



Crystal structure and Hirshfeld surface analysis of bis(μ -4-*tert*-butoxy-4-oxobut-2-en-2-olato)bis[(4-*tert*-butoxy-4-oxobut-2-en-2-olato)ethanolzinc(II)]

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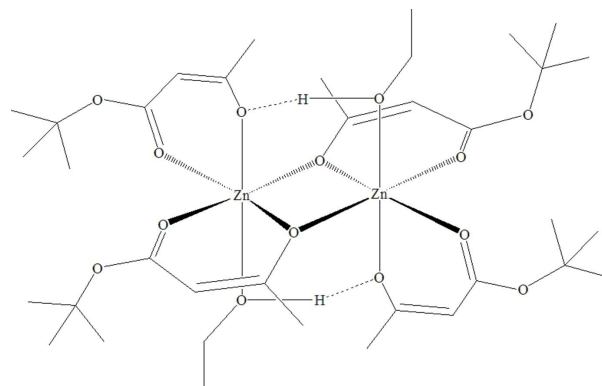
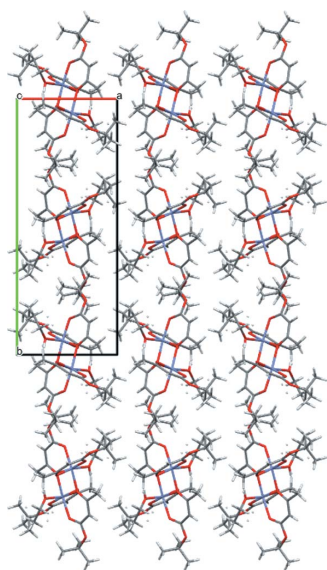
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The molecular and crystal structure of the title binuclear Zn²⁺ complex, [Zn₂(C₈H₁₃O₃)₄(C₂H₅OH)₂], with enolated anionic *tert*-butylacetoacetate and ethanol was analysed. The coordination polyhedra of the Zn atoms are distorted octahedra formed by six oxygen atoms that belong to three ligand molecules and a coordinated ethanol molecule. In the crystal phase, alternating layers can be distinguished parallel to the *ac* plane. A Hirshfeld surface analysis showed that there are no strong intermolecular interactions in the structure. The most significant contributions to the overall crystal packing are from H···H intermolecular contacts.

1. Chemical context

Metal complexes with β -dicarbonyl ligands are widely used for obtaining metal oxides and, less often, metal films by the metal–organic chemical vapor deposition (MOCVD) process and its variations (Wei *et al.*, 2014; Han *et al.*, 2017, 2018; Nayak *et al.*, 2007; Cosham *et al.*, 2017; Kawazoe *et al.*, 2006; Kamata *et al.*, 1994), for the catalysis of reduction, oxidation, and oligomerization of unsaturated compounds and cross-coupling reacti& Nobile *et al.*, 1994). They also exhibit antiviral activity (Sechi *et al.*, 2006), in which interest has increased significantly in recent years. In addition, β -dicarbonyl complexes of zinc are studied as luminescent materials and antioxidants (Aliaga-Alcalde *et al.*, 2012; Nie *et al.*, 2014; Turra *et al.*, 2010).

Our research group is developing coordination compounds soluble in non-polar organic solvents, including metal complexes of acetoacetic acid esters (Koval *et al.*, 2009), which can potentially be used as environmentally friendly additives to industrial products. Previously, we reported the structure of



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Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.031 (3)	Zn1—O4	2.076 (2)
Zn1—O2	2.039 (3)	Zn1—O5	2.072 (3)
Zn1—O4 ⁱ	2.141 (3)	Zn1—O7	2.201 (3)
O1—Zn1—O2	90.99 (11)	O2—Zn1—O7	93.30 (12)
O1—Zn1—O4	90.61 (11)	O4—Zn1—O7	86.49 (12)
O1—Zn1—O5	97.46 (12)	O5—Zn1—O4	88.08 (11)
O2—Zn1—O5	85.30 (11)	O5—Zn1—O7	94.74 (12)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

a trimeric zinc complex synthesized in a rather complicated way using diethyl zinc (Shtokvish *et al.*, 2014). After that, we developed a much simpler and relatively more efficient method for the synthesis of cobalt and nickel ketoesterates (Shtokvish *et al.*, 2015, 2017, Shtokvysh *et al.*, 2018). The use of this method for the synthesis of Zn complexes made it possible to obtain dimeric complexes with cyclohexylacetoacetate (Shtokvysh *et al.*, 2020) and *tert*-butylacetoacetate. In the present work, we report the synthesis and structural analysis of the new complex $[\text{Zn}_2(\text{C}_8\text{H}_{10}\text{O}_3)_4(\text{C}_2\text{H}_5\text{OH})_2]$.

2. Structural commentary

The title compound, systematic name bis(μ -4-*tert*-butoxy-4-oxobut-2-en-2-olato)bis[(4-*tert*-butoxy-4-oxobut-2-en-2-olato)ethanolzinc(II)], is a binuclear complex that resides on a special position with the unit cell's central inversion centre being close to the refined zinc(II) atom and directly in between this and the symmetry-generated zinc atom [symmetry code: (i) $-x + 1, -y + 1, -z + 1$] (Fig. 1). The coordination polyhedron of the Zn centre is a distorted octahedron formed by six oxygen atoms. One bidentate acetylacetonate type ligand (O1, O2) binds only to one zinc centre. Its oxygen atoms occupy an axial (O1) and an equatorial position (O2). The second bidentate ligand (O4, O5) binds the zinc centre only equatorially, while O4 also binds the symmetry-generated second zinc atom of the binuclear

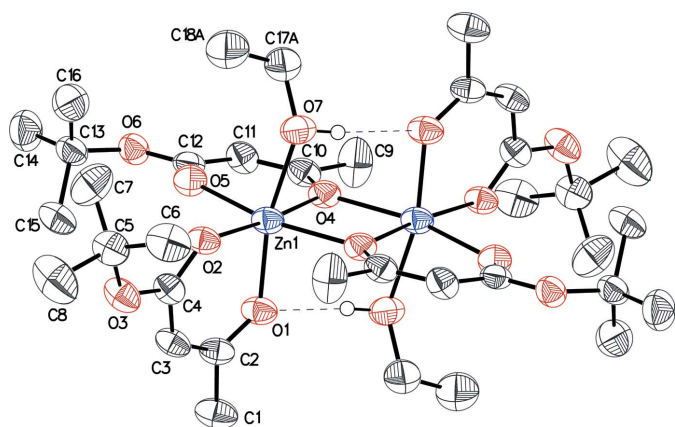


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids. H atoms and the minor occupancy disordered component have been omitted for clarity. Unlabelled atoms are related by the symmetry operation $1 - x, 1 - y, 1 - z$.

Table 2
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H7 ⁱ ···O1 ⁱ	0.86 (1)	2.01 (1)	2.861 (4)	171 (4)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

complex. This also means that the symmetry-generated O4ⁱ atom occupies the fourth equatorial position. The octahedral coordination sphere is completed by axially coordinated ethanol (O7). The bonds of zinc atoms with the enol atom of the bridging ligand are not equivalent. The Zn1—O4 bond length in the chelate is shorter than the Zn1—O4ⁱ bond length with the symmetry-generated bridging ligand [2.076 (2) and 2.141 (3) Å, respectively; Table 1]. The Zn—O bond lengths of terminal ligands (O1, O2) are shorter than the Zn—O bonds of bridging ligands (O4, O5) with ranges of 2.031 (3) to 2.039 (3) and of 2.072 (3) to 2.076 (2) Å, respectively (Table 1). The Zn1—O7 bond length (the bond between the zinc atom and the oxygen of the coordinated ethanol molecule) is the longest in the coordination polyhedron at 2.201 (3) Å (Table 1). The values of the O—Zn—O bond angles lie in the range 85.30 (11) to 97.46 (12)° (Table 1). The connection between the nuclei of the complex is additionally stabilized by two intramolecular hydrogen bonds between the hydrogen atoms of the hydroxyl groups of ethanol and the enol oxygen atoms of the terminal ligands belonging to another nucleus (Table 2).

3. Supramolecular features

There are no short intermolecular contacts between neighbouring molecules in the crystal phase. However, visually we can distinguish alternating layers parallel to the *ac* plane (Fig. 2*a*). Molecules in the layer are oriented identically with

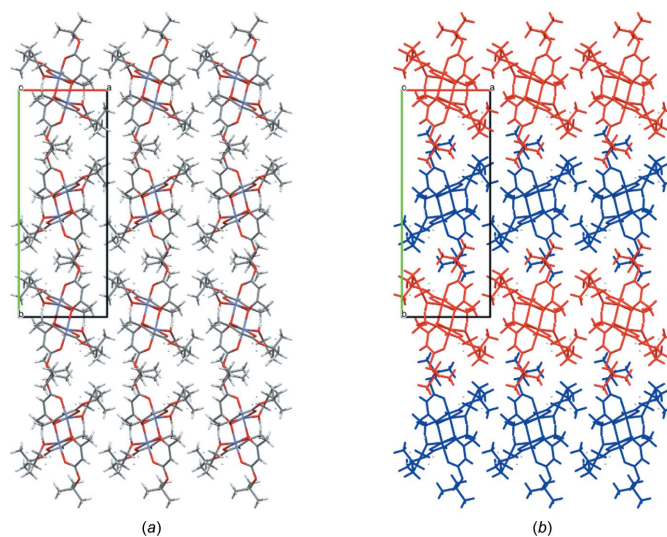


Figure 2
(*a*) Crystal packing of the title compound and (*b*) differently coloured layers in the same projection.

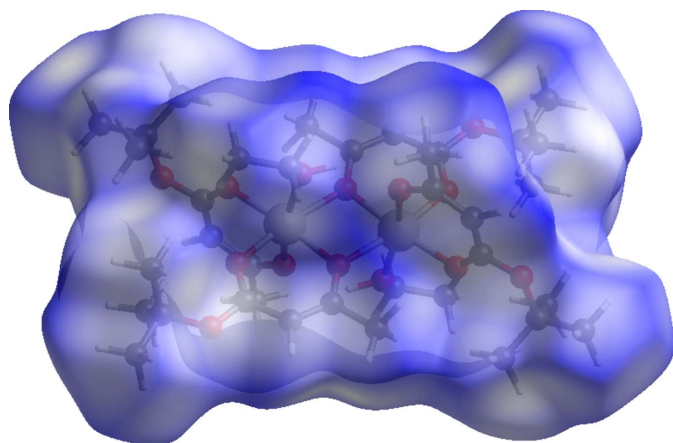


Figure 3
A projection of d_{norm} mapped on the Hirshfeld surface, showing the intermolecular interactions within the molecule.

respect to each other and mirrored with respect to the molecules of the neighbouring layer (Fig. 2*b*).

4. Hirshfeld surface analysis and finger print plots

A Hirshfeld surface analysis was performed and the associated two-dimensional fingerprint plots were generated using *Crystal Explorer 21.5* software (Spackman *et al.*, 2021), with a standard resolution of the three-dimensional d_{norm} surfaces plotted over a fixed colour scale of 0.0290 (white) to 1.706 (blue) a.u. (Fig. 3). Usually contacts shorter than the sums of van der Waals radii are shown in red, those longer in blue, and those approximately equal as white spots. There are no red

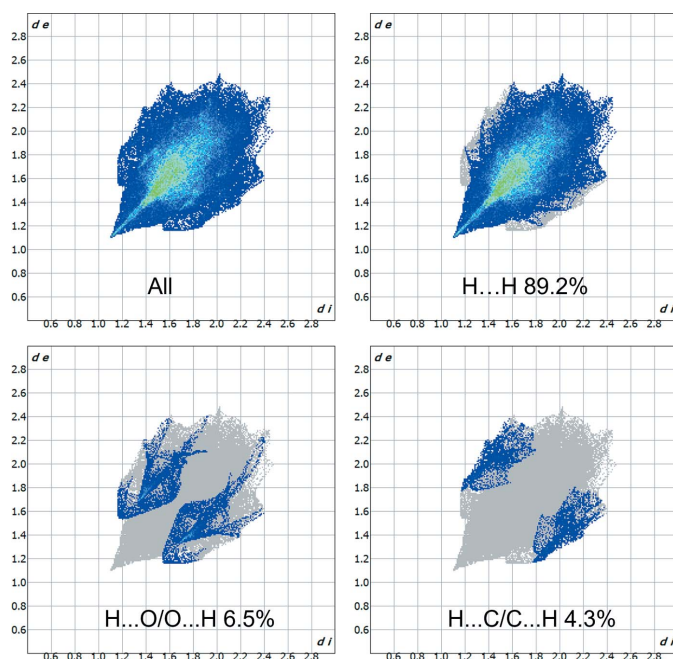


Figure 4
The overall two-dimensional fingerprint plot and those delineated into specified interactions.

spots on the d_{norm} surface. This indicates that there are no strong intermolecular interactions in the structure.

The overall two-dimensional fingerprint plot, and those decomposed into various interactions are given Fig. 4. The most significant contributions to the overall crystal packing are from H...H (89.2%) proximities, which are located mostly in the middle region of the fingerprint plot. There is also a small contribution from H...O/O...H (6.5%) and H...C/C...H (4.3%) intermolecular ‘contacts’.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.43, update November 2022; Groom *et al.*, 2016; ConQuest 2022.3.0; Bruno *et al.*, 2002) for binuclear complexes with different acetoacetic esters yielded seven structures that are very similar to the title compound. Among these structures are three structures with the metal being cobalt (refcodes BENNUG, BENPAO; Shtokvish *et al.*, 2017; WARHAB; Shtokvish *et al.*, 2015), three structures with nickel (refcodes WOCXOE, WOCXUK, WOCYAR; Shtokvish *et al.*, 2018) and one with zinc (refcode GARBOU; Shtokvish *et al.*, 2020). The coordination centres in all cases have an octahedral geometric environment. The M –O bond lengths (1.997 to 2.082 Å) are consistently shorter in the terminal ligand than the M –O bond lengths (2.088 to 2.184 Å) of the bridging ligands.

6. Synthesis and crystallization

The title compound was synthesized in accordance with the methodology reported earlier (Shtokvish *et al.*, 2015). ZnCl_2 (0.1 g, 7 mmol) was dissolved in 2 ml of ethanol (azeotrope with water, 95.6% alcohol). Then liquid *tert*-butyl acetoacetate was added to the solution (0.244 ml, 14 mmol). The components were then mixed. The test tube with the reaction mixture was placed in a container together with a vessel containing triethylamine (0.4 ml, 28 mmol). The container was sealed and left in the refrigerator for 1–2 days at a temperature of 281 K. The structural study was performed for a crystal taken directly and immediately from the reaction mixture, since this compound is prone to degradation. The crystals were filtered on a P2 (P100) fritted glass filter (to separate thin powders of by-products and degradation products), then washed several times with ethanol and dried in air for no more than 1 h. The yield is 0.078 g, which is 25.3% of the theoretical value. The obtained crystals can be stored at 261 K and below.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were placed in calculated positions [$C-H = 0.93$ Å (0.96 Å for C-methyl)] and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C-methyl})$.

The C atoms of the coordinated ethanol molecule are disordered over two positions with an occupancy of 50%. Restraints were applied to the bond lengths in the disordered

Table 3

Experimental details.

Crystal data	
Chemical formula	[Zn ₂ (C ₈ H ₁₃ O ₃) ₄ (C ₂ H ₆ O) ₂]
<i>M_r</i>	851.61
Crystal system, space group	Monoclinic, <i>P2₁/c</i>
Temperature (K)	295
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.1689 (5), 22.8882 (10), 11.0743 (5)
β (°)	103.043 (5)
<i>V</i> (Å ³)	2264.10 (19)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.12
Crystal size (mm)	0.5 × 0.4 × 0.2
Data collection	
Diffraction	Xcalibur, Sapphire3
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2018)
<i>T_{min}</i> , <i>T_{max}</i>	0.460, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	18037, 4622, 3257
<i>R_{int}</i>	0.051
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.625
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.061, 0.154, 1.09
No. of reflections	4622
No. of parameters	268
No. of restraints	53
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.56, -0.34

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL2019/3* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2020).

parts (O—C = 1.45 Å, C—C = 1.49 Å) within a standard deviation of 0.02 Å. The position of the O-bound hydrogen atom was determined from the electron-density map. The O-bound hydrogen atom was refined freely with full occupancy restraining only the O—H bond length to 0.86 Å within a standard deviation of 0.02 Å.

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Computing details

Data collection: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018); data reduction: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018); program(s) used to solve structure: *olex2.solve* 1.5 (Bourhis *et al.*, 2015); program(s) used to refine structure: *SHELXL2019/3* (Sheldrick, 2015); molecular graphics: *Olex2* 1.5 (Dolomanov *et al.*, 2009), *Mercury* 2022.3.0 (Macrae *et al.*, 2020); software used to prepare material for publication: *Olex2* 1.5 (Dolomanov *et al.*, 2009).

Bis(μ -4-*tert*-butoxy-4-oxobut-2-en-2-olato)bis[(4-*tert*-butoxy-4-oxobut-2-en-2-olato)ethanolzinc(II)]

Crystal data

$[\text{Zn}_2(\text{C}_8\text{H}_{15}\text{O}_3)_4(\text{C}_2\text{H}_6\text{O})_2]$

$M_r = 851.61$

Monoclinic, $P2_1/c$

$a = 9.1689$ (5) Å

$b = 22.8882$ (10) Å

$c = 11.0743$ (5) Å

$\beta = 103.043$ (5)°

$V = 2264.10$ (19) Å³

$Z = 2$

$F(000) = 904$

$D_x = 1.249$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2231 reflections

$\theta = 3.7\text{--}21.8^\circ$

$\mu = 1.12$ mm⁻¹

$T = 295$ K

Block, colourless

$0.5 \times 0.4 \times 0.2$ mm

Data collection

Xcalibur, Sapphire3

diffractometer

Detector resolution: 16.1827 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrysAlisPro*; Rigaku OD, 2018)

$T_{\min} = 0.460$, $T_{\max} = 1.000$

18037 measured reflections

4622 independent reflections

3257 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 3.2^\circ$

$h = -11 \rightarrow 11$

$k = -28 \rightarrow 28$

$l = -8 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.061$

$wR(F^2) = 0.154$

$S = 1.09$

4622 reflections

268 parameters

53 restraints

Primary atom site location: iterative

Hydrogen site location: mixed

H atoms treated by a mixture of independent

and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2 + 0.6818P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.56$ e Å⁻³

$\Delta\rho_{\min} = -0.34$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Zn1	0.54544 (5)	0.44504 (2)	0.42445 (4)	0.0662 (2)	
O1	0.3922 (3)	0.47158 (13)	0.2720 (3)	0.0764 (8)	
O2	0.6833 (3)	0.41548 (12)	0.3169 (2)	0.0671 (7)	
O3	0.7330 (3)	0.38286 (15)	0.1401 (3)	0.0882 (9)	
O4	0.3987 (3)	0.46505 (12)	0.5364 (2)	0.0672 (7)	
O5	0.4756 (3)	0.35898 (12)	0.4248 (3)	0.0772 (8)	
O6	0.3134 (3)	0.28661 (12)	0.4379 (2)	0.0738 (7)	
O7	0.7190 (4)	0.43704 (14)	0.5970 (3)	0.0911 (9)	
C1	0.2636 (5)	0.4793 (2)	0.0629 (4)	0.0938 (15)	
H1A	0.172653	0.468769	0.086530	0.141*	
H1B	0.266070	0.461221	-0.014835	0.141*	
H1C	0.267881	0.521015	0.054530	0.141*	
C2	0.3957 (4)	0.45897 (18)	0.1606 (4)	0.0672 (10)	
C3	0.5095 (4)	0.42909 (19)	0.1243 (4)	0.0706 (11)	
H3	0.496600	0.421072	0.040242	0.085*	
C4	0.6431 (4)	0.40970 (17)	0.2033 (4)	0.0666 (10)	
C5	0.8841 (5)	0.3624 (2)	0.1982 (5)	0.0897 (14)	
C6	0.9817 (5)	0.4121 (3)	0.2556 (6)	0.1108 (18)	
H6A	0.963480	0.445332	0.201407	0.166*	
H6B	1.084927	0.400825	0.268616	0.166*	
H6C	0.959237	0.422025	0.333682	0.166*	
C7	0.8762 (7)	0.3149 (3)	0.2906 (7)	0.131 (2)	
H7A	0.845972	0.331407	0.360811	0.197*	
H7B	0.972864	0.297042	0.317296	0.197*	
H7C	0.804662	0.285930	0.252621	0.197*	
C8	0.9363 (7)	0.3385 (4)	0.0867 (6)	0.155 (3)	
H8A	0.862961	0.311646	0.042344	0.233*	
H8B	1.030025	0.318583	0.114494	0.233*	
H8C	0.948707	0.370145	0.033114	0.233*	
C9	0.1984 (7)	0.4577 (2)	0.6368 (6)	0.123 (2)	
H9A	0.256051	0.467295	0.717969	0.184*	
H9B	0.120541	0.430766	0.643732	0.184*	
H9C	0.154656	0.492652	0.596048	0.184*	
C10	0.2986 (5)	0.43028 (19)	0.5624 (4)	0.0705 (11)	
C11	0.2793 (5)	0.37331 (19)	0.5304 (4)	0.0739 (11)	
H11	0.203184	0.353451	0.556179	0.089*	
C12	0.3643 (5)	0.34110 (17)	0.4612 (3)	0.0652 (10)	
C13	0.3831 (5)	0.24431 (19)	0.3696 (4)	0.0776 (12)	
C14	0.2860 (7)	0.1908 (2)	0.3683 (5)	0.1141 (19)	

H14A	0.285700	0.179792	0.451860	0.171*	
H14B	0.325115	0.159240	0.327984	0.171*	
H14C	0.185651	0.199405	0.324153	0.171*	
C15	0.3773 (8)	0.2664 (3)	0.2393 (4)	0.122 (2)	
H15A	0.275191	0.274108	0.198153	0.183*	
H15B	0.418317	0.237424	0.193851	0.183*	
H15C	0.434563	0.301784	0.243508	0.183*	
C16	0.5409 (6)	0.2315 (2)	0.4396 (5)	0.1051 (17)	
H16A	0.601067	0.265992	0.441878	0.158*	
H16B	0.581885	0.200646	0.398803	0.158*	
H16C	0.540080	0.219781	0.522665	0.158*	
C17A	0.7360 (17)	0.3935 (4)	0.6946 (9)	0.120 (2)	0.502 (9)
H17A	0.640986	0.375180	0.695965	0.144*	0.502 (9)
H17B	0.777579	0.410583	0.775206	0.144*	0.502 (9)
C17B	0.7398 (17)	0.3790 (2)	0.6508 (10)	0.119 (2)	0.498 (9)
H17C	0.758504	0.352034	0.588523	0.142*	0.498 (9)
H17D	0.647661	0.367100	0.672769	0.142*	0.498 (9)
C18A	0.8418 (16)	0.3510 (6)	0.6591 (14)	0.151 (3)	0.502 (9)
H18A	0.939453	0.368299	0.671692	0.226*	0.502 (9)
H18B	0.807363	0.340685	0.573319	0.226*	0.502 (9)
H18C	0.846888	0.316516	0.709264	0.226*	0.502 (9)
C18B	0.8644 (15)	0.3742 (6)	0.7627 (12)	0.142 (3)	0.498 (9)
H18D	0.941201	0.349365	0.744778	0.212*	0.498 (9)
H18E	0.827299	0.357902	0.829736	0.212*	0.498 (9)
H18F	0.905194	0.412323	0.785632	0.212*	0.498 (9)
H7	0.692 (4)	0.4672 (10)	0.633 (3)	0.079 (14)*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0695 (3)	0.0780 (3)	0.0560 (3)	0.0014 (2)	0.0247 (2)	0.0122 (2)
O1	0.0709 (18)	0.101 (2)	0.0607 (17)	0.0149 (15)	0.0226 (14)	0.0153 (15)
O2	0.0607 (15)	0.0879 (18)	0.0556 (16)	0.0049 (13)	0.0193 (13)	0.0093 (14)
O3	0.0650 (18)	0.133 (3)	0.0683 (19)	0.0093 (17)	0.0196 (15)	-0.0132 (18)
O4	0.0752 (17)	0.0740 (16)	0.0594 (16)	-0.0039 (14)	0.0297 (14)	0.0126 (13)
O5	0.0866 (19)	0.0788 (18)	0.0735 (19)	-0.0078 (16)	0.0333 (16)	0.0084 (14)
O6	0.0857 (19)	0.0751 (18)	0.0636 (17)	-0.0105 (15)	0.0233 (15)	-0.0032 (14)
O7	0.110 (2)	0.090 (2)	0.073 (2)	0.0219 (18)	0.0186 (18)	0.0182 (16)
C1	0.067 (3)	0.141 (4)	0.072 (3)	0.006 (3)	0.012 (2)	0.020 (3)
C2	0.058 (2)	0.086 (3)	0.059 (2)	-0.008 (2)	0.015 (2)	0.016 (2)
C3	0.058 (2)	0.106 (3)	0.050 (2)	-0.004 (2)	0.0160 (19)	0.002 (2)
C4	0.062 (2)	0.081 (3)	0.063 (3)	-0.009 (2)	0.026 (2)	-0.001 (2)
C5	0.067 (3)	0.120 (4)	0.085 (3)	0.015 (3)	0.023 (3)	-0.001 (3)
C6	0.063 (3)	0.155 (5)	0.113 (4)	-0.004 (3)	0.019 (3)	0.009 (4)
C7	0.114 (5)	0.112 (4)	0.171 (7)	0.034 (4)	0.039 (5)	0.020 (4)
C8	0.090 (4)	0.257 (9)	0.123 (5)	0.050 (5)	0.032 (4)	-0.049 (5)
C9	0.135 (5)	0.100 (4)	0.169 (6)	-0.036 (3)	0.108 (5)	-0.027 (4)
C10	0.074 (3)	0.086 (3)	0.058 (2)	-0.010 (2)	0.027 (2)	0.008 (2)

C11	0.078 (3)	0.084 (3)	0.067 (3)	-0.020 (2)	0.031 (2)	-0.002 (2)
C12	0.075 (3)	0.073 (3)	0.046 (2)	-0.003 (2)	0.0083 (19)	0.0114 (18)
C13	0.097 (3)	0.084 (3)	0.053 (2)	-0.007 (3)	0.020 (2)	-0.001 (2)
C14	0.144 (5)	0.089 (3)	0.113 (4)	-0.024 (3)	0.037 (4)	-0.018 (3)
C15	0.186 (6)	0.125 (4)	0.056 (3)	0.002 (4)	0.030 (4)	-0.001 (3)
C16	0.109 (4)	0.107 (4)	0.103 (4)	0.005 (3)	0.032 (4)	-0.001 (3)
C17A	0.140 (4)	0.111 (4)	0.095 (4)	0.033 (4)	-0.005 (4)	-0.002 (3)
C17B	0.138 (4)	0.109 (4)	0.095 (4)	0.038 (4)	-0.003 (4)	0.000 (3)
C18A	0.159 (6)	0.139 (6)	0.132 (6)	0.027 (6)	-0.014 (6)	0.004 (6)
C18B	0.157 (6)	0.135 (6)	0.114 (6)	0.032 (5)	-0.008 (6)	0.006 (5)

Geometric parameters (Å, °)

Zn1—O1	2.031 (3)	C8—H8B	0.9600
Zn1—O2	2.039 (3)	C8—H8C	0.9600
Zn1—O4 ⁱ	2.141 (3)	C9—H9A	0.9600
Zn1—O4	2.076 (2)	C9—H9B	0.9600
Zn1—O5	2.072 (3)	C9—H9C	0.9600
Zn1—O7	2.201 (3)	C9—C10	1.503 (6)
O1—C2	1.273 (5)	C10—C11	1.352 (6)
O2—C4	1.235 (5)	C11—H11	0.9300
O3—C4	1.345 (5)	C11—C12	1.417 (6)
O3—C5	1.467 (5)	C13—C14	1.512 (6)
O4—C10	1.295 (4)	C13—C15	1.519 (6)
O5—C12	1.248 (5)	C13—C16	1.508 (6)
O6—C12	1.336 (5)	C14—H14A	0.9600
O6—C13	1.461 (5)	C14—H14B	0.9600
O7—C17A	1.452 (2)	C14—H14C	0.9600
O7—C17B	1.450 (2)	C15—H15A	0.9600
O7—H7	0.860 (2)	C15—H15B	0.9600
C1—H1A	0.9600	C15—H15C	0.9600
C1—H1B	0.9600	C16—H16A	0.9600
C1—H1C	0.9600	C16—H16B	0.9600
C1—C2	1.505 (6)	C16—H16C	0.9600
C2—C3	1.381 (5)	C17A—H17A	0.9700
C3—H3	0.9300	C17A—H17B	0.9700
C3—C4	1.407 (6)	C17A—C18A	1.489 (2)
C5—C6	1.498 (7)	C17B—H17C	0.9700
C5—C7	1.506 (7)	C17B—H17D	0.9700
C5—C8	1.522 (7)	C17B—C18B	1.487 (2)
C6—H6A	0.9600	C18A—H18A	0.9600
C6—H6B	0.9600	C18A—H18B	0.9600
C6—H6C	0.9600	C18A—H18C	0.9600
C7—H7A	0.9600	C18B—H18D	0.9600
C7—H7B	0.9600	C18B—H18E	0.9600
C7—H7C	0.9600	C18B—H18F	0.9600
C8—H8A	0.9600		

O1—Zn1—O2	90.99 (11)	H8A—C8—H8C	109.5
O1—Zn1—O4 ⁱ	88.27 (12)	H8B—C8—H8C	109.5
O1—Zn1—O4	90.61 (11)	H9A—C9—H9B	109.5
O1—Zn1—O5	97.46 (12)	H9A—C9—H9C	109.5
O1—Zn1—O7	167.36 (12)	H9B—C9—H9C	109.5
O2—Zn1—O4	173.35 (10)	C10—C9—H9A	109.5
O2—Zn1—O4 ⁱ	106.60 (10)	C10—C9—H9B	109.5
O2—Zn1—O5	85.30 (11)	C10—C9—H9C	109.5
O2—Zn1—O7	93.30 (12)	O4—C10—C9	114.6 (4)
O4—Zn1—O4 ⁱ	79.90 (10)	O4—C10—C11	126.3 (4)
O4 ⁱ —Zn1—O7	79.11 (11)	C11—C10—C9	119.1 (4)
O4—Zn1—O7	86.49 (12)	C10—C11—H11	117.0
O5—Zn1—O4	88.08 (11)	C10—C11—C12	126.0 (4)
O5—Zn1—O4 ⁱ	166.76 (10)	C12—C11—H11	117.0
O5—Zn1—O7	94.74 (12)	O5—C12—O6	121.2 (4)
C2—O1—Zn1	125.0 (3)	O5—C12—C11	126.4 (4)
C4—O2—Zn1	123.2 (3)	O6—C12—C11	112.3 (4)
C4—O3—C5	123.2 (3)	O6—C13—C14	102.5 (4)
Zn1—O4—Zn1 ⁱ	100.10 (10)	O6—C13—C15	110.2 (4)
C10—O4—Zn1 ⁱ	134.0 (3)	O6—C13—C16	110.1 (4)
C10—O4—Zn1	125.8 (3)	C14—C13—C15	111.5 (4)
C12—O5—Zn1	126.0 (3)	C16—C13—C14	110.0 (4)
C12—O6—C13	123.0 (3)	C16—C13—C15	112.2 (4)
Zn1—O7—H7	96 (3)	C13—C14—H14A	109.5
C17A—O7—Zn1	129.7 (7)	C13—C14—H14B	109.5
C17A—O7—H7	102 (3)	C13—C14—H14C	109.5
C17B—O7—Zn1	115.8 (5)	H14A—C14—H14B	109.5
C17B—O7—H7	125 (3)	H14A—C14—H14C	109.5
H1A—C1—H1B	109.5	H14B—C14—H14C	109.5
H1A—C1—H1C	109.5	C13—C15—H15A	109.5
H1B—C1—H1C	109.5	C13—C15—H15B	109.5
C2—C1—H1A	109.5	C13—C15—H15C	109.5
C2—C1—H1B	109.5	H15A—C15—H15B	109.5
C2—C1—H1C	109.5	H15A—C15—H15C	109.5
O1—C2—C1	115.7 (4)	H15B—C15—H15C	109.5
O1—C2—C3	125.4 (4)	C13—C16—H16A	109.5
C3—C2—C1	118.8 (4)	C13—C16—H16B	109.5
C2—C3—H3	117.1	C13—C16—H16C	109.5
C2—C3—C4	125.7 (4)	H16A—C16—H16B	109.5
C4—C3—H3	117.1	H16A—C16—H16C	109.5
O2—C4—O3	120.1 (4)	H16B—C16—H16C	109.5
O2—C4—C3	128.1 (4)	O7—C17A—H17A	111.2
O3—C4—C3	111.7 (4)	O7—C17A—H17B	111.2
O3—C5—C6	111.0 (4)	O7—C17A—C18A	102.6 (8)
O3—C5—C7	110.1 (4)	H17A—C17A—H17B	109.2
O3—C5—C8	101.4 (4)	C18A—C17A—H17A	111.2
C6—C5—C7	112.0 (5)	C18A—C17A—H17B	111.2
C6—C5—C8	110.5 (5)	O7—C17B—H17C	108.6

C7—C5—C8	111.4 (5)	O7—C17B—H17D	108.6
C5—C6—H6A	109.5	O7—C17B—C18B	114.5 (8)
C5—C6—H6B	109.5	H17C—C17B—H17D	107.6
C5—C6—H6C	109.5	C18B—C17B—H17C	108.6
H6A—C6—H6B	109.5	C18B—C17B—H17D	108.6
H6A—C6—H6C	109.5	C17A—C18A—H18A	109.5
H6B—C6—H6C	109.5	C17A—C18A—H18B	109.5
C5—C7—H7A	109.5	C17A—C18A—H18C	109.5
C5—C7—H7B	109.5	H18A—C18A—H18B	109.5
C5—C7—H7C	109.5	H18A—C18A—H18C	109.5
H7A—C7—H7B	109.5	H18B—C18A—H18C	109.5
H7A—C7—H7C	109.5	C17B—C18B—H18D	109.5
H7B—C7—H7C	109.5	C17B—C18B—H18E	109.5
C5—C8—H8A	109.5	C17B—C18B—H18F	109.5
C5—C8—H8B	109.5	H18D—C18B—H18E	109.5
C5—C8—H8C	109.5	H18D—C18B—H18F	109.5
H8A—C8—H8B	109.5	H18E—C18B—H18F	109.5
Zn1—O1—C2—C1	175.2 (3)	C2—C3—C4—O2	0.0 (7)
Zn1—O1—C2—C3	-5.2 (6)	C2—C3—C4—O3	-178.9 (4)
Zn1—O2—C4—O3	-171.2 (3)	C4—O3—C5—C6	-60.4 (6)
Zn1—O2—C4—C3	10.0 (6)	C4—O3—C5—C7	64.2 (6)
Zn1 ⁱ —O4—C10—C9	-0.3 (6)	C4—O3—C5—C8	-177.8 (5)
Zn1—O4—C10—C9	-174.9 (4)	C5—O3—C4—O2	-3.7 (6)
Zn1 ⁱ —O4—C10—C11	-179.5 (3)	C5—O3—C4—C3	175.2 (4)
Zn1—O4—C10—C11	5.9 (6)	C9—C10—C11—C12	-179.8 (5)
Zn1—O5—C12—O6	168.2 (3)	C10—C11—C12—O5	4.4 (7)
Zn1—O5—C12—C11	-12.6 (6)	C10—C11—C12—O6	-176.3 (4)
Zn1—O7—C17A—C18A	95.5 (12)	C12—O6—C13—C14	-180.0 (4)
Zn1—O7—C17B—C18B	176.2 (11)	C12—O6—C13—C15	-61.2 (5)
O1—C2—C3—C4	-2.8 (7)	C12—O6—C13—C16	63.0 (5)
O4—C10—C11—C12	-0.6 (8)	C13—O6—C12—O5	0.2 (6)
C1—C2—C3—C4	176.8 (4)	C13—O6—C12—C11	-179.1 (4)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H7 [⋯] O1 ⁱ	0.86 (1)	2.01 (1)	2.861 (4)	171 (4)

Symmetry code: (i) $-x+1, -y+1, -z+1$.