(1)
C(21)	26(2)	25(2)	17(2)	2(1)	6(2)	−13(2)
C(22)	16(2)	28(2)	20(2)	−3(1)	6(1)	−7(1)
C(23)	12(2)	17(2)	17(2)	−3(1)	1(1)	−5(1)
C(24)	23(2)	14(2)	19(2)	2(1)	1(1)	0(1)
C(25)	39(3)	15(2)	31(2)	1(2)	5(2)	3(2)
C(26)	25(2)	27(2)	27(2)	4(2)	−6(2)	1(2)
C(27)	11(2)	21(2)	22(2)	−3(1)	0(1)	−1(1)
C(28)	26(2)	25(2)	37(2)	−10(2)	−10(2)	8(2)
C(29)	14(2)	28(2)	29(2)	−6(2)	4(2)	0(1)
C(30)	12(1)	10(1)	10(1)	−1(1)	1(1)	−1(1)
C(31)	15(2)	10(1)	12(1)	−2(1)	1(1)	−2(1)
C(32)	12(1)	11(1)	10(1)	−2(1)	−1(1)	−1(1)
C(33)	21(2)	12(1)	16(2)	0(1)	3(1)	−5(1)
C(34)	24(2)	16(2)	11(1)	−3(1)	0(1)	−6(1)
C(35)	13(1)	11(1)	10(1)	−4(1)	3(1)	−1(1)
C(36)	16(2)	18(2)	11(1)	−2(1)	2(1)	−4(1)
C(37)	19(2)	21(2)	11(1)	−1(1)	3(1)	−4(1)
C(38)	22(2)	19(2)	14(2)	−4(1)	8(1)	−4(1)
C(39)	16(2)	17(2)	18(2)	−4(1)	7(1)	−2(1)
C(40)	12(1)	14(1)	15(1)	−2(1)	4(1)	−2(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(41)	18(2)	22(2)	12(1)	−1(1)	0(1)	3(1)
C(42)	29(2)	25(2)	19(2)	2(2)	0(2)	5(2)
C(43)	17(2)	30(2)	25(2)	−4(2)	2(2)	−3(2)
C(44)	10(1)	19(2)	19(2)	−2(1)	3(1)	−2(1)
C(45)	14(2)	25(2)	30(2)	−9(2)	−3(2)	2(1)
C(46)	17(2)	18(2)	32(2)	−1(2)	1(2)	1(1)
C(47)	14(1)	10(1)	9(1)	0(1)	−1(1)	−3(1)
C(48)	16(2)	11(1)	13(1)	−3(1)	1(1)	−2(1)
C(49)	20(2)	15(2)	12(1)	0(1)	2(1)	−3(1)
C(50)	24(2)	16(2)	12(1)	3(1)	−2(1)	−3(1)
C(51)	18(2)	16(2)	13(1)	3(1)	−3(1)	0(1)
C(52)	14(1)	14(1)	12(1)	1(1)	−1(1)	−2(1)
C(53)	17(2)	16(2)	14(1)	−1(1)	4(1)	1(1)
C(54)	28(2)	20(2)	18(2)	−4(1)	9(2)	3(2)
C(55)	17(2)	25(2)	22(2)	−2(1)	2(1)	2(1)
C(56)	15(2)	17(2)	20(2)	4(1)	2(1)	3(1)
C(57)	21(2)	40(3)	54(3)	−13(2)	9(2)	−9(2)
C(58)	21(2)	25(2)	33(2)	2(2)	7(2)	8(2)
C(59)	17(2)	20(2)	18(2)	−2(1)	3(1)	5(1)
C(60)	16(2)	23(2)	23(2)	−4(1)	−6(1)	1(1)
C(61)	9(1)	21(2)	19(2)	0(1)	0(1)	1(1)
C(62)	17(2)	14(2)	22(2)	−2(1)	2(1)	3(1)
C(63)	14(1)	11(1)	12(1)	−1(1)	2(1)	−3(1)
C(64)	25(2)	13(1)	15(2)	−4(1)	5(1)	−9(1)
C(65)	32(2)	17(2)	16(2)	−2(1)	7(2)	−13(2)
C(66)	32(2)	16(2)	19(2)	2(1)	5(2)	−7(2)
C(67)	24(2)	17(2)	14(2)	3(1)	0(1)	−5(1)
C(68)	17(2)	14(1)	13(1)	0(1)	1(1)	−4(1)
C(69)	14(2)	19(2)	13(1)	−2(1)	4(1)	0(1)
C(70)	20(2)	25(2)	17(2)	−3(1)	6(1)	0(1)
C(71)	22(2)	36(2)	18(2)	−3(2)	6(1)	−13(2)
C(72)	28(2)	21(2)	13(2)	−2(1)	6(1)	−6(1)
C11	29(2)	33(2)	24(2)	12(2)	7(2)	1(2)
C21	35(2)	30(2)	22(2)	−1(2)	8(2)	−16(2)
C31	24(2)	65(4)	30(2)	12(2)	7(2)	−4(2)
C41	69(4)	37(3)	31(3)	7(2)	17(3)	15(3)
C51	83(5)	31(2)	17(2)	−2(2)	6(2)	−15(3)
C61	41(3)	45(3)	18(2)	11(2)	−8(2)	−24(2)
C71	53(4)	65(4)	54(4)	27(3)	21(3)	26(3)

Table 4: Bond lengths [Å] for mw_097_3m.

Sb(1)–N(7)	2.113(3)
Sb(1)–Ga(1)	2.6477(4)
Sb(1)–Sb(2)	2.7987(4)
Sb(2)–N(7)	2.099(3)
Sb(2)–Ga(2)	2.6950(5)
Ga(1)–N(5)	1.856(3)
Ga(1)–N(1)	1.986(3)
Ga(1)–N(2)	2.026(3)
Ga(2)–N(6)	1.858(3)
Ga(2)–N(3)	2.009(3)
Ga(2)–N(4)	2.015(3)
N(1)–C(1)	1.346(4)
N(1)–C(6)	1.448(4)
N(2)–C(3)	1.326(4)
N(2)–C(18)	1.441(4)
N(3)–C(30)	1.340(4)
N(3)–C(35)	1.446(4)
N(4)–C(32)	1.340(4)
N(4)–C(47)	1.441(4)
N(5)–C(60)	1.443(5)
N(5)–C(59)	1.446(5)
N(6)–C(61)	1.444(5)
N(6)–C(62)	1.450(5)
N(7)–C(63)	1.469(4)
C(1)–C(2)	1.399(5)
C(1)–C(4)	1.510(5)
C(2)–C(3)	1.417(5)
C(3)–C(5)	1.516(5)
C(6)–C(11)	1.411(5)
C(6)–C(7)	1.413(5)
C(7)–C(8)	1.400(5)
C(7)–C(12)	1.519(5)
C(8)–C(9)	1.390(5)
C(9)–C(10)	1.388(6)
C(10)–C(11)	1.397(5)
C(11)–C(15)	1.527(6)
C(12)–C(14)	1.524(6)
C(12)–C(13)	1.533(5)
C(15)–C(17)	1.537(7)
C(15)–C(16)	1.538(7)
C(18)–C(23)	1.409(5)
C(18)–C(19)	1.410(5)
C(19)–C(20)	1.403(5)
C(19)–C(24)	1.519(6)
C(20)–C(21)	1.386(6)
C(21)–C(22)	1.381(6)
C(22)–C(23)	1.401(5)
C(23)–C(27)	1.522(6)
C(24)–C(26)	1.529(6)
C(24)–C(25)	1.542(6)
C(27)–C(29)	1.533(6)
C(27)–C(28)	1.545(6)
C(30)–C(31)	1.395(5)

Table 4: (continued)

C(30)–C(33)	1.521(5)
C(31)–C(32)	1.407(5)
C(32)–C(34)	1.507(5)
C(35)–C(36)	1.402(5)
C(35)–C(40)	1.414(5)
C(36)–C(37)	1.394(5)
C(36)–C(41)	1.524(5)
C(37)–C(38)	1.388(6)
C(38)–C(39)	1.378(6)
C(39)–C(40)	1.390(5)
C(40)–C(44)	1.525(5)
C(41)–C(43)	1.541(6)
C(41)–C(42)	1.544(6)
C(44)–C(46)	1.537(5)
C(44)–C(45)	1.542(5)
C(47)–C(52)	1.413(5)
C(47)–C(48)	1.417(5)
C(48)–C(49)	1.399(5)
C(48)–C(53)	1.528(5)
C(49)–C(50)	1.389(5)
C(50)–C(51)	1.383(5)
C(51)–C(52)	1.397(5)
C(52)–C(56)	1.525(5)
C(53)–C(55)	1.535(6)
C(53)–C(54)	1.535(5)
C(56)–C(57)	1.526(6)
C(56)–C(58)	1.533(6)
C(63)–C(69)	1.534(5)
C(63)–C(68)	1.536(5)
C(63)–C(64)	1.542(5)
C(64)–C(65)	1.533(5)
C(65)–C(66)	1.529(6)
C(65)–C(71)	1.535(7)
C(66)–C(67)	1.534(5)
C(67)–C(68)	1.537(5)
C(67)–C(72)	1.540(6)
C(69)–C(70)	1.541(5)
C(70)–C(72)	1.531(6)
C(70)–C(71)	1.537(6)
C11–C21	1.392(7)
C11–C61	1.405(7)
C11–C71	1.505(8)
C21–C31	1.393(8)
C31–C41	1.372(9)
C41–C51	1.365(10)
C51–C61	1.367(9)

Table 5: Bond angles [°] for mw_097_3m.

N(7)–Sb(1)–Ga(1)	98.55(8)
N(7)–Sb(1)–Sb(2)	48.13(8)
Ga(1)–Sb(1)–Sb(2)	107.115(13)
N(7)–Sb(2)–Ga(2)	115.24(8)
N(7)–Sb(2)–Sb(1)	48.56(8)
Ga(2)–Sb(2)–Sb(1)	104.194(12)
N(5)–Ga(1)–N(1)	112.80(13)
N(5)–Ga(1)–N(2)	102.86(13)
N(1)–Ga(1)–N(2)	91.74(12)
N(5)–Ga(1)–Sb(1)	120.71(9)
N(1)–Ga(1)–Sb(1)	109.13(9)
N(2)–Ga(1)–Sb(1)	115.88(8)
N(6)–Ga(2)–N(3)	108.69(13)
N(6)–Ga(2)–N(4)	105.11(13)
N(3)–Ga(2)–N(4)	91.13(11)
N(6)–Ga(2)–Sb(2)	124.15(9)
N(3)–Ga(2)–Sb(2)	105.67(8)
N(4)–Ga(2)–Sb(2)	116.86(8)
C(1)–N(1)–C(6)	118.1(3)
C(1)–N(1)–Ga(1)	121.7(2)
C(6)–N(1)–Ga(1)	120.2(2)
C(3)–N(2)–C(18)	119.1(3)
C(3)–N(2)–Ga(1)	121.7(2)
C(18)–N(2)–Ga(1)	119.0(2)
C(30)–N(3)–C(35)	117.4(3)
C(30)–N(3)–Ga(2)	121.8(2)
C(35)–N(3)–Ga(2)	120.6(2)
C(32)–N(4)–C(47)	118.5(3)
C(32)–N(4)–Ga(2)	121.6(2)
C(47)–N(4)–Ga(2)	119.6(2)
C(60)–N(5)–C(59)	112.3(3)
C(60)–N(5)–Ga(1)	123.8(2)
C(59)–N(5)–Ga(1)	122.2(2)
C(61)–N(6)–C(62)	111.7(3)
C(61)–N(6)–Ga(2)	124.5(2)
C(62)–N(6)–Ga(2)	123.4(2)
C(63)–N(7)–Sb(2)	131.9(2)
C(63)–N(7)–Sb(1)	122.2(2)
Sb(2)–N(7)–Sb(1)	83.30(10)
N(1)–C(1)–C(2)	123.3(3)
N(1)–C(1)–C(4)	119.4(3)
C(2)–C(1)–C(4)	117.3(3)
C(1)–C(2)–C(3)	127.6(3)
N(2)–C(3)–C(2)	123.1(3)
N(2)–C(3)–C(5)	121.6(3)
C(2)–C(3)–C(5)	115.3(3)
C(11)–C(6)–C(7)	120.6(3)
C(11)–C(6)–N(1)	119.3(3)
C(7)–C(6)–N(1)	120.1(3)
C(8)–C(7)–C(6)	118.5(3)
C(8)–C(7)–C(12)	119.6(3)
C(6)–C(7)–C(12)	121.9(3)
C(9)–C(8)–C(7)	121.4(3)

Table 5: (continued)

C(10)–C(9)–C(8)	119.5(3)
C(9)–C(10)–C(11)	121.4(4)
C(10)–C(11)–C(6)	118.7(3)
C(10)–C(11)–C(15)	119.1(3)
C(6)–C(11)–C(15)	122.2(3)
C(7)–C(12)–C(14)	110.4(3)
C(7)–C(12)–C(13)	112.2(3)
C(14)–C(12)–C(13)	109.6(3)
C(11)–C(15)–C(17)	111.0(4)
C(11)–C(15)–C(16)	111.9(4)
C(17)–C(15)–C(16)	110.0(4)
C(23)–C(18)–C(19)	121.2(3)
C(23)–C(18)–N(2)	117.8(3)
C(19)–C(18)–N(2)	121.0(3)
C(20)–C(19)–C(18)	118.2(4)
C(20)–C(19)–C(24)	118.3(3)
C(18)–C(19)–C(24)	123.6(3)
C(21)–C(20)–C(19)	120.9(4)
C(22)–C(21)–C(20)	120.4(4)
C(21)–C(22)–C(23)	120.9(4)
C(22)–C(23)–C(18)	118.4(4)
C(22)–C(23)–C(27)	120.0(3)
C(18)–C(23)–C(27)	121.6(3)
C(19)–C(24)–C(26)	111.2(3)
C(19)–C(24)–C(25)	111.7(3)
C(26)–C(24)–C(25)	109.9(3)
C(23)–C(27)–C(29)	113.1(3)
C(23)–C(27)–C(28)	109.8(3)
C(29)–C(27)–C(28)	111.6(3)
N(3)–C(30)–C(31)	123.2(3)
N(3)–C(30)–C(33)	120.2(3)
C(31)–C(30)–C(33)	116.6(3)
C(30)–C(31)–C(32)	127.2(3)
N(4)–C(32)–C(31)	124.0(3)
N(4)–C(32)–C(34)	119.9(3)
C(31)–C(32)–C(34)	116.1(3)
C(36)–C(35)–C(40)	121.3(3)
C(36)–C(35)–N(3)	120.8(3)
C(40)–C(35)–N(3)	117.9(3)
C(37)–C(36)–C(35)	118.0(3)
C(37)–C(36)–C(41)	119.5(3)
C(35)–C(36)–C(41)	122.6(3)
C(38)–C(37)–C(36)	121.3(4)
C(39)–C(38)–C(37)	120.0(3)
C(38)–C(39)–C(40)	121.1(3)
C(39)–C(40)–C(35)	118.2(3)
C(39)–C(40)–C(44)	120.5(3)
C(35)–C(40)–C(44)	121.3(3)
C(36)–C(41)–C(43)	109.6(3)
C(36)–C(41)–C(42)	112.2(3)
C(43)–C(41)–C(42)	110.4(3)
C(40)–C(44)–C(46)	113.0(3)
C(40)–C(44)–C(45)	111.5(3)

Table 5: (continued)

C(46)–C(44)–C(45)	110.6(3)
C(52)–C(47)–C(48)	120.7(3)
C(52)–C(47)–N(4)	119.1(3)
C(48)–C(47)–N(4)	120.1(3)
C(49)–C(48)–C(47)	117.8(3)
C(49)–C(48)–C(53)	118.9(3)
C(47)–C(48)–C(53)	123.2(3)
C(50)–C(49)–C(48)	121.7(3)
C(51)–C(50)–C(49)	119.8(3)
C(50)–C(51)–C(52)	121.0(3)
C(51)–C(52)–C(47)	118.9(3)
C(51)–C(52)–C(56)	119.7(3)
C(47)–C(52)–C(56)	121.4(3)
C(48)–C(53)–C(55)	111.1(3)
C(48)–C(53)–C(54)	111.6(3)
C(55)–C(53)–C(54)	109.2(3)
C(52)–C(56)–C(57)	111.8(3)
C(52)–C(56)–C(58)	113.4(3)
C(57)–C(56)–C(58)	110.3(4)
N(7)–C(63)–C(69)	115.4(3)
N(7)–C(63)–C(68)	109.4(3)
C(69)–C(63)–C(68)	108.2(3)
N(7)–C(63)–C(64)	106.1(3)
C(69)–C(63)–C(64)	109.1(3)
C(68)–C(63)–C(64)	108.5(3)
C(65)–C(64)–C(63)	110.9(3)
C(66)–C(65)–C(64)	109.4(3)
C(66)–C(65)–C(71)	110.0(3)
C(64)–C(65)–C(71)	108.7(3)
C(65)–C(66)–C(67)	109.5(3)
C(66)–C(67)–C(68)	109.8(3)
C(66)–C(67)–C(72)	109.2(3)
C(68)–C(67)–C(72)	109.3(3)
C(63)–C(68)–C(67)	110.4(3)
C(63)–C(69)–C(70)	110.3(3)
C(72)–C(70)–C(71)	109.4(3)
C(72)–C(70)–C(69)	108.9(3)
C(71)–C(70)–C(69)	109.9(3)
C(65)–C(71)–C(70)	109.5(3)
C(70)–C(72)–C(67)	109.5(3)
C21–C11–C61	117.5(5)
C21–C11–C71	120.6(5)
C61–C11–C71	121.8(6)
C11–C21–C31	120.1(5)
C41–C31–C21	120.7(5)
C51–C41–C31	119.6(6)
C41–C51–C61	120.7(5)
C51–C61–C11	121.2(5)

Crystal structure of mw_130_4m_sq

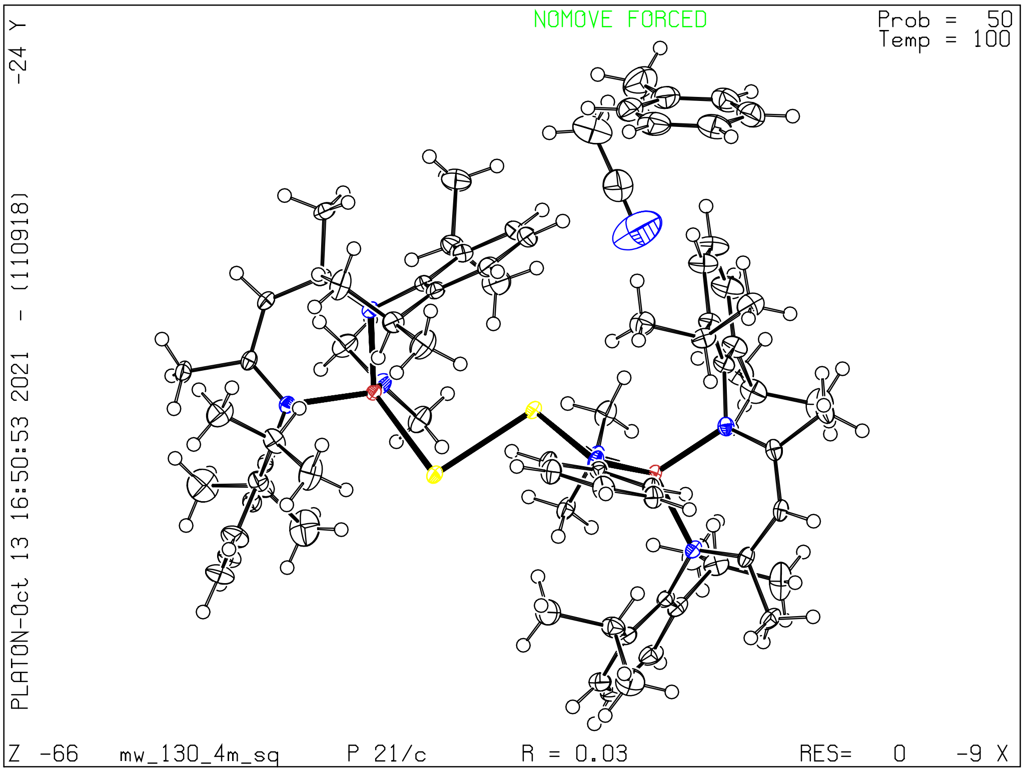

Table 1: Crystal data and structure refinement for mw_130_4m_sq.

Identification code	mw_130_4m_sq
Empirical Formula	$C_{77}H_{110}Ga_2N_8Sb_2$
Formula weight	1530.66 Da
Density (calculated)	$1.250\,g\cdot cm^{-3}$
$F(000)$	3168
Temperature	100(2) K
Crystal size	0.407 × 0.211 × 0.150 mm
Crystal appearance	red plate
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 13.6969(16)$ Å
	$b = 28.763(3)$ Å
	$c = 20.711(3)$ Å
	$\alpha = 90°$
	$\beta = 94.587(5)°$
	$\gamma = 90°$
Unit cell volume	8133.4(17) $Å^3$
Z	4
Cell measurement refections used	8909
θ range for cell measurement	2.38° to 33.13°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.726° to 34.165°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.5% (95.1%)
Index ranges	$-21 \leq h \leq 21$
	$-44 \leq k \leq 44$
	$-32 \leq l \leq 32$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.355\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.62
R_{merg} before/after correction	0.0795/0.0483
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	285425
Independent reflections	31986 ($R_{int} = 0.0430$)
Reflections with $I > 2\sigma(I)$	25883
Data / retraints / parameter	31986 / 0 / 831
Goodness-of-fit on F^2	1.060
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 6.8349P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0299$
	$wR2 = 0.0674$
R indices [all data]	$R1 = 0.0462$
	$wR2 = 0.0752$
Largest diff. peak and hole	0.899 and −0.545 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

SQUEEZE

The structure contains highly disordered solvent – likely a mixture of toluene and acetonitril. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run. (For details see: A. L. Spek, *Acta Cryst. A46* **(1990)**, 194–201). Since the nature and amount of the solvent is not clear it was not included in the sum formula.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_130_4m_sq. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	3135(1)	8145(1)	3820(1)	15(1)
Sb(2)	1569(1)	8595(1)	3277(1)	19(1)
Ga(1)	3073(1)	7070(1)	3914(1)	13(1)
Ga(2)	2624(1)	9252(1)	2842(1)	13(1)
N(1)	4168(1)	6755(1)	4386(1)	16(1)
N(2)	2264(1)	6523(1)	3767(1)	15(1)
N(3)	1802(1)	9821(1)	2652(1)	14(1)
N(4)	3604(1)	9609(1)	3412(1)	16(1)
N(5)	3284(1)	7464(1)	3169(1)	17(1)
N(6)	3238(1)	9135(1)	2079(1)	21(1)
N(7)	2557(1)	7586(1)	4314(1)	16(1)
C(1)	4009(1)	6369(1)	4717(1)	17(1)
C(2)	3133(1)	6115(1)	4648(1)	18(1)
C(3)	2355(1)	6162(1)	4174(1)	17(1)
C(4)	4787(1)	6178(1)	5199(1)	24(1)
C(5)	1590(1)	5782(1)	4132(1)	24(1)
C(6)	5123(1)	6978(1)	4448(1)	19(1)
C(7)	5762(1)	6897(1)	3953(1)	26(1)
C(8)	6640(1)	7144(1)	3983(1)	36(1)
C(9)	6888(2)	7452(1)	4482(1)	38(1)
C(10)	6271(1)	7515(1)	4972(1)	30(1)
C(11)	5379(1)	7277(1)	4969(1)	21(1)
C(12)	5507(1)	6550(1)	3411(1)	28(1)
C(13)	5720(2)	6050(1)	3630(1)	41(1)
C(14)	6040(2)	6648(1)	2799(1)	35(1)
C(15)	4757(1)	7340(1)	5541(1)	22(1)
C(16)	5327(2)	7178(1)	6174(1)	32(1)
C(17)	4429(2)	7843(1)	5623(1)	31(1)
C(18)	1541(1)	6503(1)	3221(1)	17(1)
C(19)	1835(1)	6319(1)	2636(1)	20(1)
C(20)	1135(1)	6296(1)	2108(1)	26(1)
C(21)	196(1)	6466(1)	2151(1)	28(1)
C(22)	−69(1)	6656(1)	2726(1)	27(1)
C(23)	592(1)	6672(1)	3277(1)	21(1)
C(24)	2884(1)	6168(1)	2569(1)	26(1)
C(25)	3059(2)	5662(1)	2733(1)	49(1)
C(26)	3239(2)	6272(1)	1902(1)	37(1)
C(27)	264(1)	6874(1)	3901(1)	27(1)
C(28)	−604(2)	6604(1)	4138(1)	40(1)
C(29)	−1(2)	7391(1)	3828(1)	37(1)
C(30)	2203(1)	10240(1)	2633(1)	16(1)
C(31)	3165(1)	10337(1)	2888(1)	18(1)
C(32)	3785(1)	10056(1)	3291(1)	17(1)
C(33)	1634(1)	10647(1)	2335(1)	22(1)
C(34)	4695(1)	10284(1)	3607(1)	26(1)
C(35)	761(1)	9774(1)	2499(1)	16(1)
C(36)	383(1)	9671(1)	1864(1)	20(1)
C(37)	−631(1)	9644(1)	1738(1)	28(1)
C(38)	−1251(1)	9717(1)	2224(1)	35(1)
C(39)	−870(1)	9803(1)	2850(1)	32(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(40)	135(1)	9828(1)	3003(1)	21(1)
C(41)	1032(1)	9592(1)	1313(1)	29(1)
C(42)	868(2)	9104(1)	1032(1)	51(1)
C(43)	836(2)	9955(1)	781(1)	47(1)
C(44)	528(1)	9924(1)	3699(1)	25(1)
C(45)	48(2)	9614(1)	4183(1)	38(1)
C(46)	417(2)	10432(1)	3880(1)	35(1)
C(47)	4194(1)	9368(1)	3913(1)	19(1)
C(48)	5085(1)	9159(1)	3779(1)	24(1)
C(49)	5608(1)	8913(1)	4278(1)	31(1)
C(50)	5271(1)	8873(1)	4881(1)	33(1)
C(51)	4394(1)	9077(1)	5008(1)	28(1)
C(52)	3840(1)	9329(1)	4533(1)	21(1)
C(53)	5490(1)	9184(1)	3119(1)	29(1)
C(54)	5444(2)	8705(1)	2794(1)	40(1)
C(55)	6545(1)	9370(1)	3164(1)	41(1)
C(56)	2884(1)	9554(1)	4687(1)	23(1)
C(57)	2986(2)	10074(1)	4791(1)	36(1)
C(58)	2449(2)	9338(1)	5276(1)	36(1)
C(59)	2469(1)	7453(1)	2658(1)	23(1)
C(60)	4215(1)	7493(1)	2861(1)	26(1)
C(61)	3749(1)	9480(1)	1731(1)	28(1)
C(62)	3187(2)	8697(1)	1737(1)	28(1)
C(63)	2112(1)	7608(1)	4892(1)	15(1)
C(64)	1694(1)	8022(1)	5105(1)	20(1)
C(65)	1252(1)	8040(1)	5685(1)	24(1)
C(66)	1206(1)	7649(1)	6076(1)	24(1)
C(67)	1598(1)	7235(1)	5868(1)	21(1)
C(68)	2046(1)	7212(1)	5289(1)	18(1)
C11	8409(2)	8369(1)	5354(1)	40(1)
C21	7735(2)	8630(1)	5676(2)	46(1)
C31	7392(2)	8473(1)	6250(1)	44(1)
C41	7705(2)	8056(1)	6515(1)	44(1)
C51	8378(2)	7793(1)	6205(1)	41(1)
C61	8722(2)	7953(1)	5630(1)	38(1)
C71	8782(2)	8527(1)	4724(2)	62(1)
C12	8082(2)	8115(1)	2682(2)	61(1)
N12	7536(3)	7827(1)	2656(2)	106(1)
C22	8759(3)	8482(2)	2689(2)	95(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_130_4m_sq.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	18(1)	11(1)	16(1)	−1(1)	2(1)	−1(1)
Sb(2)	17(1)	13(1)	27(1)	4(1)	2(1)	−2(1)
Ga(1)	16(1)	10(1)	12(1)	0(1)	2(1)	1(1)
Ga(2)	14(1)	11(1)	15(1)	0(1)	2(1)	0(1)
N(1)	18(1)	15(1)	14(1)	0(1)	1(1)	2(1)
N(2)	19(1)	12(1)	15(1)	0(1)	1(1)	−2(1)
N(3)	15(1)	13(1)	14(1)	1(1)	3(1)	0(1)
N(4)	16(1)	14(1)	18(1)	1(1)	1(1)	−2(1)
N(5)	23(1)	13(1)	14(1)	1(1)	4(1)	−1(1)
N(6)	24(1)	17(1)	22(1)	−4(1)	10(1)	−1(1)
N(7)	24(1)	11(1)	16(1)	−1(1)	6(1)	2(1)
C(1)	21(1)	18(1)	13(1)	−1(1)	2(1)	6(1)
C(2)	24(1)	14(1)	16(1)	3(1)	2(1)	3(1)
C(3)	23(1)	12(1)	15(1)	−1(1)	5(1)	1(1)
C(4)	26(1)	26(1)	21(1)	4(1)	−2(1)	7(1)
C(5)	32(1)	17(1)	24(1)	3(1)	3(1)	−7(1)
C(6)	16(1)	25(1)	17(1)	0(1)	3(1)	0(1)
C(7)	20(1)	36(1)	20(1)	−2(1)	4(1)	1(1)
C(8)	22(1)	58(1)	28(1)	−4(1)	9(1)	−5(1)
C(9)	25(1)	58(1)	33(1)	−7(1)	6(1)	−16(1)
C(10)	25(1)	41(1)	24(1)	−5(1)	2(1)	−9(1)
C(11)	19(1)	27(1)	16(1)	−1(1)	2(1)	−2(1)
C(12)	25(1)	38(1)	22(1)	−8(1)	7(1)	4(1)
C(13)	52(1)	40(1)	32(1)	−6(1)	14(1)	10(1)
C(14)	31(1)	50(1)	25(1)	−6(1)	11(1)	7(1)
C(15)	25(1)	26(1)	17(1)	−4(1)	4(1)	−5(1)
C(16)	42(1)	35(1)	19(1)	1(1)	2(1)	−8(1)
C(17)	36(1)	28(1)	28(1)	−9(1)	2(1)	−1(1)
C(18)	21(1)	14(1)	16(1)	1(1)	−1(1)	−4(1)
C(19)	28(1)	16(1)	16(1)	0(1)	1(1)	−6(1)
C(20)	35(1)	25(1)	17(1)	0(1)	−1(1)	−10(1)
C(21)	33(1)	27(1)	24(1)	4(1)	−9(1)	−12(1)
C(22)	24(1)	25(1)	31(1)	3(1)	−6(1)	−6(1)
C(23)	22(1)	17(1)	24(1)	1(1)	−1(1)	−4(1)
C(24)	30(1)	30(1)	17(1)	−6(1)	5(1)	−2(1)
C(25)	56(2)	39(1)	54(1)	17(1)	24(1)	19(1)
C(26)	52(1)	30(1)	31(1)	−2(1)	21(1)	0(1)
C(27)	20(1)	30(1)	30(1)	−4(1)	3(1)	1(1)
C(28)	32(1)	45(1)	45(1)	2(1)	15(1)	−1(1)
C(29)	32(1)	31(1)	48(1)	−8(1)	3(1)	4(1)
C(30)	21(1)	13(1)	14(1)	1(1)	4(1)	0(1)
C(31)	21(1)	13(1)	20(1)	2(1)	3(1)	−3(1)
C(32)	19(1)	15(1)	18(1)	−1(1)	2(1)	−4(1)
C(33)	26(1)	15(1)	26(1)	5(1)	2(1)	1(1)
C(34)	26(1)	20(1)	30(1)	2(1)	−5(1)	−9(1)
C(35)	16(1)	14(1)	18(1)	3(1)	2(1)	1(1)
C(36)	21(1)	20(1)	20(1)	0(1)	−1(1)	1(1)
C(37)	23(1)	31(1)	29(1)	−2(1)	−6(1)	−1(1)
C(38)	17(1)	46(1)	42(1)	−1(1)	−1(1)	−4(1)
C(39)	18(1)	45(1)	35(1)	2(1)	6(1)	−1(1)
C(40)	18(1)	24(1)	21(1)	4(1)	5(1)	1(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(41)	27(1)	42(1)	17(1)	−6(1)	−2(1)	5(1)
C(42)	72(2)	45(1)	36(1)	−16(1)	6(1)	14(1)
C(43)	56(2)	59(2)	26(1)	6(1)	9(1)	0(1)
C(44)	23(1)	35(1)	18(1)	6(1)	7(1)	6(1)
C(45)	59(1)	30(1)	27(1)	7(1)	21(1)	6(1)
C(46)	48(1)	34(1)	24(1)	2(1)	4(1)	−6(1)
C(47)	18(1)	15(1)	23(1)	2(1)	−4(1)	−3(1)
C(48)	19(1)	19(1)	34(1)	−1(1)	−3(1)	−3(1)
C(49)	20(1)	24(1)	49(1)	4(1)	−9(1)	0(1)
C(50)	30(1)	26(1)	40(1)	10(1)	−17(1)	−4(1)
C(51)	33(1)	23(1)	26(1)	6(1)	−10(1)	−8(1)
C(52)	24(1)	17(1)	22(1)	2(1)	−6(1)	−5(1)
C(53)	18(1)	30(1)	39(1)	−2(1)	4(1)	1(1)
C(54)	32(1)	37(1)	53(1)	−12(1)	13(1)	2(1)
C(55)	21(1)	48(1)	56(1)	3(1)	6(1)	−6(1)
C(56)	27(1)	26(1)	16(1)	2(1)	−1(1)	−3(1)
C(57)	50(1)	22(1)	38(1)	3(1)	10(1)	4(1)
C(58)	51(1)	30(1)	29(1)	2(1)	13(1)	−5(1)
C(59)	37(1)	14(1)	16(1)	1(1)	−3(1)	−2(1)
C(60)	33(1)	21(1)	25(1)	1(1)	15(1)	1(1)
C(61)	30(1)	27(1)	27(1)	−3(1)	13(1)	−5(1)
C(62)	40(1)	21(1)	26(1)	−7(1)	11(1)	1(1)
C(63)	16(1)	14(1)	16(1)	−2(1)	2(1)	0(1)
C(64)	26(1)	15(1)	20(1)	−2(1)	6(1)	3(1)
C(65)	29(1)	22(1)	22(1)	−4(1)	7(1)	5(1)
C(66)	27(1)	29(1)	18(1)	−1(1)	8(1)	4(1)
C(67)	24(1)	22(1)	18(1)	2(1)	4(1)	2(1)
C(68)	21(1)	15(1)	18(1)	0(1)	3(1)	2(1)
C11	29(1)	37(1)	53(1)	−6(1)	3(1)	−7(1)
C21	32(1)	29(1)	75(2)	−10(1)	−4(1)	−1(1)
C31	30(1)	47(1)	57(1)	−26(1)	4(1)	−2(1)
C41	34(1)	61(2)	36(1)	−12(1)	−1(1)	−5(1)
C51	34(1)	45(1)	42(1)	−4(1)	−5(1)	1(1)
C61	26(1)	44(1)	43(1)	−11(1)	2(1)	3(1)
C71	60(2)	53(2)	75(2)	12(2)	17(2)	−14(1)
C12	56(2)	50(2)	75(2)	−1(1)	−6(2)	4(1)
N12	105(3)	82(2)	134(3)	−23(2)	37(3)	−35(2)
C22	51(2)	86(3)	141(4)	4(3)	−30(2)	−11(2)

Table 4: Bond lengths [Å] for mw_130_4m_sq.

Sb(1)–N(7)	2.0955(13)
Sb(1)–N(5)	2.3949(13)
Sb(1)–Sb(2)	2.6750(3)
Sb(1)–Ga(1)	3.0988(4)
Sb(2)–Ga(2)	2.5842(3)
Ga(1)–N(7)	1.8649(12)
Ga(1)–N(2)	1.9341(12)
Ga(1)–N(1)	1.9472(13)
Ga(1)–N(5)	1.9545(13)
Ga(2)–N(6)	1.8775(13)
Ga(2)–N(4)	1.9994(13)
Ga(2)–N(3)	2.0085(12)
N(1)–C(1)	1.333(2)
N(1)–C(6)	1.454(2)
N(2)–C(3)	1.3377(19)
N(2)–C(18)	1.443(2)
N(3)–C(30)	1.3266(18)
N(3)–C(35)	1.4420(19)
N(4)–C(32)	1.3350(19)
N(4)–C(47)	1.441(2)
N(5)–C(60)	1.472(2)
N(5)–C(59)	1.476(2)
N(6)–C(61)	1.440(2)
N(6)–C(62)	1.444(2)
N(7)–C(63)	1.3880(19)
C(1)–C(2)	1.402(2)
C(1)–C(4)	1.504(2)
C(2)–C(3)	1.396(2)
C(3)–C(5)	1.512(2)
C(6)–C(11)	1.404(2)
C(6)–C(7)	1.418(2)
C(7)–C(8)	1.394(3)
C(7)–C(12)	1.520(3)
C(8)–C(9)	1.384(3)
C(9)–C(10)	1.384(3)
C(10)–C(11)	1.399(2)
C(11)–C(15)	1.524(2)
C(12)–C(13)	1.531(3)
C(12)–C(14)	1.538(3)
C(15)–C(17)	1.529(3)
C(15)–C(16)	1.542(3)
C(18)–C(23)	1.403(2)
C(18)–C(19)	1.410(2)
C(19)–C(20)	1.396(2)
C(19)–C(24)	1.517(3)
C(20)–C(21)	1.385(3)
C(21)–C(22)	1.385(3)
C(22)–C(23)	1.400(2)
C(23)–C(27)	1.517(2)
C(24)–C(25)	1.508(3)
C(24)–C(26)	1.529(3)
C(27)–C(28)	1.533(3)
C(27)–C(29)	1.534(3)

Table 4: (continued)

C(30)–C(31)	1.407(2)
C(30)–C(33)	1.510(2)
C(31)–C(32)	1.400(2)
C(32)–C(34)	1.512(2)
C(35)–C(36)	1.405(2)
C(35)–C(40)	1.412(2)
C(36)–C(37)	1.395(2)
C(36)–C(41)	1.518(2)
C(37)–C(38)	1.383(3)
C(38)–C(39)	1.380(3)
C(39)–C(40)	1.390(2)
C(40)–C(44)	1.522(2)
C(41)–C(43)	1.528(3)
C(41)–C(42)	1.528(3)
C(44)–C(46)	1.520(3)
C(44)–C(45)	1.528(3)
C(47)–C(48)	1.407(2)
C(47)–C(52)	1.413(2)
C(48)–C(49)	1.402(3)
C(48)–C(53)	1.517(3)
C(49)–C(50)	1.369(3)
C(50)–C(51)	1.381(3)
C(51)–C(52)	1.397(2)
C(52)–C(56)	1.517(2)
C(53)–C(54)	1.532(3)
C(53)–C(55)	1.537(3)
C(56)–C(57)	1.515(3)
C(56)–C(58)	1.533(3)
C(63)–C(64)	1.408(2)
C(63)–C(68)	1.411(2)
C(64)–C(65)	1.389(2)
C(65)–C(66)	1.388(2)
C(66)–C(67)	1.391(2)
C(67)–C(68)	1.391(2)
C11–C61	1.379(3)
C11–C21	1.400(3)
C11–C71	1.508(4)
C21–C31	1.389(4)
C31–C41	1.374(4)
C41–C51	1.389(3)
C51–C61	1.394(3)
C12–N12	1.114(4)
C12–C22	1.404(5)

Table 5: Bond angles [°] for mw_130_4m_sq.

N(7)–Sb(1)–N(5)	72.54(5)
N(7)–Sb(1)–Sb(2)	104.79(4)
N(5)–Sb(1)–Sb(2)	105.11(3)
N(7)–Sb(1)–Ga(1)	35.93(3)
N(5)–Sb(1)–Ga(1)	39.10(3)
Sb(2)–Sb(1)–Ga(1)	118.960(7)
Ga(2)–Sb(2)–Sb(1)	92.794(10)
N(7)–Ga(1)–N(2)	118.96(6)
N(7)–Ga(1)–N(1)	116.80(6)
N(2)–Ga(1)–N(1)	96.25(5)
N(7)–Ga(1)–N(5)	88.57(5)
N(2)–Ga(1)–N(5)	117.79(5)
N(1)–Ga(1)–N(5)	120.64(6)
N(7)–Ga(1)–Sb(1)	41.25(4)
N(2)–Ga(1)–Sb(1)	145.06(4)
N(1)–Ga(1)–Sb(1)	118.16(4)
N(5)–Ga(1)–Sb(1)	50.61(4)
N(6)–Ga(2)–N(4)	105.33(6)
N(6)–Ga(2)–N(3)	105.25(6)
N(4)–Ga(2)–N(3)	92.10(5)
N(6)–Ga(2)–Sb(2)	117.55(4)
N(4)–Ga(2)–Sb(2)	122.50(4)
N(3)–Ga(2)–Sb(2)	110.12(4)
C(1)–N(1)–C(6)	120.33(13)
C(1)–N(1)–Ga(1)	119.71(11)
C(6)–N(1)–Ga(1)	119.40(10)
C(3)–N(2)–C(18)	119.14(12)
C(3)–N(2)–Ga(1)	120.54(10)
C(18)–N(2)–Ga(1)	120.31(9)
C(30)–N(3)–C(35)	119.00(12)
C(30)–N(3)–Ga(2)	121.25(10)
C(35)–N(3)–Ga(2)	119.68(9)
C(32)–N(4)–C(47)	119.76(13)
C(32)–N(4)–Ga(2)	120.60(11)
C(47)–N(4)–Ga(2)	119.28(9)
C(60)–N(5)–C(59)	108.83(13)
C(60)–N(5)–Ga(1)	124.21(11)
C(59)–N(5)–Ga(1)	113.71(10)
C(60)–N(5)–Sb(1)	108.20(10)
C(59)–N(5)–Sb(1)	109.17(9)
Ga(1)–N(5)–Sb(1)	90.29(5)
C(61)–N(6)–C(62)	111.10(13)
C(61)–N(6)–Ga(2)	124.53(11)
C(62)–N(6)–Ga(2)	124.18(11)
C(63)–N(7)–Ga(1)	128.90(10)
C(63)–N(7)–Sb(1)	126.53(10)
Ga(1)–N(7)–Sb(1)	102.81(6)
N(1)–C(1)–C(2)	123.75(14)
N(1)–C(1)–C(4)	120.60(15)
C(2)–C(1)–C(4)	115.65(14)
C(3)–C(2)–C(1)	128.22(14)
N(2)–C(3)–C(2)	123.21(14)
N(2)–C(3)–C(5)	119.70(14)

Table 5: (continued)

C(2)–C(3)–C(5)	117.10(14)
C(11)–C(6)–C(7)	121.72(15)
C(11)–C(6)–N(1)	120.38(13)
C(7)–C(6)–N(1)	117.85(14)
C(8)–C(7)–C(6)	117.65(17)
C(8)–C(7)–C(12)	120.86(16)
C(6)–C(7)–C(12)	121.49(16)
C(9)–C(8)–C(7)	121.25(17)
C(10)–C(9)–C(8)	120.29(18)
C(9)–C(10)–C(11)	121.07(18)
C(10)–C(11)–C(6)	117.93(15)
C(10)–C(11)–C(15)	118.71(15)
C(6)–C(11)–C(15)	123.31(14)
C(7)–C(12)–C(13)	111.80(17)
C(7)–C(12)–C(14)	113.15(17)
C(13)–C(12)–C(14)	108.89(16)
C(11)–C(15)–C(17)	112.67(15)
C(11)–C(15)–C(16)	110.39(15)
C(17)–C(15)–C(16)	108.90(15)
C(23)–C(18)–C(19)	122.19(15)
C(23)–C(18)–N(2)	120.22(14)
C(19)–C(18)–N(2)	117.57(14)
C(20)–C(19)–C(18)	117.67(16)
C(20)–C(19)–C(24)	120.70(15)
C(18)–C(19)–C(24)	121.58(14)
C(21)–C(20)–C(19)	121.11(17)
C(22)–C(21)–C(20)	120.20(16)
C(21)–C(22)–C(23)	121.16(17)
C(22)–C(23)–C(18)	117.60(16)
C(22)–C(23)–C(27)	119.46(16)
C(18)–C(23)–C(27)	122.94(15)
C(25)–C(24)–C(19)	112.99(16)
C(25)–C(24)–C(26)	109.62(16)
C(19)–C(24)–C(26)	113.49(16)
C(23)–C(27)–C(28)	111.65(16)
C(23)–C(27)–C(29)	111.70(16)
C(28)–C(27)–C(29)	109.85(16)
N(3)–C(30)–C(31)	123.18(13)
N(3)–C(30)–C(33)	120.87(14)
C(31)–C(30)–C(33)	115.95(13)
C(32)–C(31)–C(30)	127.84(14)
N(4)–C(32)–C(31)	123.74(14)
N(4)–C(32)–C(34)	119.77(14)
C(31)–C(32)–C(34)	116.48(13)
C(36)–C(35)–C(40)	121.05(14)
C(36)–C(35)–N(3)	120.56(13)
C(40)–C(35)–N(3)	118.38(13)
C(37)–C(36)–C(35)	118.22(15)
C(37)–C(36)–C(41)	119.05(15)
C(35)–C(36)–C(41)	122.73(15)
C(38)–C(37)–C(36)	121.07(17)
C(39)–C(38)–C(37)	120.15(17)
C(38)–C(39)–C(40)	121.13(18)

Table 5: (continued)

C(39)–C(40)–C(35)	118.28(16)
C(39)–C(40)–C(44)	119.63(15)
C(35)–C(40)–C(44)	122.07(14)
C(36)–C(41)–C(43)	111.10(17)
C(36)–C(41)–C(42)	110.37(18)
C(43)–C(41)–C(42)	109.90(18)
C(46)–C(44)–C(40)	111.92(15)
C(46)–C(44)–C(45)	109.98(15)
C(40)–C(44)–C(45)	112.20(17)
C(48)–C(47)–C(52)	120.79(15)
C(48)–C(47)–N(4)	120.60(15)
C(52)–C(47)–N(4)	118.57(14)
C(49)–C(48)–C(47)	118.00(18)
C(49)–C(48)–C(53)	119.10(17)
C(47)–C(48)–C(53)	122.89(16)
C(50)–C(49)–C(48)	121.75(18)
C(49)–C(50)–C(51)	119.89(17)
C(50)–C(51)–C(52)	121.26(18)
C(51)–C(52)–C(47)	118.31(17)
C(51)–C(52)–C(56)	120.17(16)
C(47)–C(52)–C(56)	121.52(14)
C(48)–C(53)–C(54)	110.44(17)
C(48)–C(53)–C(55)	111.78(17)
C(54)–C(53)–C(55)	110.14(17)
C(57)–C(56)–C(52)	112.32(15)
C(57)–C(56)–C(58)	109.00(16)
C(52)–C(56)–C(58)	113.05(15)
N(7)–C(63)–C(64)	121.80(13)
N(7)–C(63)–C(68)	121.26(13)
C(64)–C(63)–C(68)	116.94(13)
C(65)–C(64)–C(63)	121.26(15)
C(66)–C(65)–C(64)	121.14(15)
C(65)–C(66)–C(67)	118.50(15)
C(66)–C(67)–C(68)	120.94(15)
C(67)–C(68)–C(63)	121.20(14)
C61–C11–C21	117.6(2)
C61–C11–C71	120.3(2)
C21–C11–C71	122.1(2)
C31–C21–C11	121.0(2)
C41–C31–C21	120.7(2)
C31–C41–C51	119.3(2)
C41–C51–C61	119.8(2)
C11–C61–C51	121.8(2)
N12–C12–C22	177.8(5)

Crystal structure of mw_143_4m

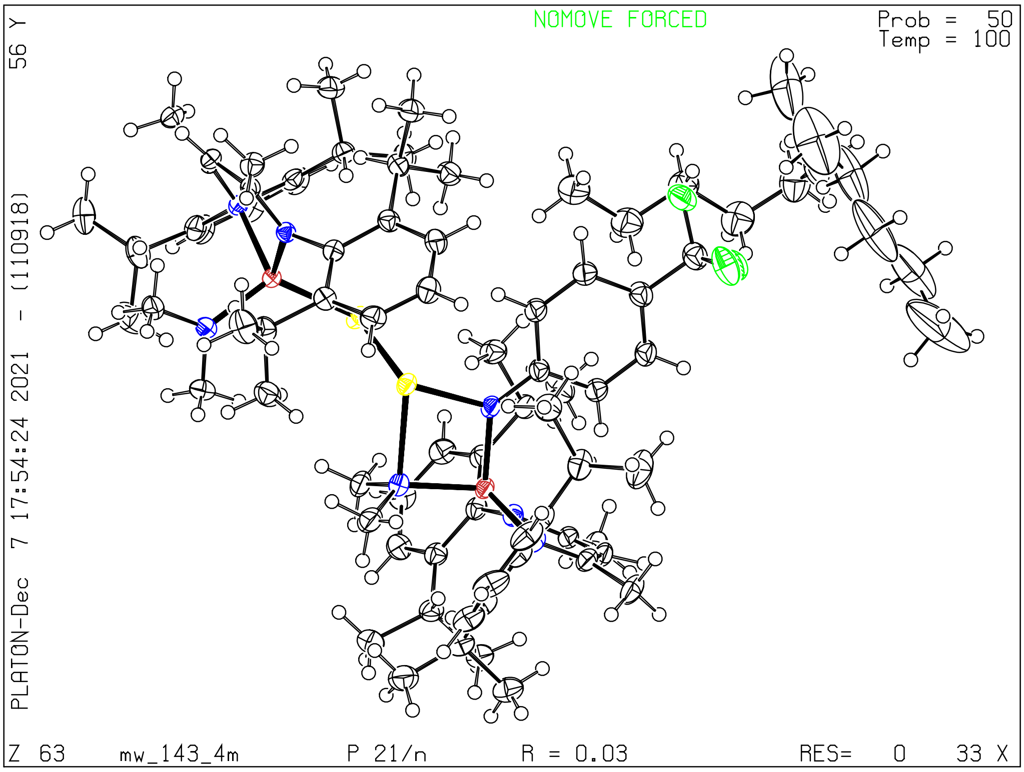

Table 1: Crystal data and structure refinement for mw_143_4m.

Identification code	mw_143_4m
Empirical Formula	$C_{78}H_{119}F_3Ga_2N_7Sb_2$
Formula weight	1594.73 Da
Density (calculated)	$1.338\,g\cdot cm^{-3}$
$F(000)$	3308
Temperature	100(2) K
Crystal size	0.186 × 0.064 × 0.063 mm
Crystal appearance	orange tablet
Wavelength (CuK_α)	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	$a = 12.1758(10)$ Å
	$b = 27.211(2)$ Å
	$c = 24.248(2)$ Å
	$\alpha = 90°$
	$\beta = 99.805(3)°$
	$\gamma = 90°$
Unit cell volume	7916.1(11) $Å^3$
Z	4
Cell measurement refections used	9912
θ range for cell measurement	2.46° to 79.73°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	2.461° to 80.082°
Completeness to $\theta = 67.679°$ (to θ_{max})	100.0% (99.1%)
Index ranges	$-15 \leq h \leq 14$
	$-34 \leq k \leq 34$
	$-30 \leq l \leq 30$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$6.527\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.54
R_{merg} before/after correction	0.1444/0.0748
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	249345
Independent reflections	17136 ($R_{int} = 0.0710$)
Reflections with $I > 2\sigma(I)$	15060
Data / retraints / parameter	17136 / 129 / 884
Goodness-of-fit on F^2	1.051
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 8.8255P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0322$
	$wR2 = 0.0824$
R indices [all data]	$R1 = 0.0398$
	$wR2 = 0.0893$
Largest diff. peak and hole	1.063 and -0.593 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

The bond lengths of the solvent molecules were restrained to be equal (`SADI`) and `RIGU` restraints were applied to their atoms' displacement parameters. One n-hexane molecule is disordered over a centre of inversion. Additional `SIMU` restraints were used for the refinement of the displacement parameters of this molecule. The local symmetry was ignored in the refinement (negative `PART`). The displacement ellipsiods suggest further disorder that could not be resolved.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_143_4m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	828(1)	1320(1)	2748(1)	26(1)
Sb(2)	2936(1)	1509(1)	2658(1)	23(1)
Ga(1)	1248(1)	472(1)	3217(1)	19(1)
Ga(2)	3088(1)	2282(1)	1704(1)	22(1)
F(1)	2670(2)	4222(1)	3856(1)	47(1)
F(2)	4222(2)	3920(1)	4252(1)	56(1)
F(3)	2707(2)	3689(1)	4512(1)	52(1)
N(1)	2294(2)	384(1)	3943(1)	20(1)
N(2)	−72(2)	294(1)	3579(1)	21(1)
N(3)	1462(2)	−65(1)	2768(1)	28(1)
N(4)	4483(2)	2569(1)	1565(1)	25(1)
N(5)	2105(2)	2706(1)	1190(1)	24(1)
N(6)	2869(2)	1573(1)	1656(1)	29(1)
N(7)	2903(2)	2264(1)	2455(1)	25(1)
C(1)	2094(2)	53(1)	4319(1)	22(1)
C(2)	1049(2)	−164(1)	4315(1)	24(1)
C(3)	18(2)	−20(1)	4002(1)	23(1)
C(4)	3026(2)	−96(1)	4786(1)	30(1)
C(5)	−1009(2)	−240(1)	4179(1)	29(1)
C(6)	3318(2)	662(1)	4044(1)	22(1)
C(7)	4243(2)	509(1)	3814(1)	26(1)
C(8)	5187(2)	806(1)	3888(1)	31(1)
C(9)	5230(2)	1241(1)	4187(1)	33(1)
C(10)	4325(2)	1382(1)	4427(1)	31(1)
C(11)	3359(2)	1096(1)	4365(1)	26(1)
C(12)	4244(2)	27(1)	3494(1)	30(1)
C(13)	5207(3)	−302(1)	3767(2)	46(1)
C(14)	4310(3)	118(1)	2879(1)	38(1)
C(15)	2410(2)	1250(1)	4666(1)	27(1)
C(16)	2779(3)	1242(1)	5302(1)	36(1)
C(17)	1970(2)	1764(1)	4485(1)	32(1)
C(18)	−1145(2)	479(1)	3316(1)	24(1)
C(19)	−1808(2)	210(1)	2888(1)	29(1)
C(20)	−2803(2)	424(1)	2617(1)	34(1)
C(21)	−3147(2)	876(1)	2770(1)	37(1)
C(22)	−2499(2)	1132(1)	3201(1)	33(1)
C(23)	−1483(2)	945(1)	3478(1)	25(1)
C(24)	−1511(2)	−298(1)	2711(1)	37(1)
C(25)	−2409(3)	−671(1)	2816(2)	45(1)
C(27)	−779(2)	1242(1)	3941(1)	26(1)
C(26)	−1374(3)	−306(2)	2099(2)	53(1)
C(28)	−994(3)	1083(1)	4518(1)	41(1)
C(29)	−954(2)	1798(1)	3870(1)	32(1)
C(30)	2443(2)	3157(1)	1080(1)	26(1)
C(31)	3545(2)	3316(1)	1210(1)	28(1)
C(32)	4501(2)	3037(1)	1400(1)	29(1)
C(33)	1598(3)	3527(1)	792(1)	33(1)
C(34)	5602(3)	3297(1)	1412(1)	39(1)
C(35)	984(2)	2549(1)	955(1)	25(1)
C(36)	837(2)	2279(1)	454(1)	27(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(37)	−227(2)	2112(1)	238(1)	33(1)
C(38)	−1119(2)	2207(1)	508(1)	37(1)
C(39)	−959(2)	2479(1)	995(1)	34(1)
C(40)	89(2)	2659(1)	1231(1)	28(1)
C(41)	1816(2)	2161(1)	156(1)	29(1)
C(42)	2082(3)	2594(1)	−206(1)	41(1)
C(43)	1647(3)	1701(1)	−210(1)	38(1)
C(44)	226(2)	2957(1)	1770(1)	30(1)
C(45)	−651(3)	3369(1)	1737(1)	45(1)
C(46)	136(3)	2634(1)	2274(1)	34(1)
C(47)	5530(2)	2302(1)	1695(1)	30(1)
C(48)	5847(2)	2002(1)	1275(1)	32(1)
C(49)	6851(3)	1742(1)	1401(1)	41(1)
C(50)	7522(3)	1791(2)	1922(2)	46(1)
C(51)	7200(3)	2088(1)	2322(1)	43(1)
C(52)	6198(2)	2346(1)	2228(1)	33(1)
C(53)	5132(2)	1961(1)	699(1)	33(1)
C(54)	5327(3)	2392(1)	320(1)	41(1)
C(55)	5312(3)	1480(1)	398(2)	44(1)
C(56)	5881(3)	2658(1)	2691(1)	39(1)
C(57)	6795(4)	3040(2)	2903(2)	67(1)
C(58)	5678(2)	2345(1)	3189(1)	35(1)
C(59)	1568(3)	−561(1)	2975(1)	32(1)
C(60)	1547(3)	−35(1)	2179(1)	33(1)
C(61)	1776(3)	1404(1)	1365(1)	35(1)
C(62)	3731(3)	1237(1)	1524(2)	43(1)
C(63)	2935(2)	2633(1)	2839(1)	25(1)
C(64)	3051(2)	3131(1)	2691(1)	30(1)
C(65)	3101(3)	3503(1)	3082(1)	32(1)
C(66)	3028(2)	3402(1)	3637(1)	31(1)
C(67)	2899(2)	2916(1)	3791(1)	32(1)
C(68)	2848(2)	2544(1)	3403(1)	30(1)
C(69)	3148(3)	3804(1)	4059(1)	37(1)
C11	−222(4)	3186(2)	3794(2)	55(1)
C21	−183(3)	3676(1)	3498(2)	51(1)
C31	−162(3)	4114(1)	3883(2)	48(1)
C41	−64(3)	4606(1)	3600(2)	55(1)
C51	−77(4)	5056(2)	3974(2)	64(1)
C61	959(5)	5100(2)	4420(2)	77(1)
C12	3780(20)	4294(6)	5904(11)	129(9)
C22	4700(20)	4479(9)	5630(9)	141(9)
C32	4308(15)	4868(6)	5199(9)	109(6)
C42	5305(18)	5000(10)	4927(12)	134(8)
C52	5110(20)	5396(9)	4489(10)	141(8)
C62	6150(20)	5530(11)	4234(12)	186(11)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_143_4m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	27(1)	22(1)	31(1)	8(1)	8(1)	1(1)
Sb(2)	26(1)	20(1)	24(1)	4(1)	3(1)	−2(1)
Ga(1)	21(1)	18(1)	19(1)	1(1)	4(1)	−1(1)
Ga(2)	25(1)	19(1)	21(1)	3(1)	2(1)	−4(1)
F(1)	70(1)	30(1)	39(1)	−1(1)	4(1)	14(1)
F(2)	53(1)	48(1)	60(1)	−24(1)	−10(1)	−1(1)
F(3)	89(2)	38(1)	32(1)	−4(1)	17(1)	2(1)
N(1)	21(1)	20(1)	20(1)	0(1)	2(1)	0(1)
N(2)	20(1)	19(1)	23(1)	1(1)	5(1)	−1(1)
N(3)	40(1)	22(1)	23(1)	−2(1)	10(1)	1(1)
N(4)	26(1)	25(1)	24(1)	6(1)	2(1)	−5(1)
N(5)	27(1)	21(1)	21(1)	2(1)	1(1)	−2(1)
N(6)	36(1)	22(1)	29(1)	0(1)	9(1)	−4(1)
N(7)	32(1)	20(1)	22(1)	3(1)	3(1)	−4(1)
C(1)	26(1)	19(1)	21(1)	0(1)	4(1)	2(1)
C(2)	30(1)	21(1)	21(1)	4(1)	6(1)	−1(1)
C(3)	27(1)	20(1)	24(1)	−2(1)	8(1)	−4(1)
C(4)	32(1)	29(1)	26(1)	5(1)	0(1)	1(1)
C(5)	28(1)	29(1)	31(1)	2(1)	10(1)	−4(1)
C(6)	21(1)	23(1)	22(1)	2(1)	1(1)	0(1)
C(7)	23(1)	27(1)	26(1)	−1(1)	2(1)	1(1)
C(8)	22(1)	39(2)	32(1)	−2(1)	6(1)	−2(1)
C(9)	24(1)	38(2)	37(2)	−5(1)	2(1)	−9(1)
C(10)	31(1)	31(1)	30(1)	−6(1)	2(1)	−7(1)
C(11)	25(1)	28(1)	23(1)	−2(1)	2(1)	−2(1)
C(12)	23(1)	29(1)	40(2)	−6(1)	8(1)	2(1)
C(13)	38(2)	38(2)	60(2)	−5(2)	3(2)	14(1)
C(14)	35(2)	42(2)	39(2)	−11(1)	12(1)	−4(1)
C(15)	29(1)	25(1)	27(1)	−4(1)	6(1)	−1(1)
C(16)	45(2)	37(2)	28(1)	0(1)	10(1)	2(1)
C(17)	36(1)	31(1)	30(1)	−1(1)	7(1)	4(1)
C(18)	21(1)	25(1)	25(1)	4(1)	7(1)	−3(1)
C(19)	23(1)	28(1)	34(1)	0(1)	4(1)	−5(1)
C(20)	25(1)	34(2)	40(2)	4(1)	−2(1)	−7(1)
C(21)	22(1)	35(2)	53(2)	11(1)	−1(1)	0(1)
C(22)	24(1)	29(1)	45(2)	7(1)	7(1)	2(1)
C(23)	22(1)	25(1)	31(1)	5(1)	10(1)	−1(1)
C(24)	27(1)	35(2)	46(2)	−11(1)	−4(1)	1(1)
C(25)	42(2)	30(2)	59(2)	−6(1)	−8(2)	−4(1)
C(27)	28(1)	24(1)	28(1)	2(1)	9(1)	5(1)
C(26)	40(2)	70(3)	48(2)	−23(2)	3(2)	−1(2)
C(28)	60(2)	37(2)	29(1)	2(1)	17(1)	2(1)
C(29)	36(1)	24(1)	36(1)	1(1)	3(1)	5(1)
C(30)	35(1)	21(1)	21(1)	3(1)	3(1)	−1(1)
C(31)	39(1)	19(1)	26(1)	3(1)	4(1)	−6(1)
C(32)	34(1)	29(1)	22(1)	4(1)	2(1)	−10(1)
C(33)	38(2)	26(1)	34(1)	10(1)	1(1)	3(1)
C(34)	39(2)	35(2)	40(2)	10(1)	0(1)	−17(1)
C(35)	27(1)	22(1)	23(1)	5(1)	0(1)	−1(1)
C(36)	28(1)	27(1)	24(1)	3(1)	1(1)	−1(1)
C(37)	32(1)	37(2)	29(1)	−3(1)	−1(1)	−4(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(38)	26(1)	44(2)	39(2)	−1(1)	−1(1)	−3(1)
C(39)	28(1)	36(2)	36(2)	2(1)	7(1)	2(1)
C(40)	31(1)	24(1)	27(1)	5(1)	4(1)	1(1)
C(41)	30(1)	33(1)	24(1)	1(1)	4(1)	−3(1)
C(42)	50(2)	42(2)	31(2)	1(1)	13(1)	−8(1)
C(43)	44(2)	41(2)	30(1)	−5(1)	10(1)	−2(1)
C(44)	37(1)	26(1)	28(1)	3(1)	5(1)	4(1)
C(45)	62(2)	33(2)	37(2)	1(1)	3(2)	17(2)
C(46)	39(2)	34(2)	30(1)	6(1)	7(1)	5(1)
C(47)	25(1)	32(1)	32(1)	10(1)	4(1)	−7(1)
C(48)	26(1)	38(2)	34(1)	12(1)	7(1)	−4(1)
C(49)	33(2)	48(2)	45(2)	14(1)	14(1)	3(1)
C(50)	28(1)	65(2)	47(2)	24(2)	8(1)	5(1)
C(51)	30(1)	56(2)	40(2)	21(2)	−3(1)	−8(1)
C(52)	29(1)	35(2)	34(1)	12(1)	−1(1)	−10(1)
C(53)	30(1)	38(2)	32(1)	5(1)	9(1)	0(1)
C(54)	45(2)	46(2)	33(2)	9(1)	9(1)	2(1)
C(55)	49(2)	44(2)	42(2)	4(1)	18(1)	4(1)
C(56)	43(2)	34(2)	34(2)	6(1)	−10(1)	−7(1)
C(57)	90(3)	51(2)	52(2)	7(2)	−11(2)	−35(2)
C(58)	34(1)	39(2)	30(1)	4(1)	−2(1)	0(1)
C(59)	43(2)	24(1)	30(1)	−2(1)	8(1)	2(1)
C(60)	41(2)	35(2)	24(1)	−2(1)	11(1)	0(1)
C(61)	49(2)	28(1)	27(1)	3(1)	1(1)	−15(1)
C(62)	56(2)	26(1)	53(2)	4(1)	32(2)	2(1)
C(63)	28(1)	23(1)	24(1)	0(1)	1(1)	−3(1)
C(64)	40(1)	25(1)	22(1)	4(1)	2(1)	−2(1)
C(65)	44(2)	22(1)	31(1)	3(1)	4(1)	0(1)
C(66)	38(1)	28(1)	26(1)	−1(1)	1(1)	1(1)
C(67)	40(2)	31(1)	26(1)	2(1)	4(1)	−2(1)
C(68)	41(2)	25(1)	24(1)	2(1)	4(1)	−3(1)
C(69)	48(2)	29(1)	33(2)	1(1)	2(1)	3(1)
C11	67(2)	56(2)	42(2)	−1(2)	10(2)	−7(2)
C21	57(2)	55(2)	39(2)	3(2)	4(2)	−4(2)
C31	51(2)	49(2)	44(2)	5(2)	6(2)	−1(2)
C41	55(2)	54(2)	51(2)	11(2)	−3(2)	3(2)
C51	70(3)	44(2)	77(3)	7(2)	5(2)	5(2)
C61	92(4)	55(3)	78(3)	−1(2)	−6(3)	6(2)
C12	170(20)	51(6)	134(15)	−18(7)	−57(13)	10(8)
C22	152(17)	105(13)	124(14)	−20(9)	−89(12)	39(11)
C32	126(14)	59(8)	114(11)	−40(7)	−59(9)	43(9)
C42	108(16)	130(16)	143(14)	−104(10)	−40(10)	16(12)
C52	133(14)	139(17)	150(15)	−101(10)	21(12)	11(11)
C62	111(14)	290(30)	163(19)	−165(18)	37(14)	−42(18)

Table 4: Bond lengths [Å] for mw_143_4m.

Sb(1)–Ga(1)	2.5834(4)
Sb(1)–Sb(2)	2.6627(3)
Sb(2)–N(7)	2.111(2)
Sb(2)–N(6)	2.424(2)
Sb(2)–Ga(2)	3.1569(4)
Ga(1)–N(3)	1.867(2)
Ga(1)–N(1)	2.003(2)
Ga(1)–N(2)	2.016(2)
Ga(2)–N(7)	1.874(2)
Ga(2)–N(6)	1.949(2)
Ga(2)–N(4)	1.949(2)
Ga(2)–N(5)	1.951(2)
F(1)–C(69)	1.334(4)
F(2)–C(69)	1.350(4)
F(3)–C(69)	1.339(4)
N(1)–C(1)	1.333(3)
N(1)–C(6)	1.443(3)
N(2)–C(3)	1.324(3)
N(2)–C(18)	1.444(3)
N(3)–C(59)	1.439(3)
N(3)–C(60)	1.453(3)
N(4)–C(32)	1.335(3)
N(4)–C(47)	1.455(3)
N(5)–C(30)	1.335(3)
N(5)–C(35)	1.451(3)
N(6)–C(62)	1.469(4)
N(6)–C(61)	1.470(4)
N(7)–C(63)	1.366(3)
C(1)–C(2)	1.402(3)
C(1)–C(4)	1.515(3)
C(2)–C(3)	1.408(4)
C(3)–C(5)	1.515(3)
C(6)–C(7)	1.404(3)
C(6)–C(11)	1.409(4)
C(7)–C(8)	1.391(4)
C(7)–C(12)	1.522(4)
C(8)–C(9)	1.384(4)
C(9)–C(10)	1.386(4)
C(10)–C(11)	1.397(4)
C(11)–C(15)	1.527(4)
C(12)–C(14)	1.529(4)
C(12)–C(13)	1.533(4)
C(15)–C(16)	1.531(4)
C(15)–C(17)	1.534(4)
C(18)–C(19)	1.406(4)
C(18)–C(23)	1.409(4)
C(19)–C(20)	1.403(4)
C(19)–C(24)	1.511(4)
C(20)–C(21)	1.370(5)
C(21)–C(22)	1.384(4)
C(22)–C(23)	1.399(4)
C(23)–C(27)	1.523(4)
C(24)–C(26)	1.521(5)

Table 4: (continued)

C(24)–C(25)	1.545(5)
C(27)–C(28)	1.529(4)
C(27)–C(29)	1.534(4)
C(30)–C(31)	1.394(4)
C(30)–C(33)	1.521(4)
C(31)–C(32)	1.400(4)
C(32)–C(34)	1.512(4)
C(35)–C(40)	1.404(4)
C(35)–C(36)	1.406(4)
C(36)–C(37)	1.389(4)
C(36)–C(41)	1.529(4)
C(37)–C(38)	1.385(4)
C(38)–C(39)	1.379(4)
C(39)–C(40)	1.396(4)
C(40)–C(44)	1.523(4)
C(41)–C(43)	1.529(4)
C(41)–C(42)	1.537(4)
C(44)–C(46)	1.524(4)
C(44)–C(45)	1.540(4)
C(47)–C(48)	1.409(4)
C(47)–C(52)	1.410(4)
C(48)–C(49)	1.400(4)
C(48)–C(53)	1.520(4)
C(49)–C(50)	1.388(5)
C(50)–C(51)	1.370(5)
C(51)–C(52)	1.394(4)
C(52)–C(56)	1.508(5)
C(53)–C(55)	1.532(4)
C(53)–C(54)	1.533(4)
C(56)–C(58)	1.532(4)
C(56)–C(57)	1.547(5)
C(63)–C(68)	1.411(4)
C(63)–C(64)	1.414(4)
C(64)–C(65)	1.380(4)
C(65)–C(66)	1.392(4)
C(66)–C(67)	1.390(4)
C(66)–C(69)	1.488(4)
C(67)–C(68)	1.376(4)
C11–C21	1.520(5)
C21–C31	1.512(5)
C31–C41	1.518(5)
C41–C51	1.524(6)
C51–C61	1.520(6)
C12–C22	1.482(13)
C22–C32	1.507(12)
C32–C42	1.519(13)
C42–C52	1.503(14)
C52–C62	1.546(13)

Table 5: Bond angles [°] for mw_143_4m.

Ga(1)–Sb(1)–Sb(2)	95.018(9)
N(7)–Sb(2)–N(6)	72.53(8)
N(7)–Sb(2)–Sb(1)	103.11(6)
N(6)–Sb(2)–Sb(1)	103.17(6)
N(7)–Sb(2)–Ga(2)	35.06(6)
N(6)–Sb(2)–Ga(2)	38.10(5)
Sb(1)–Sb(2)–Ga(2)	111.511(8)
N(3)–Ga(1)–N(1)	106.66(9)
N(3)–Ga(1)–N(2)	105.39(9)
N(1)–Ga(1)–N(2)	91.38(8)
N(3)–Ga(1)–Sb(1)	118.63(7)
N(1)–Ga(1)–Sb(1)	122.83(6)
N(2)–Ga(1)–Sb(1)	107.11(6)
N(7)–Ga(2)–N(6)	89.60(9)
N(7)–Ga(2)–N(4)	115.52(9)
N(6)–Ga(2)–N(4)	120.08(10)
N(7)–Ga(2)–N(5)	118.27(9)
N(6)–Ga(2)–N(5)	118.98(10)
N(4)–Ga(2)–N(5)	96.38(9)
N(7)–Ga(2)–Sb(2)	40.31(7)
N(6)–Ga(2)–Sb(2)	50.13(7)
N(4)–Ga(2)–Sb(2)	123.72(6)
N(5)–Ga(2)–Sb(2)	139.07(6)
C(1)–N(1)–C(6)	119.4(2)
C(1)–N(1)–Ga(1)	121.27(16)
C(6)–N(1)–Ga(1)	119.24(15)
C(3)–N(2)–C(18)	121.1(2)
C(3)–N(2)–Ga(1)	121.65(17)
C(18)–N(2)–Ga(1)	116.84(15)
C(59)–N(3)–C(60)	112.2(2)
C(59)–N(3)–Ga(1)	123.07(17)
C(60)–N(3)–Ga(1)	124.78(18)
C(32)–N(4)–C(47)	118.9(2)
C(32)–N(4)–Ga(2)	119.55(19)
C(47)–N(4)–Ga(2)	121.24(16)
C(30)–N(5)–C(35)	119.5(2)
C(30)–N(5)–Ga(2)	119.65(18)
C(35)–N(5)–Ga(2)	120.74(16)
C(62)–N(6)–C(61)	108.8(2)
C(62)–N(6)–Ga(2)	122.25(19)
C(61)–N(6)–Ga(2)	116.30(18)
C(62)–N(6)–Sb(2)	105.70(19)
C(61)–N(6)–Sb(2)	109.34(16)
Ga(2)–N(6)–Sb(2)	91.77(9)
C(63)–N(7)–Ga(2)	130.37(17)
C(63)–N(7)–Sb(2)	124.09(17)
Ga(2)–N(7)–Sb(2)	104.63(10)
N(1)–C(1)–C(2)	123.5(2)
N(1)–C(1)–C(4)	119.4(2)
C(2)–C(1)–C(4)	117.1(2)
C(1)–C(2)–C(3)	127.6(2)
N(2)–C(3)–C(2)	123.2(2)
N(2)–C(3)–C(5)	120.8(2)

Table 5: (continued)

C(2)–C(3)–C(5)	116.0(2)
C(7)–C(6)–C(11)	120.8(2)
C(7)–C(6)–N(1)	120.3(2)
C(11)–C(6)–N(1)	118.8(2)
C(8)–C(7)–C(6)	118.5(2)
C(8)–C(7)–C(12)	119.6(2)
C(6)–C(7)–C(12)	121.9(2)
C(9)–C(8)–C(7)	121.4(3)
C(8)–C(9)–C(10)	119.7(3)
C(9)–C(10)–C(11)	121.0(3)
C(10)–C(11)–C(6)	118.5(2)
C(10)–C(11)–C(15)	119.1(2)
C(6)–C(11)–C(15)	122.4(2)
C(7)–C(12)–C(14)	111.2(2)
C(7)–C(12)–C(13)	110.5(2)
C(14)–C(12)–C(13)	110.6(2)
C(11)–C(15)–C(16)	111.2(2)
C(11)–C(15)–C(17)	111.7(2)
C(16)–C(15)–C(17)	109.2(2)
C(19)–C(18)–C(23)	121.0(2)
C(19)–C(18)–N(2)	120.5(2)
C(23)–C(18)–N(2)	118.4(2)
C(20)–C(19)–C(18)	118.1(3)
C(20)–C(19)–C(24)	118.4(3)
C(18)–C(19)–C(24)	123.4(2)
C(21)–C(20)–C(19)	121.6(3)
C(20)–C(21)–C(22)	119.7(3)
C(21)–C(22)–C(23)	121.5(3)
C(22)–C(23)–C(18)	118.0(3)
C(22)–C(23)–C(27)	120.2(2)
C(18)–C(23)–C(27)	121.9(2)
C(19)–C(24)–C(26)	111.1(3)
C(19)–C(24)–C(25)	110.1(3)
C(26)–C(24)–C(25)	110.5(3)
C(23)–C(27)–C(28)	111.3(2)
C(23)–C(27)–C(29)	112.9(2)
C(28)–C(27)–C(29)	109.8(2)
N(5)–C(30)–C(31)	123.8(2)
N(5)–C(30)–C(33)	119.5(2)
C(31)–C(30)–C(33)	116.7(2)
C(30)–C(31)–C(32)	128.5(2)
N(4)–C(32)–C(31)	124.0(2)
N(4)–C(32)–C(34)	120.1(3)
C(31)–C(32)–C(34)	115.9(2)
C(40)–C(35)–C(36)	121.9(2)
C(40)–C(35)–N(5)	120.2(2)
C(36)–C(35)–N(5)	117.9(2)
C(37)–C(36)–C(35)	118.1(3)
C(37)–C(36)–C(41)	120.4(2)
C(35)–C(36)–C(41)	121.5(2)
C(38)–C(37)–C(36)	121.1(3)
C(39)–C(38)–C(37)	119.9(3)
C(38)–C(39)–C(40)	121.6(3)

Table 5: (continued)

C(39)–C(40)–C(35)	117.4(3)
C(39)–C(40)–C(44)	119.7(2)
C(35)–C(40)–C(44)	122.8(2)
C(43)–C(41)–C(36)	114.0(2)
C(43)–C(41)–C(42)	108.5(2)
C(36)–C(41)–C(42)	111.5(2)
C(40)–C(44)–C(46)	111.7(2)
C(40)–C(44)–C(45)	111.6(2)
C(46)–C(44)–C(45)	108.6(2)
C(48)–C(47)–C(52)	121.7(3)
C(48)–C(47)–N(4)	118.1(2)
C(52)–C(47)–N(4)	120.1(3)
C(49)–C(48)–C(47)	118.1(3)
C(49)–C(48)–C(53)	120.4(3)
C(47)–C(48)–C(53)	121.5(3)
C(50)–C(49)–C(48)	120.5(3)
C(51)–C(50)–C(49)	120.3(3)
C(50)–C(51)–C(52)	122.1(3)
C(51)–C(52)–C(47)	117.3(3)
C(51)–C(52)–C(56)	119.4(3)
C(47)–C(52)–C(56)	123.3(3)
C(48)–C(53)–C(55)	113.3(3)
C(48)–C(53)–C(54)	111.7(3)
C(55)–C(53)–C(54)	108.6(3)
C(52)–C(56)–C(58)	111.7(3)
C(52)–C(56)–C(57)	111.4(3)
C(58)–C(56)–C(57)	108.4(3)
N(7)–C(63)–C(68)	122.3(2)
N(7)–C(63)–C(64)	121.7(2)
C(68)–C(63)–C(64)	116.0(2)
C(65)–C(64)–C(63)	121.5(2)
C(64)–C(65)–C(66)	121.1(3)
C(67)–C(66)–C(65)	118.4(3)
C(67)–C(66)–C(69)	121.2(3)
C(65)–C(66)–C(69)	120.3(3)
C(68)–C(67)–C(66)	120.6(3)
C(67)–C(68)–C(63)	122.3(3)
F(1)–C(69)–F(3)	106.9(3)
F(1)–C(69)–F(2)	105.4(3)
F(3)–C(69)–F(2)	105.6(3)
F(1)–C(69)–C(66)	112.9(2)
F(3)–C(69)–C(66)	112.7(3)
F(2)–C(69)–C(66)	112.7(3)
C31–C21–C11	113.5(3)
C21–C31–C41	114.3(3)
C31–C41–C51	115.5(3)
C61–C51–C41	113.3(4)
C12–C22–C32	112.1(17)
C22–C32–C42	106.6(16)
C52–C42–C32	115.8(15)
C42–C52–C62	114(2)

Crystal structure of mw_130_1m

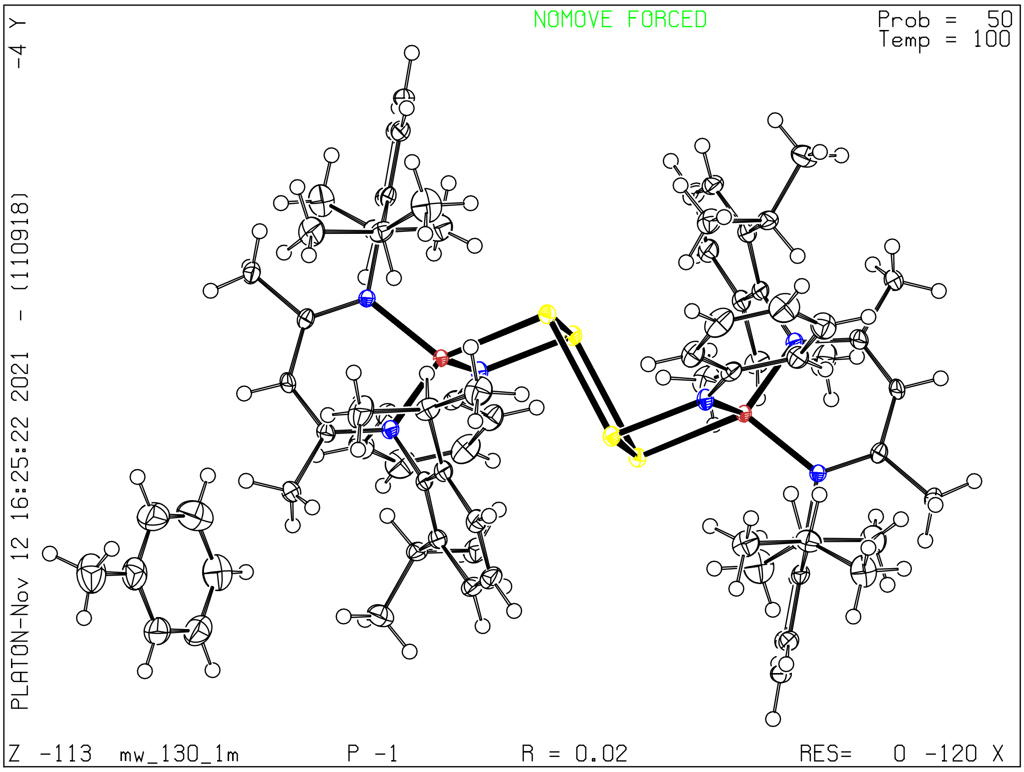

Table 1: Crystal data and structure refinement for mw_130_1m.

Identification code	mw_130_1m
Empirical Formula	$C_{84} H_{108} Ga_2 N_6 Sb_4$
Formula weight	1828.20 Da
Density (calculated)	$1.530\,g \cdot cm^{-3}$
$F(000)$	920
Temperature	100(2) K
Crystal size	0.235 × 0.079 × 0.048 mm
Crystal appearance	orange tablet
Wavelength (CuK_α)	1.54178 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 12.0886(4)$ Å
	$b = 12.3645(4)$ Å
	$c = 14.1831(9)$ Å
	$\alpha = 86.028(5)°$
	$\beta = 75.849(4)°$
	$\gamma = 74.786(2)°$
Unit cell volume	$1983.53(16)$ Å^3
Z	1
Cell measurement refections used	9683
θ range for cell measurement	3.21° to 79.77°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	3.213° to 80.427°
Completeness to $\theta = 67.679°$ (to θ_{max})	99.9% (98.8%)
Index ranges	$-15 \leq h \leq 13$
	$-15 \leq k \leq 15$
	$-18 \leq l \leq 18$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$11.749\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.42
R_{merg} before/after correction	0.1392/0.0731
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	109962
Independent reflections	8602 ($R_{int} = 0.0499$)
Reflections with $I > 2\sigma(I)$	8438
Data / retraints / parameter	8602 / 0 / 444
Goodness-of-fit on F^2	1.049
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 1.5381P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0230$
	$wR2 = 0.0623$
R indices [all data]	$R1 = 0.0235$
	$wR2 = 0.0627$
Largest diff. peak and hole	1.578 and -0.766 Å^{-3}

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_130_1m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	6328(1)	5820(1)	9350(1)	16(1)
Sb(2)	6135(1)	3917(1)	10566(1)	17(1)
Ga(1)	7192(1)	4038(1)	8244(1)	12(1)
N(1)	6740(1)	3905(1)	7027(1)	15(1)
N(2)	8900(1)	3656(1)	7651(1)	13(1)
N(3)	6788(1)	3032(1)	9266(1)	16(1)
C(1)	7497(2)	3342(2)	6259(1)	17(1)
C(2)	8697(2)	2890(2)	6208(1)	17(1)
C(3)	9372(2)	3091(2)	6820(1)	15(1)
C(4)	7054(2)	3192(2)	5384(1)	23(1)
C(5)	10689(2)	2638(2)	6487(1)	21(1)
C(6)	5543(2)	4433(2)	6965(1)	16(1)
C(7)	4709(2)	3798(2)	7107(1)	18(1)
C(8)	3555(2)	4354(2)	7060(1)	22(1)
C(9)	3253(2)	5487(2)	6858(2)	24(1)
C(10)	4089(2)	6099(2)	6701(1)	21(1)
C(11)	5248(2)	5593(2)	6760(1)	18(1)
C(12)	5005(2)	2543(2)	7316(1)	20(1)
C(13)	4615(2)	1884(2)	6632(2)	31(1)
C(14)	4449(2)	2306(2)	8373(2)	27(1)
C(15)	6154(2)	6280(2)	6579(2)	22(1)
C(16)	6833(2)	6232(2)	5520(2)	37(1)
C(17)	5624(2)	7501(2)	6902(2)	33(1)
C(18)	9666(2)	4008(2)	8143(1)	15(1)
C(19)	10226(2)	3285(2)	8788(1)	17(1)
C(20)	10967(2)	3672(2)	9227(1)	21(1)
C(21)	11133(2)	4736(2)	9045(2)	23(1)
C(22)	10558(2)	5444(2)	8418(1)	21(1)
C(23)	9821(2)	5100(2)	7953(1)	16(1)
C(24)	10074(2)	2107(2)	9021(2)	22(1)
C(25)	11262(2)	1229(2)	8782(2)	34(1)
C(26)	9472(2)	1992(2)	10098(2)	28(1)
C(27)	9241(2)	5869(2)	7229(2)	20(1)
C(28)	10017(2)	5706(2)	6197(2)	32(1)
C(29)	8892(3)	7103(2)	7509(2)	39(1)
C(30)	6898(2)	1889(2)	9231(1)	18(1)
C(31)	7523(2)	1273(2)	8383(2)	21(1)
C(32)	7580(2)	142(2)	8325(2)	29(1)
C(33)	7022(2)	−416(2)	9107(2)	34(1)
C(34)	6424(2)	174(2)	9951(2)	31(1)
C(35)	6364(2)	1299(2)	10020(2)	24(1)
C11	8053(2)	699(2)	3574(2)	38(1)
C21	7094(2)	226(2)	3790(2)	36(1)
C31	6771(2)	−270(2)	4689(2)	41(1)
C41	7390(3)	−279(2)	5389(2)	44(1)
C51	8343(3)	186(3)	5179(3)	51(1)
C61	8673(3)	657(2)	4277(2)	46(1)
C71	8403(3)	1247(3)	2614(2)	52(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_130_1m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	16(1)	19(1)	14(1)	−2(1)	−1(1)	−6(1)
Sb(2)	16(1)	25(1)	8(1)	1(1)	−2(1)	−6(1)
Ga(1)	12(1)	17(1)	7(1)	1(1)	−1(1)	−5(1)
N(1)	14(1)	22(1)	9(1)	2(1)	−2(1)	−6(1)
N(2)	13(1)	17(1)	10(1)	1(1)	−1(1)	−6(1)
N(3)	18(1)	20(1)	9(1)	2(1)	0(1)	−6(1)
C(1)	20(1)	22(1)	10(1)	2(1)	−2(1)	−9(1)
C(2)	18(1)	22(1)	9(1)	−2(1)	0(1)	−7(1)
C(3)	15(1)	17(1)	12(1)	3(1)	1(1)	−6(1)
C(4)	21(1)	39(1)	11(1)	−3(1)	−3(1)	−10(1)
C(5)	16(1)	29(1)	15(1)	−3(1)	0(1)	−3(1)
C(6)	14(1)	26(1)	7(1)	2(1)	−2(1)	−6(1)
C(7)	18(1)	28(1)	9(1)	1(1)	−3(1)	−9(1)
C(8)	16(1)	37(1)	16(1)	2(1)	−4(1)	−10(1)
C(9)	16(1)	38(1)	17(1)	4(1)	−5(1)	−5(1)
C(10)	20(1)	30(1)	12(1)	4(1)	−4(1)	−4(1)
C(11)	18(1)	27(1)	8(1)	3(1)	−2(1)	−7(1)
C(12)	18(1)	26(1)	17(1)	1(1)	−3(1)	−11(1)
C(13)	33(1)	36(1)	29(1)	−5(1)	−9(1)	−15(1)
C(14)	25(1)	34(1)	21(1)	6(1)	−1(1)	−12(1)
C(15)	21(1)	26(1)	20(1)	10(1)	−7(1)	−8(1)
C(16)	34(1)	44(1)	29(1)	7(1)	8(1)	−18(1)
C(17)	34(1)	28(1)	35(1)	6(1)	−3(1)	−12(1)
C(18)	13(1)	22(1)	10(1)	−1(1)	0(1)	−7(1)
C(19)	15(1)	24(1)	12(1)	1(1)	−1(1)	−7(1)
C(20)	16(1)	33(1)	14(1)	1(1)	−4(1)	−6(1)
C(21)	19(1)	36(1)	17(1)	−3(1)	−3(1)	−13(1)
C(22)	19(1)	26(1)	17(1)	−3(1)	1(1)	−12(1)
C(23)	13(1)	21(1)	12(1)	−1(1)	3(1)	−6(1)
C(24)	28(1)	23(1)	20(1)	6(1)	−10(1)	−9(1)
C(25)	39(1)	28(1)	29(1)	2(1)	−6(1)	−2(1)
C(26)	30(1)	32(1)	23(1)	10(1)	−7(1)	−12(1)
C(27)	19(1)	22(1)	21(1)	6(1)	−3(1)	−10(1)
C(28)	36(1)	43(1)	18(1)	9(1)	−5(1)	−11(1)
C(29)	49(2)	23(1)	43(2)	4(1)	−10(1)	−5(1)
C(30)	14(1)	22(1)	18(1)	4(1)	−4(1)	−6(1)
C(31)	22(1)	21(1)	19(1)	2(1)	−3(1)	−9(1)
C(32)	31(1)	23(1)	32(1)	−2(1)	−6(1)	−6(1)
C(33)	38(1)	20(1)	44(1)	6(1)	−9(1)	−10(1)
C(34)	29(1)	27(1)	36(1)	14(1)	−4(1)	−10(1)
C(35)	23(1)	26(1)	21(1)	7(1)	−2(1)	−6(1)
C11	39(1)	26(1)	42(1)	−10(1)	2(1)	−6(1)
C21	29(1)	33(1)	44(1)	−10(1)	−7(1)	−3(1)
C31	30(1)	34(1)	53(2)	−7(1)	0(1)	−8(1)
C41	51(2)	36(1)	40(2)	1(1)	−6(1)	−7(1)
C51	55(2)	46(2)	59(2)	−4(1)	−25(2)	−13(1)
C61	40(2)	41(1)	59(2)	−10(1)	−8(1)	−17(1)
C71	61(2)	39(2)	50(2)	−7(1)	7(2)	−17(1)

Table 4: Bond lengths [Å] for mw_130_1m.

Sb(1)–Ga(1)	2.6221(3)
Sb(1)–Sb(2)	2.8449(2)
Sb(1)–Sb(2)#1	2.8837(2)
Sb(2)–N(3)	2.0818(16)
Ga(1)–N(3)	1.8998(16)
Ga(1)–N(1)	1.9632(16)
Ga(1)–N(2)	1.9720(16)
N(1)–C(1)	1.338(2)
N(1)–C(6)	1.445(2)
N(2)–C(3)	1.333(2)
N(2)–C(18)	1.450(2)
N(3)–C(30)	1.388(3)
C(1)–C(2)	1.397(3)
C(1)–C(4)	1.507(3)
C(2)–C(3)	1.401(3)
C(3)–C(5)	1.508(3)
C(6)–C(7)	1.403(3)
C(6)–C(11)	1.412(3)
C(7)–C(8)	1.400(3)
C(7)–C(12)	1.522(3)
C(8)–C(9)	1.380(3)
C(9)–C(10)	1.383(3)
C(10)–C(11)	1.397(3)
C(11)–C(15)	1.519(3)
C(12)–C(14)	1.529(3)
C(12)–C(13)	1.537(3)
C(15)–C(16)	1.523(3)
C(15)–C(17)	1.532(3)
C(18)–C(19)	1.403(3)
C(18)–C(23)	1.410(3)
C(19)–C(20)	1.400(3)
C(19)–C(24)	1.519(3)
C(20)–C(21)	1.380(3)
C(21)–C(22)	1.385(3)
C(22)–C(23)	1.390(3)
C(23)–C(27)	1.523(3)
C(24)–C(25)	1.534(3)
C(24)–C(26)	1.537(3)
C(27)–C(29)	1.526(3)
C(27)–C(28)	1.527(3)
C(30)–C(31)	1.407(3)
C(30)–C(35)	1.408(3)
C(31)–C(32)	1.390(3)
C(32)–C(33)	1.390(3)
C(33)–C(34)	1.381(4)
C(34)–C(35)	1.383(3)
C11–C61	1.377(4)
C11–C21	1.392(4)
C11–C71	1.495(4)
C21–C31	1.388(4)
C31–C41	1.379(4)
C41–C51	1.379(5)
C51–C61	1.379(5)

#1 -x+1,-y+1,-z+2

Table 5: Bond angles [°] for mw_130_1m.

Ga(1)–Sb(1)–Sb(2)	72.465(7)
Ga(1)–Sb(1)–Sb(2)#1	98.214(7)
Sb(2)–Sb(1)–Sb(2)#1	85.018(6)
N(3)–Sb(2)–Sb(1)	84.17(4)
N(3)–Sb(2)–Sb(1)#1	96.58(5)
Sb(1)–Sb(2)–Sb(1)#1	94.982(6)
N(3)–Ga(1)–N(1)	116.89(7)
N(3)–Ga(1)–N(2)	111.87(7)
N(1)–Ga(1)–N(2)	94.61(6)
N(3)–Ga(1)–Sb(1)	94.25(5)
N(1)–Ga(1)–Sb(1)	123.26(5)
N(2)–Ga(1)–Sb(1)	117.24(5)
C(1)–N(1)–C(6)	119.12(15)
C(1)–N(1)–Ga(1)	122.47(13)
C(6)–N(1)–Ga(1)	118.41(12)
C(3)–N(2)–C(18)	119.14(15)
C(3)–N(2)–Ga(1)	122.59(13)
C(18)–N(2)–Ga(1)	118.27(12)
C(30)–N(3)–Ga(1)	129.42(13)
C(30)–N(3)–Sb(2)	121.90(12)
Ga(1)–N(3)–Sb(2)	108.66(8)
N(1)–C(1)–C(2)	123.82(17)
N(1)–C(1)–C(4)	119.20(18)
C(2)–C(1)–C(4)	116.97(17)
C(1)–C(2)–C(3)	128.31(17)
N(2)–C(3)–C(2)	123.14(17)
N(2)–C(3)–C(5)	120.61(17)
C(2)–C(3)–C(5)	116.25(16)
C(7)–C(6)–C(11)	121.77(18)
C(7)–C(6)–N(1)	120.15(17)
C(11)–C(6)–N(1)	118.08(17)
C(8)–C(7)–C(6)	117.90(19)
C(8)–C(7)–C(12)	119.16(18)
C(6)–C(7)–C(12)	122.93(18)
C(9)–C(8)–C(7)	121.0(2)
C(8)–C(9)–C(10)	120.48(19)
C(9)–C(10)–C(11)	121.0(2)
C(10)–C(11)–C(6)	117.83(19)
C(10)–C(11)–C(15)	120.13(18)
C(6)–C(11)–C(15)	122.02(18)
C(7)–C(12)–C(14)	110.60(17)
C(7)–C(12)–C(13)	112.40(17)
C(14)–C(12)–C(13)	109.83(18)
C(11)–C(15)–C(16)	111.79(19)
C(11)–C(15)–C(17)	113.21(18)
C(16)–C(15)–C(17)	110.09(19)
C(19)–C(18)–C(23)	121.44(17)
C(19)–C(18)–N(2)	120.85(17)
C(23)–C(18)–N(2)	117.71(16)
C(20)–C(19)–C(18)	117.88(18)
C(20)–C(19)–C(24)	118.96(18)
C(18)–C(19)–C(24)	123.15(17)
C(21)–C(20)–C(19)	121.32(19)

Table 5: (continued)

C(20)–C(21)–C(22)	119.97(19)
C(21)–C(22)–C(23)	121.19(19)
C(22)–C(23)–C(18)	118.18(18)
C(22)–C(23)–C(27)	120.56(17)
C(18)–C(23)–C(27)	121.21(17)
C(19)–C(24)–C(25)	111.36(19)
C(19)–C(24)–C(26)	111.23(17)
C(25)–C(24)–C(26)	109.06(18)
C(23)–C(27)–C(29)	112.96(18)
C(23)–C(27)–C(28)	111.64(17)
C(29)–C(27)–C(28)	110.25(19)
N(3)–C(30)–C(31)	120.89(17)
N(3)–C(30)–C(35)	122.21(18)
C(31)–C(30)–C(35)	116.86(19)
C(32)–C(31)–C(30)	121.14(19)
C(33)–C(32)–C(31)	120.8(2)
C(34)–C(33)–C(32)	118.6(2)
C(33)–C(34)–C(35)	121.1(2)
C(34)–C(35)–C(30)	121.3(2)
C61–C11–C21	118.0(3)
C61–C11–C71	120.4(3)
C21–C11–C71	121.5(3)
C31–C21–C11	120.9(3)
C41–C31–C21	119.9(3)
C31–C41–C51	119.4(3)
C61–C51–C41	120.3(3)
C11–C61–C51	121.4(3)

#1 -x+1,-y+1,-z+2

Crystal structure of mw_145_1m

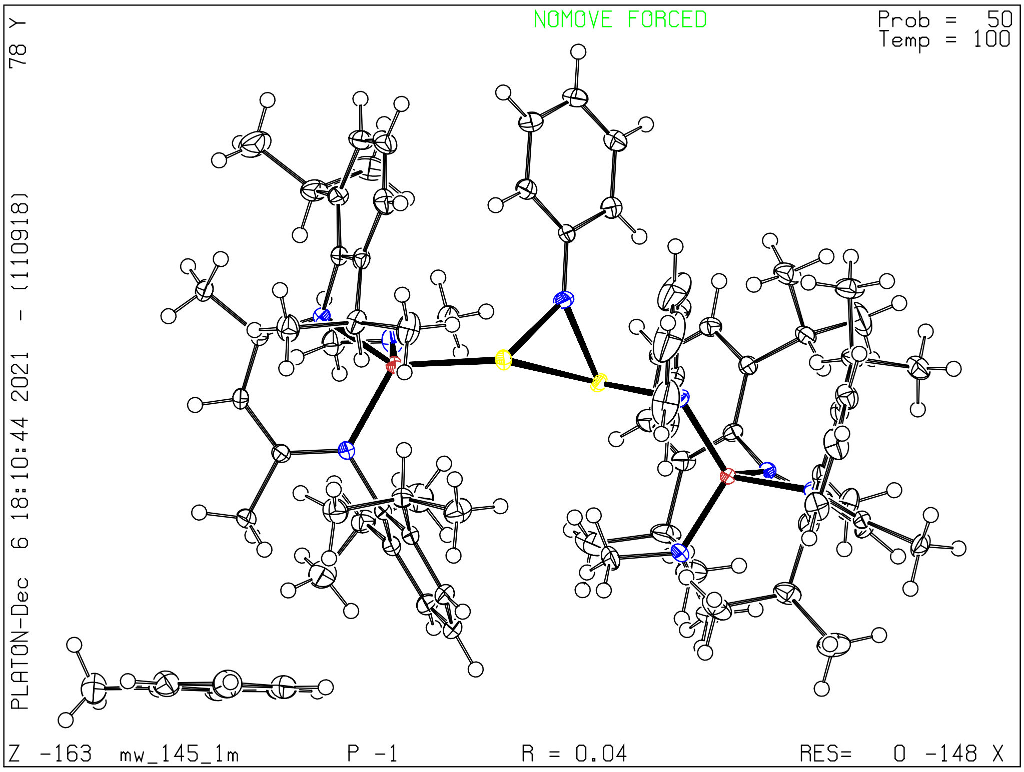

Table 1: Crystal data and structure refinement for mw_145_1m.

Identification code	mw_145_1m
Empirical Formula	$C_{81}\,H_{112}\,Ga_2\,N_8\,Sb_2$
Formula weight	1580.72 Da
Density (calculated)	$1.361\,g\cdot cm^{-3}$
$F(000)$	1636
Temperature	100(2) K
Crystal size	0.185 × 0.071 × 0.045 mm
Crystal appearance	orange needle
Wavelength (MoK_α)	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 11.6222(9)$ Å
	$b = 17.8727(14)$ Å
	$c = 19.5796(16)$ Å
	$\alpha = 108.099(4)°$
	$\beta = 90.076(4)°$
	$\gamma = 93.817(4)°$
Unit cell volume	3856.2(5) $Å^3$
Z	2
Cell measurement refections used	9560
θ range for cell measurement	2.63° to 27.10°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.202° to 33.269°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.6%)
Index ranges	$-17 \leq h \leq 17$
	$-27 \leq k \leq 27$
	$-30 \leq l \leq 30$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.431\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.68
R_{merg} before/after correction	0.0767/0.0677
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	311665
Independent reflections	29569 ($R_{int} = 0.1010$)
Reflections with $I > 2\sigma(I)$	21328
Data / retraints / parameter	29569 / 0 / 863
Goodness-of-fit on F^2	1.031
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 3.1079P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0393$
	$wR2 = 0.0747$
R indices [all data]	$R1 = 0.0720$
	$wR2 = 0.0856$
Largest diff. peak and hole	1.203 and −0.884 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_145_1m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	2993(1)	7447(1)	3293(1)	15(1)
Sb(2)	969(1)	7734(1)	2637(1)	14(1)
Ga(1)	2092(1)	6679(1)	4150(1)	12(1)
Ga(2)	1069(1)	7585(1)	891(1)	12(1)
N(1)	2207(2)	5512(1)	3761(1)	14(1)
N(2)	3204(2)	6769(1)	4964(1)	14(1)
N(3)	−556(2)	7822(1)	839(1)	14(1)
N(4)	1562(2)	7983(1)	97(1)	13(1)
N(5)	638(2)	6865(1)	4535(1)	20(1)
N(6)	1181(2)	6504(1)	580(1)	19(1)
N(7)	1969(2)	8399(1)	3480(1)	19(1)
N(8)	1682(2)	8105(1)	1826(1)	14(1)
C(1)	2448(2)	5085(1)	4185(1)	15(1)
C(2)	2870(2)	5408(1)	4894(1)	17(1)
C(3)	3307(2)	6185(1)	5240(1)	15(1)
C(4)	2298(2)	4194(1)	3905(1)	21(1)
C(5)	3923(2)	6329(1)	5956(1)	21(1)
C(6)	1934(2)	5106(1)	3010(1)	16(1)
C(7)	813(2)	4768(1)	2787(1)	18(1)
C(8)	605(2)	4380(1)	2054(1)	23(1)
C(9)	1464(2)	4319(1)	1561(1)	24(1)
C(10)	2560(2)	4661(1)	1784(1)	22(1)
C(11)	2813(2)	5066(1)	2509(1)	17(1)
C(12)	−165(2)	4804(2)	3307(1)	24(1)
C(13)	−757(2)	3986(2)	3226(2)	32(1)
C(14)	−1058(2)	5356(2)	3208(2)	34(1)
C(15)	4024(2)	5440(1)	2742(1)	19(1)
C(16)	4739(2)	4916(2)	3038(2)	27(1)
C(17)	4681(2)	5675(2)	2153(1)	29(1)
C(18)	3839(2)	7522(1)	5274(1)	15(1)
C(19)	3385(2)	8109(1)	5841(1)	19(1)
C(20)	3991(2)	8850(1)	6078(1)	24(1)
C(21)	5000(2)	9008(2)	5768(2)	27(1)
C(22)	5450(2)	8414(2)	5217(1)	24(1)
C(23)	4897(2)	7666(1)	4966(1)	17(1)
C(24)	2264(2)	7976(2)	6192(1)	26(1)
C(25)	2437(3)	8085(2)	6995(2)	42(1)
C(26)	1373(2)	8517(2)	6076(2)	35(1)
C(27)	5449(2)	7005(1)	4405(1)	19(1)
C(28)	6179(2)	6545(2)	4765(1)	26(1)
C(29)	6195(2)	7287(2)	3879(2)	31(1)
C(30)	−1026(2)	7856(1)	233(1)	16(1)
C(31)	−390(2)	7848(1)	−376(1)	18(1)
C(32)	807(2)	7962(1)	−422(1)	16(1)
C(33)	−2307(2)	7926(2)	169(1)	28(1)
C(34)	1225(2)	8082(2)	−1114(1)	23(1)
C(35)	−1211(2)	7979(1)	1487(1)	15(1)
C(36)	−1784(2)	7360(1)	1674(1)	21(1)
C(37)	−2342(2)	7537(2)	2332(1)	25(1)
C(38)	−2297(2)	8302(2)	2798(1)	23(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(39)	−1730(2)	8904(1)	2605(1)	18(1)
C(40)	−1192(2)	8761(1)	1943(1)	15(1)
C(41)	−1808(3)	6506(2)	1191(2)	32(1)
C(42)	−3001(4)	6228(2)	816(2)	59(1)
C(43)	−1522(3)	5952(2)	1611(2)	41(1)
C(44)	−679(2)	9448(1)	1719(1)	22(1)
C(45)	−1657(3)	9917(2)	1569(2)	44(1)
C(46)	166(2)	9994(2)	2278(1)	27(1)
C(47)	2753(2)	8230(1)	30(1)	16(1)
C(48)	3509(2)	7689(1)	−379(1)	20(1)
C(49)	4651(2)	7959(2)	−424(1)	26(1)
C(50)	5036(2)	8730(2)	−81(2)	28(1)
C(51)	4286(2)	9254(2)	328(1)	24(1)
C(52)	3135(2)	9020(1)	391(1)	18(1)
C(53)	3142(2)	6827(2)	−770(1)	26(1)
C(54)	3404(3)	6598(2)	−1577(2)	36(1)
C(55)	3726(3)	6271(2)	−440(2)	34(1)
C(56)	2323(2)	9610(1)	840(1)	19(1)
C(57)	1512(2)	9895(2)	371(1)	26(1)
C(58)	2958(2)	10332(2)	1381(1)	29(1)
C(59)	131(2)	6458(2)	5006(1)	24(1)
C(60)	−126(2)	7416(2)	4397(1)	24(1)
C(61)	1620(2)	6032(1)	991(1)	25(1)
C(62)	618(2)	6023(1)	−88(1)	25(1)
C(63)	1905(2)	9098(1)	4027(1)	16(1)
C(64)	1044(2)	9607(1)	4019(1)	21(1)
C(65)	983(2)	10315(1)	4563(1)	24(1)
C(66)	1774(2)	10537(1)	5130(1)	26(1)
C(67)	2632(2)	10042(2)	5149(1)	25(1)
C(68)	2705(2)	9327(1)	4605(1)	22(1)
C(69)	2884(2)	8330(1)	1897(1)	20(1)
C(70)	3289(2)	9042(2)	2396(1)	30(1)
C(71)	4464(3)	9262(2)	2454(2)	53(1)
C(72)	5241(3)	8795(3)	2020(2)	59(1)
C(73)	4850(2)	8089(2)	1536(2)	47(1)
C(74)	3681(2)	7853(2)	1477(2)	29(1)
C11	2483(2)	1938(1)	3078(1)	24(1)
C21	1667(2)	2234(2)	2730(1)	27(1)
C31	2002(3)	2632(2)	2250(1)	30(1)
C41	3150(3)	2732(2)	2105(2)	35(1)
C51	3973(3)	2442(2)	2448(2)	34(1)
C61	3643(2)	2052(2)	2932(2)	30(1)
C71	2127(2)	1496(2)	3593(2)	33(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_145_1m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	16(1)	16(1)	15(1)	7(1)	0(1)	2(1)
Sb(2)	16(1)	16(1)	11(1)	5(1)	−1(1)	0(1)
Ga(1)	14(1)	12(1)	12(1)	4(1)	0(1)	2(1)
Ga(2)	14(1)	11(1)	10(1)	3(1)	0(1)	1(1)
N(1)	17(1)	12(1)	14(1)	5(1)	−1(1)	2(1)
N(2)	16(1)	13(1)	12(1)	4(1)	0(1)	0(1)
N(3)	15(1)	13(1)	12(1)	4(1)	1(1)	0(1)
N(4)	15(1)	13(1)	13(1)	4(1)	2(1)	2(1)
N(5)	17(1)	24(1)	24(1)	11(1)	7(1)	7(1)
N(6)	28(1)	11(1)	18(1)	4(1)	−4(1)	3(1)
N(7)	25(1)	16(1)	14(1)	1(1)	−6(1)	5(1)
N(8)	15(1)	16(1)	11(1)	4(1)	−2(1)	0(1)
C(1)	16(1)	13(1)	16(1)	4(1)	0(1)	1(1)
C(2)	21(1)	17(1)	16(1)	9(1)	−2(1)	1(1)
C(3)	15(1)	16(1)	14(1)	6(1)	1(1)	2(1)
C(4)	28(1)	14(1)	20(1)	5(1)	−6(1)	−1(1)
C(5)	27(1)	21(1)	17(1)	9(1)	−5(1)	−2(1)
C(6)	21(1)	12(1)	14(1)	4(1)	−2(1)	3(1)
C(7)	21(1)	15(1)	19(1)	7(1)	−3(1)	1(1)
C(8)	28(1)	20(1)	20(1)	6(1)	−8(1)	−3(1)
C(9)	40(1)	19(1)	15(1)	5(1)	−7(1)	1(1)
C(10)	32(1)	20(1)	14(1)	5(1)	1(1)	4(1)
C(11)	23(1)	14(1)	16(1)	6(1)	−1(1)	4(1)
C(12)	22(1)	25(1)	23(1)	6(1)	−5(1)	−3(1)
C(13)	30(1)	34(2)	32(1)	12(1)	−4(1)	−12(1)
C(14)	24(1)	36(2)	39(2)	9(1)	−3(1)	4(1)
C(15)	21(1)	17(1)	17(1)	4(1)	2(1)	3(1)
C(16)	23(1)	26(1)	31(1)	8(1)	−1(1)	8(1)
C(17)	28(1)	33(1)	24(1)	7(1)	6(1)	−2(1)
C(18)	18(1)	15(1)	14(1)	6(1)	−2(1)	1(1)
C(19)	21(1)	17(1)	18(1)	4(1)	−4(1)	1(1)
C(20)	28(1)	16(1)	25(1)	1(1)	−6(1)	2(1)
C(21)	28(1)	18(1)	34(1)	9(1)	−12(1)	−6(1)
C(22)	20(1)	23(1)	31(1)	13(1)	−5(1)	−4(1)
C(23)	16(1)	19(1)	17(1)	9(1)	−4(1)	−1(1)
C(24)	28(1)	24(1)	21(1)	2(1)	6(1)	3(1)
C(25)	56(2)	42(2)	22(1)	3(1)	10(1)	−1(2)
C(26)	27(1)	28(1)	42(2)	−2(1)	7(1)	6(1)
C(27)	14(1)	26(1)	19(1)	10(1)	0(1)	0(1)
C(28)	26(1)	30(1)	27(1)	12(1)	4(1)	10(1)
C(29)	22(1)	47(2)	30(1)	22(1)	5(1)	2(1)
C(30)	14(1)	16(1)	17(1)	6(1)	−3(1)	0(1)
C(31)	20(1)	20(1)	12(1)	4(1)	−4(1)	1(1)
C(32)	21(1)	13(1)	13(1)	4(1)	1(1)	3(1)
C(33)	18(1)	44(2)	27(1)	18(1)	−4(1)	2(1)
C(34)	28(1)	28(1)	13(1)	9(1)	2(1)	3(1)
C(35)	13(1)	16(1)	14(1)	3(1)	0(1)	0(1)
C(36)	21(1)	18(1)	20(1)	3(1)	5(1)	−2(1)
C(37)	28(1)	21(1)	23(1)	6(1)	7(1)	−5(1)
C(38)	23(1)	26(1)	17(1)	4(1)	6(1)	0(1)
C(39)	19(1)	17(1)	18(1)	3(1)	2(1)	3(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(40)	15(1)	15(1)	16(1)	4(1)	0(1)	3(1)
C(41)	49(2)	17(1)	25(1)	0(1)	14(1)	−9(1)
C(42)	99(3)	29(2)	42(2)	7(1)	−28(2)	−23(2)
C(43)	45(2)	21(1)	50(2)	2(1)	−3(1)	2(1)
C(44)	33(1)	12(1)	19(1)	4(1)	6(1)	3(1)
C(45)	55(2)	30(2)	56(2)	26(2)	−11(2)	4(1)
C(46)	30(1)	18(1)	29(1)	5(1)	6(1)	−4(1)
C(47)	17(1)	18(1)	16(1)	9(1)	3(1)	2(1)
C(48)	20(1)	21(1)	19(1)	8(1)	4(1)	2(1)
C(49)	21(1)	29(1)	31(1)	14(1)	10(1)	8(1)
C(50)	16(1)	32(1)	40(2)	19(1)	6(1)	1(1)
C(51)	22(1)	22(1)	29(1)	11(1)	−1(1)	−2(1)
C(52)	18(1)	19(1)	18(1)	9(1)	0(1)	0(1)
C(53)	27(1)	21(1)	27(1)	3(1)	10(1)	5(1)
C(54)	40(2)	33(2)	28(1)	−2(1)	11(1)	7(1)
C(55)	41(2)	20(1)	42(2)	8(1)	13(1)	12(1)
C(56)	21(1)	15(1)	21(1)	5(1)	3(1)	−1(1)
C(57)	30(1)	19(1)	30(1)	8(1)	2(1)	6(1)
C(58)	34(1)	20(1)	27(1)	0(1)	4(1)	−6(1)
C(59)	22(1)	28(1)	23(1)	11(1)	6(1)	3(1)
C(60)	22(1)	28(1)	26(1)	11(1)	3(1)	9(1)
C(61)	34(1)	18(1)	25(1)	11(1)	2(1)	10(1)
C(62)	34(1)	14(1)	23(1)	1(1)	−2(1)	−1(1)
C(63)	22(1)	12(1)	14(1)	6(1)	0(1)	0(1)
C(64)	23(1)	20(1)	20(1)	6(1)	−1(1)	3(1)
C(65)	30(1)	18(1)	24(1)	5(1)	2(1)	5(1)
C(66)	35(1)	16(1)	23(1)	1(1)	0(1)	−1(1)
C(67)	31(1)	20(1)	22(1)	3(1)	−8(1)	−4(1)
C(68)	26(1)	17(1)	22(1)	5(1)	−5(1)	1(1)
C(69)	19(1)	26(1)	17(1)	12(1)	−4(1)	−4(1)
C(70)	31(1)	36(2)	22(1)	10(1)	−7(1)	−14(1)
C(71)	43(2)	78(3)	38(2)	26(2)	−21(2)	−35(2)
C(72)	18(1)	117(4)	59(2)	56(2)	−16(1)	−23(2)
C(73)	17(1)	86(3)	54(2)	45(2)	4(1)	9(2)
C(74)	21(1)	45(2)	29(1)	21(1)	2(1)	7(1)
C11	30(1)	20(1)	20(1)	3(1)	−6(1)	−3(1)
C21	29(1)	23(1)	26(1)	1(1)	−6(1)	2(1)
C31	46(2)	19(1)	22(1)	0(1)	−9(1)	7(1)
C41	54(2)	23(1)	25(1)	5(1)	2(1)	2(1)
C51	34(1)	35(2)	33(2)	10(1)	2(1)	−1(1)
C61	27(1)	27(1)	34(1)	9(1)	−6(1)	−2(1)
C71	29(1)	38(2)	38(2)	18(1)	−7(1)	−7(1)

Table 4: Bond lengths [Å] for mw_145_1m.

Sb(1)–N(7)	2.0795(19)
Sb(1)–Ga(1)	2.6540(3)
Sb(1)–Sb(2)	2.8291(3)
Sb(2)–N(7)	2.0194(19)
Sb(2)–N(8)	2.0582(18)
Ga(1)–N(5)	1.8585(18)
Ga(1)–N(1)	1.9999(18)
Ga(1)–N(2)	2.0111(18)
Ga(2)–N(6)	1.8500(18)
Ga(2)–N(8)	1.8900(17)
Ga(2)–N(4)	1.9719(18)
Ga(2)–N(3)	1.9729(17)
N(1)–C(1)	1.332(3)
N(1)–C(6)	1.446(3)
N(2)–C(3)	1.327(3)
N(2)–C(18)	1.443(3)
N(3)–C(30)	1.325(3)
N(3)–C(35)	1.443(3)
N(4)–C(32)	1.332(3)
N(4)–C(47)	1.444(3)
N(5)–C(59)	1.446(3)
N(5)–C(60)	1.453(3)
N(6)–C(61)	1.447(3)
N(6)–C(62)	1.450(3)
N(7)–C(63)	1.377(3)
N(8)–C(69)	1.421(3)
C(1)–C(2)	1.401(3)
C(1)–C(4)	1.512(3)
C(2)–C(3)	1.403(3)
C(3)–C(5)	1.514(3)
C(6)–C(11)	1.408(3)
C(6)–C(7)	1.408(3)
C(7)–C(8)	1.400(3)
C(7)–C(12)	1.519(3)
C(8)–C(9)	1.375(4)
C(9)–C(10)	1.383(4)
C(10)–C(11)	1.400(3)
C(11)–C(15)	1.523(3)
C(12)–C(14)	1.530(4)
C(12)–C(13)	1.536(4)
C(15)–C(16)	1.532(3)
C(15)–C(17)	1.533(3)
C(18)–C(19)	1.402(3)
C(18)–C(23)	1.414(3)
C(19)–C(20)	1.399(3)
C(19)–C(24)	1.512(3)
C(20)–C(21)	1.375(4)
C(21)–C(22)	1.388(4)
C(22)–C(23)	1.386(3)
C(23)–C(27)	1.519(3)
C(24)–C(26)	1.526(4)
C(24)–C(25)	1.534(4)
C(27)–C(29)	1.527(3)

Table 4: (continued)

C(27)–C(28)	1.531(3)
C(30)–C(31)	1.400(3)
C(30)–C(33)	1.510(3)
C(31)–C(32)	1.400(3)
C(32)–C(34)	1.511(3)
C(35)–C(36)	1.398(3)
C(35)–C(40)	1.404(3)
C(36)–C(37)	1.399(3)
C(36)–C(41)	1.524(3)
C(37)–C(38)	1.385(3)
C(38)–C(39)	1.377(3)
C(39)–C(40)	1.397(3)
C(40)–C(44)	1.513(3)
C(41)–C(43)	1.521(4)
C(41)–C(42)	1.545(5)
C(44)–C(46)	1.523(4)
C(44)–C(45)	1.536(4)
C(47)–C(48)	1.408(3)
C(47)–C(52)	1.409(3)
C(48)–C(49)	1.394(3)
C(48)–C(53)	1.524(3)
C(49)–C(50)	1.375(4)
C(50)–C(51)	1.387(4)
C(51)–C(52)	1.392(3)
C(52)–C(56)	1.527(3)
C(53)–C(55)	1.535(4)
C(53)–C(54)	1.540(4)
C(56)–C(57)	1.530(3)
C(56)–C(58)	1.535(3)
C(63)–C(64)	1.401(3)
C(63)–C(68)	1.404(3)
C(64)–C(65)	1.384(3)
C(65)–C(66)	1.382(4)
C(66)–C(67)	1.384(4)
C(67)–C(68)	1.394(3)
C(69)–C(74)	1.391(4)
C(69)–C(70)	1.392(4)
C(70)–C(71)	1.390(4)
C(71)–C(72)	1.377(6)
C(72)–C(73)	1.370(6)
C(73)–C(74)	1.390(4)
C11–C21	1.390(4)
C11–C61	1.392(4)
C11–C71	1.506(4)
C21–C31	1.386(4)
C31–C41	1.376(4)
C41–C51	1.384(4)
C51–C61	1.381(4)

Table 5: Bond angles [°] for mw_145_1m.

N(7)–Sb(1)–Ga(1)	102.47(6)
N(7)–Sb(1)–Sb(2)	45.48(5)
Ga(1)–Sb(1)–Sb(2)	100.628(9)
N(7)–Sb(2)–N(8)	100.23(8)
N(7)–Sb(2)–Sb(1)	47.24(5)
N(8)–Sb(2)–Sb(1)	100.05(5)
N(5)–Ga(1)–N(1)	108.29(8)
N(5)–Ga(1)–N(2)	107.74(8)
N(1)–Ga(1)–N(2)	91.79(7)
N(5)–Ga(1)–Sb(1)	121.79(6)
N(1)–Ga(1)–Sb(1)	113.01(5)
N(2)–Ga(1)–Sb(1)	110.00(5)
N(6)–Ga(2)–N(8)	114.68(8)
N(6)–Ga(2)–N(4)	107.31(8)
N(8)–Ga(2)–N(4)	118.88(8)
N(6)–Ga(2)–N(3)	109.71(8)
N(8)–Ga(2)–N(3)	109.60(7)
N(4)–Ga(2)–N(3)	94.73(7)
C(1)–N(1)–C(6)	118.54(18)
C(1)–N(1)–Ga(1)	121.72(14)
C(6)–N(1)–Ga(1)	119.55(13)
C(3)–N(2)–C(18)	120.64(18)
C(3)–N(2)–Ga(1)	122.29(15)
C(18)–N(2)–Ga(1)	116.94(13)
C(30)–N(3)–C(35)	120.87(18)
C(30)–N(3)–Ga(2)	121.31(14)
C(35)–N(3)–Ga(2)	117.80(13)
C(32)–N(4)–C(47)	118.88(18)
C(32)–N(4)–Ga(2)	119.69(14)
C(47)–N(4)–Ga(2)	121.17(13)
C(59)–N(5)–C(60)	111.98(18)
C(59)–N(5)–Ga(1)	122.92(15)
C(60)–N(5)–Ga(1)	125.10(16)
C(61)–N(6)–C(62)	112.29(19)
C(61)–N(6)–Ga(2)	126.75(16)
C(62)–N(6)–Ga(2)	120.13(15)
C(63)–N(7)–Sb(2)	137.12(15)
C(63)–N(7)–Sb(1)	134.49(15)
Sb(2)–N(7)–Sb(1)	87.28(7)
C(69)–N(8)–Ga(2)	117.66(14)
C(69)–N(8)–Sb(2)	116.21(13)
Ga(2)–N(8)–Sb(2)	115.91(9)
N(1)–C(1)–C(2)	124.0(2)
N(1)–C(1)–C(4)	120.15(19)
C(2)–C(1)–C(4)	115.82(19)
C(1)–C(2)–C(3)	127.7(2)
N(2)–C(3)–C(2)	122.96(19)
N(2)–C(3)–C(5)	120.91(19)
C(2)–C(3)–C(5)	116.12(19)
C(11)–C(6)–C(7)	121.0(2)
C(11)–C(6)–N(1)	118.29(19)
C(7)–C(6)–N(1)	120.73(19)
C(8)–C(7)–C(6)	118.0(2)

Table 5: (continued)

C(8)–C(7)–C(12)	119.2(2)
C(6)–C(7)–C(12)	122.8(2)
C(9)–C(8)–C(7)	121.6(2)
C(8)–C(9)–C(10)	120.0(2)
C(9)–C(10)–C(11)	120.9(2)
C(10)–C(11)–C(6)	118.5(2)
C(10)–C(11)–C(15)	120.0(2)
C(6)–C(11)–C(15)	121.5(2)
C(7)–C(12)–C(14)	110.7(2)
C(7)–C(12)–C(13)	112.3(2)
C(14)–C(12)–C(13)	109.7(2)
C(11)–C(15)–C(16)	111.89(19)
C(11)–C(15)–C(17)	113.7(2)
C(16)–C(15)–C(17)	110.3(2)
C(19)–C(18)–C(23)	121.0(2)
C(19)–C(18)–N(2)	120.66(19)
C(23)–C(18)–N(2)	118.31(19)
C(20)–C(19)–C(18)	118.0(2)
C(20)–C(19)–C(24)	119.3(2)
C(18)–C(19)–C(24)	122.6(2)
C(21)–C(20)–C(19)	121.7(2)
C(20)–C(21)–C(22)	119.4(2)
C(23)–C(22)–C(21)	121.5(2)
C(22)–C(23)–C(18)	118.3(2)
C(22)–C(23)–C(27)	120.7(2)
C(18)–C(23)–C(27)	120.9(2)
C(19)–C(24)–C(26)	110.5(2)
C(19)–C(24)–C(25)	112.0(2)
C(26)–C(24)–C(25)	110.8(2)
C(23)–C(27)–C(29)	113.9(2)
C(23)–C(27)–C(28)	110.69(19)
C(29)–C(27)–C(28)	108.84(19)
N(3)–C(30)–C(31)	123.44(19)
N(3)–C(30)–C(33)	120.8(2)
C(31)–C(30)–C(33)	115.74(19)
C(30)–C(31)–C(32)	127.9(2)
N(4)–C(32)–C(31)	124.44(19)
N(4)–C(32)–C(34)	120.0(2)
C(31)–C(32)–C(34)	115.55(19)
C(36)–C(35)–C(40)	121.4(2)
C(36)–C(35)–N(3)	120.45(19)
C(40)–C(35)–N(3)	117.99(19)
C(35)–C(36)–C(37)	118.3(2)
C(35)–C(36)–C(41)	122.4(2)
C(37)–C(36)–C(41)	119.4(2)
C(38)–C(37)–C(36)	121.0(2)
C(39)–C(38)–C(37)	119.9(2)
C(38)–C(39)–C(40)	121.3(2)
C(39)–C(40)–C(35)	118.1(2)
C(39)–C(40)–C(44)	119.7(2)
C(35)–C(40)–C(44)	122.11(19)
C(43)–C(41)–C(36)	111.7(2)
C(43)–C(41)–C(42)	108.6(2)

Table 5: (continued)

C(36)–C(41)–C(42)	111.2(3)
C(40)–C(44)–C(46)	113.0(2)
C(40)–C(44)–C(45)	109.3(2)
C(46)–C(44)–C(45)	109.8(2)
C(48)–C(47)–C(52)	121.3(2)
C(48)–C(47)–N(4)	120.5(2)
C(52)–C(47)–N(4)	118.19(19)
C(49)–C(48)–C(47)	118.1(2)
C(49)–C(48)–C(53)	118.7(2)
C(47)–C(48)–C(53)	123.3(2)
C(50)–C(49)–C(48)	121.4(2)
C(49)–C(50)–C(51)	119.9(2)
C(50)–C(51)–C(52)	121.3(2)
C(51)–C(52)–C(47)	118.0(2)
C(51)–C(52)–C(56)	120.3(2)
C(47)–C(52)–C(56)	121.74(19)
C(48)–C(53)–C(55)	111.6(2)
C(48)–C(53)–C(54)	111.9(2)
C(55)–C(53)–C(54)	109.1(2)
C(52)–C(56)–C(57)	112.14(19)
C(52)–C(56)–C(58)	113.3(2)
C(57)–C(56)–C(58)	108.6(2)
N(7)–C(63)–C(64)	120.8(2)
N(7)–C(63)–C(68)	121.2(2)
C(64)–C(63)–C(68)	117.9(2)
C(65)–C(64)–C(63)	121.1(2)
C(66)–C(65)–C(64)	120.7(2)
C(65)–C(66)–C(67)	119.2(2)
C(66)–C(67)–C(68)	120.8(2)
C(67)–C(68)–C(63)	120.3(2)
C(74)–C(69)–C(70)	118.4(2)
C(74)–C(69)–N(8)	121.4(2)
C(70)–C(69)–N(8)	120.2(2)
C(71)–C(70)–C(69)	119.8(3)
C(72)–C(71)–C(70)	121.3(3)
C(73)–C(72)–C(71)	119.2(3)
C(72)–C(73)–C(74)	120.3(3)
C(73)–C(74)–C(69)	121.0(3)
C21–C11–C61	118.4(2)
C21–C11–C71	121.0(2)
C61–C11–C71	120.6(2)
C31–C21–C11	120.7(3)
C41–C31–C21	120.3(3)
C31–C41–C51	119.7(3)
C61–C51–C41	120.1(3)
C51–C61–C11	120.8(3)

Crystal structure of mw_150_2m

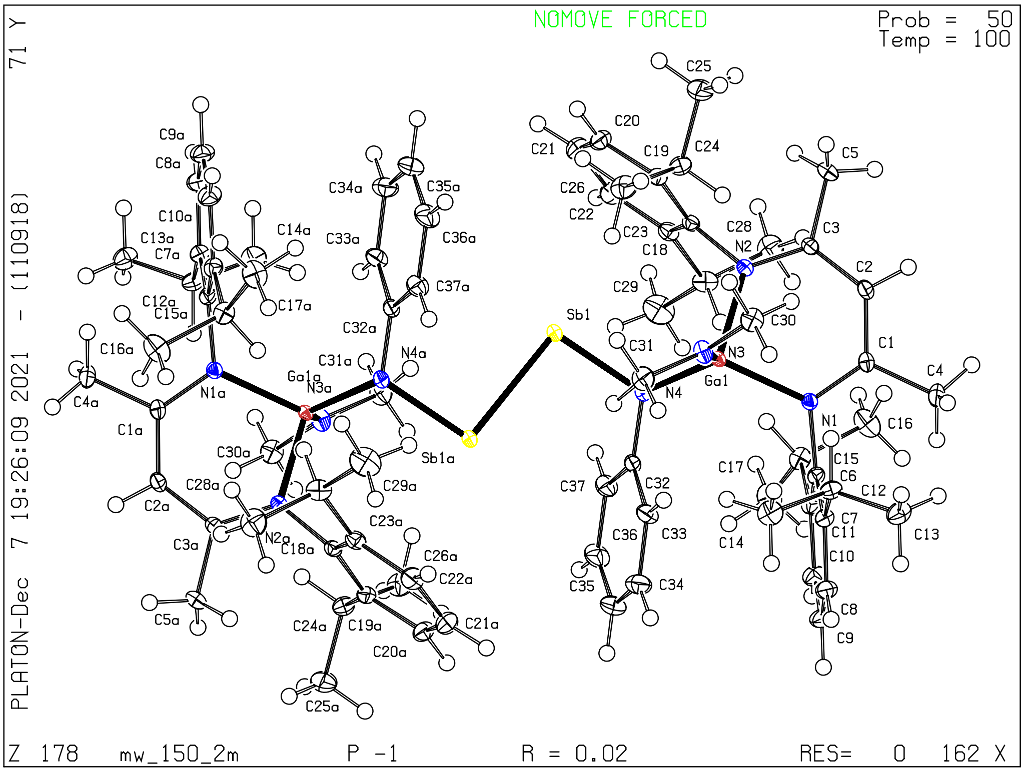

Table 1: Crystal data and structure refinement for mw_150_2m.

Identification code	mw_150_2m
Empirical Formula	$C_{74}H_{104}Ga_2N_8Sb_2$
Formula weight	1488.59 Da
Density (calculated)	$1.410\,g \cdot cm^{-3}$
$F(000)$	768
Temperature	100(2) K
Crystal size	0.184 × 0.182 × 0.116 mm
Crystal appearance	dark brown block
Wavelength (MoK_α)	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 10.4552(4)$ Å
	$b = 11.9732(4)$ Å
	$c = 14.9227(5)$ Å
	$\alpha = 93.2189(14)°$
	$\beta = 97.3354(14)°$
	$\gamma = 107.9954(14)°$
Unit cell volume	1753.06(11) $Å^3$
Z	1
Cell measurement refections used	9032
θ range for cell measurement	2.59° to 33.50°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	2.072° to 33.595°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.2%)
Index ranges	$-16 \leq h \leq 16$
	$-18 \leq k \leq 18$
	$-23 \leq l \leq 23$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.569\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.65
R_{merg} before/after correction	0.0465/0.0317
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	139632
Independent reflections	13767 ($R_{int} = 0.0193$)
Reflections with $I > 2\sigma(I)$	12730
Data / retraints / parameter	13767 / 0 / 400
Goodness-of-fit on F^2	1.079
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2 + 0.8077P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0191$
	$wR2 = 0.0525$
R indices [all data]	$R1 = 0.0219$
	$wR2 = 0.0543$
Largest diff. peak and hole	0.928 and -0.313 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_150_2m. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	4592(1)	5544(1)	4317(1)	15(1)
Ga(1)	3332(1)	3902(1)	2369(1)	8(1)
N(1)	1910(1)	2644(1)	1563(1)	11(1)
N(2)	2853(1)	5206(1)	1806(1)	11(1)
N(3)	5027(1)	3901(1)	2129(1)	15(1)
N(4)	3174(1)	4038(1)	3609(1)	12(1)
C(1)	1530(1)	2844(1)	714(1)	12(1)
C(2)	1799(1)	3973(1)	412(1)	14(1)
C(3)	2311(1)	5071(1)	937(1)	12(1)
C(4)	736(1)	1825(1)	16(1)	17(1)
C(5)	2201(1)	6130(1)	462(1)	18(1)
C(6)	1395(1)	1473(1)	1847(1)	12(1)
C(7)	2047(1)	628(1)	1700(1)	13(1)
C(8)	1552(1)	−467(1)	2039(1)	17(1)
C(9)	435(1)	−724(1)	2489(1)	19(1)
C(10)	−210(1)	114(1)	2618(1)	18(1)
C(11)	259(1)	1227(1)	2313(1)	14(1)
C(12)	3269(1)	844(1)	1201(1)	15(1)
C(13)	2985(1)	−67(1)	375(1)	21(1)
C(14)	4533(1)	815(1)	1827(1)	22(1)
C(15)	−431(1)	2149(1)	2490(1)	16(1)
C(16)	−1349(1)	2275(1)	1643(1)	24(1)
C(17)	−1266(1)	1911(1)	3274(1)	23(1)
C(18)	3228(1)	6331(1)	2340(1)	12(1)
C(19)	4507(1)	7175(1)	2335(1)	14(1)
C(20)	4888(1)	8196(1)	2938(1)	18(1)
C(21)	4029(1)	8385(1)	3522(1)	21(1)
C(22)	2754(1)	7559(1)	3503(1)	19(1)
C(23)	2331(1)	6518(1)	2920(1)	14(1)
C(24)	5496(1)	7015(1)	1718(1)	16(1)
C(25)	5826(1)	8012(1)	1097(1)	24(1)
C(26)	6814(1)	6963(1)	2266(1)	22(1)
C(27)	948(1)	5600(1)	2913(1)	18(1)
C(28)	−92(1)	5714(1)	2134(1)	26(1)
C(29)	404(1)	5627(1)	3815(1)	31(1)
C(30)	5390(1)	3943(1)	1227(1)	19(1)
C(31)	6113(1)	3832(1)	2804(1)	19(1)
C(32)	2761(1)	3042(1)	4097(1)	12(1)
C(33)	3163(1)	2053(1)	3950(1)	17(1)
C(34)	2713(1)	1062(1)	4425(1)	24(1)
C(35)	1879(1)	1062(1)	5075(1)	26(1)
C(36)	1491(1)	2054(1)	5242(1)	24(1)
C(37)	1919(1)	3032(1)	4763(1)	18(1)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_150_2m.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	20(1)	12(1)	10(1)	2(1)	−3(1)	4(1)
Ga(1)	8(1)	10(1)	8(1)	1(1)	1(1)	3(1)
N(1)	10(1)	11(1)	10(1)	1(1)	1(1)	3(1)
N(2)	11(1)	12(1)	10(1)	2(1)	1(1)	4(1)
N(3)	10(1)	21(1)	14(1)	2(1)	2(1)	6(1)
N(4)	14(1)	13(1)	9(1)	2(1)	1(1)	3(1)
C(1)	10(1)	15(1)	10(1)	0(1)	0(1)	4(1)
C(2)	15(1)	16(1)	9(1)	2(1)	0(1)	5(1)
C(3)	11(1)	13(1)	11(1)	3(1)	2(1)	4(1)
C(4)	17(1)	18(1)	13(1)	−3(1)	−2(1)	3(1)
C(5)	22(1)	17(1)	14(1)	6(1)	1(1)	7(1)
C(6)	10(1)	11(1)	12(1)	1(1)	1(1)	2(1)
C(7)	13(1)	12(1)	14(1)	1(1)	3(1)	3(1)
C(8)	19(1)	13(1)	18(1)	2(1)	4(1)	4(1)
C(9)	21(1)	14(1)	22(1)	4(1)	6(1)	2(1)
C(10)	16(1)	16(1)	20(1)	3(1)	7(1)	1(1)
C(11)	11(1)	14(1)	14(1)	1(1)	2(1)	2(1)
C(12)	14(1)	12(1)	19(1)	2(1)	5(1)	5(1)
C(13)	24(1)	17(1)	22(1)	−1(1)	9(1)	5(1)
C(14)	16(1)	23(1)	28(1)	2(1)	3(1)	9(1)
C(15)	12(1)	18(1)	18(1)	0(1)	5(1)	5(1)
C(16)	22(1)	36(1)	22(1)	7(1)	6(1)	18(1)
C(17)	19(1)	32(1)	20(1)	3(1)	8(1)	10(1)
C(18)	14(1)	11(1)	11(1)	2(1)	1(1)	6(1)
C(19)	15(1)	12(1)	14(1)	3(1)	1(1)	4(1)
C(20)	19(1)	12(1)	21(1)	0(1)	0(1)	4(1)
C(21)	28(1)	15(1)	20(1)	−2(1)	2(1)	9(1)
C(22)	26(1)	18(1)	18(1)	1(1)	5(1)	12(1)
C(23)	16(1)	15(1)	14(1)	3(1)	4(1)	8(1)
C(24)	14(1)	14(1)	18(1)	3(1)	4(1)	3(1)
C(25)	27(1)	22(1)	22(1)	8(1)	8(1)	4(1)
C(26)	14(1)	22(1)	30(1)	5(1)	3(1)	4(1)
C(27)	17(1)	18(1)	23(1)	4(1)	9(1)	9(1)
C(28)	16(1)	31(1)	30(1)	3(1)	2(1)	6(1)
C(29)	28(1)	40(1)	29(1)	8(1)	17(1)	12(1)
C(30)	16(1)	22(1)	18(1)	1(1)	7(1)	5(1)
C(31)	11(1)	22(1)	23(1)	2(1)	0(1)	7(1)
C(32)	13(1)	14(1)	10(1)	2(1)	1(1)	4(1)
C(33)	22(1)	18(1)	14(1)	5(1)	5(1)	9(1)
C(34)	35(1)	17(1)	23(1)	6(1)	5(1)	10(1)
C(35)	33(1)	22(1)	22(1)	11(1)	5(1)	2(1)
C(36)	24(1)	28(1)	18(1)	9(1)	8(1)	5(1)
C(37)	19(1)	21(1)	15(1)	4(1)	6(1)	6(1)

Table 4: Bond lengths [Å] for mw_150_2m.

Sb(1)–N(4)	2.0727(8)
Sb(1)–Sb(1)#1	2.66878(14)
Ga(1)–N(3)	1.8524(8)
Ga(1)–N(4)	1.8818(8)
Ga(1)–N(1)	1.9700(8)
Ga(1)–N(2)	1.9785(8)
N(1)–C(1)	1.3362(12)
N(1)–C(6)	1.4468(12)
N(2)–C(3)	1.3270(11)
N(2)–C(18)	1.4416(12)
N(3)–C(30)	1.4445(13)
N(3)–C(31)	1.4447(13)
N(4)–C(32)	1.4137(12)
C(1)–C(2)	1.4057(13)
C(1)–C(4)	1.5074(13)
C(2)–C(3)	1.4031(13)
C(3)–C(5)	1.5151(13)
C(6)–C(7)	1.4061(13)
C(6)–C(11)	1.4150(13)
C(7)–C(8)	1.4019(13)
C(7)–C(12)	1.5214(14)
C(8)–C(9)	1.3822(15)
C(9)–C(10)	1.3883(15)
C(10)–C(11)	1.3945(14)
C(11)–C(15)	1.5224(14)
C(12)–C(14)	1.5282(15)
C(12)–C(13)	1.5328(15)
C(15)–C(16)	1.5313(16)
C(15)–C(17)	1.5342(15)
C(18)–C(19)	1.4062(13)
C(18)–C(23)	1.4128(13)
C(19)–C(20)	1.3951(14)
C(19)–C(24)	1.5163(14)
C(20)–C(21)	1.3860(16)
C(21)–C(22)	1.3884(17)
C(22)–C(23)	1.3952(14)
C(23)–C(27)	1.5208(15)
C(24)–C(26)	1.5303(16)
C(24)–C(25)	1.5346(15)
C(27)–C(29)	1.5283(16)
C(27)–C(28)	1.5297(17)
C(32)–C(33)	1.3889(14)
C(32)–C(37)	1.4073(14)
C(33)–C(34)	1.4023(15)
C(34)–C(35)	1.3846(18)
C(35)–C(36)	1.3884(19)
C(36)–C(37)	1.3901(15)

#1 -x+1,-y+1,-z+1

Table 5: Bond angles [°] for mw_150_2m.

N(4)–Sb(1)–Sb(1)#1	95.83(2)
N(3)–Ga(1)–N(4)	114.86(4)
N(3)–Ga(1)–N(1)	109.30(4)
N(4)–Ga(1)–N(1)	117.88(3)
N(3)–Ga(1)–N(2)	109.88(4)
N(4)–Ga(1)–N(2)	108.28(3)
N(1)–Ga(1)–N(2)	94.62(3)
C(1)–N(1)–C(6)	119.80(8)
C(1)–N(1)–Ga(1)	119.27(6)
C(6)–N(1)–Ga(1)	120.53(6)
C(3)–N(2)–C(18)	121.15(8)
C(3)–N(2)–Ga(1)	120.47(6)
C(18)–N(2)–Ga(1)	118.11(6)
C(30)–N(3)–C(31)	112.52(8)
C(30)–N(3)–Ga(1)	122.81(7)
C(31)–N(3)–Ga(1)	124.65(7)
C(32)–N(4)–Ga(1)	122.29(6)
C(32)–N(4)–Sb(1)	116.72(6)
Ga(1)–N(4)–Sb(1)	112.55(4)
N(1)–C(1)–C(2)	124.02(8)
N(1)–C(1)–C(4)	120.09(9)
C(2)–C(1)–C(4)	115.87(8)
C(3)–C(2)–C(1)	128.01(8)
N(2)–C(3)–C(2)	123.43(8)
N(2)–C(3)–C(5)	120.20(8)
C(2)–C(3)–C(5)	116.37(8)
C(7)–C(6)–C(11)	121.24(9)
C(7)–C(6)–N(1)	120.81(8)
C(11)–C(6)–N(1)	117.88(8)
C(8)–C(7)–C(6)	118.20(9)
C(8)–C(7)–C(12)	118.35(8)
C(6)–C(7)–C(12)	123.44(8)
C(9)–C(8)–C(7)	121.19(10)
C(8)–C(9)–C(10)	119.96(9)
C(9)–C(10)–C(11)	121.28(9)
C(10)–C(11)–C(6)	118.10(9)
C(10)–C(11)–C(15)	120.53(9)
C(6)–C(11)–C(15)	121.36(9)
C(7)–C(12)–C(14)	111.41(9)
C(7)–C(12)–C(13)	111.51(8)
C(14)–C(12)–C(13)	109.11(9)
C(11)–C(15)–C(16)	112.09(9)
C(11)–C(15)–C(17)	113.36(9)
C(16)–C(15)–C(17)	108.80(9)
C(19)–C(18)–C(23)	121.29(9)
C(19)–C(18)–N(2)	120.26(8)
C(23)–C(18)–N(2)	118.22(8)
C(20)–C(19)–C(18)	118.23(9)
C(20)–C(19)–C(24)	118.75(9)
C(18)–C(19)–C(24)	123.01(9)
C(21)–C(20)–C(19)	121.24(10)
C(20)–C(21)–C(22)	119.96(10)
C(21)–C(22)–C(23)	121.04(10)

Table 5: (continued)

C(22)–C(23)–C(18)	118.21(9)
C(22)–C(23)–C(27)	121.12(9)
C(18)–C(23)–C(27)	120.66(9)
C(19)–C(24)–C(26)	111.31(9)
C(19)–C(24)–C(25)	111.05(9)
C(26)–C(24)–C(25)	109.67(9)
C(23)–C(27)–C(29)	113.45(10)
C(23)–C(27)–C(28)	111.15(9)
C(29)–C(27)–C(28)	110.34(10)
C(33)–C(32)–C(37)	117.60(9)
C(33)–C(32)–N(4)	122.31(9)
C(37)–C(32)–N(4)	120.08(9)
C(32)–C(33)–C(34)	121.44(10)
C(35)–C(34)–C(33)	120.26(11)
C(34)–C(35)–C(36)	118.93(10)
C(35)–C(36)–C(37)	120.94(11)
C(36)–C(37)–C(32)	120.80(10)

#1 -x+1,-y+1,-z+1

Crystal structure of mw_089_1fsm

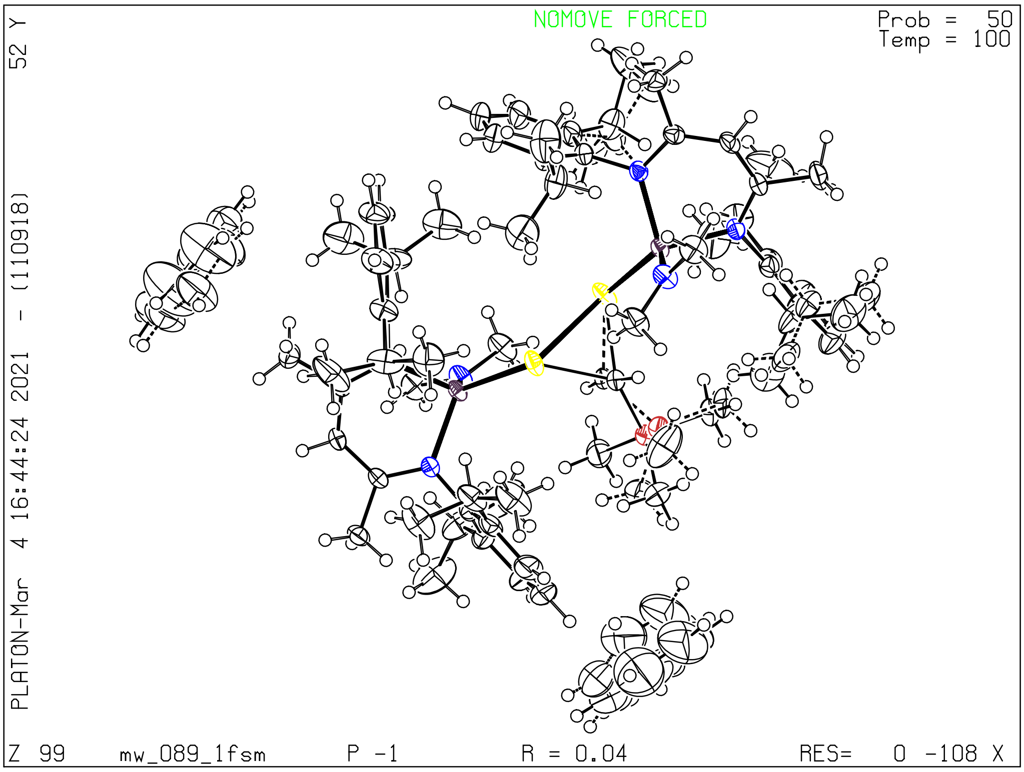

Table 1: Crystal data and structure refinement for mw_089_1fsm.

Identification code	mw_089_1fsm
Empirical Formula	$C_{78}H_{116}Ga_2N_6Sb_2Si$
Formula weight	1548.79 Da
Density (calculated)	$1.295\,g \cdot cm^{-3}$
$F(000)$	1608
Temperature	100(2) K
Crystal size	0.321 × 0.316 × 0.107 mm
Crystal appearance	orange tablet
Wavelength (MoK_{α})	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 10.919(2)$ Å
	$b = 14.343(3)$ Å
	$c = 26.014(6)$ Å
	$\alpha = 83.994(15)°$
	$\beta = 78.718(10)°$
	$\gamma = 88.053(10)°$
Unit cell volume	3972.9(16) $Å^3$
Z	2
Cell measurement refections used	8951
θ range for cell measurement	2.36° to 30.61°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.902° to 33.568°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.0%)
Index ranges	$-16 \le h \le 16$
	$-22 \le k \le 22$
	$-40 \le l \le 40$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.401\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.59
R_{merg} before/after correction	0.0986/0.0730
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	238703
Independent reflections	31007 ($R_{int} = 0.0652$)
Reflections with $I > 2\sigma(I)$	23633
Data / retraints / parameter	31007 / 1030 / 1048
Goodness-of-fit on F^2	1.063
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 4.0886P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0402$
	$wR2 = 0.0841$
R indices [all data]	$R1 = 0.0628$
	$wR2 = 0.0942$
Largest diff. peak and hole	3.087 and -3.509 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

The benzene molecules are highly disordered and were modelled with two alternate positions. No further alternate positions could be found although the anisotropic displacememnt parameters suggest that this is just a crude model. This can also be concluded from the unrealistically short bond lengths. All bond lengths and angles were restraint to be equal (`SADI`) and the atoms were restrained to lie on a mutual plane (`FLAT`). `DFIX` restraints were not suitable to improve the unrealistic bond lengths. The displacement parameters of the benzenes' atoms were restrained with `RIGU` and `SIMU`. Two iso-propyl groups are disordered over two positions. Their atoms' displacement parameters were restrained with `RIGU` in both cases and additionally with `SIMU` in one case. The $CHSiMe_3$ group is disordered over two positions. All its corresponding bond lengths were restrained to be equal (`SADI`) and `RIGU` restraints were applied to the displacement parameters.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_089_1fsm. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	3621(1)	6668(1)	2630(1)	31(1)
C(1)	2614(2)	6188(1)	4574(1)	26(1)
Si(1)	3745(2)	4828(1)	1764(1)	41(1)
C(63)	3669(4)	6072(3)	1906(1)	31(1)
C(64)	3039(11)	4717(7)	1178(3)	76(3)
C(65)	5423(6)	4458(5)	1616(2)	70(2)
C(66)	2867(6)	4058(3)	2324(2)	56(1)
Si(1')	3972(3)	5085(2)	1595(1)	46(1)
C(63')	2897(6)	5704(4)	2099(2)	31(1)
C(64')	3290(17)	5024(12)	1006(4)	77(4)
C(65')	5600(9)	5591(9)	1416(5)	97(4)
C(66')	4219(12)	3898(6)	1901(3)	80(3)
N(1)	2536(2)	6537(1)	4085(1)	24(1)
Ga(1)	2572(1)	5696(1)	3517(1)	23(1)
Sb(2)	1827(1)	6912(1)	1994(1)	33(1)
C(2)	3064(2)	5289(1)	4700(1)	26(1)
N(2)	3684(1)	4754(1)	3838(1)	22(1)
Ga(2)	2728(1)	8280(1)	1274(1)	22(1)
N(5)	1058(2)	5078(1)	3614(1)	33(1)
C(5)	4318(2)	3839(2)	4606(1)	33(1)
N(4)	2252(2)	8189(1)	573(1)	25(1)
C(4)	2232(2)	6780(2)	5028(1)	38(1)
N(3)	1699(2)	9439(1)	1391(1)	24(1)
C(3)	3663(2)	4655(1)	4353(1)	23(1)
N(6)	4412(2)	8613(1)	1118(1)	33(1)
C(6)	2326(2)	7536(1)	3998(1)	29(1)
C(9)	1926(3)	9464(2)	3925(1)	48(1)
C(8)	3126(3)	9101(2)	3890(1)	47(1)
C(7)	3359(2)	8138(2)	3923(1)	37(1)
C(10)	937(3)	8870(2)	3977(1)	44(1)
C(11)	1112(2)	7900(2)	4010(1)	35(1)
C(12)	4693(2)	7776(2)	3894(1)	50(1)
C(14)	5567(3)	8192(3)	3398(1)	61(1)
C(13)	5208(3)	7971(3)	4376(2)	79(1)
C(15)	−17(2)	7277(2)	4055(1)	46(1)
C(16)	−954(3)	7357(3)	4572(2)	79(1)
C(17)	−657(3)	7525(2)	3589(2)	65(1)
C(18)	4420(2)	4102(2)	3513(1)	29(1)
C(19)	5597(2)	4395(2)	3222(1)	40(1)
C(20)	6289(3)	3754(3)	2901(1)	60(1)
C(21)	5847(3)	2887(3)	2868(1)	64(1)
C(22)	4708(3)	2611(2)	3156(1)	54(1)
C(23)	3967(2)	3206(2)	3489(1)	39(1)
C(24)	6106(2)	5343(2)	3276(1)	45(1)
C(25)	6672(3)	5315(3)	3772(1)	61(1)
C(26)	7053(3)	5742(3)	2794(1)	70(1)
C(27)	2729(3)	2845(2)	3807(1)	58(1)
C(28)	2904(4)	1912(2)	4145(2)	88(1)
C(29)	1787(4)	2728(3)	3455(2)	106(2)
C(30)	1576(2)	10062(1)	986(1)	27(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(31)	1811(2)	9847(2)	464(1)	30(1)
C(32)	2012(2)	8967(2)	278(1)	29(1)
C(33)	1155(2)	11056(2)	1077(1)	38(1)
C(34)	1945(3)	8933(2)	−294(1)	47(1)
C(35)	1150(2)	9664(2)	1915(1)	29(1)
C(36)	−112(2)	9423(2)	2115(1)	38(1)
C(37)	−661(3)	9680(2)	2613(1)	52(1)
C(38)	0(3)	10143(2)	2905(1)	56(1)
C(39)	1241(3)	10348(2)	2710(1)	50(1)
C(40)	1851(2)	10108(2)	2214(1)	37(1)
C(41)	−835(17)	8792(13)	1801(7)	37(3)
C(42)	−1492(18)	9454(13)	1448(8)	59(4)
C(43)	−1790(30)	8149(19)	2125(10)	55(4)
C(41')	−911(14)	9044(13)	1801(6)	45(3)
C(42')	−1859(15)	9744(14)	1603(7)	70(3)
C(43')	−1590(20)	8156(14)	2128(8)	57(3)
C(44)	3219(3)	10336(2)	2027(1)	50(1)
C(45)	3456(4)	11391(3)	2001(2)	76(1)
C(46)	4011(3)	9788(3)	2381(2)	72(1)
C(47)	2288(2)	7302(2)	350(1)	31(1)
C(48)	1189(2)	6774(2)	443(1)	39(1)
C(49)	1227(3)	5941(2)	208(1)	52(1)
C(50)	2303(4)	5626(2)	−98(1)	58(1)
C(51)	3376(3)	6137(2)	−173(1)	58(1)
C(52)	3399(3)	6988(2)	47(1)	47(1)
C(53)	−25(3)	7103(2)	770(1)	52(1)
C(54)	−834(4)	7659(4)	431(2)	101(2)
C(55)	−776(4)	6318(3)	1112(2)	75(1)
C(56)	4624(9)	7439(10)	10(7)	55(2)
C(57)	5185(14)	7700(10)	−573(7)	80(3)
C(58)	5560(8)	6869(12)	280(7)	77(3)
C(56')	4599(14)	7665(13)	−164(8)	44(3)
C(57')	4995(17)	7884(13)	−758(8)	58(4)
C(58')	5632(16)	7191(19)	65(10)	66(5)
C(59)	418(2)	4688(2)	4128(1)	39(1)
C(60)	240(2)	5161(2)	3237(1)	43(1)
C(61)	4881(2)	9390(2)	741(1)	42(1)
C(62)	5342(2)	8252(2)	1409(1)	45(1)
C11	2771(19)	8513(12)	6086(8)	108(5)
C21	1628(14)	8355(8)	5986(5)	66(3)
C31	1155(10)	8938(9)	5625(6)	62(3)
C41	1828(16)	9666(10)	5351(7)	74(3)
C51	2985(16)	9816(13)	5443(10)	143(7)
C61	3413(17)	9287(14)	5836(13)	162(8)
C12	8580(14)	3022(7)	1275(4)	111(4)
C22	8160(10)	2321(9)	1649(4)	97(3)
C32	8756(10)	2128(8)	2069(4)	92(3)
C42	9722(12)	2661(9)	2115(5)	117(4)
C52	10156(17)	3355(10)	1727(6)	159(6)
C62	9569(19)	3530(7)	1310(5)	154(6)
C13	8205(18)	2945(15)	1462(9)	123(7)
C23	8330(20)	2188(12)	1810(10)	115(7)

Table 2: (continued)

	x	y	z	U_{eq}
C33	9060(30)	2247(16)	2173(10)	130(9)
C43	9660(20)	3050(20)	2191(7)	125(7)
C53	9530(20)	3808(17)	1846(8)	135(7)
C63	8780(20)	3757(13)	1492(9)	128(7)
C14	3239(17)	8619(14)	5983(6)	96(5)
C24	2043(19)	8323(11)	6077(7)	87(4)
C34	1246(14)	8712(17)	5770(9)	94(5)
C44	1649(16)	9379(18)	5371(8)	91(5)
C54	2836(18)	9699(13)	5286(6)	100(5)
C64	3648(12)	9285(13)	5584(7)	107(5)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_089_1fsm.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	25(1)	48(1)	19(1)	6(1)	−5(1)	−5(1)
C(1)	25(1)	27(1)	24(1)	−1(1)	−4(1)	−5(1)
Si(1)	65(1)	34(1)	26(1)	−9(1)	−16(1)	20(1)
C(63)	37(2)	35(2)	20(1)	−2(1)	−4(1)	8(1)
C(64)	128(7)	77(5)	35(4)	−26(3)	−41(5)	49(5)
C(65)	85(4)	78(4)	49(3)	−22(3)	−16(3)	47(3)
C(66)	95(4)	33(2)	43(2)	−6(2)	−20(2)	3(2)
Si(1')	74(2)	37(1)	24(1)	−4(1)	−6(1)	22(1)
C(63')	46(3)	27(2)	18(2)	−1(2)	−4(2)	5(2)
C(64')	102(9)	104(12)	36(6)	−35(6)	−34(6)	48(8)
C(65')	79(6)	116(9)	87(8)	−41(7)	24(6)	−6(6)
C(66')	133(9)	51(4)	49(5)	2(4)	−11(5)	49(5)
N(1)	23(1)	23(1)	25(1)	2(1)	−6(1)	−2(1)
Ga(1)	18(1)	29(1)	21(1)	5(1)	−7(1)	−5(1)
Sb(2)	32(1)	34(1)	33(1)	14(1)	−15(1)	−9(1)
C(2)	31(1)	28(1)	18(1)	2(1)	−7(1)	−4(1)
N(2)	20(1)	27(1)	20(1)	1(1)	−4(1)	−3(1)
Ga(2)	20(1)	26(1)	19(1)	3(1)	−5(1)	−3(1)
N(5)	23(1)	44(1)	32(1)	6(1)	−9(1)	−12(1)
C(5)	38(1)	29(1)	31(1)	4(1)	−13(1)	3(1)
N(4)	30(1)	26(1)	21(1)	−1(1)	−7(1)	−2(1)
C(4)	46(1)	37(1)	28(1)	−5(1)	−1(1)	1(1)
N(3)	24(1)	27(1)	20(1)	1(1)	−2(1)	−1(1)
C(3)	22(1)	24(1)	23(1)	4(1)	−8(1)	−4(1)
N(6)	23(1)	40(1)	34(1)	7(1)	−4(1)	−7(1)
C(6)	29(1)	24(1)	34(1)	2(1)	−10(1)	−1(1)
C(9)	58(2)	26(1)	64(2)	−1(1)	−25(1)	2(1)
C(8)	50(2)	30(1)	65(2)	3(1)	−24(1)	−12(1)
C(7)	35(1)	29(1)	49(1)	4(1)	−15(1)	−6(1)
C(10)	42(1)	32(1)	59(2)	1(1)	−18(1)	9(1)
C(11)	32(1)	30(1)	43(1)	3(1)	−10(1)	1(1)
C(12)	32(1)	33(1)	85(2)	5(1)	−18(1)	−10(1)
C(14)	40(1)	80(2)	65(2)	−9(2)	−16(1)	−10(2)
C(13)	49(2)	114(3)	71(2)	37(2)	−28(2)	−6(2)
C(15)	24(1)	35(1)	74(2)	4(1)	−8(1)	1(1)
C(16)	43(2)	87(3)	92(3)	16(2)	8(2)	−2(2)
C(17)	41(2)	62(2)	99(3)	−4(2)	−30(2)	−10(1)
C(18)	26(1)	41(1)	21(1)	−2(1)	−6(1)	6(1)
C(19)	25(1)	60(2)	30(1)	10(1)	−4(1)	10(1)
C(20)	39(1)	88(2)	42(1)	10(2)	8(1)	29(2)
C(21)	71(2)	73(2)	42(2)	−9(2)	−1(1)	40(2)
C(22)	66(2)	52(2)	46(2)	−21(1)	−17(1)	26(1)
C(23)	40(1)	42(1)	39(1)	−15(1)	−13(1)	8(1)
C(24)	21(1)	66(2)	43(1)	20(1)	−4(1)	−3(1)
C(25)	35(1)	89(2)	58(2)	22(2)	−18(1)	−25(1)
C(26)	32(1)	105(3)	60(2)	38(2)	1(1)	−10(2)
C(27)	47(2)	42(2)	86(2)	−32(2)	−5(2)	−9(1)
C(28)	94(3)	38(2)	118(4)	−18(2)	17(3)	−23(2)
C(29)	58(2)	109(3)	176(5)	−98(4)	−41(3)	4(2)
C(30)	26(1)	25(1)	27(1)	3(1)	−3(1)	−1(1)
C(31)	38(1)	28(1)	24(1)	7(1)	−7(1)	−1(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(32)	35(1)	33(1)	19(1)	2(1)	−8(1)	−1(1)
C(33)	48(1)	28(1)	36(1)	1(1)	−1(1)	4(1)
C(34)	72(2)	48(1)	22(1)	1(1)	−16(1)	1(1)
C(35)	33(1)	32(1)	22(1)	0(1)	−2(1)	2(1)
C(36)	34(1)	52(1)	25(1)	3(1)	1(1)	2(1)
C(37)	43(1)	75(2)	29(1)	3(1)	7(1)	10(1)
C(38)	67(2)	71(2)	24(1)	−7(1)	2(1)	20(2)
C(39)	68(2)	54(2)	30(1)	−16(1)	−8(1)	8(1)
C(40)	47(1)	38(1)	28(1)	−8(1)	−5(1)	0(1)
C(41)	33(4)	44(6)	31(4)	1(4)	−4(3)	−7(4)
C(42)	49(6)	70(8)	59(7)	24(5)	−25(5)	−17(5)
C(43)	30(7)	66(7)	64(7)	27(6)	−13(5)	−8(4)
C(41')	31(3)	58(7)	41(3)	−4(4)	12(2)	−12(4)
C(42')	55(6)	88(8)	66(6)	27(6)	−29(5)	−20(5)
C(43')	32(6)	62(5)	72(6)	−8(5)	1(4)	−6(4)
C(44)	51(2)	62(2)	40(1)	−22(1)	−7(1)	−17(1)
C(45)	95(3)	73(2)	64(2)	−16(2)	−14(2)	−39(2)
C(46)	52(2)	91(3)	79(2)	−20(2)	−23(2)	−4(2)
C(47)	40(1)	29(1)	28(1)	−5(1)	−13(1)	−1(1)
C(48)	46(1)	35(1)	41(1)	−4(1)	−22(1)	−4(1)
C(49)	66(2)	42(1)	56(2)	−9(1)	−30(2)	−11(1)
C(50)	91(2)	40(1)	53(2)	−20(1)	−29(2)	−2(2)
C(51)	71(2)	51(2)	55(2)	−27(1)	−10(2)	5(2)
C(52)	51(2)	45(1)	48(2)	−21(1)	−5(1)	−1(1)
C(53)	37(1)	51(2)	71(2)	−9(1)	−17(1)	−12(1)
C(54)	43(2)	116(4)	136(4)	30(3)	−23(2)	8(2)
C(55)	68(2)	82(3)	75(2)	−12(2)	−7(2)	−32(2)
C(56)	50(3)	52(5)	54(5)	−22(4)	21(3)	−5(3)
C(57)	83(6)	69(5)	70(6)	−1(5)	28(5)	−8(4)
C(58)	43(3)	108(7)	81(7)	−24(6)	−8(4)	−7(4)
C(56')	43(4)	43(6)	42(6)	−11(5)	4(4)	−4(4)
C(57')	69(7)	48(7)	44(6)	−3(5)	21(5)	1(5)
C(58')	58(6)	83(11)	60(9)	−38(7)	−9(6)	24(6)
C(59)	30(1)	44(1)	41(1)	6(1)	−1(1)	−14(1)
C(60)	29(1)	53(2)	51(1)	5(1)	−20(1)	−13(1)
C(61)	32(1)	44(1)	46(1)	7(1)	0(1)	−13(1)
C(62)	24(1)	66(2)	43(1)	6(1)	−9(1)	−7(1)
C11	92(10)	119(10)	131(12)	−10(8)	−68(10)	3(8)
C21	62(6)	72(5)	63(6)	−14(4)	−12(4)	15(5)
C31	56(4)	64(6)	67(7)	−13(4)	−12(4)	12(3)
C41	85(7)	58(6)	85(7)	−12(5)	−24(5)	0(5)
C51	129(10)	123(11)	193(18)	27(11)	−79(10)	−60(9)
C61	126(11)	180(14)	202(19)	27(13)	−102(12)	−58(10)
C12	175(10)	82(6)	74(6)	1(4)	−30(7)	52(5)
C22	93(6)	119(7)	67(5)	10(5)	−4(4)	55(5)
C32	90(5)	120(7)	50(4)	11(4)	4(4)	61(4)
C42	140(9)	111(8)	103(7)	−35(5)	−32(7)	56(6)
C52	205(14)	113(9)	172(11)	−21(7)	−60(9)	−11(9)
C62	236(15)	71(6)	153(10)	24(6)	−54(10)	5(7)
C13	128(13)	127(13)	95(14)	14(11)	15(10)	−2(10)
C23	124(17)	86(9)	107(17)	−8(9)	43(10)	33(10)
C33	128(18)	128(14)	104(16)	16(13)	26(11)	68(12)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C43	126(13)	160(16)	77(9)	−21(10)	1(8)	68(12)
C53	136(15)	133(13)	130(14)	−7(10)	−20(10)	26(11)
C63	129(15)	110(11)	136(15)	41(11)	−29(11)	5(10)
C14	89(9)	103(10)	96(8)	17(6)	−37(7)	22(7)
C24	90(10)	91(8)	81(8)	−22(6)	−13(7)	21(8)
C34	85(8)	116(14)	86(12)	−40(8)	−21(6)	25(7)
C44	93(9)	103(14)	86(9)	−35(8)	−35(8)	35(8)
C54	119(10)	104(10)	85(8)	13(6)	−49(7)	3(8)
C64	89(7)	132(10)	97(9)	25(7)	−34(6)	2(7)

Table 4: Bond lengths [Å] for mw_089_1fsm.

Sb(1)–C(63)	2.139(3)
Sb(1)–C(63')	2.311(6)
Sb(1)–Ga(1)	2.6431(6)
Sb(1)–Sb(2)	2.7912(5)
C(1)–N(1)	1.335(2)
C(1)–C(2)	1.394(3)
C(1)–C(4)	1.511(3)
Si(1)–C(63)	1.855(4)
Si(1)–C(66)	1.859(5)
Si(1)–C(64)	1.861(7)
Si(1)–C(65)	1.867(6)
C(63)–Sb(2)	2.294(4)
Si(1')–C(66')	1.837(7)
Si(1')–C(64')	1.840(10)
Si(1')–C(63')	1.859(6)
Si(1')–C(65')	1.895(10)
C(63')–Sb(2)	2.081(5)
N(1)–C(6)	1.444(3)
N(1)–Ga(1)	1.9976(18)
Ga(1)–N(5)	1.8630(17)
Ga(1)–N(2)	2.0115(16)
Sb(2)–Ga(2)	2.6400(6)
C(2)–C(3)	1.403(3)
N(2)–C(3)	1.327(2)
N(2)–C(18)	1.444(3)
Ga(2)–N(6)	1.8707(18)
Ga(2)–N(3)	1.9918(17)
Ga(2)–N(4)	2.0092(16)
N(5)–C(60)	1.444(3)
N(5)–C(59)	1.447(3)
C(5)–C(3)	1.510(3)
N(4)–C(32)	1.336(3)
N(4)–C(47)	1.448(3)
N(3)–C(30)	1.333(2)
N(3)–C(35)	1.444(3)
N(6)–C(62)	1.434(3)
N(6)–C(61)	1.442(3)
C(6)–C(11)	1.404(3)
C(6)–C(7)	1.415(3)
C(9)–C(10)	1.375(4)
C(9)–C(8)	1.384(4)
C(8)–C(7)	1.392(3)
C(7)–C(12)	1.520(3)
C(10)–C(11)	1.394(3)
C(11)–C(15)	1.526(3)
C(12)–C(14)	1.525(4)
C(12)–C(13)	1.525(5)
C(15)–C(17)	1.519(4)
C(15)–C(16)	1.534(5)
C(18)–C(23)	1.404(3)
C(18)–C(19)	1.411(3)
C(19)–C(20)	1.407(4)
C(19)–C(24)	1.516(4)

Table 4: (continued)

C(20)–C(21)	1.366(5)
C(21)–C(22)	1.368(5)
C(22)–C(23)	1.403(4)
C(23)–C(27)	1.517(4)
C(24)–C(26)	1.533(3)
C(24)–C(25)	1.534(4)
C(27)–C(29)	1.529(5)
C(27)–C(28)	1.549(5)
C(30)–C(31)	1.396(3)
C(30)–C(33)	1.511(3)
C(31)–C(32)	1.395(3)
C(32)–C(34)	1.510(3)
C(35)–C(40)	1.402(3)
C(35)–C(36)	1.415(3)
C(36)–C(37)	1.398(3)
C(36)–C(41')	1.459(17)
C(36)–C(41)	1.60(2)
C(37)–C(38)	1.376(5)
C(38)–C(39)	1.381(4)
C(39)–C(40)	1.402(3)
C(40)–C(44)	1.513(4)
C(41)–C(43)	1.49(3)
C(41)–C(42)	1.513(16)
C(41')–C(42')	1.541(14)
C(41')–C(43')	1.58(2)
C(44)–C(46)	1.525(5)
C(44)–C(45)	1.537(4)
C(47)–C(52)	1.400(4)
C(47)–C(48)	1.407(3)
C(48)–C(49)	1.394(4)
C(48)–C(53)	1.518(4)
C(49)–C(50)	1.375(5)
C(50)–C(51)	1.373(5)
C(51)–C(52)	1.404(4)
C(52)–C(56)	1.487(10)
C(52)–C(56')	1.629(19)
C(53)–C(55)	1.516(5)
C(53)–C(54)	1.517(5)
C(56)–C(58)	1.520(11)
C(56)–C(57)	1.532(9)
C(56')–C(58')	1.488(17)
C(56')–C(57')	1.523(14)
C11–C21	1.354(9)
C11–C61	1.367(11)
C21–C31	1.359(9)
C31–C41	1.352(9)
C41–C51	1.358(10)
C51–C61	1.359(11)
C12–C62	1.346(10)
C12–C22	1.349(9)
C22–C32	1.378(8)
C32–C42	1.354(10)
C42–C52	1.368(10)

Table 4: (continued)

C52–C62	1.361(10)
C13–C63	1.357(11)
C13–C23	1.360(11)
C23–C33	1.354(12)
C33–C43	1.357(12)
C43–C53	1.359(11)
C53–C63	1.355(11)
C14–C64	1.352(10)
C14–C24	1.356(10)
C24–C34	1.360(10)
C34–C44	1.352(11)
C44–C54	1.359(11)
C54–C64	1.370(10)

Table 5: Bond angles [°] for mw_089_1fsm.

C(63)–Sb(1)–Ga(1)	118.22(10)
C(63')–Sb(1)–Ga(1)	94.17(13)
C(63)–Sb(1)–Sb(2)	53.48(9)
C(63')–Sb(1)–Sb(2)	46.99(13)
Ga(1)–Sb(1)–Sb(2)	107.135(18)
N(1)–C(1)–C(2)	123.61(18)
N(1)–C(1)–C(4)	120.26(19)
C(2)–C(1)–C(4)	116.12(18)
C(63)–Si(1)–C(66)	111.7(2)
C(63)–Si(1)–C(64)	109.5(3)
C(66)–Si(1)–C(64)	107.7(4)
C(63)–Si(1)–C(65)	108.2(3)
C(66)–Si(1)–C(65)	110.6(3)
C(64)–Si(1)–C(65)	109.1(4)
Si(1)–C(63)–Sb(1)	130.33(19)
Si(1)–C(63)–Sb(2)	121.4(2)
Sb(1)–C(63)–Sb(2)	77.97(11)
C(66')–Si(1')–C(64')	110.1(7)
C(66')–Si(1')–C(63')	106.6(4)
C(64')–Si(1')–C(63')	111.0(6)
C(66')–Si(1')–C(65')	103.7(6)
C(64')–Si(1')–C(65')	111.5(7)
C(63')–Si(1')–C(65')	113.6(4)
Si(1')–C(63')–Sb(2)	128.7(3)
Si(1')–C(63')–Sb(1)	122.1(3)
Sb(2)–C(63')–Sb(1)	78.72(18)
C(1)–N(1)–C(6)	117.04(17)
C(1)–N(1)–Ga(1)	120.99(14)
C(6)–N(1)–Ga(1)	121.79(13)
N(5)–Ga(1)–N(1)	110.14(8)
N(5)–Ga(1)–N(2)	103.64(8)
N(1)–Ga(1)–N(2)	92.17(7)
N(5)–Ga(1)–Sb(1)	124.22(6)
N(1)–Ga(1)–Sb(1)	106.03(5)
N(2)–Ga(1)–Sb(1)	116.00(5)
C(63')–Sb(2)–Ga(2)	119.69(16)
C(63)–Sb(2)–Ga(2)	94.28(9)
C(63')–Sb(2)–Sb(1)	54.29(16)
C(63)–Sb(2)–Sb(1)	48.55(9)
Ga(2)–Sb(2)–Sb(1)	103.577(16)
C(1)–C(2)–C(3)	127.91(17)
C(3)–N(2)–C(18)	118.94(16)
C(3)–N(2)–Ga(1)	121.35(13)
C(18)–N(2)–Ga(1)	119.36(12)
N(6)–Ga(2)–N(3)	108.25(8)
N(6)–Ga(2)–N(4)	105.39(8)
N(3)–Ga(2)–N(4)	92.33(7)
N(6)–Ga(2)–Sb(2)	123.35(6)
N(3)–Ga(2)–Sb(2)	109.72(5)
N(4)–Ga(2)–Sb(2)	113.31(5)
C(60)–N(5)–C(59)	111.46(18)
C(60)–N(5)–Ga(1)	124.16(15)
C(59)–N(5)–Ga(1)	122.18(15)

Table 5: (continued)

C(32)–N(4)–C(47)	118.16(17)
C(32)–N(4)–Ga(2)	120.02(14)
C(47)–N(4)–Ga(2)	121.50(13)
C(30)–N(3)–C(35)	118.20(17)
C(30)–N(3)–Ga(2)	120.39(13)
C(35)–N(3)–Ga(2)	121.24(13)
N(2)–C(3)–C(2)	123.78(17)
N(2)–C(3)–C(5)	121.20(18)
C(2)–C(3)–C(5)	115.01(17)
C(62)–N(6)–C(61)	111.19(19)
C(62)–N(6)–Ga(2)	125.27(15)
C(61)–N(6)–Ga(2)	122.74(15)
C(11)–C(6)–C(7)	120.9(2)
C(11)–C(6)–N(1)	120.41(18)
C(7)–C(6)–N(1)	118.66(18)
C(10)–C(9)–C(8)	119.9(2)
C(9)–C(8)–C(7)	121.4(2)
C(8)–C(7)–C(6)	117.9(2)
C(8)–C(7)–C(12)	119.3(2)
C(6)–C(7)–C(12)	122.8(2)
C(9)–C(10)–C(11)	121.3(2)
C(10)–C(11)–C(6)	118.5(2)
C(10)–C(11)–C(15)	118.9(2)
C(6)–C(11)–C(15)	122.6(2)
C(7)–C(12)–C(14)	112.1(2)
C(7)–C(12)–C(13)	111.9(3)
C(14)–C(12)–C(13)	109.1(2)
C(17)–C(15)–C(11)	110.3(2)
C(17)–C(15)–C(16)	109.9(3)
C(11)–C(15)–C(16)	111.8(3)
C(23)–C(18)–C(19)	121.5(2)
C(23)–C(18)–N(2)	120.54(19)
C(19)–C(18)–N(2)	118.0(2)
C(20)–C(19)–C(18)	117.1(3)
C(20)–C(19)–C(24)	122.0(2)
C(18)–C(19)–C(24)	120.9(2)
C(21)–C(20)–C(19)	121.9(3)
C(20)–C(21)–C(22)	120.4(3)
C(21)–C(22)–C(23)	121.1(3)
C(22)–C(23)–C(18)	118.0(3)
C(22)–C(23)–C(27)	118.3(3)
C(18)–C(23)–C(27)	123.6(2)
C(19)–C(24)–C(26)	114.4(3)
C(19)–C(24)–C(25)	111.1(2)
C(26)–C(24)–C(25)	109.8(2)
C(23)–C(27)–C(29)	111.6(3)
C(23)–C(27)–C(28)	111.3(3)
C(29)–C(27)–C(28)	110.6(3)
N(3)–C(30)–C(31)	123.24(19)
N(3)–C(30)–C(33)	120.32(19)
C(31)–C(30)–C(33)	116.44(18)
C(32)–C(31)–C(30)	128.13(18)
N(4)–C(32)–C(31)	123.85(18)

Table 5: (continued)

N(4)–C(32)–C(34)	120.5(2)
C(31)–C(32)–C(34)	115.66(19)
C(40)–C(35)–C(36)	121.5(2)
C(40)–C(35)–N(3)	120.68(19)
C(36)–C(35)–N(3)	117.84(19)
C(37)–C(36)–C(35)	117.8(2)
C(37)–C(36)–C(41')	118.3(6)
C(35)–C(36)–C(41')	123.3(6)
C(37)–C(36)–C(41)	121.5(7)
C(35)–C(36)–C(41)	120.4(7)
C(38)–C(37)–C(36)	121.5(3)
C(37)–C(38)–C(39)	119.8(2)
C(38)–C(39)–C(40)	121.7(3)
C(35)–C(40)–C(39)	117.7(2)
C(35)–C(40)–C(44)	123.2(2)
C(39)–C(40)–C(44)	119.1(2)
C(43)–C(41)–C(42)	107.4(15)
C(43)–C(41)–C(36)	116.4(17)
C(42)–C(41)–C(36)	107.1(11)
C(36)–C(41')–C(42')	115.4(10)
C(36)–C(41')–C(43')	108.3(14)
C(42')–C(41')–C(43')	111.1(13)
C(40)–C(44)–C(46)	110.7(3)
C(40)–C(44)–C(45)	112.0(3)
C(46)–C(44)–C(45)	110.1(3)
C(52)–C(47)–C(48)	121.3(2)
C(52)–C(47)–N(4)	120.0(2)
C(48)–C(47)–N(4)	118.7(2)
C(49)–C(48)–C(47)	118.0(3)
C(49)–C(48)–C(53)	119.9(2)
C(47)–C(48)–C(53)	122.1(2)
C(50)–C(49)–C(48)	121.7(3)
C(51)–C(50)–C(49)	119.7(3)
C(50)–C(51)–C(52)	121.6(3)
C(47)–C(52)–C(51)	117.8(3)
C(47)–C(52)–C(56)	123.1(4)
C(51)–C(52)–C(56)	118.6(4)
C(47)–C(52)–C(56')	122.3(6)
C(51)–C(52)–C(56')	118.4(6)
C(55)–C(53)–C(54)	109.8(3)
C(55)–C(53)–C(48)	113.8(3)
C(54)–C(53)–C(48)	111.8(3)
C(52)–C(56)–C(58)	115.6(8)
C(52)–C(56)–C(57)	108.5(8)
C(58)–C(56)–C(57)	110.4(7)
C(58')–C(56')–C(57')	110.8(11)
C(58')–C(56')–C(52)	105.1(9)
C(57')–C(56')–C(52)	117.1(12)
C21–C11–C61	119.1(8)
C11–C21–C31	120.1(8)
C41–C31–C21	120.7(8)
C31–C41–C51	119.4(8)
C41–C51–C61	120.0(8)

Table 5: (continued)

C51–C61–C11	120.0(8)
C62–C12–C22	120.6(7)
C12–C22–C32	119.2(8)
C42–C32–C22	120.2(7)
C32–C42–C52	119.8(8)
C62–C52–C42	119.3(8)
C12–C62–C52	120.7(8)
C63–C13–C23	119.6(10)
C33–C23–C13	119.6(10)
C23–C33–C43	120.8(10)
C33–C43–C53	119.6(10)
C63–C53–C43	119.6(10)
C53–C63–C13	120.8(10)
C64–C14–C24	120.6(8)
C14–C24–C34	119.4(9)
C44–C34–C24	120.3(9)
C34–C44–C54	120.5(8)
C44–C54–C64	119.0(8)
C14–C64–C54	120.0(9)

Crystal structure of mw_099_tw5

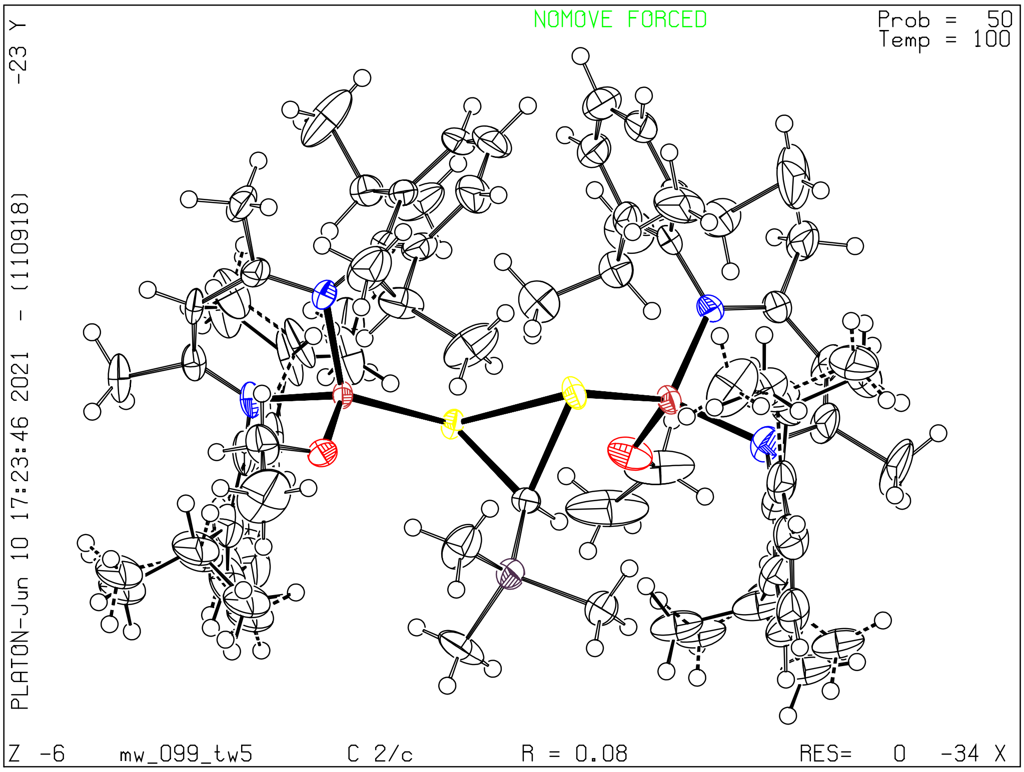

Table 1: Crystal data and structure refinement for mw_099_tw5.

Identification code	mw_099_tw5
Empirical Formula	$C_{66}\,H_{102}\,Ga_2\,N_4\,O_2\,Sb_2\,Si$
Formula weight	1394.54 Da
Density (calculated)	$1.318\,g\cdot cm^{-3}$
$F(000)$	5760
Temperature	100(2) K
Crystal size	0.451 × 0.429 × 0.344 mm
Crystal appearance	orange block
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$C2/c$
Unit cell dimensions	$a = 59.557(6)$ Å
	$b = 11.8135(12)$ Å
	$c = 21.011(2)$ Å
	$\alpha = 90°$
	$\beta = 108.078(3)°$
	$\gamma = 90°$
Unit cell volume	14053(3) $Å^3$
Z	8
Cell measurement refections used	9799
θ range for cell measurement	2.63° to 32.65°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	0.719° to 30.506°
Completeness to $\theta = 25.242°$ (to θ_{max})	97.0% (92.0%)
Index ranges	$-84 \leq h \leq 80$
	$0 \leq k \leq 16$
	$0 \leq l \leq 30$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.578\,mm^{-1}$
Absorption correction computing	TWINABS
Max./min. transmission	0.75/0.46
R_{merg} before/after correction	0.1129/0.0784 and 0.1278/0.0682
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	151709
Independent reflections	25033 ($R_{int} = 0.0753$)
Reflections with $I > 2\sigma(I)$	20170
Data / retraints / parameter	25033 / 889 / 827
Goodness-of-fit on F^2	1.125
Weighting details	$w = 1/[\sigma^2(F_o^2) + 293.6031P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0755$
	$wR2 = 0.1676$
R indices [all data]	$R1 = 0.0995$
	$wR2 = 0.1812$
Largest diff. peak and hole	2.377 and $-1.587\,Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

Two isopropyl groups and a complete diisopropyl phenyl moiety are disordered over two positions. All corresponding bond lengths and angles were restrained to be equal (`SADI`) and `RIGU` an `SIMU` restraints were applied to the displacement parameters of the disordered atoms. For two isopropyl groups and the ispo C atom of the phenyl ring common displacement parameters were used for both orientation (`EADP`).

Twinning

The model was refined as a 2-component twin against HKLF5 data.

Weak data

The combination of twinning and a long axis led to serious problems with overlapping reflections and part of the frames could not be integrated successfully. Considering the low quality of the data, the twinning and the vast disorder quantitative results should not be discussed.

Table 2: Atom coordinates ($\times10^4$) and equivalent isotropic displacement parameters ($\times10^3$) for mw_099_tw5. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	3915(1)	8062(1)	5163(1)	30(1)
Sb(2)	3576(1)	6703(1)	4276(1)	25(1)
Ga(1)	4267(1)	7306(1)	4782(1)	25(1)
Ga(2)	3180(1)	7565(1)	4367(1)	21(1)
Si(1)	3737(1)	5853(2)	6052(1)	38(1)
O(1)	4189(1)	5938(5)	4393(3)	45(2)
O(2)	3093(1)	7397(5)	5120(3)	33(1)
N(1)	4396(1)	8257(6)	4206(3)	30(2)
N(2)	4574(1)	7113(7)	5494(3)	38(2)
N(3)	3083(1)	9121(6)	4072(3)	25(1)
N(4)	2918(1)	6836(6)	3654(3)	27(1)
C(1)	4620(2)	8186(8)	4235(5)	40(2)
C(2)	4788(2)	7596(11)	4740(6)	61(3)
C(3)	4774(2)	7196(11)	5331(5)	54(3)
C(4)	4706(2)	8755(12)	3708(6)	62(3)
C(5)	5007(2)	6842(18)	5853(7)	112(7)
C(6)	4251(2)	9069(7)	3739(4)	33(2)
C(7)	4140(2)	8768(8)	3071(4)	36(2)
C(8)	4017(2)	9613(9)	2638(5)	41(2)
C(9)	4005(2)	10710(10)	2851(5)	51(3)
C(10)	4106(2)	10972(8)	3516(6)	49(3)
C(11)	4232(2)	10170(8)	3972(5)	44(2)
C(12)	4145(2)	7571(8)	2821(5)	40(2)
C(13)	4212(3)	7519(11)	2178(6)	65(3)
C(14)	3907(2)	7013(9)	2722(5)	51(3)
C(15)	4346(2)	10498(9)	4707(6)	63(3)
C(16)	4569(2)	11200(13)	4780(9)	103(6)
C(17)	4182(3)	11143(9)	4992(6)	70(4)
C(18)	4590(1)	6802(9)	6170(4)	36(2)
C(19)	4618(2)	5676(9)	6375(4)	46(2)
C(20)	4636(2)	5434(11)	7049(5)	52(3)
C(21)	4625(2)	6260(12)	7478(5)	58(3)
C(22)	4593(2)	7381(11)	7264(5)	54(3)
C(23)	4574(2)	7668(10)	6610(5)	49(3)
C(24')	4650(7)	4788(18)	5893(13)	58(3)
C(25')	4435(5)	4010(30)	5725(19)	58(3)
C(26')	4877(5)	4150(20)	6257(15)	58(3)
C(24)	4607(4)	4636(12)	5930(10)	58(3)
C(25)	4356(4)	4127(18)	5675(13)	58(3)
C(26)	4783(4)	3673(15)	6215(10)	58(3)
C(27)	4526(8)	9020(40)	6380(30)	56(9)
C(28)	4758(9)	9690(50)	6570(40)	87(14)
C(29)	4350(12)	9590(50)	6680(30)	80(12)
C(27')	4567(6)	8790(30)	6400(20)	46(8)
C(28')	4807(6)	9250(50)	6390(20)	77(10)
C(29')	4453(9)	9620(30)	6770(16)	62(9)
C(30)	2855(2)	9341(7)	3784(4)	29(2)
C(31)	2683(1)	8521(7)	3513(4)	30(2)
C(32)	2719(1)	7364(8)	3408(4)	31(2)
C(33)	2775(2)	10567(8)	3721(5)	44(2)

Table 2: (continued)

	x	y	z	U_{eq}
C(34)	2502(2)	6735(9)	2992(5)	44(2)
C(35)	3252(1)	10033(7)	4151(4)	26(2)
C(36)	3335(2)	10615(7)	4763(4)	38(2)
C(37)	3489(2)	11522(9)	4794(5)	54(3)
C(38)	3558(2)	11847(9)	4263(6)	58(3)
C(39)	3482(2)	11243(8)	3674(5)	43(2)
C(40)	3327(1)	10331(7)	3615(4)	29(2)
C(41)	3263(2)	10311(8)	5371(4)	47(3)
C(42)	3123(2)	11235(13)	5570(6)	71(4)
C(43)	3485(3)	10063(12)	5968(5)	72(4)
C(44)	3244(2)	9689(8)	2960(4)	36(2)
C(45)	3107(3)	10430(13)	2372(5)	82(5)
C(46)	3445(2)	9148(11)	2763(5)	61(3)
C(47)	2935(9)	5656(18)	3480(20)	40(3)
C(48)	2891(5)	4830(20)	3904(12)	44(5)
C(49)	2926(5)	3692(19)	3781(13)	58(5)
C(50)	3030(5)	3396(17)	3297(13)	63(5)
C(51)	3090(4)	4229(19)	2904(12)	54(5)
C(52)	3054(5)	5368(18)	3018(14)	45(5)
C(53)	2760(4)	5057(19)	4406(10)	63(3)
C(54)	2543(4)	4258(18)	4220(11)	63(3)
C(55)	2914(4)	4820(20)	5131(10)	63(3)
C(56)	3097(5)	6310(20)	2583(11)	48(6)
C(57)	2890(5)	6660(30)	1970(15)	65(8)
C(58)	3306(5)	5960(30)	2346(16)	61(8)
C(47')	2957(15)	5720(30)	3470(30)	40(3)
C(48')	2871(8)	4770(30)	3732(18)	44(6)
C(49')	2919(8)	3690(30)	3530(18)	57(7)
C(50')	3011(8)	3570(20)	2999(19)	65(7)
C(51')	3055(7)	4520(30)	2662(18)	56(7)
C(52')	3025(9)	5610(30)	2890(20)	48(7)
C(56')	3126(9)	6520(40)	2550(20)	56(9)
C(55')	2941(5)	4420(30)	5018(18)	63(3)
C(54')	2520(5)	4630(30)	4282(19)	63(3)
C(53')	2780(5)	4850(30)	4335(15)	63(3)
C(57')	2897(8)	7030(40)	2080(20)	55(9)
C(58')	3296(9)	6260(70)	2150(30)	78(15)
C(59)	4316(3)	5273(10)	4091(6)	80(5)
C(60)	4181(4)	4256(10)	3775(7)	113(8)
C(61)	2879(2)	7755(10)	5193(4)	44(2)
C(62)	2867(3)	7582(16)	5876(6)	90(5)
C(63)	3801(2)	6314(7)	5297(4)	31(2)
C(64)	4020(2)	5827(9)	6741(5)	48(3)
C(65)	3619(2)	4413(9)	5901(5)	61(3)
C(66)	3537(2)	6788(11)	6341(5)	58(3)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_099_tw5.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	20(1)	25(1)	47(1)	−7(1)	14(1)	−5(1)
Sb(2)	17(1)	33(1)	24(1)	0(1)	5(1)	2(1)
Ga(1)	20(1)	24(1)	32(1)	−2(1)	10(1)	−2(1)
Ga(2)	14(1)	23(1)	25(1)	−3(1)	3(1)	−2(1)
Si(1)	30(1)	46(2)	32(1)	10(1)	2(1)	−6(1)
O(1)	70(5)	28(3)	46(4)	−8(3)	29(3)	−5(3)
O(2)	32(3)	38(3)	24(3)	8(2)	3(2)	−3(3)
N(1)	24(3)	33(4)	38(4)	9(3)	15(3)	−1(3)
N(2)	29(4)	58(5)	32(4)	8(3)	15(3)	7(4)
N(3)	21(3)	30(3)	21(3)	−1(2)	2(2)	2(3)
N(4)	19(3)	33(4)	27(3)	−14(3)	3(2)	−7(3)
C(1)	27(4)	46(5)	50(5)	13(4)	18(4)	2(4)
C(2)	22(4)	101(10)	67(7)	41(7)	26(5)	26(5)
C(3)	22(4)	90(9)	55(6)	27(6)	20(4)	15(5)
C(4)	30(5)	93(9)	68(7)	35(7)	21(5)	10(6)
C(5)	21(5)	230(20)	91(9)	93(12)	22(6)	36(9)
C(6)	23(4)	33(4)	44(5)	6(4)	10(3)	−8(3)
C(7)	27(4)	47(5)	38(5)	2(4)	14(4)	1(4)
C(8)	35(5)	54(6)	38(5)	10(4)	17(4)	8(4)
C(9)	48(6)	54(6)	52(6)	18(5)	14(5)	13(5)
C(10)	39(5)	28(5)	72(7)	6(5)	6(5)	−7(4)
C(11)	38(5)	30(4)	55(6)	3(4)	1(4)	−14(4)
C(12)	40(5)	41(5)	43(5)	−6(4)	17(4)	0(4)
C(13)	82(9)	68(8)	63(7)	−5(6)	49(7)	9(7)
C(14)	58(7)	51(6)	52(6)	−11(5)	27(5)	−2(5)
C(15)	71(8)	29(5)	63(7)	−11(5)	−16(6)	−10(5)
C(16)	46(8)	80(10)	158(15)	−45(10)	−6(9)	−23(7)
C(17)	101(11)	32(6)	65(7)	−6(5)	8(7)	−23(6)
C(18)	22(4)	56(6)	28(4)	5(4)	4(3)	3(4)
C(19)	33(5)	73(7)	31(5)	7(5)	9(4)	10(5)
C(20)	51(6)	67(7)	33(5)	16(5)	5(4)	4(5)
C(21)	40(6)	100(10)	29(5)	10(6)	3(4)	−12(6)
C(22)	48(6)	78(8)	33(5)	−9(5)	7(4)	−17(6)
C(23)	32(5)	69(7)	38(5)	−3(5)	0(4)	−6(5)
C(24’)	89(10)	34(5)	56(4)	12(4)	29(5)	23(5)
C(25’)	89(10)	34(5)	56(4)	12(4)	29(5)	23(5)
C(26’)	89(10)	34(5)	56(4)	12(4)	29(5)	23(5)
C(24)	89(10)	34(5)	56(4)	12(4)	29(5)	23(5)
C(25)	89(10)	34(5)	56(4)	12(4)	29(5)	23(5)
C(26)	89(10)	34(5)	56(4)	12(4)	29(5)	23(5)
C(27)	72(18)	26(15)	65(17)	1(13)	15(15)	6(13)
C(28)	90(20)	40(20)	110(30)	20(20)	10(19)	−9(16)
C(29)	90(30)	80(20)	60(20)	−38(18)	0(19)	30(20)
C(27’)	46(13)	35(15)	52(12)	−6(12)	7(10)	−13(11)
C(28’)	56(14)	60(20)	110(20)	−4(17)	12(13)	−23(13)
C(29’)	80(20)	46(12)	44(12)	−11(9)	−3(13)	6(15)
C(30)	30(4)	37(5)	19(3)	3(3)	6(3)	2(3)
C(31)	12(3)	46(5)	28(4)	−3(3)	−1(3)	−1(3)
C(32)	22(4)	51(5)	20(3)	−8(3)	7(3)	−7(4)
C(33)	30(5)	45(6)	49(5)	5(4)	0(4)	12(4)
C(34)	19(4)	70(7)	41(5)	−22(5)	6(3)	−8(4)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(35)	24(4)	27(4)	24(4)	2(3)	4(3)	−1(3)
C(36)	47(5)	29(4)	29(4)	3(3)	−1(4)	0(4)
C(37)	55(7)	52(6)	43(5)	−3(5)	−3(5)	−26(5)
C(38)	62(7)	42(5)	62(6)	10(5)	8(5)	−26(5)
C(39)	38(5)	41(5)	52(6)	19(4)	18(4)	−5(4)
C(40)	26(4)	30(4)	33(4)	9(3)	14(3)	6(3)
C(41)	80(8)	37(5)	21(4)	−4(4)	9(4)	−16(5)
C(42)	63(8)	106(11)	44(6)	22(7)	16(6)	17(8)
C(43)	94(10)	89(9)	34(5)	9(6)	19(6)	42(8)
C(44)	35(5)	39(5)	41(5)	6(4)	22(4)	6(4)
C(45)	82(10)	109(11)	35(5)	−14(6)	−12(6)	54(9)
C(46)	69(8)	80(8)	40(5)	25(5)	28(5)	39(7)
C(47)	21(8)	37(4)	56(5)	−28(4)	3(4)	−7(4)
C(48)	35(10)	38(7)	53(11)	−24(7)	3(9)	−6(7)
C(49)	50(10)	43(7)	80(15)	−30(9)	19(11)	−11(7)
C(50)	51(10)	52(9)	86(14)	−31(9)	22(11)	−6(8)
C(51)	31(9)	47(10)	85(13)	−37(9)	18(10)	−4(8)
C(52)	14(7)	49(9)	71(11)	−30(8)	11(8)	−1(7)
C(53)	78(6)	22(7)	89(6)	0(5)	26(5)	−5(4)
C(54)	78(6)	22(7)	89(6)	0(5)	26(5)	−5(4)
C(55)	78(6)	22(7)	89(6)	0(5)	26(5)	−5(4)
C(56)	30(8)	82(15)	43(8)	−51(9)	28(6)	−33(9)
C(57)	43(9)	110(30)	52(11)	−43(13)	28(8)	−19(13)
C(58)	45(10)	92(19)	60(17)	−42(15)	39(11)	−19(10)
C(47')	21(8)	37(4)	56(5)	−28(4)	3(4)	−7(4)
C(48')	22(11)	34(8)	62(15)	−25(10)	−6(11)	−12(8)
C(49')	53(14)	34(8)	76(17)	−29(12)	7(14)	−11(10)
C(50')	61(14)	43(11)	86(17)	−32(12)	16(15)	−6(11)
C(51')	41(14)	43(13)	82(16)	−37(10)	16(13)	−6(11)
C(52')	35(15)	45(12)	61(12)	−35(10)	7(11)	−6(11)
C(56')	40(14)	71(19)	63(16)	−25(14)	26(11)	−40(13)
C(55')	78(6)	22(7)	89(6)	0(5)	26(5)	−5(4)
C(54')	78(6)	22(7)	89(6)	0(5)	26(5)	−5(4)
C(53')	78(6)	22(7)	89(6)	0(5)	26(5)	−5(4)
C(57')	57(14)	60(20)	53(19)	−37(15)	26(13)	−26(14)
C(58')	53(18)	130(40)	50(20)	−20(20)	21(16)	0(20)
C(59)	170(16)	38(6)	45(6)	1(5)	52(8)	20(8)
C(60)	250(20)	28(6)	64(9)	−9(6)	49(11)	2(9)
C(61)	40(5)	66(7)	30(4)	−4(4)	19(4)	−11(5)
C(62)	92(11)	149(15)	44(7)	20(8)	41(7)	19(11)
C(63)	31(4)	28(4)	30(4)	6(3)	4(3)	−5(3)
C(64)	42(6)	54(6)	38(5)	9(4)	−3(4)	−7(5)
C(65)	85(9)	53(6)	42(5)	2(5)	16(5)	−43(6)
C(66)	50(6)	92(9)	33(5)	9(5)	15(4)	17(6)

Table 4: Bond lengths [Å] for mw_099_tw5.

Sb(1)–C(63)	2.219(8)
Sb(1)–Ga(1)	2.6230(10)
Sb(1)–Sb(2)	2.7912(7)
Sb(2)–C(63)	2.196(8)
Sb(2)–Ga(2)	2.6269(10)
Ga(1)–O(1)	1.806(6)
Ga(1)–N(1)	1.971(7)
Ga(1)–N(2)	1.982(7)
Ga(2)–O(2)	1.823(6)
Ga(2)–N(3)	1.969(7)
Ga(2)–N(4)	1.994(6)
Si(1)–C(63)	1.824(8)
Si(1)–C(65)	1.831(10)
Si(1)–C(64)	1.851(9)
Si(1)–C(66)	1.860(11)
O(1)–C(59)	1.375(14)
O(2)–C(61)	1.392(11)
N(1)–C(1)	1.319(11)
N(1)–C(6)	1.450(11)
N(2)–C(3)	1.342(11)
N(2)–C(18)	1.441(11)
N(3)–C(30)	1.332(10)
N(3)–C(35)	1.449(10)
N(4)–C(32)	1.295(10)
N(4)–C(47')	1.42(3)
N(4)–C(47)	1.45(2)
C(1)–C(2)	1.399(13)
C(1)–C(4)	1.516(13)
C(2)–C(3)	1.356(14)
C(3)–C(5)	1.538(14)
C(6)–C(7)	1.400(12)
C(6)–C(11)	1.406(13)
C(7)–C(8)	1.395(13)
C(7)–C(12)	1.512(13)
C(8)–C(9)	1.380(15)
C(9)–C(10)	1.374(15)
C(10)–C(11)	1.391(13)
C(11)–C(15)	1.531(14)
C(12)–C(14)	1.518(14)
C(12)–C(13)	1.523(14)
C(15)–C(17)	1.504(19)
C(15)–C(16)	1.533(18)
C(18)–C(19)	1.392(14)
C(18)–C(23)	1.403(14)
C(19)–C(20)	1.416(13)
C(19)–C(24')	1.510(17)
C(19)–C(24)	1.533(15)
C(20)–C(21)	1.345(16)
C(21)–C(22)	1.393(17)
C(22)–C(23)	1.385(14)
C(23)–C(27')	1.40(5)
C(23)–C(27)	1.67(6)
C(24')–C(25')	1.527(16)

Table 4: (continued)

C(24')–C(26')	1.528(16)
C(24)–C(26)	1.537(14)
C(24)–C(25)	1.543(15)
C(27)–C(28)	1.529(16)
C(27)–C(29)	1.531(16)
C(27')–C(29')	1.528(15)
C(27')–C(28')	1.534(15)
C(30)–C(31)	1.394(11)
C(30)–C(33)	1.517(13)
C(31)–C(32)	1.411(13)
C(32)–C(34)	1.514(11)
C(35)–C(40)	1.376(11)
C(35)–C(36)	1.406(11)
C(36)–C(37)	1.398(13)
C(36)–C(41)	1.510(13)
C(37)–C(38)	1.362(16)
C(38)–C(39)	1.378(15)
C(39)–C(40)	1.402(12)
C(40)–C(44)	1.514(12)
C(41)–C(42)	1.512(17)
C(41)–C(43)	1.541(15)
C(44)–C(46)	1.525(13)
C(44)–C(45)	1.528(14)
C(47)–C(48)	1.400(14)
C(47)–C(52)	1.404(14)
C(48)–C(49)	1.399(13)
C(48)–C(53)	1.519(16)
C(49)–C(50)	1.389(13)
C(50)–C(51)	1.399(14)
C(51)–C(52)	1.395(13)
C(52)–C(56)	1.515(16)
C(53)–C(55)	1.542(15)
C(53)–C(54)	1.546(15)
C(56)–C(58)	1.533(14)
C(56)–C(57)	1.539(15)
C(47')–C(52')	1.403(15)
C(47')–C(48')	1.404(16)
C(48')–C(49')	1.402(15)
C(48')–C(53')	1.529(18)
C(49')–C(50')	1.395(14)
C(50')–C(51')	1.395(14)
C(51')–C(52')	1.401(14)
C(52')–C(56')	1.521(18)
C(56')–C(58')	1.539(17)
C(56')–C(57')	1.540(17)
C(55')–C(53')	1.545(16)
C(54')–C(53')	1.541(16)
C(59)–C(60)	1.48(2)
C(61)–C(62)	1.475(13)

Table 5: Bond angles [°] for mw_099_tw5.

C(63)–Sb(1)–Ga(1)	91.6(2)
C(63)–Sb(1)–Sb(2)	50.4(2)
Ga(1)–Sb(1)–Sb(2)	94.69(3)
C(63)–Sb(2)–Ga(2)	107.4(2)
C(63)–Sb(2)–Sb(1)	51.2(2)
Ga(2)–Sb(2)–Sb(1)	102.00(3)
O(1)–Ga(1)–N(1)	109.1(3)
O(1)–Ga(1)–N(2)	106.6(3)
N(1)–Ga(1)–N(2)	95.0(3)
O(1)–Ga(1)–Sb(1)	108.9(2)
N(1)–Ga(1)–Sb(1)	119.6(2)
N(2)–Ga(1)–Sb(1)	116.4(2)
O(2)–Ga(2)–N(3)	103.9(3)
O(2)–Ga(2)–N(4)	103.7(3)
N(3)–Ga(2)–N(4)	94.7(3)
O(2)–Ga(2)–Sb(2)	121.67(19)
N(3)–Ga(2)–Sb(2)	121.5(2)
N(4)–Ga(2)–Sb(2)	106.81(19)
C(63)–Si(1)–C(65)	107.4(4)
C(63)–Si(1)–C(64)	107.5(4)
C(65)–Si(1)–C(64)	109.2(5)
C(63)–Si(1)–C(66)	115.7(5)
C(65)–Si(1)–C(66)	110.9(6)
C(64)–Si(1)–C(66)	106.0(5)
C(59)–O(1)–Ga(1)	128.2(8)
C(61)–O(2)–Ga(2)	125.4(5)
C(1)–N(1)–C(6)	116.9(7)
C(1)–N(1)–Ga(1)	121.1(6)
C(6)–N(1)–Ga(1)	122.0(5)
C(3)–N(2)–C(18)	118.4(8)
C(3)–N(2)–Ga(1)	118.8(6)
C(18)–N(2)–Ga(1)	122.6(5)
C(30)–N(3)–C(35)	118.9(7)
C(30)–N(3)–Ga(2)	118.9(6)
C(35)–N(3)–Ga(2)	122.2(5)
C(32)–N(4)–C(47')	123(4)
C(32)–N(4)–C(47)	119(2)
C(32)–N(4)–Ga(2)	119.9(5)
C(47')–N(4)–Ga(2)	117(4)
C(47)–N(4)–Ga(2)	120(2)
N(1)–C(1)–C(2)	122.8(8)
N(1)–C(1)–C(4)	120.5(8)
C(2)–C(1)–C(4)	116.7(8)
C(3)–C(2)–C(1)	129.4(9)
N(2)–C(3)–C(2)	124.9(9)
N(2)–C(3)–C(5)	118.4(9)
C(2)–C(3)–C(5)	116.6(9)
C(7)–C(6)–C(11)	121.4(8)
C(7)–C(6)–N(1)	120.5(8)
C(11)–C(6)–N(1)	118.1(8)
C(8)–C(7)–C(6)	117.4(9)
C(8)–C(7)–C(12)	120.4(8)
C(6)–C(7)–C(12)	122.1(8)

Table 5: (continued)

C(9)–C(8)–C(7)	122.1(9)
C(10)–C(9)–C(8)	119.3(9)
C(9)–C(10)–C(11)	121.4(10)
C(10)–C(11)–C(6)	118.3(9)
C(10)–C(11)–C(15)	119.9(9)
C(6)–C(11)–C(15)	121.8(9)
C(7)–C(12)–C(14)	109.7(8)
C(7)–C(12)–C(13)	112.5(9)
C(14)–C(12)–C(13)	110.6(9)
C(17)–C(15)–C(11)	112.9(10)
C(17)–C(15)–C(16)	109.8(10)
C(11)–C(15)–C(16)	109.7(12)
C(19)–C(18)–C(23)	121.3(8)
C(19)–C(18)–N(2)	120.8(8)
C(23)–C(18)–N(2)	117.9(9)
C(18)–C(19)–C(20)	117.8(9)
C(18)–C(19)–C(24')	119.0(13)
C(20)–C(19)–C(24')	123.0(14)
C(18)–C(19)–C(24)	126.8(10)
C(20)–C(19)–C(24)	115.1(12)
C(21)–C(20)–C(19)	121.4(11)
C(20)–C(21)–C(22)	120.3(10)
C(23)–C(22)–C(21)	120.9(11)
C(22)–C(23)–C(27')	122.0(19)
C(22)–C(23)–C(18)	118.3(10)
C(27')–C(23)–C(18)	119.2(18)
C(22)–C(23)–C(27)	118(2)
C(18)–C(23)–C(27)	123(2)
C(19)–C(24')–C(25')	108(2)
C(19)–C(24')–C(26')	106(2)
C(25')–C(24')–C(26')	111.3(15)
C(19)–C(24)–C(26)	117.4(15)
C(19)–C(24)–C(25)	112.2(16)
C(26)–C(24)–C(25)	108.4(12)
C(28)–C(27)–C(29)	110.6(16)
C(28)–C(27)–C(23)	111(3)
C(29)–C(27)–C(23)	112(4)
C(23)–C(27')–C(29')	115(3)
C(23)–C(27')–C(28')	114(2)
C(29')–C(27')–C(28')	110.1(14)
N(3)–C(30)–C(31)	124.4(8)
N(3)–C(30)–C(33)	118.3(8)
C(31)–C(30)–C(33)	117.2(8)
C(30)–C(31)–C(32)	127.6(7)
N(4)–C(32)–C(31)	124.6(7)
N(4)–C(32)–C(34)	120.4(8)
C(31)–C(32)–C(34)	114.9(8)
C(40)–C(35)–C(36)	120.9(8)
C(40)–C(35)–N(3)	119.0(7)
C(36)–C(35)–N(3)	120.1(7)
C(37)–C(36)–C(35)	117.1(8)
C(37)–C(36)–C(41)	119.7(8)
C(35)–C(36)–C(41)	123.2(8)

Table 5: (continued)

C(38)–C(37)–C(36)	122.7(9)
C(37)–C(38)–C(39)	119.4(9)
C(38)–C(39)–C(40)	120.1(9)
C(35)–C(40)–C(39)	119.8(8)
C(35)–C(40)–C(44)	121.2(7)
C(39)–C(40)–C(44)	119.0(8)
C(36)–C(41)–C(42)	112.9(8)
C(36)–C(41)–C(43)	109.8(10)
C(42)–C(41)–C(43)	108.7(8)
C(40)–C(44)–C(46)	113.2(8)
C(40)–C(44)–C(45)	113.0(8)
C(46)–C(44)–C(45)	106.7(8)
C(48)–C(47)–C(52)	120.3(12)
C(48)–C(47)–N(4)	117.7(18)
C(52)–C(47)–N(4)	119.8(17)
C(49)–C(48)–C(47)	118.9(10)
C(49)–C(48)–C(53)	115.8(18)
C(47)–C(48)–C(53)	124.1(18)
C(50)–C(49)–C(48)	120.2(10)
C(49)–C(50)–C(51)	120.5(10)
C(52)–C(51)–C(50)	119.7(10)
C(51)–C(52)–C(47)	119.3(10)
C(51)–C(52)–C(56)	122.8(17)
C(47)–C(52)–C(56)	117.0(17)
C(48)–C(53)–C(55)	112(2)
C(48)–C(53)–C(54)	107(2)
C(55)–C(53)–C(54)	109.6(12)
C(52)–C(56)–C(58)	108(2)
C(52)–C(56)–C(57)	117(3)
C(58)–C(56)–C(57)	108.8(12)
C(52')–C(47')–C(48')	120.1(15)
C(52')–C(47')–N(4)	116(3)
C(48')–C(47')–N(4)	122(3)
C(49')–C(48')–C(47')	118.3(13)
C(49')–C(48')–C(53')	118(3)
C(47')–C(48')–C(53')	122(3)
C(50')–C(49')–C(48')	119.9(11)
C(49')–C(50')–C(51')	120.8(11)
C(50')–C(51')–C(52')	119.5(11)
C(51')–C(52')–C(47')	119.2(12)
C(51')–C(52')–C(56')	112(3)
C(47')–C(52')–C(56')	128(3)
C(52')–C(56')–C(58')	123(5)
C(52')–C(56')–C(57')	100(4)
C(58')–C(56')–C(57')	108.9(16)
C(48')–C(53')–C(54')	122(3)
C(48')–C(53')–C(55')	118(3)
C(54')–C(53')–C(55')	109.3(15)
O(1)–C(59)–C(60)	111.7(15)
O(2)–C(61)–C(62)	112.9(9)
Si(1)–C(63)–Sb(2)	133.1(5)
Si(1)–C(63)–Sb(1)	122.9(4)
Sb(2)–C(63)–Sb(1)	78.4(2)

Crystal structure of mw_112_3frm

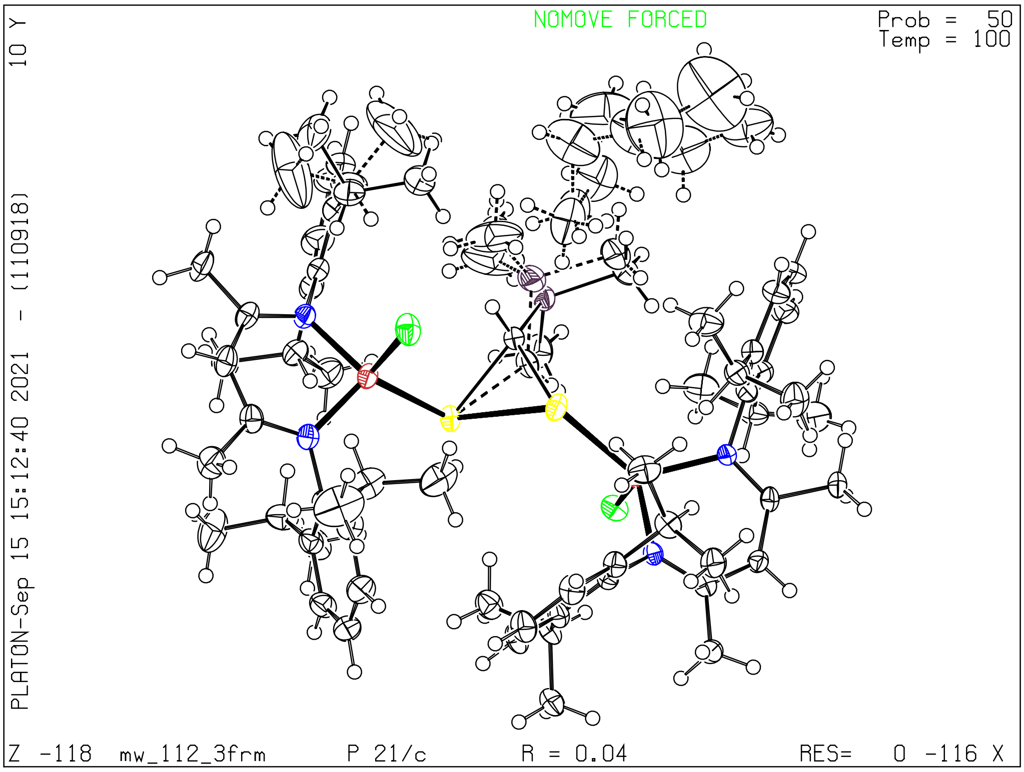

Table 1: Crystal data and structure refinement for mw_112_3frm.

Identification code	mw_112_3frm
Empirical Formula	$C_{64.50}\,H_{98}\,Cl_2\,Ga_2\,N_4\,Sb_2\,Si$
Formula weight	1411.39 Da
Density (calculated)	$1.348\,g\cdot cm^{-3}$
$F(000)$	2900
Temperature	100(2) K
Crystal size	$0.338 \times 0.053 \times 0.040$ mm
Crystal appearance	orange needle
Wavelength (CuK_α)	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 19.7547(17)$ Å
	$b = 10.5843(9)$ Å
	$c = 33.512(3)$ Å
	$\alpha = 90°$
	$\beta = 96.970(4)°$
	$\gamma = 90°$
Unit cell volume	$6955.1(10)\,Å^3$
Z	4
Cell measurement refections used	9539
θ range for cell measurement	2.66° to 79.98°
Diffractometer used for measurement	Bruker D8 Venture (Photon II detector)
Diffractometer control software	Bruker APEX3(v2017.3-0)
Measurement method	Data collection strategy APEX 3/Queen
θ range for data collection	2.253° to 80.760°
Completeness to $\theta = 67.679°$ (to θ_{max})	100.0% (98.9%)
Index ranges	$-25 \leq h \leq 25$
	$-13 \leq k \leq 11$
	$-42 \leq l \leq 42$
Computing data reduction	Bruker APEX3(v2017.3-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$8.131\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.48
R_{merg} before/after correction	0.1608/0.1004
Computing structure solution	Bruker APEX3(v2017.3-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	273985
Independent reflections	15129 ($R_{int} = 0.1275$)
Reflections with $I > 2\sigma(I)$	12943
Data / retraints / parameter	15129 / 348 / 838
Goodness-of-fit on F^2	1.028
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 11.7785P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0359$
	$wR2 = 0.0847$
R indices [all data]	$R1 = 0.0454$
	$wR2 = 0.0902$
Largest diff. peak and hole	1.844 and $-1.943\,Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The hydrogen atoms of the solvents' and minor disorder components' methyl groups were placed in ideally staggered positions (`AFIX 33`).

Disorder

The $CHSi(CH_3)_3$ group and an isopropyl group are disordered over two positions. The corresponding bond length and angles of these groups were restrained to be equal (`SADI`) and `RIGU` restraints were applied to their atoms. For C12, C12', C59 and C59' additional `SIMU` restraints were used. Despite the rather large displacement ellipsoids no further alternate orientations could be identified. The solvent molecule is highly disordered over a centre of inversion and was crudely modelled with two alternate positions. Its bond length were restrained to be equal to 1.54 Å (`DFIX`) and its bond angles to be equal (`SADI`). `RIGU`, `SIMU` and `ISOR` restraints were applied to it displacement parameters. Due to their close proximity C1_1 and C1_2 were refined with common displacement parameters (`EADP`).

Formation of ice

During the measurement ice formed on the crystal and the resulting reflections and ring patterns disturbed the integration leading to a rather high R_{int}.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_112_3frm. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	2635(1)	−150(1)	3591(1)	25(1)
Sb(2)	2427(1)	2197(1)	3942(1)	30(1)
Ga(1)	3494(1)	565(1)	3098(1)	25(1)
Ga(2)	1319(1)	1742(1)	4294(1)	20(1)
Cl(1)	3918(1)	2501(1)	3212(1)	38(1)
Cl(2)	968(1)	−241(1)	4350(1)	29(1)
N(1)	4312(1)	−470(3)	3056(1)	27(1)
N(2)	3155(1)	490(2)	2528(1)	26(1)
N(3)	1180(1)	2464(2)	4825(1)	21(1)
N(4)	540(1)	2641(2)	4001(1)	20(1)
C(1)	4577(2)	−561(3)	2707(1)	31(1)
C(2)	4257(2)	−68(3)	2345(1)	35(1)
C(3)	3588(2)	339(3)	2254(1)	31(1)
C(4)	5242(2)	−1242(4)	2689(1)	41(1)
C(5)	3350(2)	599(4)	1814(1)	45(1)
C(6)	4666(2)	−1137(3)	3398(1)	31(1)
C(7)	5241(2)	−582(4)	3622(1)	42(1)
C(8)	5604(2)	−1320(5)	3918(1)	54(1)
C(9)	5408(2)	−2523(6)	3995(1)	60(1)
C(10)	4826(2)	−3033(5)	3784(1)	49(1)
C(11)	4441(2)	−2343(4)	3485(1)	34(1)
C(12)	5440(6)	790(20)	3559(4)	53(3)
C(13)	5295(3)	1598(6)	3920(2)	60(2)
C(14)	6207(3)	914(9)	3513(3)	85(3)
C(12')	5520(20)	720(80)	3594(11)	53(5)
C(13')	5910(30)	1280(60)	3980(10)	200(30)
C(14')	5940(30)	940(50)	3246(11)	160(30)
C(15)	3809(2)	−2931(3)	3253(1)	33(1)
C(16)	3396(2)	−3735(4)	3514(1)	45(1)
C(17)	3984(2)	−3702(5)	2895(1)	54(1)
C(18)	2436(2)	650(3)	2387(1)	28(1)
C(19)	2171(2)	1845(3)	2293(1)	34(1)
C(20)	1483(2)	1941(4)	2136(1)	38(1)
C(21)	1077(2)	884(4)	2080(1)	38(1)
C(22)	1340(2)	−294(3)	2185(1)	34(1)
C(23)	2024(2)	−438(3)	2343(1)	29(1)
C(24)	2593(2)	3036(3)	2362(1)	45(1)
C(25)	2366(2)	3785(4)	2710(2)	64(1)
C(26)	2563(3)	3849(5)	1980(2)	76(2)
C(27)	2304(2)	−1746(3)	2440(1)	38(1)
C(28)	2441(3)	−2431(4)	2060(2)	61(1)
C(29)	1839(2)	−2529(4)	2677(1)	46(1)
C(30)	562(2)	2830(3)	4893(1)	23(1)
C(31)	−1(2)	2926(3)	4597(1)	23(1)
C(32)	−2(2)	2938(3)	4181(1)	22(1)
C(33)	421(2)	3207(4)	5312(1)	33(1)
C(34)	−660(2)	3342(3)	3935(1)	28(1)
C(35)	1732(2)	2527(3)	5153(1)	25(1)
C(36)	1789(2)	1599(3)	5454(1)	29(1)
C(37)	2303(2)	1763(4)	5778(1)	37(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(38)	2734(2)	2788(4)	5797(1)	40(1)
C(39)	2676(2)	3676(4)	5496(1)	36(1)
C(40)	2178(2)	3564(3)	5162(1)	29(1)
C(41)	1332(2)	441(3)	5445(1)	34(1)
C(42)	997(2)	309(5)	5834(1)	48(1)
C(43)	1730(2)	−748(4)	5375(1)	48(1)
C(44)	2113(2)	4578(3)	4838(1)	30(1)
C(45)	1655(2)	5655(4)	4951(1)	46(1)
C(46)	2800(2)	5054(4)	4740(1)	46(1)
C(47)	531(2)	2973(3)	3582(1)	23(1)
C(48)	322(2)	2079(3)	3282(1)	27(1)
C(49)	306(2)	2450(3)	2883(1)	34(1)
C(50)	483(2)	3655(3)	2783(1)	37(1)
C(51)	694(2)	4525(3)	3078(1)	32(1)
C(52)	724(2)	4206(3)	3484(1)	26(1)
C(53)	101(2)	754(3)	3377(1)	28(1)
C(54)	−639(2)	504(3)	3194(1)	35(1)
C(55)	578(2)	−233(3)	3231(1)	38(1)
C(56)	950(2)	5198(3)	3801(1)	30(1)
C(57)	437(2)	6287(4)	3795(1)	39(1)
C(58)	1653(2)	5737(4)	3751(1)	40(1)
Si(1)	3406(1)	−124(2)	4583(1)	30(1)
C(59)	3215(2)	815(4)	4115(1)	25(1)
C(60)	3380(4)	874(6)	5037(2)	45(2)
C(61)	4285(2)	−776(6)	4587(2)	52(2)
C(62)	2804(3)	−1485(4)	4585(1)	41(1)
C(59')	2851(8)	165(14)	4215(4)	27(3)
C(60')	4340(11)	1000(30)	4301(8)	108(13)
C(61')	3946(16)	−1562(15)	4612(10)	121(14)
C(62')	3593(19)	830(30)	5037(7)	111(17)
Si(1')	3681(5)	114(7)	4533(2)	41(2)
C11	4376(9)	4042(15)	4351(4)	69(4)
C21	4644(8)	3550(15)	4748(5)	86(4)
C31	5287(10)	4300(30)	4890(8)	146(10)
C41	5060(20)	5620(20)	4979(9)	165(12)
C51	5110(30)	5710(40)	5436(9)	201(16)
C12	4420(40)	3720(60)	4460(20)	69(4)
C22	5150(30)	4090(70)	4637(19)	95(14)
C32	5040(40)	5230(60)	4910(15)	94(14)
C42	4610(30)	4670(60)	5223(17)	97(16)
C52	4630(40)	5710(80)	5550(20)	103(18)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_112_3frm.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	31(1)	24(1)	22(1)	−2(1)	9(1)	−1(1)
Sb(2)	28(1)	26(1)	37(1)	−6(1)	14(1)	−1(1)
Ga(1)	26(1)	24(1)	29(1)	−3(1)	10(1)	−1(1)
Ga(2)	24(1)	19(1)	19(1)	−1(1)	6(1)	0(1)
Cl(1)	46(1)	28(1)	40(1)	−7(1)	15(1)	−10(1)
Cl(2)	36(1)	21(1)	31(1)	2(1)	0(1)	−2(1)
N(1)	24(1)	29(1)	27(1)	−2(1)	7(1)	−1(1)
N(2)	29(1)	23(1)	26(1)	1(1)	6(1)	1(1)
N(3)	21(1)	24(1)	18(1)	−2(1)	3(1)	0(1)
N(4)	25(1)	19(1)	18(1)	1(1)	4(1)	−1(1)
C(1)	28(2)	30(2)	37(2)	1(1)	13(1)	0(1)
C(2)	40(2)	38(2)	30(2)	4(1)	17(1)	3(1)
C(3)	39(2)	28(2)	26(2)	3(1)	8(1)	2(1)
C(4)	35(2)	51(2)	41(2)	2(2)	20(2)	10(2)
C(5)	50(2)	57(2)	29(2)	12(2)	10(2)	9(2)
C(6)	24(2)	40(2)	28(2)	−5(1)	5(1)	5(1)
C(7)	27(2)	60(3)	38(2)	−12(2)	8(1)	−1(2)
C(8)	31(2)	89(4)	39(2)	−14(2)	−5(2)	7(2)
C(9)	38(2)	93(4)	44(2)	8(2)	−7(2)	17(2)
C(10)	41(2)	61(3)	44(2)	14(2)	4(2)	13(2)
C(11)	30(2)	42(2)	32(2)	2(1)	7(1)	7(1)
C(12)	31(4)	68(5)	62(4)	−23(4)	5(3)	−13(4)
C(13)	41(3)	68(4)	69(4)	−32(3)	5(3)	−12(3)
C(14)	43(3)	107(6)	114(7)	−50(6)	39(4)	−31(4)
C(12')	34(9)	65(9)	55(8)	−2(8)	−12(7)	0(8)
C(13')	180(50)	300(80)	110(20)	−100(40)	20(20)	−150(50)
C(14')	270(60)	120(40)	110(20)	−60(30)	110(30)	−120(40)
C(15)	30(2)	31(2)	38(2)	1(1)	6(1)	6(1)
C(16)	41(2)	48(2)	48(2)	5(2)	10(2)	0(2)
C(17)	47(2)	60(3)	57(3)	−21(2)	17(2)	−9(2)
C(18)	30(2)	25(2)	28(2)	−1(1)	2(1)	2(1)
C(19)	38(2)	27(2)	37(2)	4(1)	7(1)	4(1)
C(20)	40(2)	32(2)	43(2)	2(2)	1(2)	10(2)
C(21)	33(2)	41(2)	39(2)	−2(2)	−1(1)	10(2)
C(22)	36(2)	32(2)	33(2)	−5(1)	−2(1)	−1(1)
C(23)	33(2)	24(2)	30(2)	−3(1)	1(1)	1(1)
C(24)	42(2)	23(2)	70(3)	9(2)	9(2)	0(2)
C(25)	44(2)	31(2)	118(4)	−26(2)	12(3)	−3(2)
C(26)	75(3)	40(3)	111(5)	40(3)	9(3)	−1(2)
C(27)	37(2)	22(2)	52(2)	−2(1)	−7(2)	0(1)
C(28)	72(3)	30(2)	88(4)	−12(2)	34(3)	7(2)
C(29)	67(3)	26(2)	44(2)	1(2)	−6(2)	−4(2)
C(30)	28(2)	24(2)	18(1)	0(1)	8(1)	2(1)
C(31)	22(1)	27(2)	22(1)	0(1)	5(1)	1(1)
C(32)	24(1)	18(1)	24(1)	1(1)	4(1)	−2(1)
C(33)	32(2)	44(2)	23(2)	−8(1)	6(1)	7(1)
C(34)	27(2)	32(2)	25(2)	4(1)	4(1)	3(1)
C(35)	26(2)	27(2)	22(1)	−4(1)	0(1)	2(1)
C(36)	26(2)	40(2)	22(1)	3(1)	3(1)	2(1)
C(37)	32(2)	51(2)	26(2)	4(1)	−1(1)	1(2)
C(38)	30(2)	59(2)	29(2)	−6(2)	−6(1)	−1(2)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(39)	30(2)	41(2)	37(2)	−8(2)	−2(1)	−4(1)
C(40)	27(2)	31(2)	28(2)	−6(1)	4(1)	2(1)
C(41)	34(2)	38(2)	27(2)	9(1)	−2(1)	−4(1)
C(42)	44(2)	62(3)	39(2)	19(2)	8(2)	−4(2)
C(43)	47(2)	44(2)	51(2)	9(2)	−2(2)	−3(2)
C(44)	31(2)	26(2)	33(2)	−4(1)	3(1)	−2(1)
C(45)	57(2)	34(2)	49(2)	−2(2)	10(2)	9(2)
C(46)	40(2)	48(2)	51(2)	6(2)	5(2)	−13(2)
C(47)	26(1)	25(2)	18(1)	4(1)	4(1)	2(1)
C(48)	33(2)	28(2)	20(1)	0(1)	4(1)	1(1)
C(49)	49(2)	33(2)	18(1)	1(1)	4(1)	2(1)
C(50)	51(2)	37(2)	22(2)	9(1)	8(1)	3(2)
C(51)	42(2)	28(2)	28(2)	8(1)	10(1)	2(1)
C(52)	32(2)	24(2)	23(1)	5(1)	6(1)	2(1)
C(53)	39(2)	26(2)	18(1)	−1(1)	0(1)	−3(1)
C(54)	41(2)	34(2)	29(2)	−7(1)	2(1)	−4(1)
C(55)	46(2)	29(2)	36(2)	−3(1)	1(2)	2(2)
C(56)	37(2)	23(2)	28(2)	5(1)	4(1)	−5(1)
C(57)	42(2)	35(2)	41(2)	−8(2)	7(2)	3(2)
C(58)	37(2)	31(2)	50(2)	4(2)	3(2)	−7(1)
Si(1)	30(1)	38(1)	22(1)	−1(1)	3(1)	10(1)
C(59)	24(2)	27(2)	23(2)	−4(1)	3(1)	1(1)
C(60)	46(4)	62(4)	25(2)	−5(2)	−2(2)	6(2)
C(61)	39(3)	78(4)	40(3)	8(3)	4(2)	25(3)
C(62)	54(3)	38(2)	31(2)	8(2)	11(2)	7(2)
C(59')	41(6)	25(6)	15(5)	7(5)	6(5)	0(5)
C(60')	46(12)	200(30)	75(17)	60(20)	−2(11)	−25(17)
C(61')	100(20)	84(13)	160(30)	8(16)	−70(20)	30(15)
C(62')	50(20)	230(40)	50(14)	−60(20)	1(11)	10(20)
Si(1')	37(4)	59(4)	27(3)	0(2)	2(3)	−2(3)
C11	88(8)	46(8)	81(9)	6(6)	38(7)	3(7)
C21	96(10)	70(9)	94(10)	18(8)	20(8)	17(7)
C31	124(17)	100(13)	200(20)	28(16)	−24(15)	−1(12)
C41	220(30)	96(13)	180(20)	−10(17)	40(20)	−27(18)
C51	300(50)	140(30)	170(20)	50(20)	20(30)	−20(40)
C12	88(8)	46(8)	81(9)	6(6)	38(7)	3(7)
C22	130(20)	80(20)	80(30)	30(20)	−10(20)	−30(20)
C32	130(30)	60(20)	90(30)	44(18)	−10(20)	−10(20)
C42	120(30)	70(30)	100(30)	60(20)	0(20)	20(30)
C52	80(40)	110(40)	120(40)	20(30)	10(30)	−10(30)

Table 4: Bond lengths [Å] for mw_112_3frm.

Sb(1)–C(59')	2.107(14)
Sb(1)–C(59)	2.225(4)
Sb(1)–Ga(1)	2.6213(4)
Sb(1)–Sb(2)	2.7991(3)
Sb(2)–C(59)	2.164(4)
Sb(2)–C(59')	2.446(15)
Sb(2)–Ga(2)	2.6521(4)
Ga(1)–N(2)	1.949(3)
Ga(1)–N(1)	1.971(3)
Ga(1)–Cl(1)	2.2280(9)
Ga(2)–N(4)	1.966(2)
Ga(2)–N(3)	1.987(2)
Ga(2)–Cl(2)	2.2264(8)
N(1)–C(1)	1.340(4)
N(1)–C(6)	1.452(4)
N(2)–C(3)	1.336(4)
N(2)–C(18)	1.452(4)
N(3)–C(30)	1.326(4)
N(3)–C(35)	1.454(4)
N(4)–C(32)	1.330(4)
N(4)–C(47)	1.447(3)
C(1)–C(2)	1.400(5)
C(1)–C(4)	1.506(5)
C(2)–C(3)	1.389(5)
C(3)–C(5)	1.518(5)
C(6)–C(11)	1.394(5)
C(6)–C(7)	1.410(5)
C(7)–C(8)	1.393(6)
C(7)–C(12')	1.49(7)
C(7)–C(12)	1.53(2)
C(8)–C(9)	1.364(8)
C(9)–C(10)	1.384(6)
C(10)–C(11)	1.391(5)
C(11)–C(15)	1.520(5)
C(12)–C(13)	1.537(10)
C(12)–C(14)	1.548(9)
C(12')–C(14')	1.540(17)
C(12')–C(13')	1.543(16)
C(15)–C(17)	1.524(5)
C(15)–C(16)	1.526(5)
C(18)–C(19)	1.390(5)
C(18)–C(23)	1.407(5)
C(19)–C(20)	1.401(5)
C(19)–C(24)	1.514(5)
C(20)–C(21)	1.376(5)
C(21)–C(22)	1.380(5)
C(22)–C(23)	1.398(5)
C(23)–C(27)	1.513(5)
C(24)–C(25)	1.524(6)
C(24)–C(26)	1.535(6)
C(27)–C(28)	1.518(6)
C(27)–C(29)	1.529(6)
C(30)–C(31)	1.402(4)

Table 4: (continued)

C(30)–C(33)	1.518(4)
C(31)–C(32)	1.393(4)
C(32)–C(34)	1.513(4)
C(35)–C(36)	1.401(4)
C(35)–C(40)	1.405(5)
C(36)–C(37)	1.405(4)
C(36)–C(41)	1.520(5)
C(37)–C(38)	1.375(5)
C(38)–C(39)	1.375(5)
C(39)–C(40)	1.402(4)
C(40)–C(44)	1.522(5)
C(41)–C(43)	1.517(6)
C(41)–C(42)	1.537(5)
C(44)–C(46)	1.522(5)
C(44)–C(45)	1.530(5)
C(47)–C(48)	1.404(4)
C(47)–C(52)	1.410(4)
C(48)–C(49)	1.393(4)
C(48)–C(53)	1.513(4)
C(49)–C(50)	1.374(5)
C(50)–C(51)	1.380(5)
C(51)–C(52)	1.394(4)
C(52)–C(56)	1.522(4)
C(53)–C(55)	1.526(5)
C(53)–C(54)	1.539(5)
C(56)–C(58)	1.529(5)
C(56)–C(57)	1.534(5)
Si(1)–C(59)	1.856(4)
Si(1)–C(60)	1.860(5)
Si(1)–C(61)	1.867(5)
Si(1)–C(62)	1.868(5)
C(59')–Si(1')	1.846(18)
C(60')–Si(1')	1.850(13)
C(61')–Si(1')	1.860(13)
C(62')–Si(1')	1.880(13)
C11–C21	1.466(15)
C21–C31	1.525(17)
C31–C41	1.502(18)
C41–C51	1.527(19)
C12–C22	1.54(2)
C22–C32	1.55(2)
C32–C42	1.54(2)
C42–C52	1.54(2)

Table 5: Bond angles [°] for mw_112_3frm.

C(59')–Sb(1)–Ga(1)	120.7(4)
C(59)–Sb(1)–Ga(1)	93.10(10)
C(59')–Sb(1)–Sb(2)	57.8(4)
C(59)–Sb(1)–Sb(2)	49.42(10)
Ga(1)–Sb(1)–Sb(2)	98.484(12)
C(59)–Sb(2)–Ga(2)	111.29(11)
C(59')–Sb(2)–Ga(2)	86.4(4)
C(59)–Sb(2)–Sb(1)	51.33(10)
C(59')–Sb(2)–Sb(1)	46.8(3)
Ga(2)–Sb(2)–Sb(1)	101.324(11)
N(2)–Ga(1)–N(1)	95.38(11)
N(2)–Ga(1)–Cl(1)	106.44(8)
N(1)–Ga(1)–Cl(1)	103.30(8)
N(2)–Ga(1)–Sb(1)	115.78(8)
N(1)–Ga(1)–Sb(1)	118.94(8)
Cl(1)–Ga(1)–Sb(1)	114.56(3)
N(4)–Ga(2)–N(3)	94.30(10)
N(4)–Ga(2)–Cl(2)	105.40(7)
N(3)–Ga(2)–Cl(2)	101.96(8)
N(4)–Ga(2)–Sb(2)	109.18(7)
N(3)–Ga(2)–Sb(2)	122.70(7)
Cl(2)–Ga(2)–Sb(2)	119.46(3)
C(1)–N(1)–C(6)	116.9(3)
C(1)–N(1)–Ga(1)	120.8(2)
C(6)–N(1)–Ga(1)	122.3(2)
C(3)–N(2)–C(18)	118.3(3)
C(3)–N(2)–Ga(1)	120.4(2)
C(18)–N(2)–Ga(1)	121.3(2)
C(30)–N(3)–C(35)	118.5(2)
C(30)–N(3)–Ga(2)	119.85(19)
C(35)–N(3)–Ga(2)	121.56(18)
C(32)–N(4)–C(47)	117.8(2)
C(32)–N(4)–Ga(2)	120.89(19)
C(47)–N(4)–Ga(2)	121.25(19)
N(1)–C(1)–C(2)	123.1(3)
N(1)–C(1)–C(4)	120.3(3)
C(2)–C(1)–C(4)	116.6(3)
C(3)–C(2)–C(1)	128.5(3)
N(2)–C(3)–C(2)	123.9(3)
N(2)–C(3)–C(5)	119.8(3)
C(2)–C(3)–C(5)	116.3(3)
C(11)–C(6)–C(7)	121.9(3)
C(11)–C(6)–N(1)	118.3(3)
C(7)–C(6)–N(1)	119.8(3)
C(8)–C(7)–C(6)	117.2(4)
C(8)–C(7)–C(12')	114(2)
C(6)–C(7)–C(12')	129(2)
C(8)–C(7)–C(12)	120.9(7)
C(6)–C(7)–C(12)	121.8(6)
C(9)–C(8)–C(7)	121.7(4)
C(8)–C(9)–C(10)	120.3(4)
C(9)–C(10)–C(11)	120.8(4)
C(10)–C(11)–C(6)	118.1(4)

Table 5: (continued)

C(10)–C(11)–C(15)	119.8(4)
C(6)–C(11)–C(15)	122.0(3)
C(7)–C(12)–C(13)	110.2(9)
C(7)–C(12)–C(14)	111.5(13)
C(13)–C(12)–C(14)	107.9(6)
C(7)–C(12')–C(14')	116(4)
C(7)–C(12')–C(13')	117(5)
C(14')–C(12')–C(13')	107.9(18)
C(11)–C(15)–C(17)	111.8(3)
C(11)–C(15)–C(16)	113.5(3)
C(17)–C(15)–C(16)	109.9(3)
C(19)–C(18)–C(23)	121.6(3)
C(19)–C(18)–N(2)	120.4(3)
C(23)–C(18)–N(2)	118.0(3)
C(18)–C(19)–C(20)	118.2(3)
C(18)–C(19)–C(24)	122.6(3)
C(20)–C(19)–C(24)	119.2(3)
C(21)–C(20)–C(19)	121.0(3)
C(20)–C(21)–C(22)	120.3(3)
C(21)–C(22)–C(23)	120.7(3)
C(22)–C(23)–C(18)	118.1(3)
C(22)–C(23)–C(27)	119.5(3)
C(18)–C(23)–C(27)	122.3(3)
C(19)–C(24)–C(25)	110.0(3)
C(19)–C(24)–C(26)	112.1(4)
C(25)–C(24)–C(26)	111.2(4)
C(23)–C(27)–C(28)	110.7(3)
C(23)–C(27)–C(29)	112.4(3)
C(28)–C(27)–C(29)	110.9(3)
N(3)–C(30)–C(31)	124.5(3)
N(3)–C(30)–C(33)	120.9(3)
C(31)–C(30)–C(33)	114.6(3)
C(32)–C(31)–C(30)	127.8(3)
N(4)–C(32)–C(31)	123.3(3)
N(4)–C(32)–C(34)	120.4(3)
C(31)–C(32)–C(34)	116.4(3)
C(36)–C(35)–C(40)	122.5(3)
C(36)–C(35)–N(3)	119.9(3)
C(40)–C(35)–N(3)	117.5(3)
C(35)–C(36)–C(37)	117.1(3)
C(35)–C(36)–C(41)	123.8(3)
C(37)–C(36)–C(41)	119.1(3)
C(38)–C(37)–C(36)	121.4(3)
C(39)–C(38)–C(37)	120.5(3)
C(38)–C(39)–C(40)	121.1(3)
C(39)–C(40)–C(35)	117.4(3)
C(39)–C(40)–C(44)	120.0(3)
C(35)–C(40)–C(44)	122.5(3)
C(43)–C(41)–C(36)	110.7(3)
C(43)–C(41)–C(42)	109.8(3)
C(36)–C(41)–C(42)	111.9(3)
C(46)–C(44)–C(40)	112.8(3)
C(46)–C(44)–C(45)	112.1(3)

Table 5: (continued)

C(40)–C(44)–C(45)	110.5(3)
C(48)–C(47)–C(52)	121.5(3)
C(48)–C(47)–N(4)	119.9(3)
C(52)–C(47)–N(4)	118.6(3)
C(49)–C(48)–C(47)	117.9(3)
C(49)–C(48)–C(53)	119.3(3)
C(47)–C(48)–C(53)	122.8(3)
C(50)–C(49)–C(48)	121.3(3)
C(49)–C(50)–C(51)	120.5(3)
C(50)–C(51)–C(52)	120.8(3)
C(51)–C(52)–C(47)	118.0(3)
C(51)–C(52)–C(56)	119.2(3)
C(47)–C(52)–C(56)	122.8(3)
C(48)–C(53)–C(55)	111.3(3)
C(48)–C(53)–C(54)	111.1(3)
C(55)–C(53)–C(54)	110.4(3)
C(52)–C(56)–C(58)	111.9(3)
C(52)–C(56)–C(57)	111.9(3)
C(58)–C(56)–C(57)	109.0(3)
C(59)–Si(1)–C(60)	111.3(3)
C(59)–Si(1)–C(61)	107.3(2)
C(60)–Si(1)–C(61)	108.8(3)
C(59)–Si(1)–C(62)	110.6(2)
C(60)–Si(1)–C(62)	110.7(3)
C(61)–Si(1)–C(62)	107.9(3)
Si(1)–C(59)–Sb(2)	131.0(2)
Si(1)–C(59)–Sb(1)	116.9(2)
Sb(2)–C(59)–Sb(1)	79.24(12)
Si(1')–C(59')–Sb(1)	128.9(9)
Si(1')–C(59')–Sb(2)	118.8(8)
Sb(1)–C(59')–Sb(2)	75.5(4)
C(59')–Si(1')–C(60')	111.3(10)
C(59')–Si(1')–C(61')	109.0(11)
C(60')–Si(1')–C(61')	110.0(9)
C(59')–Si(1')–C(62')	109.6(13)
C(60')–Si(1')–C(62')	108.7(9)
C(61')–Si(1')–C(62')	108.3(9)
C11–C21–C31	107.0(14)
C41–C31–C21	106.9(16)
C31–C41–C51	106.0(17)
C12–C22–C32	103.0(18)
C42–C32–C22	103.7(18)
C32–C42–C52	103.6(19)

Crystal structure of mw_022_4m_sq

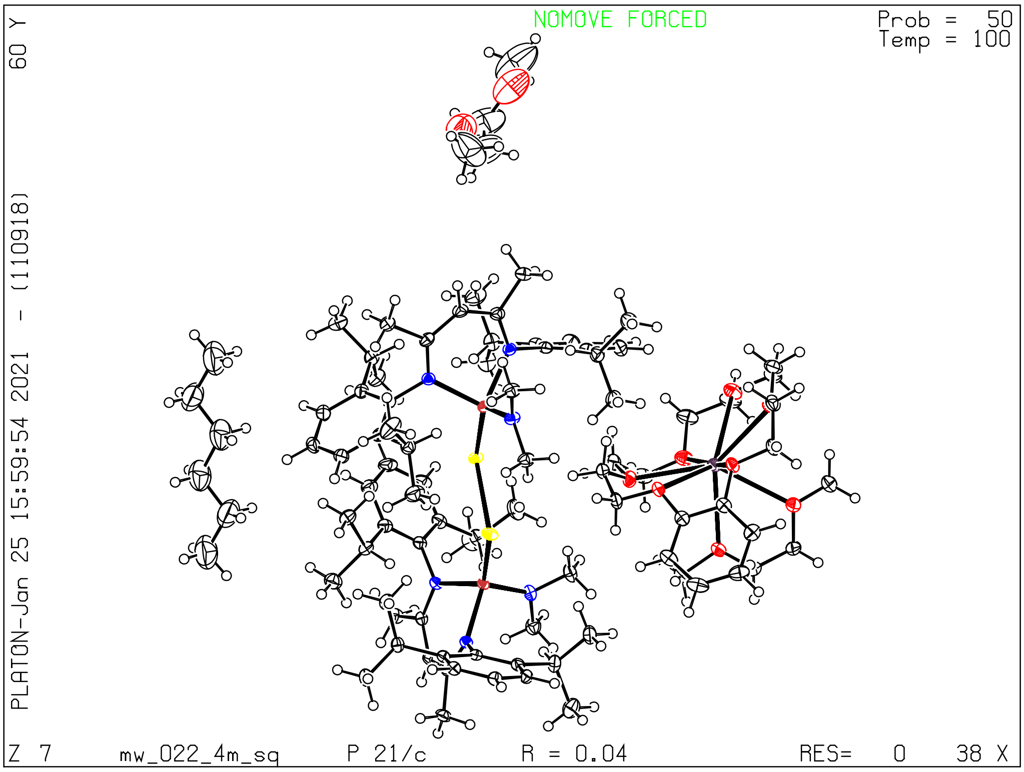

Table 1: Crystal data and structure refinement for mw_022_4m_sq.

Identification code	mw_022_4m_sq
Empirical Formula	$C_{89}\,H_{145}\,Ga_2\,K\,N_6\,O_{10}\,Sb_2$
Formula weight	1881.14 Da
Density (calculated)	$1.201\,g \cdot cm^{-3}$
$F(000)$	3936
Temperature	100(2) K
Crystal size	$0.348 \times 0.076 \times 0.070$ mm
Crystal appearance	black needle
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 19.3507(10)$ Å
	$b = 17.6402(10)$ Å
	$c = 31.0106(17)$ Å
	$\alpha = 90°$
	$\beta = 100.619(3)°$
	$\gamma = 90°$
Unit cell volume	$10404.2(10)$ Å^3
Z	4
Cell measurement refections used	9306
θ range for cell measurement	2.31° to 29.11°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.334° to 30.589°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (99.7%)
Index ranges	$-27 \leq h \leq 27$
	$-25 \leq k \leq 25$
	$-44 \leq l \leq 44$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$1.117\,mm^{-1}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.65
R_{merg} before/after correction	0.0631/0.0532
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	320168
Independent reflections	31900 ($R_{int} = 0.0746$)
Reflections with $I > 2\sigma(I)$	22902
Data / retraints / parameter	31900 / 0 / 1020
Goodness-of-fit on F^2	1.079
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 24.0495P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0438$
	$wR2 = 0.0940$
R indices [all data]	$R1 = 0.0772$
	$wR2 = 0.1102$
Largest diff. peak and hole	1.804 and -0.886 Å^{-3}

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disordered solvent

The dimethoxy ethane shows rather large displacement ellipsoids. Reducing the occupancy to 50% yields ellipsiods of realistic size but significantly increases the R-values. No residual electron density maxima giving an alternate orientation could be found, thus the model with partial occupancy was discarded.

SQUEEZE

The structure contains highly disordered solvent – possibly n-hexane or dimethoxy ethane. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run. (For details see: A. L. Spek, *Acta Cryst. A46* **(1990)**, 194–201). Since the nature and amount of the solvent is not clear it was not included in the sum formula.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_022_4m_sq. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Sb(1)	2832(1)	1687(1)	2984(1)	19(1)
Sb(2)	2247(1)	2722(1)	3468(1)	18(1)
Ga(1)	1743(1)	1318(1)	2408(1)	13(1)
Ga(2)	3342(1)	3126(1)	4043(1)	14(1)
K(1)	3322(1)	5439(1)	1809(1)	19(1)
O(1)	4750(1)	5176(1)	2039(1)	20(1)
O(2)	4264(1)	6641(1)	2013(1)	24(1)
O(3)	2822(1)	6839(1)	2039(1)	28(1)
O(4)	1886(1)	5626(1)	1724(1)	26(1)
O(5)	2585(1)	4374(1)	2192(1)	24(1)
O(6)	4013(1)	4118(1)	2266(1)	21(1)
O(7)	3803(1)	5790(1)	1037(1)	26(1)
O(8)	3001(1)	4479(1)	1109(1)	26(1)
N(1)	805(1)	1025(1)	2543(1)	15(1)
N(2)	1887(1)	263(1)	2181(1)	15(1)
N(3)	3306(1)	2769(1)	4664(1)	17(1)
N(4)	3352(1)	4230(1)	4238(1)	17(1)
N(5)	1464(1)	1922(1)	1904(1)	20(1)
N(6)	4287(1)	3016(2)	3985(1)	19(1)
C(1)	405(1)	503(2)	2309(1)	16(1)
C(2)	650(1)	−19(2)	2033(1)	17(1)
C(3)	1351(1)	−168(2)	1999(1)	17(1)
C(4)	−366(1)	463(2)	2332(1)	24(1)
C(5)	1484(2)	−876(2)	1750(1)	23(1)
C(6)	532(1)	1443(2)	2877(1)	17(1)
C(7)	162(1)	2123(2)	2777(1)	21(1)
C(8)	−75(2)	2506(2)	3118(1)	26(1)
C(9)	45(2)	2225(2)	3539(1)	28(1)
C(10)	417(2)	1557(2)	3633(1)	25(1)
C(11)	676(1)	1157(2)	3308(1)	20(1)
C(12)	34(2)	2462(2)	2323(1)	25(1)
C(13)	−749(2)	2621(2)	2150(1)	35(1)
C(14)	450(2)	3200(2)	2325(1)	36(1)
C(15)	1116(2)	448(2)	3418(1)	21(1)
C(16)	683(2)	−279(2)	3340(1)	32(1)
C(17)	1536(2)	466(2)	3886(1)	26(1)
C(18)	2592(1)	−27(2)	2201(1)	15(1)
C(19)	3010(1)	258(2)	1910(1)	18(1)
C(20)	3689(1)	−27(2)	1939(1)	19(1)
C(21)	3956(1)	−569(2)	2243(1)	19(1)
C(22)	3545(1)	−836(2)	2531(1)	18(1)
C(23)	2861(1)	−575(2)	2517(1)	17(1)
C(24)	2756(2)	848(2)	1563(1)	23(1)
C(25)	2676(2)	509(2)	1101(1)	34(1)
C(26)	3253(2)	1530(2)	1611(1)	31(1)
C(27)	2448(1)	−886(2)	2853(1)	19(1)
C(28)	2475(2)	−1756(2)	2882(1)	27(1)
C(29)	2730(2)	−560(2)	3308(1)	24(1)
C(30)	3580(1)	3173(2)	5017(1)	20(1)
C(31)	3765(2)	3939(2)	5000(1)	22(1)

Table 2: (continued)

	x	y	z	U_{eq}
C(32)	3616(2)	4445(2)	4648(1)	21(1)
C(33)	3696(2)	2816(2)	5468(1)	27(1)
C(34)	3772(2)	5274(2)	4754(1)	28(1)
C(35)	2978(2)	2057(2)	4729(1)	19(1)
C(36)	3310(2)	1366(2)	4669(1)	21(1)
C(37)	2969(2)	691(2)	4734(1)	24(1)
C(38)	2323(2)	690(2)	4863(1)	26(1)
C(39)	1998(2)	1367(2)	4919(1)	24(1)
C(40)	2307(2)	2060(2)	4848(1)	20(1)
C(41)	4042(2)	1335(2)	4552(1)	25(1)
C(42)	4595(2)	1147(3)	4960(1)	41(1)
C(43)	4096(2)	774(2)	4189(1)	38(1)
C(44)	1901(2)	2786(2)	4892(1)	22(1)
C(45)	1699(2)	2871(2)	5345(1)	33(1)
C(46)	1238(2)	2819(2)	4541(1)	29(1)
C(47)	3138(2)	4806(2)	3909(1)	19(1)
C(48)	3629(2)	5164(2)	3693(1)	22(1)
C(49)	3383(2)	5714(2)	3380(1)	30(1)
C(50)	2683(2)	5913(2)	3282(1)	32(1)
C(51)	2205(2)	5542(2)	3492(1)	30(1)
C(52)	2419(2)	4988(2)	3807(1)	23(1)
C(53)	4404(2)	4961(2)	3783(1)	24(1)
C(54)	4882(2)	5657(2)	3879(1)	34(1)
C(55)	4596(2)	4517(2)	3397(1)	29(1)
C(56)	1894(2)	4604(2)	4047(1)	26(1)
C(57)	1857(2)	5004(2)	4480(1)	40(1)
C(58)	1158(2)	4538(2)	3764(1)	35(1)
C(59)	1829(2)	2597(2)	1819(1)	27(1)
C(60)	969(2)	1694(2)	1519(1)	26(1)
C(61)	4500(2)	2571(2)	3643(1)	25(1)
C(62)	4875(2)	3169(2)	4335(1)	25(1)
C(63)	4846(1)	4488(2)	1855(1)	20(1)
C(64)	5280(2)	4351(2)	1557(1)	25(1)
C(65)	5340(2)	3617(2)	1400(1)	31(1)
C(66)	4977(2)	3029(2)	1548(1)	33(1)
C(67)	4532(2)	3162(2)	1846(1)	27(1)
C(68)	4454(2)	3894(2)	1994(1)	20(1)
C(69)	5191(2)	5798(2)	1958(1)	23(1)
C(70)	4972(2)	6463(2)	2204(1)	25(1)
C(71)	3997(2)	7294(2)	2196(1)	30(1)
C(72)	3269(2)	7437(2)	1952(1)	31(1)
C(73)	2116(2)	6939(2)	1814(1)	32(1)
C(74)	1679(2)	6292(2)	1925(1)	31(1)
C(75)	1543(2)	4960(2)	1836(1)	29(1)
C(76)	1913(2)	4618(2)	2260(1)	29(1)
C(77)	2979(2)	3987(2)	2563(1)	26(1)
C(78)	3555(2)	3565(2)	2403(1)	24(1)
C(79)	3789(2)	6557(2)	895(1)	32(1)
C(80)	3568(2)	5298(2)	677(1)	26(1)
C(81)	3524(2)	4503(2)	841(1)	24(1)
C(82)	2779(2)	3725(2)	1169(1)	29(1)
O11	1912(3)	8259(4)	5656(2)	113(2)

Table 2: (continued)

	x	y	z	U_{eq}
O21	2544(3)	6804(3)	5925(2)	99(2)
C11	1371(5)	8843(6)	5637(3)	147(4)
C21	1575(4)	7532(6)	5535(3)	123(3)
C31	2156(5)	6967(6)	5497(2)	123(3)
C41	3183(4)	6407(4)	5891(3)	122(3)
C22	111(4)	498(4)	5573(2)	85(2)
C12	495(4)	1175(4)	5764(2)	98(2)
C32	219(3)	337(4)	5113(2)	74(2)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_022_4m_sq.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	13(1)	18(1)	25(1)	−7(1)	1(1)	−1(1)
Sb(2)	14(1)	22(1)	16(1)	−4(1)	2(1)	−1(1)
Ga(1)	11(1)	12(1)	17(1)	−2(1)	3(1)	−1(1)
Ga(2)	13(1)	16(1)	13(1)	−2(1)	3(1)	−1(1)
K(1)	18(1)	17(1)	22(1)	−1(1)	4(1)	−1(1)
O(1)	18(1)	16(1)	27(1)	1(1)	6(1)	−3(1)
O(2)	26(1)	17(1)	29(1)	−6(1)	3(1)	1(1)
O(3)	26(1)	21(1)	36(1)	−2(1)	2(1)	2(1)
O(4)	22(1)	24(1)	33(1)	−6(1)	5(1)	2(1)
O(5)	22(1)	26(1)	27(1)	2(1)	10(1)	−3(1)
O(6)	23(1)	17(1)	25(1)	1(1)	6(1)	−5(1)
O(7)	32(1)	24(1)	21(1)	−2(1)	4(1)	−8(1)
O(8)	34(1)	17(1)	31(1)	−4(1)	12(1)	−3(1)
N(1)	12(1)	13(1)	20(1)	−1(1)	3(1)	0(1)
N(2)	14(1)	13(1)	18(1)	−1(1)	4(1)	1(1)
N(3)	17(1)	18(1)	16(1)	−1(1)	2(1)	−1(1)
N(4)	18(1)	19(1)	15(1)	−2(1)	3(1)	−1(1)
N(5)	18(1)	17(1)	24(1)	4(1)	3(1)	−1(1)
N(6)	14(1)	24(1)	20(1)	−5(1)	4(1)	0(1)
C(1)	13(1)	17(1)	18(1)	2(1)	2(1)	−1(1)
C(2)	14(1)	16(1)	20(1)	−3(1)	2(1)	−4(1)
C(3)	17(1)	16(1)	18(1)	1(1)	4(1)	0(1)
C(4)	15(1)	25(2)	31(2)	−5(1)	5(1)	−3(1)
C(5)	23(1)	18(2)	28(2)	−8(1)	4(1)	−6(1)
C(6)	11(1)	19(1)	23(1)	−4(1)	6(1)	−4(1)
C(7)	14(1)	20(2)	29(2)	−2(1)	6(1)	−2(1)
C(8)	19(1)	22(2)	39(2)	−9(1)	9(1)	2(1)
C(9)	23(1)	31(2)	34(2)	−14(1)	11(1)	−1(1)
C(10)	22(1)	29(2)	25(2)	−6(1)	6(1)	−3(1)
C(11)	15(1)	21(2)	24(1)	−5(1)	5(1)	−3(1)
C(12)	20(1)	20(2)	37(2)	2(1)	7(1)	6(1)
C(13)	25(2)	34(2)	45(2)	5(2)	3(1)	8(1)
C(14)	31(2)	24(2)	54(2)	6(2)	14(2)	4(1)
C(15)	22(1)	24(2)	17(1)	−1(1)	3(1)	1(1)
C(16)	39(2)	26(2)	28(2)	−2(1)	1(1)	−3(1)
C(17)	29(2)	32(2)	18(1)	0(1)	2(1)	1(1)
C(18)	15(1)	14(1)	18(1)	−3(1)	2(1)	0(1)
C(19)	19(1)	15(1)	22(1)	−1(1)	6(1)	2(1)
C(20)	17(1)	19(1)	23(1)	−1(1)	8(1)	−1(1)
C(21)	15(1)	21(1)	23(1)	−2(1)	5(1)	0(1)
C(22)	17(1)	18(1)	20(1)	1(1)	1(1)	1(1)
C(23)	16(1)	15(1)	18(1)	−2(1)	2(1)	−2(1)
C(24)	23(1)	22(2)	28(2)	8(1)	11(1)	6(1)
C(25)	36(2)	40(2)	27(2)	7(2)	5(1)	5(2)
C(26)	38(2)	24(2)	37(2)	7(1)	20(2)	1(1)
C(27)	16(1)	20(1)	23(1)	3(1)	5(1)	1(1)
C(28)	27(2)	25(2)	31(2)	5(1)	9(1)	−4(1)
C(29)	24(1)	27(2)	23(1)	1(1)	8(1)	0(1)
C(30)	16(1)	27(2)	16(1)	−2(1)	2(1)	1(1)
C(31)	22(1)	26(2)	15(1)	−4(1)	−1(1)	−2(1)
C(32)	18(1)	23(2)	22(1)	−6(1)	5(1)	−4(1)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(33)	36(2)	27(2)	16(1)	0(1)	1(1)	−5(1)
C(34)	36(2)	23(2)	24(2)	−7(1)	5(1)	−4(1)
C(35)	22(1)	21(1)	14(1)	0(1)	3(1)	−3(1)
C(36)	24(1)	24(2)	14(1)	0(1)	1(1)	2(1)
C(37)	32(2)	19(2)	19(1)	1(1)	0(1)	0(1)
C(38)	32(2)	22(2)	20(1)	4(1)	−1(1)	−7(1)
C(39)	24(1)	28(2)	20(1)	2(1)	1(1)	−7(1)
C(40)	19(1)	24(2)	16(1)	0(1)	1(1)	−4(1)
C(41)	28(2)	22(2)	25(2)	3(1)	7(1)	3(1)
C(42)	27(2)	67(3)	30(2)	2(2)	6(1)	7(2)
C(43)	46(2)	37(2)	32(2)	−6(2)	14(2)	5(2)
C(44)	17(1)	26(2)	23(1)	−1(1)	4(1)	−2(1)
C(45)	38(2)	35(2)	26(2)	−7(1)	8(1)	2(2)
C(46)	24(2)	37(2)	26(2)	0(1)	6(1)	3(1)
C(47)	22(1)	16(1)	18(1)	−4(1)	1(1)	−1(1)
C(48)	25(1)	21(2)	21(1)	−4(1)	2(1)	−6(1)
C(49)	37(2)	24(2)	27(2)	1(1)	5(1)	−9(1)
C(50)	43(2)	19(2)	30(2)	4(1)	−2(1)	−1(1)
C(51)	30(2)	25(2)	34(2)	2(1)	0(1)	3(1)
C(52)	25(1)	18(1)	25(2)	−3(1)	2(1)	1(1)
C(53)	23(1)	28(2)	22(1)	−1(1)	4(1)	−8(1)
C(54)	30(2)	38(2)	35(2)	−4(2)	4(1)	−15(2)
C(55)	24(2)	35(2)	28(2)	−2(1)	9(1)	−7(1)
C(56)	18(1)	29(2)	31(2)	2(1)	4(1)	2(1)
C(57)	35(2)	49(2)	39(2)	−8(2)	14(2)	4(2)
C(58)	23(2)	39(2)	41(2)	6(2)	2(1)	4(1)
C(59)	26(2)	19(2)	37(2)	7(1)	10(1)	0(1)
C(60)	27(2)	26(2)	24(2)	5(1)	2(1)	1(1)
C(61)	20(1)	30(2)	24(1)	−6(1)	6(1)	0(1)
C(62)	19(1)	32(2)	24(1)	−7(1)	2(1)	−2(1)
C(63)	15(1)	20(1)	23(1)	1(1)	−1(1)	1(1)
C(64)	19(1)	31(2)	26(2)	0(1)	3(1)	2(1)
C(65)	24(2)	36(2)	30(2)	−9(1)	3(1)	5(1)
C(66)	29(2)	26(2)	40(2)	−11(2)	−2(1)	5(1)
C(67)	24(1)	20(2)	36(2)	−2(1)	0(1)	−1(1)
C(68)	18(1)	21(2)	20(1)	2(1)	−2(1)	0(1)
C(69)	18(1)	21(2)	30(2)	2(1)	5(1)	−4(1)
C(70)	22(1)	23(2)	29(2)	0(1)	4(1)	−7(1)
C(71)	33(2)	22(2)	36(2)	−10(1)	9(1)	−5(1)
C(72)	36(2)	20(2)	38(2)	−3(1)	10(1)	3(1)
C(73)	30(2)	24(2)	40(2)	−6(1)	−2(1)	10(1)
C(74)	23(2)	27(2)	42(2)	−10(2)	3(1)	6(1)
C(75)	17(1)	31(2)	41(2)	−13(2)	6(1)	−3(1)
C(76)	25(2)	28(2)	36(2)	−4(1)	16(1)	−8(1)
C(77)	32(2)	23(2)	22(1)	2(1)	6(1)	−8(1)
C(78)	29(2)	20(2)	25(2)	5(1)	6(1)	−6(1)
C(79)	36(2)	27(2)	32(2)	−1(1)	8(1)	−10(1)
C(80)	32(2)	28(2)	18(1)	−3(1)	4(1)	−8(1)
C(81)	25(1)	27(2)	21(1)	−3(1)	4(1)	0(1)
C(82)	37(2)	21(2)	29(2)	−2(1)	8(1)	−8(1)
O11	92(4)	167(6)	80(3)	4(3)	14(3)	34(4)
O21	93(3)	117(4)	91(3)	−10(3)	25(3)	−12(3)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C11	157(8)	207(11)	74(5)	25(6)	15(5)	101(8)
C21	78(5)	195(10)	86(5)	−51(6)	−11(4)	3(6)
C31	132(7)	161(8)	64(4)	−20(5)	−11(4)	19(6)
C41	113(6)	60(4)	204(10)	−4(5)	61(6)	20(4)
C22	95(5)	109(5)	55(3)	−3(3)	29(3)	−38(4)
C12	102(5)	105(5)	89(5)	19(4)	21(4)	−41(4)
C32	58(3)	86(4)	81(4)	14(3)	17(3)	−18(3)

Table 4: Bond lengths [Å] for mw_022_4m_sq.

Sb(1)–Ga(1)	2.5826(4)
Sb(1)–Sb(2)	2.7359(3)
Sb(2)–Ga(2)	2.6052(4)
Ga(1)–N(5)	1.886(2)
Ga(1)–N(1)	2.004(2)
Ga(1)–N(2)	2.027(2)
Ga(2)–N(6)	1.881(2)
Ga(2)–N(3)	2.038(2)
Ga(2)–N(4)	2.038(2)
K(1)–O(8)	2.732(2)
K(1)–O(5)	2.757(2)
K(1)–O(4)	2.762(2)
K(1)–O(1)	2.763(2)
K(1)–O(2)	2.791(2)
K(1)–O(3)	2.794(2)
K(1)–O(7)	2.794(2)
K(1)–O(6)	2.920(2)
K(1)–C(63)	3.372(3)
K(1)–C(68)	3.477(3)
K(1)–C(81)	3.511(3)
K(1)–C(73)	3.531(3)
O(1)–C(63)	1.368(4)
O(1)–C(69)	1.439(3)
O(2)–C(71)	1.422(4)
O(2)–C(70)	1.424(4)
O(3)–C(72)	1.422(4)
O(3)–C(73)	1.426(4)
O(4)–C(74)	1.422(4)
O(4)–C(75)	1.423(4)
O(5)–C(76)	1.423(4)
O(5)–C(77)	1.431(4)
O(6)–C(68)	1.366(4)
O(6)–C(78)	1.434(3)
O(7)–C(79)	1.421(4)
O(7)–C(80)	1.421(4)
O(8)–C(82)	1.419(4)
O(8)–C(81)	1.426(4)
N(1)–C(1)	1.329(3)
N(1)–C(6)	1.449(3)
N(2)–C(3)	1.325(3)
N(2)–C(18)	1.446(3)
N(3)–C(30)	1.331(4)
N(3)–C(35)	1.439(4)
N(4)–C(32)	1.334(4)
N(4)–C(47)	1.445(4)
N(5)–C(59)	1.434(4)
N(5)–C(60)	1.443(4)
N(6)–C(61)	1.438(4)
N(6)–C(62)	1.445(4)
C(1)–C(2)	1.399(4)
C(1)–C(4)	1.509(4)
C(2)–C(3)	1.403(4)
C(3)–C(5)	1.516(4)

Table 4: (continued)

C(6)–C(7)	1.402(4)
C(6)–C(11)	1.407(4)
C(7)–C(8)	1.401(4)
C(7)–C(12)	1.507(4)
C(8)–C(9)	1.377(5)
C(9)–C(10)	1.384(5)
C(10)–C(11)	1.395(4)
C(11)–C(15)	1.516(4)
C(12)–C(14)	1.531(5)
C(12)–C(13)	1.537(4)
C(15)–C(16)	1.527(4)
C(15)–C(17)	1.528(4)
C(18)–C(23)	1.406(4)
C(18)–C(19)	1.412(4)
C(19)–C(20)	1.394(4)
C(19)–C(24)	1.514(4)
C(20)–C(21)	1.375(4)
C(21)–C(22)	1.383(4)
C(22)–C(23)	1.394(4)
C(23)–C(27)	1.528(4)
C(24)–C(26)	1.530(5)
C(24)–C(25)	1.534(5)
C(27)–C(29)	1.527(4)
C(27)–C(28)	1.538(4)
C(30)–C(31)	1.402(4)
C(30)–C(33)	1.511(4)
C(31)–C(32)	1.398(4)
C(32)–C(34)	1.517(4)
C(35)–C(36)	1.406(4)
C(35)–C(40)	1.414(4)
C(36)–C(37)	1.393(4)
C(36)–C(41)	1.527(4)
C(37)–C(38)	1.382(4)
C(38)–C(39)	1.375(5)
C(39)–C(40)	1.397(4)
C(40)–C(44)	1.522(4)
C(41)–C(43)	1.516(5)
C(41)–C(42)	1.534(5)
C(44)–C(46)	1.522(4)
C(44)–C(45)	1.534(4)
C(47)–C(52)	1.405(4)
C(47)–C(48)	1.410(4)
C(48)–C(49)	1.392(5)
C(48)–C(53)	1.518(4)
C(49)–C(50)	1.379(5)
C(50)–C(51)	1.390(5)
C(51)–C(52)	1.390(4)
C(52)–C(56)	1.522(4)
C(53)–C(55)	1.530(4)
C(53)–C(54)	1.534(4)
C(56)–C(57)	1.530(5)
C(56)–C(58)	1.533(4)
C(63)–C(64)	1.379(4)

Table 4: (continued)

C(63)–C(68)	1.407(4)
C(64)–C(65)	1.396(5)
C(65)–C(66)	1.378(5)
C(66)–C(67)	1.396(5)
C(67)–C(68)	1.388(4)
C(69)–C(70)	1.503(4)
C(71)–C(72)	1.493(5)
C(73)–C(74)	1.498(5)
C(75)–C(76)	1.503(5)
C(77)–C(78)	1.498(5)
C(80)–C(81)	1.500(4)
O11–C21	1.458(10)
O11–C11	1.462(9)
O21–C31	1.427(8)
O21–C41	1.441(8)
C21–C31	1.523(11)
C22–C12	1.473(8)
C22–C32	1.505(8)
C32–C32#1	1.550(11)

#1 -x,-y,-z+1

Table 5: Bond angles [°] for mw_022_4m_sq.

Ga(1)–Sb(1)–Sb(2)	100.405(10)
Ga(2)–Sb(2)–Sb(1)	101.056(10)
N(5)–Ga(1)–N(1)	100.75(10)
N(5)–Ga(1)–N(2)	105.54(10)
N(1)–Ga(1)–N(2)	91.36(9)
N(5)–Ga(1)–Sb(1)	120.25(7)
N(1)–Ga(1)–Sb(1)	125.08(7)
N(2)–Ga(1)–Sb(1)	108.96(6)
N(6)–Ga(2)–N(3)	105.18(10)
N(6)–Ga(2)–N(4)	99.83(10)
N(3)–Ga(2)–N(4)	90.84(9)
N(6)–Ga(2)–Sb(2)	126.07(7)
N(3)–Ga(2)–Sb(2)	113.41(7)
N(4)–Ga(2)–Sb(2)	115.23(7)
O(8)–K(1)–O(5)	81.91(7)
O(8)–K(1)–O(4)	85.46(7)
O(5)–K(1)–O(4)	62.04(7)
O(8)–K(1)–O(1)	99.88(7)
O(5)–K(1)–O(1)	110.27(6)
O(4)–K(1)–O(1)	170.16(7)
O(8)–K(1)–O(2)	133.97(7)
O(5)–K(1)–O(2)	142.03(7)
O(4)–K(1)–O(2)	122.27(7)
O(1)–K(1)–O(2)	59.27(6)
O(8)–K(1)–O(3)	135.42(7)
O(5)–K(1)–O(3)	105.13(7)
O(4)–K(1)–O(3)	61.87(7)
O(1)–K(1)–O(3)	117.37(7)
O(2)–K(1)–O(3)	60.86(6)
O(8)–K(1)–O(7)	61.31(6)
O(5)–K(1)–O(7)	143.21(7)
O(4)–K(1)–O(7)	112.34(7)
O(1)–K(1)–O(7)	77.50(6)
O(2)–K(1)–O(7)	73.67(6)
O(3)–K(1)–O(7)	102.07(7)
O(8)–K(1)–O(6)	84.73(7)
O(5)–K(1)–O(6)	58.27(6)
O(4)–K(1)–O(6)	120.27(7)
O(1)–K(1)–O(6)	52.69(6)
O(2)–K(1)–O(6)	105.94(6)
O(3)–K(1)–O(6)	136.90(7)
O(7)–K(1)–O(6)	113.47(7)
O(8)–K(1)–C(63)	78.14(7)
O(5)–K(1)–C(63)	99.24(7)
O(4)–K(1)–C(63)	156.90(7)
O(1)–K(1)–C(63)	23.15(6)
O(2)–K(1)–C(63)	80.74(7)
O(3)–K(1)–C(63)	140.41(7)
O(7)–K(1)–C(63)	73.73(7)
O(6)–K(1)–C(63)	42.62(6)
O(8)–K(1)–C(68)	71.89(7)
O(5)–K(1)–C(68)	75.81(7)
O(4)–K(1)–C(68)	134.53(7)

Table 5: (continued)

O(1)–K(1)–C(68)	41.95(6)
O(2)–K(1)–C(68)	101.14(7)
O(3)–K(1)–C(68)	152.67(7)
O(7)–K(1)–C(68)	90.92(7)
O(6)–K(1)–C(68)	22.57(6)
C(63)–K(1)–C(68)	23.65(7)
O(8)–K(1)–C(81)	22.23(7)
O(5)–K(1)–C(81)	101.29(7)
O(4)–K(1)–C(81)	104.10(7)
O(1)–K(1)–C(81)	83.01(7)
O(2)–K(1)–C(81)	112.33(7)
O(3)–K(1)–C(81)	137.15(7)
O(7)–K(1)–C(81)	42.63(7)
O(6)–K(1)–C(81)	85.82(7)
C(63)–K(1)–C(81)	64.40(7)
C(68)–K(1)–C(81)	66.81(7)
O(8)–K(1)–C(73)	114.46(8)
O(5)–K(1)–C(73)	96.56(8)
O(4)–K(1)–C(73)	41.98(7)
O(1)–K(1)–C(73)	139.05(7)
O(2)–K(1)–C(73)	80.45(7)
O(3)–K(1)–C(73)	22.41(7)
O(7)–K(1)–C(73)	99.33(8)
O(6)–K(1)–C(73)	147.12(8)
C(63)–K(1)–C(73)	161.12(8)
C(68)–K(1)–C(73)	169.63(8)
C(81)–K(1)–C(73)	122.28(8)
C(63)–O(1)–C(69)	118.2(2)
C(63)–O(1)–K(1)	104.28(15)
C(69)–O(1)–K(1)	115.02(16)
C(71)–O(2)–C(70)	113.8(2)
C(71)–O(2)–K(1)	115.85(18)
C(70)–O(2)–K(1)	117.72(17)
C(72)–O(3)–C(73)	112.0(3)
C(72)–O(3)–K(1)	110.80(18)
C(73)–O(3)–K(1)	109.26(18)
C(74)–O(4)–C(75)	113.2(2)
C(74)–O(4)–K(1)	114.62(18)
C(75)–O(4)–K(1)	112.60(17)
C(76)–O(5)–C(77)	113.0(2)
C(76)–O(5)–K(1)	114.68(18)
C(77)–O(5)–K(1)	115.45(17)
C(68)–O(6)–C(78)	118.4(2)
C(68)–O(6)–K(1)	102.29(16)
C(78)–O(6)–K(1)	115.70(17)
C(79)–O(7)–C(80)	110.7(2)
C(79)–O(7)–K(1)	119.08(19)
C(80)–O(7)–K(1)	115.34(17)
C(82)–O(8)–C(81)	111.6(2)
C(82)–O(8)–K(1)	120.52(18)
C(81)–O(8)–K(1)	111.30(17)
C(1)–N(1)–C(6)	119.4(2)
C(1)–N(1)–Ga(1)	121.57(18)

Table 5: (continued)

C(6)–N(1)–Ga(1)	118.78(17)
C(3)–N(2)–C(18)	118.3(2)
C(3)–N(2)–Ga(1)	121.80(18)
C(18)–N(2)–Ga(1)	119.85(17)
C(30)–N(3)–C(35)	118.1(2)
C(30)–N(3)–Ga(2)	122.3(2)
C(35)–N(3)–Ga(2)	119.67(17)
C(32)–N(4)–C(47)	118.8(2)
C(32)–N(4)–Ga(2)	122.3(2)
C(47)–N(4)–Ga(2)	118.50(17)
C(59)–N(5)–C(60)	110.7(2)
C(59)–N(5)–Ga(1)	123.1(2)
C(60)–N(5)–Ga(1)	125.0(2)
C(61)–N(6)–C(62)	111.2(2)
C(61)–N(6)–Ga(2)	122.85(19)
C(62)–N(6)–Ga(2)	123.63(19)
N(1)–C(1)–C(2)	124.1(2)
N(1)–C(1)–C(4)	119.2(2)
C(2)–C(1)–C(4)	116.6(2)
C(1)–C(2)–C(3)	127.6(2)
N(2)–C(3)–C(2)	123.5(3)
N(2)–C(3)–C(5)	119.7(2)
C(2)–C(3)–C(5)	116.7(2)
C(7)–C(6)–C(11)	121.4(3)
C(7)–C(6)–N(1)	121.0(3)
C(11)–C(6)–N(1)	117.6(2)
C(8)–C(7)–C(6)	118.0(3)
C(8)–C(7)–C(12)	119.5(3)
C(6)–C(7)–C(12)	122.5(3)
C(9)–C(8)–C(7)	121.4(3)
C(8)–C(9)–C(10)	119.7(3)
C(9)–C(10)–C(11)	121.4(3)
C(10)–C(11)–C(6)	118.0(3)
C(10)–C(11)–C(15)	121.1(3)
C(6)–C(11)–C(15)	120.9(2)
C(7)–C(12)–C(14)	109.8(3)
C(7)–C(12)–C(13)	112.4(3)
C(14)–C(12)–C(13)	109.3(3)
C(11)–C(15)–C(16)	112.9(2)
C(11)–C(15)–C(17)	112.0(2)
C(16)–C(15)–C(17)	110.4(3)
C(23)–C(18)–C(19)	120.4(2)
C(23)–C(18)–N(2)	119.9(2)
C(19)–C(18)–N(2)	119.6(2)
C(20)–C(19)–C(18)	118.4(3)
C(20)–C(19)–C(24)	118.2(2)
C(18)–C(19)–C(24)	123.4(2)
C(21)–C(20)–C(19)	121.8(3)
C(20)–C(21)–C(22)	119.3(3)
C(21)–C(22)–C(23)	121.6(3)
C(22)–C(23)–C(18)	118.5(2)
C(22)–C(23)–C(27)	118.2(2)
C(18)–C(23)–C(27)	123.2(2)

Table 5: (continued)

C(19)–C(24)–C(26)	110.8(3)
C(19)–C(24)–C(25)	111.1(3)
C(26)–C(24)–C(25)	110.5(3)
C(29)–C(27)–C(23)	110.6(2)
C(29)–C(27)–C(28)	108.6(2)
C(23)–C(27)–C(28)	112.4(2)
N(3)–C(30)–C(31)	123.4(3)
N(3)–C(30)–C(33)	120.5(3)
C(31)–C(30)–C(33)	116.1(3)
C(32)–C(31)–C(30)	128.9(3)
N(4)–C(32)–C(31)	123.4(3)
N(4)–C(32)–C(34)	120.4(3)
C(31)–C(32)–C(34)	116.2(3)
C(36)–C(35)–C(40)	120.2(3)
C(36)–C(35)–N(3)	121.0(3)
C(40)–C(35)–N(3)	118.9(3)
C(37)–C(36)–C(35)	118.8(3)
C(37)–C(36)–C(41)	119.3(3)
C(35)–C(36)–C(41)	121.9(3)
C(38)–C(37)–C(36)	121.4(3)
C(39)–C(38)–C(37)	119.6(3)
C(38)–C(39)–C(40)	121.5(3)
C(39)–C(40)–C(35)	118.5(3)
C(39)–C(40)–C(44)	118.7(3)
C(35)–C(40)–C(44)	122.8(3)
C(43)–C(41)–C(36)	113.2(3)
C(43)–C(41)–C(42)	109.8(3)
C(36)–C(41)–C(42)	110.3(3)
C(40)–C(44)–C(46)	110.4(3)
C(40)–C(44)–C(45)	112.8(3)
C(46)–C(44)–C(45)	109.2(3)
C(52)–C(47)–C(48)	121.1(3)
C(52)–C(47)–N(4)	117.5(3)
C(48)–C(47)–N(4)	121.3(3)
C(49)–C(48)–C(47)	118.0(3)
C(49)–C(48)–C(53)	119.4(3)
C(47)–C(48)–C(53)	122.5(3)
C(50)–C(49)–C(48)	121.8(3)
C(49)–C(50)–C(51)	119.2(3)
C(50)–C(51)–C(52)	121.6(3)
C(51)–C(52)–C(47)	118.2(3)
C(51)–C(52)–C(56)	121.1(3)
C(47)–C(52)–C(56)	120.7(3)
C(48)–C(53)–C(55)	110.5(2)
C(48)–C(53)–C(54)	112.8(3)
C(55)–C(53)–C(54)	109.8(3)
C(52)–C(56)–C(57)	111.5(3)
C(52)–C(56)–C(58)	112.8(3)
C(57)–C(56)–C(58)	110.3(3)
O(1)–C(63)–C(64)	125.5(3)
O(1)–C(63)–C(68)	114.3(3)
C(64)–C(63)–C(68)	120.2(3)
O(1)–C(63)–K(1)	52.57(13)

Table 5: (continued)

C(64)–C(63)–K(1)	134.0(2)
C(68)–C(63)–K(1)	82.36(17)
C(63)–C(64)–C(65)	119.8(3)
C(66)–C(65)–C(64)	120.0(3)
C(65)–C(66)–C(67)	120.7(3)
C(68)–C(67)–C(66)	119.5(3)
O(6)–C(68)–C(67)	126.3(3)
O(6)–C(68)–C(63)	114.0(3)
C(67)–C(68)–C(63)	119.7(3)
O(6)–C(68)–K(1)	55.15(13)
C(67)–C(68)–K(1)	141.2(2)
C(63)–C(68)–K(1)	73.99(16)
O(1)–C(69)–C(70)	106.0(2)
O(2)–C(70)–C(69)	107.4(2)
O(2)–C(71)–C(72)	108.2(3)
O(3)–C(72)–C(71)	109.2(3)
O(3)–C(73)–C(74)	108.8(3)
O(3)–C(73)–K(1)	48.33(14)
C(74)–C(73)–K(1)	80.29(18)
O(4)–C(74)–C(73)	108.2(3)
O(4)–C(75)–C(76)	112.2(3)
O(5)–C(76)–C(75)	107.0(2)
O(5)–C(77)–C(78)	106.8(2)
O(6)–C(78)–C(77)	107.3(2)
O(7)–C(80)–C(81)	109.6(2)
O(8)–C(81)–C(80)	108.4(3)
O(8)–C(81)–K(1)	46.47(13)
C(80)–C(81)–K(1)	82.65(17)
C21–O11–C11	109.0(7)
C31–O21–C41	110.1(6)
O11–C21–C31	107.1(7)
O21–C31–C21	109.3(6)
C12–C22–C32	112.8(5)
C22–C32–C32#1	114.4(6)

#1 -x,-y,-z+1

Crystal structure of mw_022_16m_sq

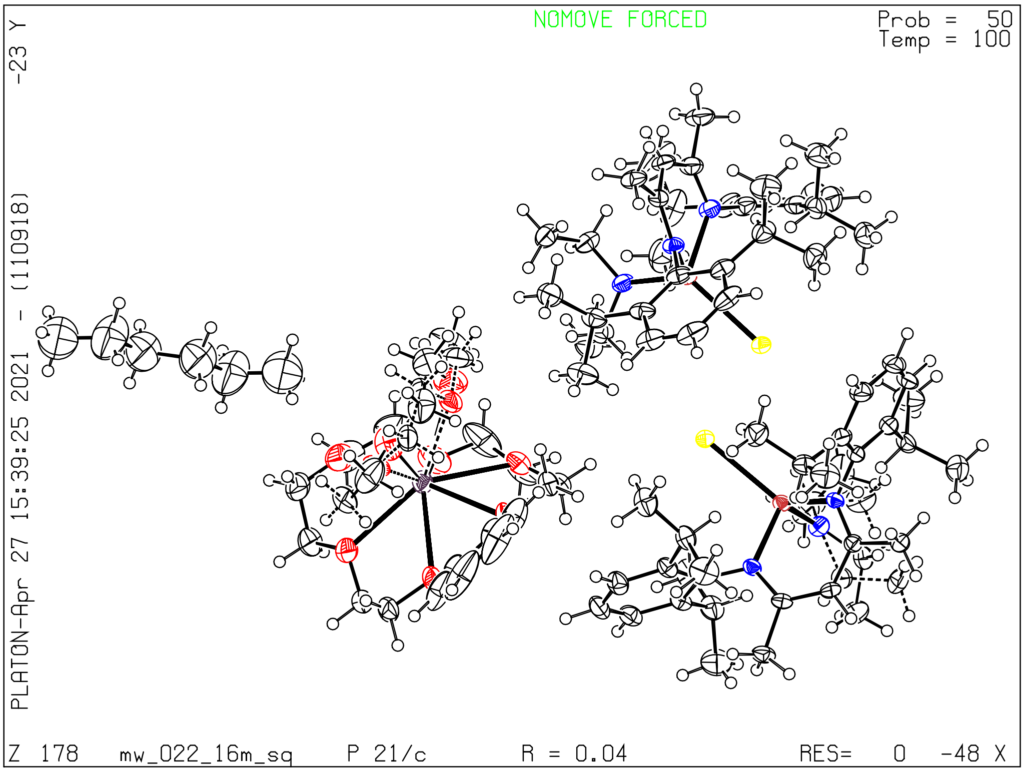

Table 1: Crystal data and structure refinement for mw_022_16m_sq.

Identification code	mw_022_16m_sq
Empirical Formula	$C_{89}\,H_{143}\,Bi_2\,Ga_2\,K\,N_6\,O_8$
Formula weight	2021.59 Da
Density (calculated)	$1.273\,\mathrm{g\cdot cm^{-3}}$
$F(000)$	4120
Temperature	100(2) K
Crystal size	$0.376 \times 0.104 \times 0.070$ mm
Crystal appearance	brownish orange needle
Wavelength (MoK_α)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 19.493(2)$ Å
	$b = 17.962(2)$ Å
	$c = 30.744(4)$ Å
	$\alpha = 90°$
	$\beta = 101.573(5)°$
	$\gamma = 90°$
Unit cell volume	10546(2) $Å^3$
Z	4
Cell measurement refections used	9450
θ range for cell measurement	2.38° to 24.76°
Diffractometer used for measurement	Bruker D8 KAPPA II (APEX II detector)
Diffractometer control software	BRUKER APEX3(v2019.1-0)
Measurement method	Data collection strategy APEX 3/QUEEN
θ range for data collection	1.320° to 30.508°
Completeness to $\theta = 25.242°$ (to θ_{max})	99.9% (100.0%)
Index ranges	$-27 \leq h \leq 27$
	$-25 \leq k \leq 25$
	$-43 \leq l \leq 43$
Computing data reduction	BRUKER APEX3(v2019.1-0)
Absorption correction	Semi-empirical from equivalents
Absorption coefficient	$3.920\,\mathrm{mm^{-1}}$
Absorption correction computing	SADABS
Max./min. transmission	0.75/0.49
R_{merg} before/after correction	0.0869/0.0636
Computing structure solution	BRUKER APEX3(v2019.1-0)
Computing structure refinement	SHELXL-2017/1 (Sheldrick, 2017)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	338181
Independent reflections	32182 ($R_{int} = 0.1112$)
Reflections with $I > 2\sigma(I)$	21665
Data / retraints / parameter	32182 / 113 / 1091
Goodness-of-fit on F^2	1.023
Weighting details	$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 20.5495P]$
	where $P = (F_o^2 + 2F_c^2)/3$
R indices $[I > 2\sigma(I)]$	$R1 = 0.0433$
	$wR2 = 0.0851$
R indices [all data]	$R1 = 0.0838$
	$wR2 = 0.0985$
Largest diff. peak and hole	4.127 and -1.746 $Å^{-3}$

Comments

Treatment of hydrogen atoms

Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent U_{ij} of the corresponding carbon atom.

Disorder

Two ethyl groups are disordered over two positions. Their corresponding bond lengths and angle were restrained to be equal (`SADI`) and `RIGU` restraints were applied to their anisotropic displacememnt parameters. Due to their close proximity C65 and C65' were refined with common displacement parameters (`EADP`). The dimethoxy ethane ligand is disordered over two positions. All corresponding bond length and angle were restrained to be equal (`SADI`). The anisotropic displacement parameters of its atoms were refined with `RIGU` restraints.

SQUEEZE

Two highly disordered solvent molecules (either n-hexane or dimethoxy ethane or a mixture of both, exact occupancy unknown) could not be modelled sufficiently. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run. (For details see: A. L. Spek, *Acta Cryst. A46* **(1990)**, 194–201). Since the nature and exact amount of the solvent is not clear it was not included in the sum formula.

Table 2: Atom coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$) for mw_022_16m_sq. U_eq is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	x	y	z	U_{eq}
Bi11	2200(1)	2280(1)	3437(1)	29(1)
Bi21	2830(1)	3352(1)	2917(1)	27(1)
Ga11	3333(1)	1810(1)	4029(1)	24(1)
Ga21	1671(1)	3768(1)	2345(1)	21(1)
N11	3322(2)	2256(2)	4644(1)	27(1)
N21	3241(2)	756(2)	4257(1)	30(1)
N31	769(2)	4080(2)	2525(1)	23(1)
N41	1858(2)	4826(2)	2161(1)	23(1)
N51	4285(2)	1825(2)	3982(1)	32(1)
N61	1334(2)	3283(2)	1793(1)	29(1)
C11	3589(2)	1878(2)	5012(1)	29(1)
C21	3714(2)	1107(2)	5018(1)	33(1)
C31	3494(2)	578(2)	4681(2)	36(1)
C41	3780(3)	2265(3)	5457(1)	38(1)
C51	3559(3)	−232(3)	4826(2)	49(1)
C61	3040(2)	2996(2)	4686(1)	31(1)
C71	3417(2)	3640(2)	4619(1)	33(1)
C81	3105(3)	4334(3)	4648(2)	45(1)
C91	2456(3)	4402(3)	4749(2)	48(1)
C101	2089(3)	3773(3)	4815(2)	45(1)
C111	2361(2)	3055(3)	4776(1)	36(1)
C121	4154(3)	3603(3)	4535(2)	39(1)
C131	4688(3)	3831(3)	4952(2)	50(1)
C141	4254(3)	4097(3)	4141(2)	52(1)
C151	1918(2)	2380(3)	4840(1)	39(1)
C161	1841(3)	2283(4)	5324(2)	62(2)
C171	1196(2)	2411(3)	4543(2)	48(1)
C181	2923(2)	169(2)	3960(1)	35(1)
C191	3322(3)	−286(3)	3734(2)	43(1)
C201	2983(3)	−861(3)	3465(2)	54(1)
C211	2282(3)	−986(3)	3426(2)	56(2)
C221	1889(3)	−529(3)	3638(2)	48(1)
C231	2194(3)	69(2)	3904(1)	37(1)
C241	4105(3)	−190(3)	3771(2)	63(2)
C251	4519(4)	−906(5)	3948(3)	101(3)
C261	4281(3)	27(4)	3326(2)	72(2)
C271	1738(2)	565(3)	4134(2)	41(1)
C281	1687(3)	265(4)	4592(2)	62(2)
C291	1010(3)	684(3)	3849(2)	47(1)
C301	390(2)	4635(2)	2306(1)	24(1)
C311	636(2)	5133(2)	2023(1)	25(1)
C321	1328(2)	5265(2)	1982(1)	24(1)
C331	−351(2)	4769(2)	2370(1)	30(1)
C341	1460(2)	5954(2)	1724(2)	33(1)
C351	503(2)	3717(2)	2880(1)	27(1)
C361	214(2)	3002(2)	2820(2)	34(1)
C371	−31(2)	2672(3)	3172(2)	43(1)
C381	9(2)	3040(3)	3571(2)	47(1)
C391	298(2)	3743(3)	3630(2)	41(1)
C401	553(2)	4091(3)	3287(1)	33(1)

Table 2: (continued)

	x	y	z	U_{eq}
C411	133(2)	2589(2)	2386(2)	37(1)
C421	−606(3)	2683(3)	2106(2)	52(1)
C431	303(3)	1751(3)	2456(2)	60(2)
C441	889(2)	4859(3)	3383(1)	37(1)
C451	405(3)	5419(3)	3552(2)	52(1)
C461	1566(3)	4775(3)	3727(2)	50(1)
C471	2561(2)	5101(2)	2187(1)	25(1)
C481	2930(2)	4949(2)	1847(1)	30(1)
C491	3583(2)	5284(2)	1875(2)	36(1)
C501	3872(2)	5734(2)	2227(2)	40(1)
C511	3520(2)	5837(2)	2568(2)	37(1)
C521	2870(2)	5517(2)	2561(1)	29(1)
C531	2667(3)	4419(3)	1472(2)	40(1)
C541	2584(3)	4775(4)	1011(2)	62(2)
C551	3162(3)	3738(3)	1507(2)	54(1)
C561	2511(2)	5608(2)	2959(1)	34(1)
C571	2061(3)	6304(3)	2930(2)	51(1)
C581	3038(3)	5604(3)	3397(2)	46(1)
C591	4509(2)	2325(2)	3666(2)	35(1)
C601	4860(3)	1957(3)	3323(2)	50(1)
C611	4858(2)	1475(3)	4294(2)	40(1)
C621	5275(3)	1975(3)	4654(2)	51(1)
C631	676(4)	3453(4)	1493(2)	32(2)
C641	741(4)	3922(5)	1091(2)	47(2)
C63'1	955(7)	3677(8)	1381(5)	35(4)
C64'1	154(6)	3599(9)	1285(5)	45(4)
C651	1710(15)	2689(11)	1655(9)	42(2)
C661	1396(7)	1919(5)	1672(8)	86(5)
C65'1	1640(30)	2570(30)	1672(19)	42(2)
C66'1	1101(14)	2031(10)	1421(7)	47(5)
K12	6668(1)	4543(1)	3147(1)	36(1)
O12	6203(2)	5974(2)	2759(1)	42(1)
O22	7583(2)	5491(2)	2872(1)	51(1)
O32	8021(2)	4045(2)	3203(1)	59(1)
O42	6902(2)	3242(2)	2706(2)	64(1)
O52	5549(2)	3581(2)	2819(1)	51(1)
O62	5330(2)	5047(2)	2973(1)	45(1)
C12	5765(3)	6264(3)	3020(2)	49(1)
C22	5312(3)	5747(3)	3154(2)	49(1)
C32	4898(3)	5951(5)	3448(2)	74(2)
C42	4915(4)	6687(6)	3592(3)	104(3)
C52	5334(4)	7199(5)	3453(3)	102(3)
C62	5766(3)	6989(3)	3162(2)	76(2)
C72	6746(3)	6443(3)	2662(2)	62(2)
C82	7279(3)	5974(4)	2515(2)	63(2)
C92	8221(3)	5164(4)	2810(2)	62(2)
C102	8478(3)	4657(4)	3200(2)	61(2)
C112	8122(4)	3475(4)	2902(2)	80(2)
C122	7554(4)	2900(4)	2897(3)	90(2)
C132	6351(4)	2703(3)	2634(3)	89(2)
C142	5682(4)	3089(3)	2479(2)	74(2)
C152	4873(3)	3889(3)	2720(2)	57(2)

Table 2: (continued)

	x	y	z	U_{eq}
C162	4833(3)	4478(3)	3045(2)	52(1)
O23	6221(5)	4212(6)	3922(2)	45(3)
O13	6975(5)	5529(5)	3887(3)	40(2)
C13	7250(7)	6256(6)	3887(4)	43(3)
C23	6487(5)	5464(7)	4175(4)	44(3)
C33	6478(11)	4636(9)	4314(4)	42(4)
C43	6308(11)	3438(7)	4024(5)	67(5)
C14	6947(7)	5947(7)	4001(4)	70(4)
O24	6369(6)	3678(6)	3867(3)	71(3)
C24	6426(10)	4862(8)	4227(4)	69(5)
O14	6874(5)	5158(6)	3955(3)	65(3)
C34	6557(7)	4019(8)	4280(3)	77(4)
C44	6587(9)	2907(7)	3892(5)	103(5)
C15	8578(5)	4422(7)	4442(3)	152(5)
C25	9291(5)	4568(7)	4530(3)	125(4)
C35	9604(4)	4989(6)	4940(3)	112(3)

Table 3: Anisotropic displacement parameters ($\times 10^3$) for mw_022_16m_sq.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi11	27(1)	35(1)	23(1)	8(1)	3(1)	0(1)
Bi21	25(1)	22(1)	33(1)	5(1)	3(1)	1(1)
Ga11	29(1)	23(1)	19(1)	2(1)	3(1)	2(1)
Ga21	24(1)	16(1)	25(1)	2(1)	6(1)	1(1)
N11	36(2)	26(2)	18(2)	2(1)	3(1)	−1(1)
N21	36(2)	25(2)	27(2)	1(1)	−1(2)	1(2)
N31	23(2)	19(2)	28(2)	6(1)	6(1)	−1(1)
N41	25(2)	17(1)	28(2)	2(1)	6(1)	−1(1)
N51	30(2)	36(2)	30(2)	9(2)	5(2)	8(2)
N61	33(2)	23(2)	31(2)	−3(1)	3(2)	2(1)
C11	31(2)	34(2)	23(2)	5(2)	5(2)	−4(2)
C21	43(2)	29(2)	22(2)	7(2)	−3(2)	2(2)
C31	45(3)	28(2)	32(2)	7(2)	1(2)	−2(2)
C41	52(3)	37(2)	21(2)	2(2)	1(2)	2(2)
C51	72(4)	30(2)	38(3)	10(2)	−6(2)	−1(2)
C61	44(2)	28(2)	18(2)	−1(2)	2(2)	6(2)
C71	55(3)	25(2)	18(2)	−1(2)	3(2)	−2(2)
C81	68(3)	28(2)	32(2)	−4(2)	−4(2)	4(2)
C91	72(4)	32(2)	33(3)	−7(2)	−7(2)	16(2)
C101	49(3)	55(3)	26(2)	−4(2)	−3(2)	19(2)
C111	43(3)	41(2)	22(2)	0(2)	3(2)	7(2)
C121	53(3)	30(2)	32(2)	1(2)	8(2)	−6(2)
C131	59(3)	49(3)	38(3)	1(2)	2(2)	−14(3)
C141	82(4)	36(3)	38(3)	1(2)	15(3)	−11(3)
C151	39(2)	52(3)	26(2)	1(2)	7(2)	5(2)
C161	72(4)	84(4)	33(3)	11(3)	14(3)	−1(3)
C171	36(3)	70(4)	39(3)	0(3)	10(2)	2(2)
C181	45(3)	24(2)	31(2)	2(2)	−4(2)	0(2)
C191	49(3)	32(2)	40(3)	−7(2)	−11(2)	11(2)
C201	62(4)	38(3)	52(3)	−16(2)	−9(3)	10(2)
C211	65(4)	33(3)	61(4)	−13(3)	−8(3)	−7(3)
C221	51(3)	39(3)	48(3)	−3(2)	−4(2)	−9(2)
C231	49(3)	28(2)	31(2)	6(2)	−2(2)	−4(2)
C241	48(3)	58(3)	74(4)	−36(3)	−6(3)	16(3)
C251	79(5)	132(7)	82(5)	−10(5)	−12(4)	56(5)
C261	50(3)	59(4)	103(6)	−5(4)	6(3)	7(3)
C271	42(3)	45(3)	33(2)	0(2)	3(2)	−14(2)
C281	76(4)	70(4)	41(3)	7(3)	14(3)	−17(3)
C291	45(3)	49(3)	47(3)	−3(2)	8(2)	−11(2)
C301	25(2)	22(2)	24(2)	0(2)	3(2)	0(2)
C311	29(2)	20(2)	25(2)	5(2)	4(2)	7(2)
C321	33(2)	18(2)	24(2)	4(2)	9(2)	3(2)
C331	25(2)	30(2)	36(2)	6(2)	6(2)	3(2)
C341	38(2)	24(2)	39(2)	11(2)	14(2)	8(2)
C351	23(2)	27(2)	32(2)	9(2)	6(2)	−1(2)
C361	24(2)	33(2)	44(3)	13(2)	5(2)	2(2)
C371	32(2)	39(3)	58(3)	27(2)	12(2)	−1(2)
C381	33(2)	60(3)	51(3)	30(3)	17(2)	5(2)
C391	36(2)	53(3)	36(2)	15(2)	11(2)	6(2)
C401	27(2)	43(2)	30(2)	12(2)	7(2)	5(2)
C411	31(2)	24(2)	55(3)	9(2)	8(2)	−5(2)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C421	43(3)	51(3)	57(3)	−1(3)	0(2)	−8(2)
C431	74(4)	29(3)	77(4)	6(3)	14(3)	4(3)
C441	42(3)	44(3)	26(2)	4(2)	11(2)	−2(2)
C451	61(3)	53(3)	47(3)	−1(3)	23(3)	6(3)
C461	43(3)	67(4)	40(3)	4(3)	4(2)	−3(3)
C471	29(2)	14(2)	33(2)	7(2)	10(2)	3(2)
C481	35(2)	24(2)	33(2)	5(2)	12(2)	−1(2)
C491	37(2)	32(2)	43(3)	6(2)	18(2)	2(2)
C501	31(2)	31(2)	60(3)	7(2)	17(2)	−3(2)
C511	37(2)	24(2)	49(3)	−3(2)	9(2)	−4(2)
C521	32(2)	20(2)	36(2)	−2(2)	11(2)	−1(2)
C531	42(3)	50(3)	32(2)	−5(2)	17(2)	−4(2)
C541	71(4)	83(4)	35(3)	4(3)	19(3)	−5(3)
C551	63(3)	50(3)	55(3)	−23(3)	29(3)	−6(3)
C561	33(2)	31(2)	38(2)	−9(2)	11(2)	−5(2)
C571	59(3)	42(3)	55(3)	−9(2)	22(3)	10(2)
C581	47(3)	51(3)	41(3)	−17(2)	11(2)	−11(2)
C591	35(2)	34(2)	37(2)	3(2)	9(2)	6(2)
C601	51(3)	55(3)	50(3)	4(3)	25(3)	6(3)
C611	37(2)	46(3)	33(2)	6(2)	1(2)	12(2)
C621	41(3)	45(3)	57(3)	10(3)	−9(2)	0(2)
C631	34(4)	25(4)	36(4)	−9(3)	5(3)	−6(3)
C641	55(5)	55(5)	28(4)	−1(3)	2(3)	7(4)
C63'1	39(7)	30(7)	33(8)	−1(6)	0(6)	−9(6)
C64'1	35(7)	54(9)	40(8)	−1(7)	−7(6)	0(6)
C651	54(6)	24(6)	45(3)	−12(4)	1(4)	9(4)
C661	58(7)	22(4)	165(16)	−17(6)	−7(8)	7(4)
C65'1	54(6)	24(6)	45(3)	−12(4)	1(4)	9(4)
C66'1	68(13)	25(7)	47(11)	−11(7)	6(8)	9(7)
K12	30(1)	44(1)	36(1)	0(1)	11(1)	−2(1)
O12	33(2)	29(2)	64(2)	0(2)	7(2)	−7(1)
O22	32(2)	69(2)	54(2)	17(2)	10(2)	1(2)
O32	45(2)	77(3)	59(2)	14(2)	22(2)	19(2)
O42	81(3)	29(2)	87(3)	2(2)	31(2)	3(2)
O52	51(2)	41(2)	59(2)	11(2)	7(2)	−14(2)
O62	30(2)	51(2)	58(2)	−5(2)	17(2)	−10(2)
C12	36(3)	41(3)	60(3)	−15(2)	−11(2)	6(2)
C22	35(3)	64(3)	46(3)	−16(3)	1(2)	6(2)
C32	46(3)	121(6)	51(3)	−28(4)	1(3)	18(4)
C42	58(4)	154(9)	83(5)	−66(6)	−24(4)	46(5)
C52	77(5)	92(6)	109(6)	−75(5)	−49(5)	48(4)
C62	53(4)	51(3)	105(5)	−32(4)	−31(4)	15(3)
C72	38(3)	39(3)	102(5)	27(3)	−6(3)	−12(2)
C82	33(3)	79(4)	73(4)	37(3)	2(3)	−9(3)
C92	35(3)	95(5)	65(4)	17(3)	27(3)	2(3)
C102	34(3)	93(5)	59(4)	16(3)	14(3)	7(3)
C112	78(5)	91(5)	77(5)	8(4)	31(4)	45(4)
C122	109(6)	54(4)	115(6)	18(4)	37(5)	42(4)
C132	117(6)	30(3)	134(7)	−5(4)	61(6)	−12(4)
C142	105(6)	47(3)	77(5)	−17(3)	32(4)	−39(4)
C152	51(3)	49(3)	64(4)	21(3)	−6(3)	−22(3)
C162	29(2)	65(4)	62(3)	20(3)	11(2)	−7(2)

Table 3: (continued)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O23	51(5)	56(6)	29(4)	4(4)	7(3)	−21(4)
O13	62(6)	20(4)	41(5)	−3(4)	17(4)	−7(4)
C13	56(8)	23(5)	49(7)	−15(5)	10(6)	−16(5)
C23	32(5)	59(7)	39(6)	−3(5)	5(4)	−10(5)
C33	42(8)	62(8)	21(6)	8(5)	5(5)	−18(7)
C43	93(12)	57(8)	44(9)	21(7)	−2(9)	−25(8)
C14	71(9)	66(7)	62(8)	−26(7)	−17(6)	2(7)
O24	94(7)	75(7)	42(5)	7(4)	12(5)	−13(6)
C24	59(8)	113(10)	34(7)	−19(7)	9(6)	−12(9)
O14	69(5)	66(6)	60(5)	−25(5)	15(4)	−12(5)
C34	77(8)	111(10)	40(5)	5(6)	5(5)	−25(8)
C44	127(13)	71(8)	123(13)	13(8)	56(11)	−10(8)
C15	121(9)	249(15)	88(7)	26(8)	29(6)	−23(9)
C25	91(7)	220(12)	67(5)	−12(7)	19(5)	10(7)
C35	85(5)	167(9)	93(6)	10(6)	42(5)	13(6)

Table 4: Bond lengths [Å] for mw_022_16m_sq.

Bi11–Ga11	2.6992(5)
Bi11–Bi21	2.9266(3)
Bi21–Ga21	2.6759(5)
Ga11–N51	1.890(4)
Ga11–N21	2.040(3)
Ga11–N11	2.057(3)
Ga21–N61	1.902(3)
Ga21–N31	2.025(3)
Ga21–N41	2.036(3)
N11–C11	1.332(5)
N11–C61	1.455(5)
N21–C31	1.336(5)
N21–C181	1.449(5)
N31–C301	1.339(5)
N31–C351	1.455(5)
N41–C321	1.328(5)
N41–C471	1.443(5)
N51–C591	1.454(5)
N51–C611	1.461(5)
N61–C651	1.41(3)
N61–C631	1.455(8)
N61–C65'1	1.49(7)
N61–C63'1	1.509(15)
C11–C21	1.406(6)
C11–C41	1.515(6)
C21–C31	1.406(6)
C31–C51	1.520(6)
C61–C111	1.408(6)
C61–C71	1.408(6)
C71–C81	1.399(6)
C71–C121	1.509(7)
C81–C91	1.368(7)
C91–C101	1.373(7)
C101–C111	1.409(6)
C111–C151	1.524(7)
C121–C131	1.535(6)
C121–C141	1.546(6)
C151–C171	1.518(6)
C151–C161	1.534(6)
C181–C191	1.404(6)
C181–C231	1.409(6)
C191–C201	1.403(6)
C191–C241	1.517(7)
C201–C211	1.367(8)
C211–C221	1.373(8)
C221–C231	1.406(6)
C231–C271	1.527(7)
C241–C261	1.526(9)
C241–C251	1.558(9)
C271–C291	1.525(7)
C271–C281	1.529(7)
C301–C311	1.399(5)
C301–C331	1.513(5)

Table 4: (continued)

C311–C321	1.399(5)
C321–C341	1.520(5)
C351–C361	1.401(6)
C351–C401	1.404(6)
C361–C371	1.400(6)
C361–C411	1.507(7)
C371–C381	1.381(7)
C381–C391	1.380(7)
C391–C401	1.400(6)
C401–C441	1.531(6)
C411–C421	1.532(6)
C411–C431	1.547(6)
C441–C461	1.524(6)
C441–C451	1.539(7)
C471–C521	1.404(6)
C471–C481	1.410(5)
C481–C491	1.393(6)
C481–C531	1.504(6)
C491–C501	1.376(7)
C501–C511	1.377(6)
C511–C521	1.387(6)
C521–C561	1.534(6)
C531–C541	1.533(7)
C531–C551	1.547(7)
C561–C571	1.519(6)
C561–C581	1.521(6)
C591–C601	1.520(6)
C611–C621	1.528(7)
C631–C641	1.521(9)
C63'1–C64'1	1.535(13)
C651–C661	1.517(13)
C65'1–C66'1	1.529(17)
K12–O14	2.673(8)
K12–O62	2.710(3)
K12–O22	2.721(3)
K12–O32	2.757(4)
K12–O23	2.762(8)
K12–O42	2.784(4)
K12–O52	2.808(3)
K12–O13	2.851(10)
K12–O24	2.858(9)
K12–O12	2.902(3)
K12–C22	3.419(5)
K12–C24	3.494(11)
O12–C12	1.385(6)
O12–C72	1.431(6)
O22–C92	1.422(6)
O22–C82	1.432(6)
O32–C102	1.417(7)
O32–C112	1.418(7)
O42–C122	1.426(8)
O42–C132	1.430(7)
O52–C152	1.404(6)

Table 4: (continued)

O52–C142	1.430(7)
O62–C22	1.378(6)
O62–C162	1.456(6)
C12–C62	1.373(7)
C12–C22	1.400(8)
C22–C32	1.377(7)
C32–C42	1.391(11)
C42–C52	1.355(13)
C52–C62	1.397(11)
C72–C82	1.476(8)
C92–C102	1.509(8)
C112–C122	1.512(10)
C132–C142	1.469(10)
C152–C162	1.468(8)
O23–C33	1.427(13)
O23–C43	1.428(12)
O13–C13	1.412(10)
O13–C23	1.427(10)
C23–C33	1.548(18)
C14–O14	1.428(10)
O24–C34	1.393(10)
O24–C44	1.446(11)
C24–O14	1.429(12)
C24–C34	1.538(19)
C15–C25	1.387(11)
C25–C35	1.490(12)
C35–C35#1	1.515(15)

#1 -x+2,-y+1,-z+1

Table 5: Bond angles [°] for mw_022_16m_sq.

Ga11–Bi11–Bi21	101.438(13)
Ga21–Bi21–Bi11	98.732(12)
N51–Ga11–N21	101.27(15)
N51–Ga11–N11	104.86(15)
N21–Ga11–N11	91.56(13)
N51–Ga11–Bi11	128.83(10)
N21–Ga11–Bi11	113.92(10)
N11–Ga11–Bi11	109.83(9)
N61–Ga21–N31	101.93(14)
N61–Ga21–N41	103.29(14)
N31–Ga21–N41	91.76(12)
N61–Ga21–Bi21	123.58(10)
N31–Ga21–Bi21	124.21(9)
N41–Ga21–Bi21	105.56(9)
C11–N11–C61	118.7(3)
C11–N11–Ga11	120.5(3)
C61–N11–Ga11	120.8(2)
C31–N21–C181	117.9(3)
C31–N21–Ga11	121.1(3)
C181–N21–Ga11	121.0(3)
C301–N31–C351	117.7(3)
C301–N31–Ga21	119.5(2)
C351–N31–Ga21	122.8(2)
C321–N41–C471	118.1(3)
C321–N41–Ga21	120.1(2)
C471–N41–Ga21	121.6(2)
C591–N51–C611	114.4(4)
C591–N51–Ga11	119.4(3)
C611–N51–Ga11	125.2(3)
C651–N61–Ga21	120.6(9)
C631–N61–Ga21	125.0(3)
C65'1–N61–Ga21	122.0(18)
C63'1–N61–Ga21	123.9(6)
N11–C11–C21	123.4(4)
N11–C11–C41	121.1(4)
C21–C11–C41	115.5(4)
C11–C21–C31	129.0(4)
N21–C31–C21	123.7(4)
N21–C31–C51	120.4(4)
C21–C31–C51	115.9(4)
C111–C61–C71	120.4(4)
C111–C61–N11	118.2(4)
C71–C61–N11	121.3(4)
C81–C71–C61	118.4(4)
C81–C71–C121	119.4(4)
C61–C71–C121	122.2(4)
C91–C81–C71	121.9(5)
C81–C91–C101	119.6(5)
C91–C101–C111	121.6(5)
C61–C111–C101	118.0(4)
C61–C111–C151	123.0(4)
C101–C111–C151	118.9(4)
C71–C121–C131	110.9(4)

Table 5: (continued)

C71–C121–C141	112.4(4)
C131–C121–C141	109.2(4)
C171–C151–C111	111.9(4)
C171–C151–C161	109.2(4)
C111–C151–C161	112.7(4)
C191–C181–C231	120.6(4)
C191–C181–N21	121.8(4)
C231–C181–N21	117.6(4)
C201–C191–C181	118.6(5)
C201–C191–C241	118.4(5)
C181–C191–C241	123.0(4)
C211–C201–C191	121.2(5)
C201–C211–C221	120.1(5)
C211–C221–C231	121.5(5)
C221–C231–C181	117.8(5)
C221–C231–C271	119.8(4)
C181–C231–C271	122.4(4)
C191–C241–C261	111.5(5)
C191–C241–C251	112.0(6)
C261–C241–C251	109.3(5)
C291–C271–C231	112.2(4)
C291–C271–C281	110.6(4)
C231–C271–C281	111.8(4)
N31–C301–C311	124.3(3)
N31–C301–C331	119.9(3)
C311–C301–C331	115.7(3)
C321–C311–C301	128.4(4)
N41–C321–C311	123.1(3)
N41–C321–C341	120.0(3)
C311–C321–C341	116.9(3)
C361–C351–C401	120.7(4)
C361–C351–N31	120.4(4)
C401–C351–N31	118.9(3)
C371–C361–C351	118.5(4)
C371–C361–C411	119.1(4)
C351–C361–C411	122.4(4)
C381–C371–C361	121.1(4)
C391–C381–C371	120.2(4)
C381–C391–C401	120.4(5)
C391–C401–C351	119.1(4)
C391–C401–C441	117.3(4)
C351–C401–C441	123.6(4)
C361–C411–C421	111.3(4)
C361–C411–C431	112.0(4)
C421–C411–C431	109.6(4)
C461–C441–C401	108.8(4)
C461–C441–C451	109.5(4)
C401–C441–C451	112.7(4)
C521–C471–C481	120.8(4)
C521–C471–N41	118.2(3)
C481–C471–N41	121.0(4)
C491–C481–C471	117.7(4)
C491–C481–C531	119.3(4)

Table 5: (continued)

C471–C481–C531	122.9(4)
C501–C491–C481	121.9(4)
C491–C501–C511	119.2(4)
C501–C511–C521	121.8(4)
C511–C521–C471	118.2(4)
C511–C521–C561	120.3(4)
C471–C521–C561	121.5(4)
C481–C531–C541	113.5(4)
C481–C531–C551	109.5(4)
C541–C531–C551	110.0(4)
C571–C561–C581	109.7(4)
C571–C561–C521	113.0(4)
C581–C561–C521	111.8(4)
N51–C591–C601	115.7(4)
N51–C611–C621	116.6(4)
N61–C631–C641	115.2(6)
N61–C63'1–C64'1	115.3(12)
N61–C651–C661	116(2)
N61–C65'1–C66'1	113(4)
O14–K12–O62	90.3(2)
O14–K12–O22	92.5(2)
O62–K12–O22	113.23(11)
O14–K12–O32	96.5(2)
O62–K12–O32	172.27(11)
O22–K12–O32	62.86(11)
O62–K12–O23	77.6(2)
O22–K12–O23	137.99(19)
O32–K12–O23	109.9(2)
O14–K12–O42	142.2(3)
O62–K12–O42	115.41(12)
O22–K12–O42	101.08(12)
O32–K12–O42	60.64(13)
O23–K12–O42	110.5(2)
O14–K12–O52	123.3(2)
O62–K12–O52	59.13(11)
O22–K12–O52	141.64(11)
O32–K12–O52	119.15(13)
O23–K12–O52	79.69(18)
O42–K12–O52	59.99(12)
O62–K12–O13	89.4(2)
O22–K12–O13	79.28(19)
O32–K12–O13	96.2(2)
O23–K12–O13	59.8(2)
O42–K12–O13	151.8(2)
O52–K12–O13	133.8(2)
O14–K12–O24	61.4(3)
O62–K12–O24	89.8(2)
O22–K12–O24	146.0(2)
O32–K12–O24	96.7(2)
O42–K12–O24	89.9(2)
O52–K12–O24	71.3(2)
O14–K12–O12	89.6(3)
O62–K12–O12	54.13(9)

Table 5: (continued)

O22–K12–O12	59.20(10)
O32–K12–O12	121.94(11)
O23–K12–O12	114.8(2)
O42–K12–O12	127.68(12)
O52–K12–O12	103.95(10)
O13–K12–O12	77.1(2)
O24–K12–O12	134.8(2)
O14–K12–C22	72.9(2)
O62–K12–C22	22.40(11)
O22–K12–C22	99.33(13)
O32–K12–C22	159.40(14)
O23–K12–C22	75.7(2)
O42–K12–C22	137.40(13)
O52–K12–C22	81.11(12)
O13–K12–C22	69.0(2)
O24–K12–C22	93.5(2)
O12–K12–C22	42.61(12)
O14–K12–C24	22.1(3)
O62–K12–C24	79.9(3)
O22–K12–C24	114.5(3)
O32–K12–C24	107.7(3)
O42–K12–C24	131.8(3)
O52–K12–C24	101.5(3)
O24–K12–C24	42.8(2)
O12–K12–C24	98.9(3)
C22–K12–C24	68.8(3)
C12–O12–C72	117.8(4)
C12–O12–K12	105.8(3)
C72–O12–K12	115.1(3)
C92–O22–C82	112.8(4)
C92–O22–K12	115.4(3)
C82–O22–K12	114.9(3)
C102–O32–C112	112.8(5)
C102–O32–K12	110.0(3)
C112–O32–K12	116.7(4)
C122–O42–C132	110.6(5)
C122–O42–K12	112.4(4)
C132–O42–K12	116.9(4)
C152–O52–C142	112.7(5)
C152–O52–K12	117.5(3)
C142–O52–K12	113.6(3)
C22–O62–C162	120.4(4)
C22–O62–K12	109.1(3)
C162–O62–K12	112.3(3)
C62–C12–O12	125.5(6)
C62–C12–C22	119.7(6)
O12–C12–C22	114.8(4)
C32–C22–O62	125.1(6)
C32–C22–C12	120.2(6)
O62–C22–C12	114.7(4)
C32–C22–K12	136.8(4)
O62–C22–K12	48.5(2)
C12–C22–K12	83.3(3)

Table 5: (continued)

C22–C32–C42	118.8(8)
C52–C42–C32	121.5(7)
C42–C52–C62	119.8(7)
C12–C62–C52	119.9(7)
O12–C72–C82	108.9(4)
O22–C82–C72	108.6(5)
O22–C92–C102	107.6(4)
O32–C102–C92	111.4(5)
O32–C102–K12	47.6(2)
C92–C102–K12	80.1(3)
O32–C112–C122	107.7(5)
O42–C122–C112	107.5(5)
O42–C132–C142	108.8(5)
O52–C142–C132	109.5(6)
O52–C152–C162	108.3(4)
O62–C162–C152	105.9(4)
O62–C162–K12	45.2(2)
C152–C162–K12	83.8(3)
C33–O23–C43	109.2(9)
C33–O23–K12	119.7(6)
C43–O23–K12	110.7(8)
C13–O13–C23	112.1(9)
C13–O13–K12	126.4(6)
C23–O13–K12	112.7(6)
O13–C23–C33	107.2(10)
O23–C33–C23	107.6(10)
O23–C43–K12	47.0(6)
C34–O24–C44	110.7(10)
C34–O24–K12	114.2(7)
C44–O24–K12	117.4(7)
O14–C24–C34	108.6(11)
O14–C24–K12	44.6(5)
C34–C24–K12	83.5(6)
C14–O14–C24	111.7(9)
C14–O14–K12	119.8(7)
C24–O14–K12	113.3(7)
O24–C34–C24	109.3(10)
C15–C25–C35	119.0(8)
C25–C35–C35#1	116.4(10)

#1 -x+2,-y+1,-z+1