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SHORT COMMUNICATION

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Direct Carboxylation of Zincocene Cp^*_2Zn**

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Keywords: Zinc / CO_2 activation / XRD

The reaction of zincocene Cp^*_2Zn with CO_2 proceeds with formation of $[Zn_4(\mu_4\text{-}O)(O_2CCp^*)_6]$ **1**, which was characterized by NMR (^1H, ^{13}C) and IR spectroscopy as well as elemental analysis and single crystal X-ray diffraction. The solid state structure of **1** is comparable to that previously observed of basic zinc acetate. In contrast to many previously reported CO_2 activation reactions, the formation of **1** occurred without the use of any additional transmetalation catalyst.

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Introduction

The effective utilization of CO_2 as C_1-feedstock in organic chemistry has received growing interest over the last decades since CO_2 is abundant, renewable, nontoxic and inexpensive.[1] Unfortunately, CO_2 is thermodynamically very stable and kinetically inert, thus limiting its use in industrial syntheses. Only highly nucleophilic reagents such as organolithium and Grignard reagents readily react with CO_2 with formation of carboxylic acids and their derivatives. However, the range of functional groups that are compatible to these reagents is somewhat limited. As a consequence, activation reactions of CO_2 via coordination to transition metal complexes, which lower the activation energy for further reactions, have been investigated in detail.[2] Recently, carboxylation reactions of organoboronic acids, organozinc and organotin reagents using CO_2 were found to be catalyzed by complexes containing late transition metals such as Pd, Rh, Ni and Pd, whose presence is essential for this purpose.[3]

Organozinc reagents RZnX (X = halide) and R_2Zn, which have been established as soft nucleophiles in various organic reactions in the past, are of particular interest, since they show a much higher tolerance toward functional groups compared to the stronger nucleophilic organolithium and -magnesium reagents. Unfortunately, only zinc hydrides, zinc alkoxides and zinc amides are known to react with CO_2 with insertion into the Zn-H, Zn-O and Zn-N bond and subsequent formation of zinc formates, zinc carbonates and zinc carbamates.[4] As a consequence, zinc amides, alkoxides and carboxylates are very actice *living single-site catalysts* for the ring-opening polymerization (ROMP) of lactide[5] and the epoxide/CO_2 copolymerization.[6] Moreover, bimetallic calcium/zinc complexes effectively catalyze the terpolymerization of epoxide, cyclic anhydrides and CO_2.[7] In remarkable contrast, insertion reactions into Zn-C bonds are less favored and typically require transition metal complexes of electron rich, late transition metals (Ni, Pd) as effective transmetalation catalyst.[8] In these carboxylation reactions, the presence of LiCl also plays a critical, yet not fully understood, role. In addition, nickel complexes such as $[Ni(\eta^2\text{-}CO(PCy_3)_2]$ were successfully used.[9] Very recently, *Kondo et al.* reported on carboxylation reactions of organozinc reagents using CO_2, in which the solvent (DMF) was found to have a crucial influence on the reaction.[10] To the best of our knowledge, this is the only report on a transition-metal-free carboxylation reaction of organozinc complexes, to date.

We started recently to investigate the activation of carbon dioxide as well as heterocumulenes such as isocyanates and carbodiimides using zinc hydride and zinc alkyl complexes.[11] Herein we report on the direct carboxylation reaction of zincocene Cp^*_2Zn with CO_2 in the absence of any transmetalation reagent. The resulting zinc oxocarboxylate $[Zn_4(\mu_4\text{-}O)(O_2CCp^*)_6]$ **1** contains a central $[Zn_4O]^{6+}$ tetrahedron, which is the characteristic structural motif in basic zinc acetate,[12] zinc carbonates and carbamates,[4] zinc phosphates and phosphonates[13] as well as in microporous metal organic frameworks (MOFs) such as MOF-5 and IRMOF-9.[14] Zinc oxocarboxylates, which are known for decades,[15] are typically prepared by solvothermal methods. Recently, Lewinski et al. reported on the synthesis of $[Zn_4(\mu_4\text{-}O)(O_2CPh)_6]$ via oxidation of the corresponding zinc carboxylate with dry oxygen,[16] whereas Redshaw et al. obtained an oxocarboxylate complex by reaction of $Zn(C_6F_5)_2$ with 3-dimethylaminobenzoic acid in the presence of trace amounts of water.[17]

Results and Discussion

Stirring a toluene solution of Cp^*_2Zn under an CO_2 atmosphere of 6 bar for 1 h at 70 °C yielded $[Zn_4(\mu_4\text{-}O)(O_2CCp^*)_6]$ **1** in about 30% yield, whereas lower yields (< 10%) were obtained under milder reaction conditions (50 °C, no CO_2 pressure, 4 h). The formation of **1** occurred with formation of Cp*H, that was unambiguously identified by *in situ* ^1H NMR spectroscopy. Cp*H is obviously formed due to partial hydrolysis/condensation reaction of Cp^*_2Zn as was previously described for the formation of zinc carbamates, which are typically synthesized by reaction of zinc alkyls, primary amines and water.[18] As a consequence, when Cp^*_2Zn was reacted with CO_2 in toluene that was not dried prior to use, **1** was obtained in higher yield of almost 80 %.

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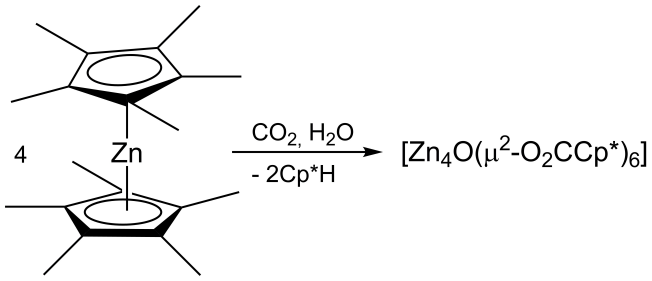

Scheme 1. Synthesis of [[$Zn_4(\mu_4$-O)($O_2CCp^*)_6$] **1**

The formation of **1** was *in situ* monitored by ^{1}H NMR spectroscopy, showing a continuously decreasing signal of the Zn-bonded Cp* group at 1.88 ppm (toluene) and steadily increasing new singlets at 1.22, 1.63 and 1.82 ppm with a relative intensity of 1:2:2, indicating the formation of a σ-bonded Cp* group. The ^{13}C NMR spectrum of **1** shows an additional signal at 184.9 ppm and the IR spectrum strong absorption bands at 1580 ($\nu(CO_2)_{as}$) and 1402 cm^{-1} ($\nu(CO_2)_s$), clearly indicating the formation of a μ^2-bonded carboxylate group. Comparable values have been reported for basic zinc pivalate (1594, 1424 cm^{-1}), benzoate (1562, 1410 cm^{-1}) and others, respectively.[19] Moreover, a very broad absorption band at 494 cm^{-1}, which most likely results from overlapping of several absorption bands, can be assigned to the asymmetric vibration of the central Zn_4O oxygen atom. Basic zinc carboxylates of the type [$Zn_4(\mu_4$-O)($O_2CR)_6$], R = Me, Et) typically show values near 530 cm^{-1} according to experimental findings and theoretical calculations.[20]

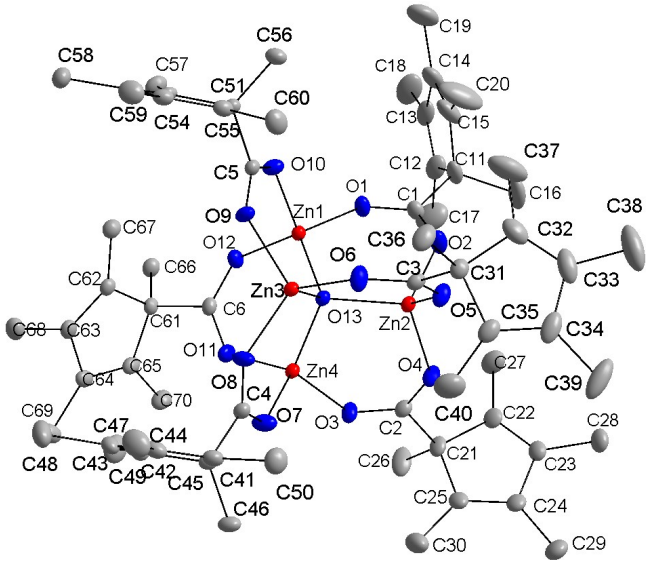

Figure 1. Molecular structure of the **1**. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Zn1-O1 1.9441(10), Zn1-O10 1.9622(10), Zn1-O12 1.9517(10), Zn1-O13 1.9458(10), C1-O1 1.2624(17), C1-O2 1.2587(18), C1-C11 1.523(2); Zn1-O13-Zn2 110.37(5), Zn1-O13-Zn3 110.48(5), Zn1-O13-Zn4 109.79(4), O1-Zn1-O10 107.75(5), O1-Zn1-O12 110.52(4), O1-Zn1-O13 110.86(4), O1-C1-O2 125.27(14).

Single crystals of **1** were obtained from a solution in toluene upon storage at -30 °C.[21] The structure of **1** shows an almost ideal T_d symmetry as was reported for basic zinc acetate.[12b] The central $[Zn_4O]^{6+}$ tetrahedron is also coordinated by six anionic Cp*CO_2 carboxylate units, which adopt μ^2-bridging positions on the edges of the $[Zn_4O]^{6+}$ tetrahedron.

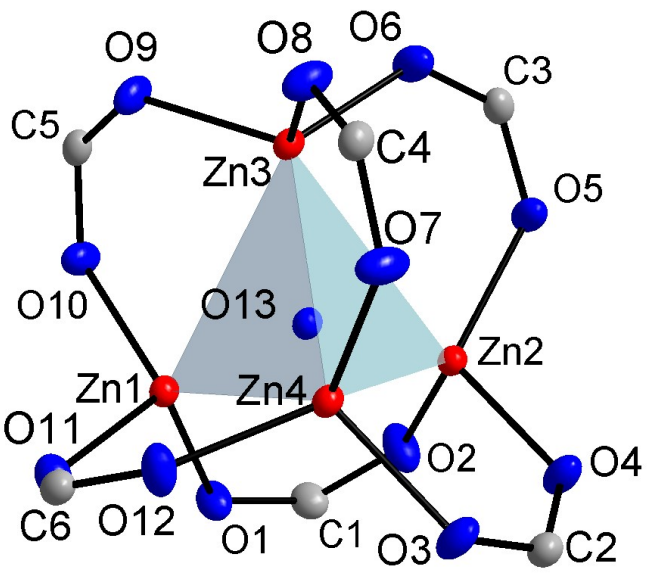

Figure 2. Projection of the tetrahedral $[Zn_4O]^{6+}$ core of **1** coordinated by six bridging carboxylate anions (Cp* groups are omitted for clarity).

The Zn atoms are also tetrahedrally coordinated by four oxygen atoms. The Zn-O distances to the central Zn_4O oxygen atom (1.9364(9) – 1.9458(10) Å) are almost identical to the Zn-O bonds of the bridging carboxylate groups (1.9271(10) – 1.9622(10) Å). The average C-O bond length of 1.26 Å clearly indicates delocalized π-electrons as was expected. The Zn-O-Zn (107.55(5) – 110.89(4)°) and O-C-O (125.20(14) – 125.43(13)°) bond angles are within the typical range previously reported for basic zinc carboxylates. Almost identical values were observed for [$Zn_4(\mu_4$-O)($O_2CMe)_6$], [$Zn_4(\mu_4$-O)($O_2CPh)_6$] and [$Zn_4(\mu_4$-O)($O_2CCMe_3)_6$], respectively.[12,19] The C-C_{Cp^*} bond lengths range from 1.520(2) to 1.5317(19) Å, which is comparable to C-C_{Cp^*} bond lengths reported very recently for the homoleptic zinc amidate complex [Zn{OC(Cp*)N*i*-Pr}$_2$]$_2$ (av. 1.54 Å).[11d]

Conclusions

In conclusion, we have reported for the first time on the direct carboxylation reaction of a Zn-C bond without the use of any transmetalation catalyst. The structure of as-formed **1** is typical for basic zinc carboxylates, consisting of a central $[Zn_4O]^{6+}$ tetrahedron, which is well known as structure-determining rigid SBU in microporous zinc-based metal organic frameworks (MOF's). The $[Zn_4O]^{6+}$ nodal regions within these materials, which are of particular interesting as novel hydrogen storage materials,[22] have been identified as the principal sites for the hydrogen gas adsorption.[23] The potential capability of **1** as molecular model for hydrogen adsorption, which seems to be generally possible according to previous findings by *Redshaw et al.*,[17] is currently under investigation. Moreover, the potential capability of **1** to serve as *single source precursor* for the solution-based and gas-phase based (MOCVD) formation of ZnO, which was shown for structurally related zinc oxocarboxylates and oxocarbamates in the past,[4e,24] will be studied in detail.

Experimental Section

All manipulations were performed under an Ar atmosphere. Cp*$_2$Zn was prepared according to literature methods.[25] ^{1}H, ^{13}C{^{1}H} NMR spectra were recorded on a Bruker DMX 300 spectrometer and are referenced to internal

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C_6D_5H (^1H: δ = 7.154; ^{13}C: δ = 128.0). IR spectra were recorded on an ALPHA-T FT-IR spectrometer equipped with a single reflection ATR sampling module. Melting points were measured in sealed capillaries and were not corrected. Elemental analyses were performed at the *Elementaranalyse Labor* of the University of Essen.

$[Zn_4(\mu_4\text{-}O)(O_2CCp^*)_6]$ **1**: 0.34 g Cp^*_2Zn (1 mmol) was dissolved in 15 ml wet toluene and stirred for 1 h at 70 °C under an CO_2 atmosphere of 6 bar in a glass autoclave. Colorless crystals of **1** were formed within 24 h after storage at -30 °C.

Yield: 0.28 g (78 %). Melting point: > 220 °C. Anal. Found (calcd) for $C_{66}H_{90}O_{13}Zn_4{*}C_7H_8$ (1444.99 g/mol): H 6.8 (6.7), C 58.6 (58.6). ^1H NMR (300 MHz, C_6D_6, 25 °C): δ = 1.22 (s, 3H, C_5Me_5), 1.63 (s, 6H, C_5Me_5), 1.82 (s, 6H, C_5Me_5). $^{13}C\{^1H\}$ NMR (125 MHz, C_6D_6, 25 °C): δ = 10.5 (C_5Me_5), 11.2 (C_5Me_5), 19.2 (C_5Me_5), 66.2 (C_5Me_5), 136.3 (C_5Me_5), 136.6 (C_5Me_5), 184.9 (CO_2). IR: ν 2968, 2911, 2854, 1580, 1441, 1402, 1383, 1356, 1327, 1292, 1260, 1110, 1062, 1018, 842, 809, 725, 696, 643, 626, 494, 465.

Supporting Information: X-ray crystallographic data of **1** are given in the electronic supplement. The crystallographic data (without structure factors) were also deposited as „supplementary publication no. CCDC-826463 at the Cambridge Crystallographic Data Centre. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre: CCDC, 12 Union Road, Cambridge, CB21EZ (Fax: (+44)1223/336033; E-mail: deposit@ccdc.cam-ak.uk).

Acknowledgments

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[21] Bruker AXS D8 Kappa diffractometer with APEX2 detector ($Mo_{K\alpha}$ radiation, λ = 0.71073 Å; *T* = 100(1) K). The structure was solved by Direct Methods (SHELXS-97, G. M. Sheldrick, *Acta Crystallogr. Sect. A* **1990**, *46*, 467) and refined by full-matrix least-squares on F^2. Semi-empirical absorption correction from equivalent reflections on basis of multi-scans (Bruker AXS APEX2) was applied. All non-hydrogen atoms were refined anisotropically and hydrogen atoms by a riding model. (SHELXL-97, *Program for Crystal Structure Refinement*, G. M. Sheldrick, Universität Göttingen, 1997; see also: Sheldrick, G. M. *Acta Crystallogr*. **2008**, *A64*, 112). **1**: $C_{66}H_{90}O_{13}Zn_2{\cdot}x\ C_7H_8$, *M* = 1444.99, colorless crystal (0.33 x 0.28 x 0.23 mm); triclinic, space group $P\bar{1}$; *a* = 12.5160(7), *b* = 15.3748(10), *c* = 19.6899(12) Å; α = 89.586(3)°, β = 76.430(3)°, γ = 88.709(3)°, *V* = 3682.2(4) Å^3; *Z* = 2; μ = 1.345 mm^{-1}; $\rho_{ber.}$ = 1.303 g cm^{-3}; 83967 reflexes ($2\theta_{max}$ = 61°), 21910 unique (R_{int} = 0.0235); 811 parameters; largest max./min. in the final difference Fourier synthesis 0.692 eÅ^{-3}/–0.376 eÅ^{-3}; max./min. transmission 0.75/0.62; R_1 = 0.0284 ($I > 2\sigma(I)$), wR_2 (all data) = 0.0747. The ADP of C20 indicates severe disorder which couldn't be resolved.

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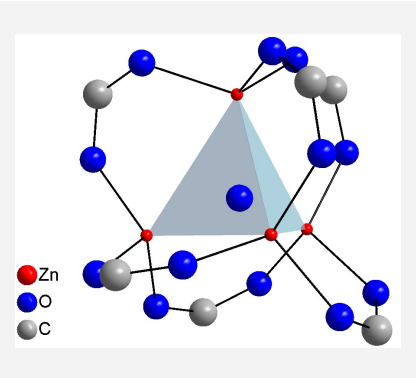
Entry for the Table of Contents

Layout 1:

CO_2 Activation

Zincocene activates CO_2 with formation of $[Zn_4(\mu_4\text{-}O)(O_2CCp^*)_6]$ **1**, whose structure is comparable to that of basic zinc acetate.



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Direct carboxylation of Zincocene Cp^*_2Zn

Keywords: Zinc / CO_2 activation / XRD

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Supporting Information

Direct Carboxylation of Zincocene Cp^*_2Zn

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Single-crystal X-ray analyses. The crystals were mounted on nylon loops in inert oil. Data were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) at 100 K. The structures were solved by Direct Methods (SHELXS-97)[1] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-97)[2]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX2). Hydrogen atoms were refined using a riding model or rigid methyl groups.

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Table 1. Crystal data and structure refinement for 1.

Identification code	sar_400m	
Empirical formula	$C_{66}H_{90}O_{13}Zn_4 * C_7H_8$	
Formula weight	1444.99 Da	
Density (calculated)	1.303 g cm^{-3}	
F(000)	1520	
Temperature	100(1) K	
Crystal size	0.33 x 0.28 x 0.23 mm	
Crystal color	colourless	
Crystal description	block	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\ \bar{1}$	
Unit cell dimensions	a = 12.5160(7) Å	α = 89.586(3)°
	b = 15.3748(10) Å	β = 76.430(3)°
	c = 19.6899(12) Å	γ = 88.709(3)°
Volume	3682.2(4) $Å^3$	
Z	2	
Cell measurement reflections used	9866	
Cell measurement theta min/max	2.38° to 30.51°	
Diffractometer control software	Bruker AXS APEX 2 Vers.3.0/2009	
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system	
Diffractometer measurement method	Data collection strategy APEX 2/COSMO	
Theta range for data collection	1.06° to 30.58°	
Completeness to theta = 30.58°	96.9 %	
Index ranges	$-17<=h<=17$, $-22<=k<=21$, $-28<=l<=28$	
Computing data reduction	Bruker AXS APEX 2 Vers.3/2009	
Absorption coefficient	1.345 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Empirical absorption correction	Bruker AXS APEX 2 Vers.3/2009	
Max. / min. transmission	0.75 / 0.62	
R(merg) before/after correction	0.0534 / 0.0336	

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Computing structure solution	Bruker AXS SHELXTL Vers. 2008/4/(c) 2008
Computing structure refinement	Bruker AXS SHELXTL Vers. 2008/4/(c) 2008
Refinement method	Full-matrix least-squares on F^2
Reflections collected	83967
Independent reflections	21910 [R(int) = 0.0235]
Data / restraints / parameters	18175 / 0 / 811
Goodness-of-fit on F^2	1.013
Weighting details	$w = 1/[\sigma^2 (Fo^2) + (0.0343*P)^2 + 2.2249*P]$ where $P = (Fo^2 + 2Fc^2)/3$
Final R indices [I>2sigma(I)]	$R1$ = 0.0284, $wR2$ = 0.0686
R indices (all data)	$R1$ = 0.0408, $wR2$ = 0.0747
Largest diff. peak and hole	0.692 and -0.376 eÅ^{-3}
Treatment of hydrogen atoms	Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent Uij 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 Uij of the corresponding carbon atom.
Comment	The ADP of C(20) indicate severe disorder which could not be resolved. Consequently atom distances given for these atoms have no significance.

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3)for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn(1)	7407(1)	2859(1)	3547(1)	13(1)
Zn(2)	9131(1)	3637(1)	2242(1)	13(1)
Zn(3)	9741(1)	1912(1)	2993(1)	13(1)
Zn(4)	7998(1)	1882(1)	2084(1)	13(1)
O(1)	6910(1)	4063(1)	3520(1)	20(1)
O(2)	8335(1)	4626(1)	2749(1)	26(1)
O(3)	7681(1)	2550(1)	1318(1)	22(1)
O(4)	8774(1)	3679(1)	1331(1)	22(1)
O(5)	10679(1)	3752(1)	2208(1)	21(1)
O(6)	11088(1)	2583(1)	2789(1)	24(1)
O(7)	9058(1)	974(1)	1696(1)	24(1)
O(8)	10051(1)	818(1)	2501(1)	21(1)
O(9)	9380(1)	1747(1)	3998(1)	19(1)
O(10)	8004(1)	2711(1)	4378(1)	19(1)
O(11)	6695(1)	1309(1)	2588(1)	22(1)
O(12)	6191(1)	2074(1)	3582(1)	19(1)
O(13)	8572(1)	2582(1)	2728(1)	13(1)
C(1)	7450(1)	4693(1)	3209(1)	19(1)
C(2)	8080(1)	3269(1)	1092(1)	17(1)
C(3)	11316(1)	3298(1)	2485(1)	17(1)
C(4)	9759(1)	582(1)	1959(1)	16(1)
C(5)	8793(1)	2226(1)	4463(1)	15(1)
C(6)	6108(1)	1443(1)	3191(1)	16(1)
C(11)	7018(1)	5607(1)	3426(1)	26(1)
C(12)	5779(1)	5695(1)	3583(1)	28(1)
C(13)	5406(1)	5943(1)	4253(1)	29(1)
C(14)	6324(2)	5990(1)	4597(1)	33(1)
C(15)	7265(2)	5784(1)	4128(1)	35(1)
C(16)	7541(2)	6284(1)	2873(1)	46(1)
C(17)	5157(2)	5525(2)	3036(1)	49(1)
C(18)	4246(2)	6150(2)	4630(1)	45(1)
C(19)	6161(2)	6227(2)	5350(1)	53(1)
C(20)	8411(2)	5711(2)	4229(2)	67(1)
C(21)	7706(1)	3662(1)	469(1)	21(1)
C(22)	7708(1)	4644(1)	487(1)	21(1)
C(23)	8410(1)	4942(1)	-86(1)	20(1)
C(24)	8942(1)	4199(1)	-516(1)	22(1)
C(25)	8568(1)	3453(1)	-199(1)	24(1)
C(26)	6581(2)	3309(1)	433(1)	35(1)
C(27)	7022(2)	5144(1)	1087(1)	31(1)
C(28)	8660(2)	5866(1)	-297(1)	28(1)
C(29)	9767(2)	4316(1)	-1197(1)	32(1)
C(30)	8869(2)	2539(1)	-425(1)	42(1)
C(31)	12468(1)	3651(1)	2432(1)	18(1)
C(32)	12414(1)	4624(1)	2546(1)	29(1)
C(33)	12959(1)	5013(1)	1956(1)	34(1)
C(34)	13384(1)	4360(1)	1422(1)	29(1)
C(35)	13105(1)	3571(1)	1676(1)	22(1)
C(36)	13065(1)	3162(1)	2922(1)	28(1)
C(37)	11804(2)	5011(2)	3220(1)	53(1)
C(38)	13120(2)	5970(1)	1825(2)	60(1)
C(39)	14014(2)	4582(2)	694(1)	47(1)

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C(40)	13328(2)	2706(1)	1321(1)	37(1)
C(41)	10268(1)	-253(1)	1604(1)	16(1)
C(42)	9682(1)	-1008(1)	2030(1)	20(1)
C(43)	10426(1)	-1497(1)	2259(1)	22(1)
C(44)	11522(1)	-1116(1)	2026(1)	21(1)
C(45)	11446(1)	-388(1)	1661(1)	18(1)
C(46)	10173(1)	-274(1)	843(1)	22(1)
C(47)	8469(2)	-1117(1)	2152(1)	35(1)
C(48)	10224(2)	-2301(1)	2700(1)	36(1)
C(49)	12526(2)	-1511(1)	2206(1)	33(1)
C(50)	12304(1)	254(1)	1360(1)	28(1)
C(51)	9038(1)	2209(1)	5189(1)	15(1)
C(52)	8268(1)	1561(1)	5640(1)	16(1)
C(53)	8879(1)	921(1)	5841(1)	17(1)
C(54)	10059(1)	1088(1)	5560(1)	18(1)
C(55)	10168(1)	1820(1)	5175(1)	17(1)
C(56)	8887(1)	3124(1)	5510(1)	21(1)
C(57)	7051(1)	1700(1)	5832(1)	22(1)
C(58)	8493(1)	138(1)	6281(1)	25(1)
C(59)	10949(1)	504(1)	5713(1)	27(1)
C(60)	11198(1)	2226(1)	4768(1)	26(1)
C(61)	5253(1)	764(1)	3489(1)	16(1)
C(62)	5802(1)	143(1)	3921(1)	16(1)
C(63)	5843(1)	-661(1)	3650(1)	18(1)
C(64)	5376(1)	-639(1)	3026(1)	19(1)
C(65)	5031(1)	175(1)	2926(1)	19(1)
C(66)	4199(1)	1192(1)	3928(1)	20(1)
C(67)	6212(1)	450(1)	4530(1)	20(1)
C(68)	6269(1)	-1479(1)	3920(1)	26(1)
C(69)	5354(1)	-1432(1)	2590(1)	26(1)
C(70)	4505(1)	520(1)	2370(1)	25(1)
C(71)	3617(2)	543(2)	9354(1)	43(1)
C(72)	2928(2)	1263(2)	9382(1)	55(1)
C(73)	3331(4)	2091(2)	9376(2)	81(1)
C(74)	4432(4)	2215(3)	9359(2)	94(1)
C(75)	5110(3)	1504(3)	9354(1)	77(1)
C(76)	4705(2)	683(2)	9352(1)	54(1)
C(77)	3193(2)	-357(2)	9319(2)	67(1)

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Table 3. Bond lengths [Å] and angles [°] for 1.

Zn(1)-O(1)	1.9441(10)	C(25)-C(30)	1.490(3)
Zn(1)-O(13)	1.9458(10)	C(31)-C(32)	1.512(2)
Zn(1)-O(12)	1.9517(10)	C(31)-C(35)	1.519(2)
Zn(1)-O(10)	1.9622(10)	C(31)-C(36)	1.534(2)
Zn(2)-O(5)	1.9347(10)	C(32)-C(33)	1.345(3)
Zn(2)-O(13)	1.9364(9)	C(32)-C(37)	1.487(3)
Zn(2)-O(2)	1.9470(11)	C(33)-C(34)	1.458(3)
Zn(2)-O(4)	1.9486(11)	C(33)-C(38)	1.502(3)
Zn(2)-Zn(4)	3.1266(3)	C(34)-C(35)	1.332(2)
Zn(3)-O(8)	1.9326(11)	C(34)-C(39)	1.506(2)
Zn(3)-O(13)	1.9381(9)	C(35)-C(40)	1.497(3)
Zn(3)-O(9)	1.9405(10)	C(41)-C(45)	1.5142(19)
Zn(3)-O(6)	1.9546(11)	C(41)-C(42)	1.525(2)
Zn(3)-Zn(4)	3.1305(3)	C(41)-C(46)	1.531(2)
Zn(4)-O(11)	1.9271(10)	C(42)-C(43)	1.341(2)
Zn(4)-O(3)	1.9299(10)	C(42)-C(47)	1.494(2)
Zn(4)-O(7)	1.9369(11)	C(43)-C(44)	1.473(2)
Zn(4)-O(13)	1.9394(10)	C(43)-C(48)	1.498(2)
O(1)-C(1)	1.2624(17)	C(44)-C(45)	1.339(2)
O(2)-C(1)	1.2587(18)	C(44)-C(49)	1.498(2)
O(3)-C(2)	1.2581(17)	C(45)-C(50)	1.490(2)
O(4)-C(2)	1.2621(17)	C(51)-C(55)	1.5167(19)
O(5)-C(3)	1.2627(17)	C(51)-C(52)	1.5282(19)
O(6)-C(3)	1.2549(17)	C(51)-C(56)	1.537(2)
O(7)-C(4)	1.2607(17)	C(52)-C(53)	1.347(2)
O(8)-C(4)	1.2635(18)	C(52)-C(57)	1.493(2)
O(9)-C(5)	1.2602(17)	C(53)-C(54)	1.478(2)
O(10)-C(5)	1.2653(17)	C(53)-C(58)	1.498(2)
O(11)-C(6)	1.2562(18)	C(54)-C(55)	1.343(2)
O(12)-C(6)	1.2654(18)	C(54)-C(59)	1.498(2)
C(1)-C(11)	1.523(2)	C(55)-C(60)	1.497(2)
C(2)-C(21)	1.528(2)	C(61)-C(65)	1.515(2)
C(3)-C(31)	1.5317(19)	C(61)-C(62)	1.528(2)
C(4)-C(41)	1.520(2)	C(61)-C(66)	1.534(2)
C(5)-C(51)	1.5312(19)	C(62)-C(63)	1.345(2)
C(6)-C(61)	1.5258(18)	C(62)-C(67)	1.493(2)
C(11)-C(12)	1.511(2)	C(63)-C(64)	1.479(2)
C(11)-C(15)	1.513(3)	C(63)-C(68)	1.498(2)
C(11)-C(16)	1.542(2)	C(64)-C(65)	1.343(2)
C(12)-C(13)	1.348(3)	C(64)-C(69)	1.500(2)
C(12)-C(17)	1.498(3)	C(65)-C(70)	1.492(2)
C(13)-C(14)	1.467(3)	C(71)-C(72)	1.381(3)
C(13)-C(18)	1.496(2)	C(71)-C(76)	1.383(3)
C(14)-C(15)	1.349(3)	C(71)-C(77)	1.501(4)
C(14)-C(19)	1.494(3)	C(72)-C(73)	1.379(4)
C(15)-C(20)	1.494(3)	C(73)-C(74)	1.388(6)
C(21)-C(22)	1.510(2)	C(74)-C(75)	1.366(5)
C(21)-C(25)	1.523(2)	C(75)-C(76)	1.371(4)
C(21)-C(26)	1.537(2)		
C(22)-C(23)	1.342(2)	O(1)-Zn(1)-O(13)	110.86(4)
C(22)-C(27)	1.493(2)	O(1)-Zn(1)-O(12)	110.52(4)
C(23)-C(24)	1.476(2)	O(13)-Zn(1)-O(12)	108.93(4)
C(23)-C(28)	1.498(2)	O(1)-Zn(1)-O(10)	107.75(5)
C(24)-C(25)	1.342(2)	O(13)-Zn(1)-O(10)	108.16(4)
C(24)-C(29)	1.501(2)	O(12)-Zn(1)-O(10)	110.59(5)

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O(5)-Zn(2)-O(13)	110.82(4)	O(3)-C(2)-C(21)	116.95(12)
O(5)-Zn(2)-O(2)	108.52(5)	O(4)-C(2)-C(21)	117.90(12)
O(13)-Zn(2)-O(2)	108.41(4)	O(6)-C(3)-O(5)	125.43(13)
O(5)-Zn(2)-O(4)	114.20(5)	O(6)-C(3)-C(31)	117.80(12)
O(13)-Zn(2)-O(4)	109.79(4)	O(5)-C(3)-C(31)	116.76(12)
O(2)-Zn(2)-O(4)	104.78(5)	O(7)-C(4)-O(8)	125.20(14)
O(5)-Zn(2)-Zn(4)	124.72(3)	O(7)-C(4)-C(41)	116.90(13)
O(13)-Zn(2)-Zn(4)	36.26(3)	O(8)-C(4)-C(41)	117.88(12)
O(2)-Zn(2)-Zn(4)	122.49(3)	O(9)-C(5)-O(10)	124.89(13)
O(4)-Zn(2)-Zn(4)	73.73(3)	O(9)-C(5)-C(51)	117.67(12)
O(8)-Zn(3)-O(13)	112.69(4)	O(10)-C(5)-C(51)	117.43(12)
O(8)-Zn(3)-O(9)	111.79(5)	O(11)-C(6)-O(12)	125.78(13)
O(13)-Zn(3)-O(9)	109.27(4)	O(11)-C(6)-C(61)	117.13(13)
O(8)-Zn(3)-O(6)	108.04(5)	O(12)-C(6)-C(61)	117.03(12)
O(13)-Zn(3)-O(6)	109.52(4)	C(12)-C(11)-C(15)	102.78(14)
O(9)-Zn(3)-O(6)	105.24(5)	C(12)-C(11)-C(1)	113.50(13)
O(8)-Zn(3)-Zn(4)	76.60(3)	C(15)-C(11)-C(1)	107.24(14)
O(13)-Zn(3)-Zn(4)	36.18(3)	C(12)-C(11)-C(16)	110.08(15)
O(9)-Zn(3)-Zn(4)	123.45(3)	C(15)-C(11)-C(16)	111.87(16)
O(6)-Zn(3)-Zn(4)	125.78(3)	C(1)-C(11)-C(16)	111.08(14)
O(11)-Zn(4)-O(3)	110.17(5)	C(13)-C(12)-C(17)	129.73(17)
O(11)-Zn(4)-O(7)	106.63(5)	C(13)-C(12)-C(11)	108.78(16)
O(3)-Zn(4)-O(7)	107.91(5)	C(17)-C(12)-C(11)	121.48(16)
O(11)-Zn(4)-O(13)	109.34(4)	C(12)-C(13)-C(14)	110.06(15)
O(3)-Zn(4)-O(13)	112.93(4)	C(12)-C(13)-C(18)	127.87(19)
O(7)-Zn(4)-O(13)	109.65(4)	C(14)-C(13)-C(18)	122.07(18)
O(11)-Zn(4)-Zn(2)	135.33(3)	C(15)-C(14)-C(13)	108.74(17)
O(3)-Zn(4)-Zn(2)	78.62(3)	C(15)-C(14)-C(19)	128.9(2)
O(7)-Zn(4)-Zn(2)	111.95(4)	C(13)-C(14)-C(19)	122.39(18)
O(13)-Zn(4)-Zn(2)	36.19(3)	C(14)-C(15)-C(20)	129.2(2)
O(11)-Zn(4)-Zn(3)	109.96(3)	C(14)-C(15)-C(11)	109.50(16)
O(3)-Zn(4)-Zn(3)	136.60(3)	C(20)-C(15)-C(11)	121.28(18)
O(7)-Zn(4)-Zn(3)	75.29(3)	C(22)-C(21)-C(25)	102.55(12)
O(13)-Zn(4)-Zn(3)	36.15(3)	C(22)-C(21)-C(2)	111.16(13)
Zn(2)-Zn(4)-Zn(3)	61.324(6)	C(25)-C(21)-C(2)	109.12(12)
C(1)-O(1)-Zn(1)	127.44(10)	C(22)-C(21)-C(26)	112.41(14)
C(1)-O(2)-Zn(2)	132.74(10)	C(25)-C(21)-C(26)	110.84(14)
C(2)-O(3)-Zn(4)	127.02(10)	C(2)-C(21)-C(26)	110.48(12)
C(2)-O(4)-Zn(2)	131.20(10)	C(23)-C(22)-C(27)	128.94(15)
C(3)-O(5)-Zn(2)	130.76(9)	C(23)-C(22)-C(21)	109.51(14)
C(3)-O(6)-Zn(3)	131.75(10)	C(27)-C(22)-C(21)	121.52(14)
C(4)-O(7)-Zn(4)	129.87(10)	C(22)-C(23)-C(24)	109.36(14)
C(4)-O(8)-Zn(3)	128.34(10)	C(22)-C(23)-C(28)	128.29(16)
C(5)-O(9)-Zn(3)	128.56(9)	C(24)-C(23)-C(28)	122.34(14)
C(5)-O(10)-Zn(1)	129.05(10)	C(25)-C(24)-C(23)	109.40(14)
C(6)-O(11)-Zn(4)	130.38(10)	C(25)-C(24)-C(29)	128.16(16)
C(6)-O(12)-Zn(1)	130.11(9)	C(23)-C(24)-C(29)	122.44(14)
Zn(2)-O(13)-Zn(3)	110.89(4)	C(24)-C(25)-C(30)	129.22(17)
Zn(2)-O(13)-Zn(4)	107.55(5)	C(24)-C(25)-C(21)	109.10(14)
Zn(3)-O(13)-Zn(4)	107.67(5)	C(30)-C(25)-C(21)	121.67(15)
Zn(2)-O(13)-Zn(1)	110.37(5)	C(32)-C(31)-C(35)	102.45(13)
Zn(3)-O(13)-Zn(1)	110.48(5)	C(32)-C(31)-C(3)	110.58(12)
Zn(4)-O(13)-Zn(1)	109.79(4)	C(35)-C(31)-C(3)	107.89(12)
O(2)-C(1)-O(1)	125.27(14)	C(32)-C(31)-C(36)	112.82(13)
O(2)-C(1)-C(11)	117.27(13)	C(35)-C(31)-C(36)	110.99(13)
O(1)-C(1)-C(11)	117.42(13)	C(3)-C(31)-C(36)	111.65(12)
O(3)-C(2)-O(4)	125.14(13)	C(33)-C(32)-C(37)	129.92(19)

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C(33)-C(32)-C(31)	108.76(16)
C(37)-C(32)-C(31)	121.31(18)
C(32)-C(33)-C(34)	109.86(15)
C(32)-C(33)-C(38)	127.6(2)
C(34)-C(33)-C(38)	122.5(2)
C(35)-C(34)-C(33)	109.65(15)
C(35)-C(34)-C(39)	127.0(2)
C(33)-C(34)-C(39)	123.31(17)
C(34)-C(35)-C(40)	129.17(16)
C(34)-C(35)-C(31)	109.26(15)
C(40)-C(35)-C(31)	121.56(14)
C(45)-C(41)-C(4)	111.85(12)
C(45)-C(41)-C(42)	102.81(12)
C(4)-C(41)-C(42)	107.16(12)
C(45)-C(41)-C(46)	111.72(12)
C(4)-C(41)-C(46)	110.82(12)
C(42)-C(41)-C(46)	112.17(12)
C(43)-C(42)-C(47)	129.24(15)
C(43)-C(42)-C(41)	108.63(13)
C(47)-C(42)-C(41)	122.12(14)
C(42)-C(43)-C(44)	109.81(13)
C(42)-C(43)-C(48)	127.36(16)
C(44)-C(43)-C(48)	122.82(15)
C(45)-C(44)-C(43)	109.52(13)
C(45)-C(44)-C(49)	127.95(15)
C(43)-C(44)-C(49)	122.51(15)
C(44)-C(45)-C(50)	129.75(14)
C(44)-C(45)-C(41)	109.17(13)
C(50)-C(45)-C(41)	121.03(13)
C(55)-C(51)-C(52)	102.78(11)
C(55)-C(51)-C(5)	112.00(12)
C(52)-C(51)-C(5)	108.03(11)
C(55)-C(51)-C(56)	111.99(12)
C(52)-C(51)-C(56)	111.54(12)
C(5)-C(51)-C(56)	110.25(12)
C(53)-C(52)-C(57)	128.97(13)
C(53)-C(52)-C(51)	108.72(12)
C(57)-C(52)-C(51)	122.21(13)
C(52)-C(53)-C(54)	109.66(12)
C(52)-C(53)-C(58)	128.23(14)
C(54)-C(53)-C(58)	122.11(13)
C(55)-C(54)-C(53)	109.46(13)
C(55)-C(54)-C(59)	128.14(14)
C(53)-C(54)-C(59)	122.39(14)
C(54)-C(55)-C(60)	128.60(14)
C(54)-C(55)-C(51)	109.36(12)
C(60)-C(55)-C(51)	122.04(13)
C(65)-C(61)-C(6)	111.91(12)
C(65)-C(61)-C(62)	102.75(12)
C(6)-C(61)-C(62)	105.87(11)
C(65)-C(61)-C(66)	112.44(11)
C(6)-C(61)-C(66)	111.15(12)
C(62)-C(61)-C(66)	112.27(12)
C(63)-C(62)-C(67)	129.28(14)
C(63)-C(62)-C(61)	108.73(13)
C(67)-C(62)-C(61)	121.98(13)
C(62)-C(63)-C(64)	109.68(13)
C(62)-C(63)-C(68)	127.31(14)
C(64)-C(63)-C(68)	123.00(14)
C(65)-C(64)-C(63)	109.38(13)
C(65)-C(64)-C(69)	128.45(15)
C(63)-C(64)-C(69)	122.16(14)
C(64)-C(65)-C(70)	129.33(15)
C(64)-C(65)-C(61)	109.44(13)
C(70)-C(65)-C(61)	121.23(14)
C(72)-C(71)-C(76)	117.7(3)
C(72)-C(71)-C(77)	120.7(2)
C(76)-C(71)-C(77)	121.6(2)
C(73)-C(72)-C(71)	120.7(3)
C(72)-C(73)-C(74)	120.5(3)
C(75)-C(74)-C(73)	119.1(3)
C(74)-C(75)-C(76)	120.1(3)
C(75)-C(76)-C(71)	121.9(3)

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Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zn(1)	14(1)	12(1)	12(1)	1(1)	-2(1)	0(1)
Zn(2)	13(1)	13(1)	13(1)	2(1)	-3(1)	0(1)
Zn(3)	15(1)	13(1)	11(1)	0(1)	-3(1)	2(1)
Zn(4)	14(1)	13(1)	12(1)	2(1)	-3(1)	0(1)
O(1)	19(1)	13(1)	25(1)	1(1)	0(1)	1(1)
O(2)	24(1)	15(1)	32(1)	-1(1)	7(1)	1(1)
O(3)	28(1)	19(1)	21(1)	8(1)	-12(1)	-4(1)
O(4)	24(1)	26(1)	20(1)	9(1)	-11(1)	-7(1)
O(5)	17(1)	26(1)	23(1)	9(1)	-7(1)	-4(1)
O(6)	19(1)	23(1)	31(1)	10(1)	-9(1)	-4(1)
O(7)	27(1)	26(1)	19(1)	-6(1)	-10(1)	12(1)
O(8)	31(1)	18(1)	16(1)	-5(1)	-10(1)	9(1)
O(9)	27(1)	17(1)	12(1)	0(1)	-3(1)	7(1)
O(10)	20(1)	24(1)	14(1)	-2(1)	-5(1)	5(1)
O(11)	24(1)	24(1)	17(1)	1(1)	0(1)	-9(1)
O(12)	18(1)	16(1)	21(1)	0(1)	-2(1)	-3(1)
O(13)	14(1)	13(1)	12(1)	2(1)	-2(1)	0(1)
C(1)	19(1)	14(1)	23(1)	-2(1)	-3(1)	1(1)
C(2)	17(1)	20(1)	15(1)	3(1)	-5(1)	1(1)
C(3)	16(1)	21(1)	13(1)	0(1)	-2(1)	-1(1)
C(4)	18(1)	16(1)	13(1)	0(1)	-2(1)	2(1)
C(5)	17(1)	14(1)	12(1)	1(1)	-3(1)	-2(1)
C(6)	16(1)	16(1)	17(1)	4(1)	-5(1)	-2(1)
C(11)	27(1)	12(1)	33(1)	-2(1)	6(1)	1(1)
C(12)	29(1)	21(1)	31(1)	6(1)	0(1)	11(1)
C(13)	30(1)	17(1)	33(1)	5(1)	6(1)	9(1)
C(14)	39(1)	18(1)	38(1)	-12(1)	-2(1)	-1(1)
C(15)	30(1)	24(1)	49(1)	-17(1)	-6(1)	-3(1)
C(16)	53(1)	15(1)	55(1)	2(1)	18(1)	-1(1)
C(17)	43(1)	63(2)	44(1)	6(1)	-17(1)	18(1)
C(18)	37(1)	40(1)	48(1)	5(1)	11(1)	20(1)
C(19)	69(2)	44(1)	45(1)	-24(1)	-9(1)	1(1)
C(20)	39(1)	84(2)	84(2)	-49(2)	-23(1)	-4(1)
C(21)	25(1)	21(1)	19(1)	8(1)	-12(1)	-3(1)
C(22)	22(1)	21(1)	21(1)	6(1)	-10(1)	3(1)
C(23)	24(1)	19(1)	21(1)	5(1)	-11(1)	0(1)
C(24)	30(1)	24(1)	16(1)	3(1)	-10(1)	-1(1)
C(25)	38(1)	21(1)	16(1)	2(1)	-12(1)	-1(1)
C(26)	35(1)	38(1)	42(1)	19(1)	-27(1)	-13(1)
C(27)	31(1)	32(1)	29(1)	4(1)	-5(1)	10(1)
C(28)	34(1)	20(1)	30(1)	8(1)	-10(1)	-2(1)
C(29)	44(1)	34(1)	18(1)	3(1)	-5(1)	-1(1)
C(30)	76(2)	24(1)	26(1)	-2(1)	-12(1)	0(1)
C(31)	16(1)	21(1)	18(1)	3(1)	-5(1)	-2(1)
C(32)	24(1)	24(1)	44(1)	-8(1)	-15(1)	0(1)
C(33)	25(1)	22(1)	60(1)	12(1)	-22(1)	-6(1)
C(34)	15(1)	38(1)	34(1)	19(1)	-10(1)	-4(1)
C(35)	14(1)	30(1)	21(1)	6(1)	-4(1)	1(1)
C(36)	23(1)	38(1)	26(1)	11(1)	-12(1)	-6(1)
C(37)	45(1)	54(1)	62(2)	-35(1)	-14(1)	7(1)
C(38)	55(1)	26(1)	108(2)	20(1)	-41(2)	-13(1)
C(39)	23(1)	74(2)	44(1)	38(1)	-10(1)	-10(1)
C(40)	34(1)	42(1)	32(1)	-7(1)	-3(1)	10(1)
C(41)	19(1)	16(1)	13(1)	-2(1)	-4(1)	3(1)
C(42)	25(1)	18(1)	18(1)	-2(1)	-5(1)	-3(1)
C(43)	34(1)	15(1)	18(1)	-1(1)	-10(1)	-2(1)
C(44)	26(1)	18(1)	20(1)	-6(1)	-10(1)	5(1)

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C(45)	18(1)	18(1)	16(1)	-4(1)	-4(1)	3(1)
C(46)	30(1)	23(1)	15(1)	-4(1)	-7(1)	6(1)
C(47)	27(1)	40(1)	38(1)	7(1)	-8(1)	-10(1)
C(48)	57(1)	22(1)	36(1)	8(1)	-20(1)	-9(1)
C(49)	34(1)	28(1)	41(1)	-2(1)	-19(1)	9(1)
C(50)	22(1)	30(1)	32(1)	3(1)	-4(1)	-3(1)
C(51)	16(1)	16(1)	12(1)	-1(1)	-3(1)	1(1)
C(52)	18(1)	19(1)	10(1)	-1(1)	-3(1)	-1(1)
C(53)	23(1)	17(1)	12(1)	-1(1)	-6(1)	-1(1)
C(54)	20(1)	19(1)	16(1)	-4(1)	-7(1)	3(1)
C(55)	16(1)	19(1)	16(1)	-4(1)	-4(1)	0(1)
C(56)	26(1)	19(1)	19(1)	-5(1)	-8(1)	3(1)
C(57)	17(1)	30(1)	18(1)	1(1)	-2(1)	-1(1)
C(58)	34(1)	21(1)	20(1)	4(1)	-8(1)	-4(1)
C(59)	28(1)	26(1)	31(1)	-2(1)	-14(1)	8(1)
C(60)	18(1)	26(1)	33(1)	-1(1)	-3(1)	-2(1)
C(61)	16(1)	15(1)	16(1)	2(1)	-3(1)	-3(1)
C(62)	14(1)	17(1)	15(1)	3(1)	-1(1)	-2(1)
C(63)	17(1)	18(1)	19(1)	2(1)	0(1)	-1(1)
C(64)	18(1)	21(1)	18(1)	-1(1)	0(1)	-6(1)
C(65)	16(1)	23(1)	16(1)	2(1)	-3(1)	-5(1)
C(66)	18(1)	21(1)	20(1)	2(1)	-3(1)	0(1)
C(67)	20(1)	22(1)	19(1)	2(1)	-5(1)	-1(1)
C(68)	28(1)	18(1)	28(1)	1(1)	-3(1)	3(1)
C(69)	24(1)	26(1)	27(1)	-6(1)	-3(1)	-5(1)
C(70)	26(1)	31(1)	22(1)	3(1)	-10(1)	-4(1)
C(71)	40(1)	60(1)	26(1)	-6(1)	-1(1)	1(1)
C(72)	53(1)	72(2)	40(1)	-10(1)	-10(1)	11(1)
C(73)	122(3)	58(2)	54(2)	-14(1)	-1(2)	16(2)
C(74)	138(4)	85(3)	46(2)	-25(2)	7(2)	-49(3)
C(75)	71(2)	121(3)	37(1)	-16(2)	-6(1)	-40(2)
C(76)	40(1)	88(2)	31(1)	2(1)	-6(1)	0(1)
C(77)	63(2)	67(2)	62(2)	-7(1)	2(1)	-10(1)

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Table 5. Hydrogen coordinates (x 10^4) and i displacement parameters (Å^2 x 10^3) for 1.

	x	y	z	U(eq)
H(16A)	7200	6857	3003	69
H(16B)	7424	6117	2416	69
H(16C)	8332	6307	2846	69
H(17A)	4372	5641	3230	73
H(17B)	5271	4916	2888	73
H(17C)	5419	5906	2632	73
H(18A)	3752	6033	4324	68
H(18B)	4180	6765	4763	68
H(18C)	4045	5788	5051	68
H(19A)	6876	6238	5471	80
H(19B)	5698	5796	5640	80
H(19C)	5803	6803	5431	80
H(20A)	8391	5714	4729	101
H(20B)	8836	6204	4001	101
H(20C)	8758	5166	4022	101
H(26A)	6028	3495	849	53
H(26B)	6623	2672	414	53
H(26C)	6374	3535	14	53
H(27A)	7354	5094	1490	46
H(27B)	6280	4909	1209	46
H(27C)	6982	5757	954	46
H(28A)	8232	6257	61	42
H(28B)	8467	5983	-744	42
H(28C)	9446	5963	-347	42
H(29A)	10034	3745	-1392	48
H(29B)	10386	4649	-1119	48
H(29C)	9419	4631	-1526	48
H(30A)	9481	2533	-840	63
H(30B)	8232	2264	-535	63
H(30C)	9088	2217	-46	63
H(36A)	13799	3399	2874	42
H(36B)	13133	2543	2798	42
H(36C)	12644	3228	3406	42
H(37A)	11909	5642	3205	80
H(37B)	12085	4758	3603	80
H(37C)	11020	4892	3294	80
H(38A)	12835	6288	2262	89
H(38B)	12725	6165	1475	89
H(38C)	13905	6082	1655	89
H(39A)	14220	4048	422	70
H(39B)	14680	4892	719	70
H(39C)	13553	4955	468	70
H(40A)	13819	2782	858	56
H(40B)	12635	2462	1270	56
H(40C)	13677	2310	1600	56
H(46A)	10544	229	591	34
H(46B)	9395	-253	829	34
H(46C)	10518	-811	620	34
H(47A)	8265	-1671	2392	52
H(47B)	8257	-1114	1703	52
H(47C)	8087	-637	2442	52
H(48A)	9436	-2422	2815	55
H(48B)	10469	-2216	3132	55
H(48C)	10632	-2794	2440	55
H(49A)	13143	-1118	2057	49
H(49B)	12707	-2070	1965	49
H(49C)	12385	-1603	2712	49
H(50A)	12144	802	1618	43

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H(50B)	12308	357	867	43
H(50C)	13026	25	1396	43
H(56A)	9025	3100	5980	31
H(56B)	8134	3337	5539	31
H(56C)	9406	3519	5217	31
H(57A)	6700	1178	6063	33
H(57B)	6788	1819	5408	33
H(57C)	6864	2197	6150	33
H(58A)	7687	142	6407	38
H(58B)	8771	150	6706	38
H(58C)	8767	-390	6015	38
H(59A)	11667	716	5463	41
H(59B)	10855	-88	5561	41
H(59C)	10905	505	6216	41
H(60A)	11834	1965	4910	39
H(60B)	11164	2853	4860	39
H(60C)	11271	2127	4268	39
H(66A)	3873	1579	3630	30
H(66B)	4376	1529	4306	30
H(66C)	3675	741	4127	30
H(67A)	6400	-55	4789	30
H(67B)	5639	804	4837	30
H(67C)	6867	799	4362	30
H(68A)	6928	-1689	3583	39
H(68B)	5704	-1923	3988	39
H(68C)	6453	-1361	4367	39
H(69A)	5095	-1269	2173	39
H(69B)	4857	-1857	2864	39
H(69C)	6096	-1689	2449	39
H(70A)	4515	64	2024	38
H(70B)	4912	1021	2142	38
H(70C)	3743	700	2579	38
H(72)	2170	1186	9404	66
H(73)	2847	2579	9388	98
H(74)	4709	2786	9346	112
H(75)	5861	1579	9354	92
H(76)	5186	195	9347	64
H(77A)	3078	-459	8851	100
H(77B)	2496	-419	9666	100
H(77C)	3734	-782	9415	100

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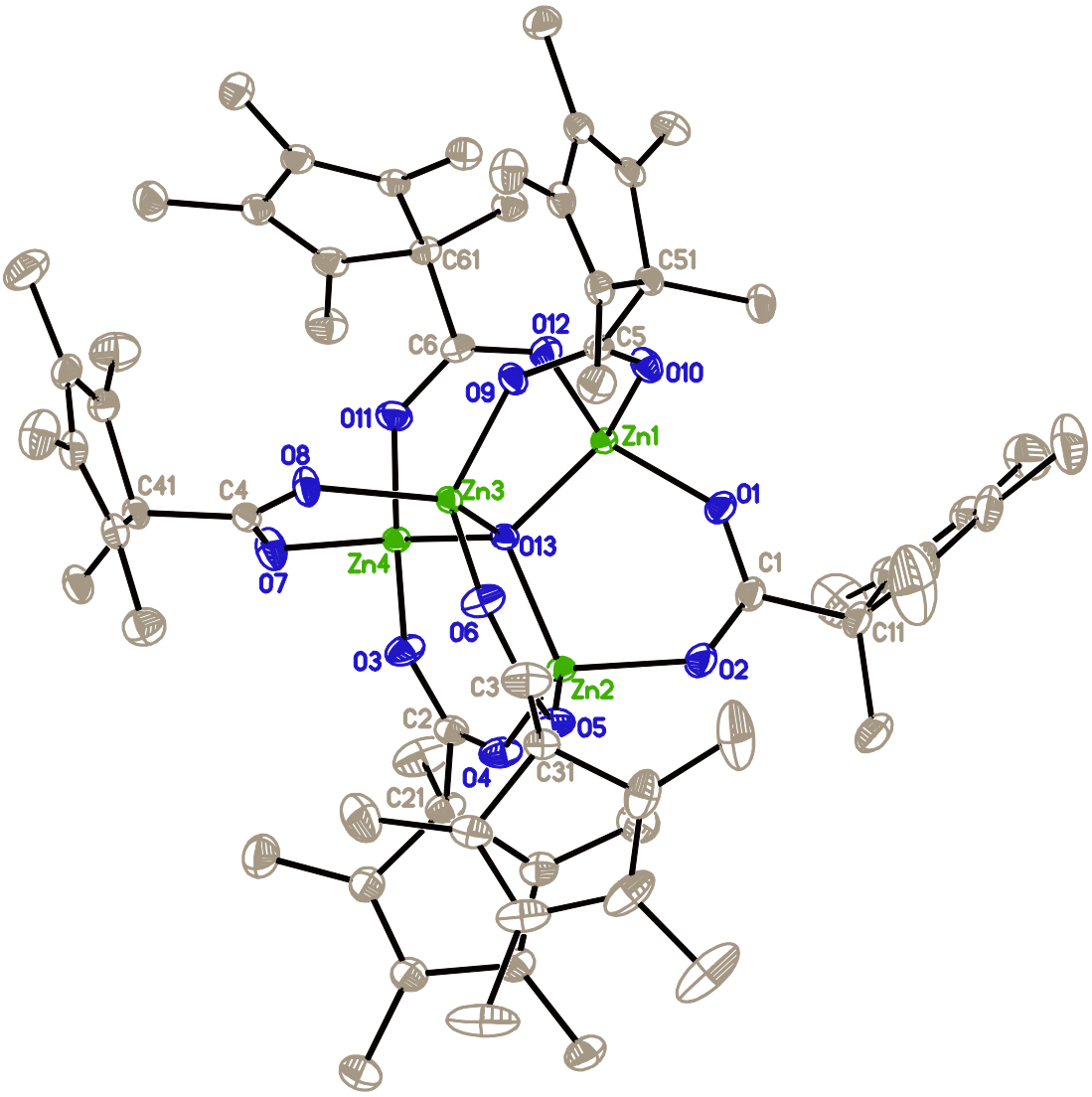
Solid state structure of **1**



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