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Chiral crystallization of a zinc(II) complex

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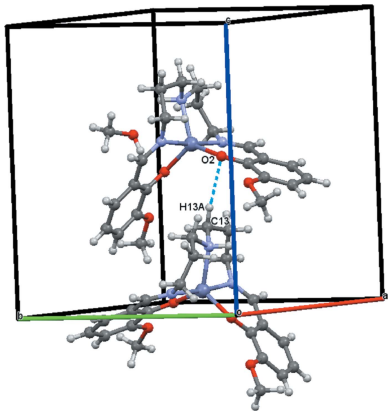
The compound, {6,6′-dimethoxy-2,2′-[(4-azaheptane-1,7-diyl)bis(nitrilomethanylidyne)]diphenolato}zinc(II) methanol monosolvate, $[Zn(C_{22}H_{27}N_3O_4)]\cdot CH_3OH$, at 298 K crystallizes in the orthorhombic space group $Pna2_1$. The Zn atom is coordinated by a pentadentate Schiff base ligand in a distorted trigonal–bipyramidal N_3O_2 geometry. The equatorial plane is formed by the two phenolic O and one amine N atom. The axial positions are occupied by two amine N atoms. The distorted bipyramidal geometry is also supported by the trigonality index (τ), which is found to be 0.85 for the molecule. In the crystal, methanol solvent molecule is connected to the complex molecule by an O—H···O hydrogen bond and the complex molecules are connected by weak supramolecular interactions, so achiral molecules generate a chiral crystal. The Hirshfeld surface analysis suggests that H···H contacts account for the largest percentage of all interactions.

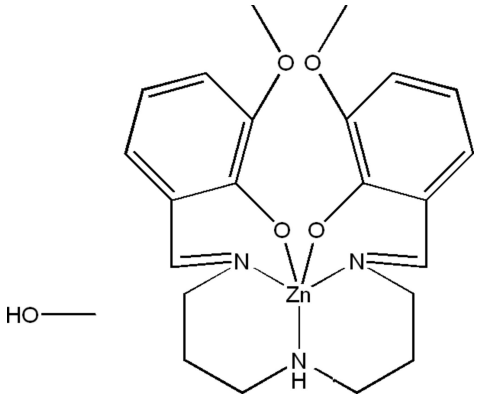
1. Chemical context

Schiff bases and their coordination compounds play an important role in metal coordination chemistry owing to their thermal stability, relevant biological properties and high synthesis flexibility (Bartyzel, 2018; Siddiqui *et al.*, 2006; Sacconi, 1966). These ligands are able to coordinate a wide variety of metal ions and to stabilize them in various oxidation states. The coordination geometry of the complexes depends upon the chemical structure of the chosen ligand, the coordination geometry preferred by the metal, the metal-to-ligand ratio, the reaction time and temperature (Thakurta *et al.*, 2010; Fleck *et al.*, 2013; Sanmartín *et al.*, 2001; Khalaji *et al.*, 2011). A number of zinc(II) complexes with different Schiff base ligands and their potential applications in sensing and as antibacterial and anticancer agents have been documented in the literature (Lui *et al.*,2019; Niu *et al.*, 2015; Tang *et al.*, 2013; AlDamen *et al.*, 2016; Iksi *et al.*, 2020). In addition, lanthanide Schiff base compounds are the subject of immense research interest because of their unique structures and their potential applications in advanced materials such as undoped semiconductors, magnetic, catalytic and florescent and non-linear optical materials (Li *et al.*, 2016; Ishikawa *et al.*, 2003; Long *et al.*, 2018*b*).

In a previous work, we reported the crystal and molecular structure of a Cu^{II} complex based on Schiff base ligand *N*1,*N*3-bis(3-methoxysalicylicylidene)diethylenetriamine where two Schiff base ligands join two Cu^{II} ions in a chelate–spacer–chelate mode, in which the protonated aliphatic secondary



amine moieties represents the spacer to form a double helix (Noor *et al.*, 2018). In an another report, we redetermined the crystal structure of an organic–inorganic salt of an Mn^{II}–Schiff base ligand complex $Mn(C_{18}H_{18}N_2O_4)(H_2O)_2]ClO_4$ at 100 K. In contrast to crystal-structure determinations at room temperature (Akitsu *et al.*, 2005, Bermejo *et al.*, 2007), positional disorder of the ethylene bridge in the Schiff base and the perchlorate anion was not observed at 100 K (Noor *et al.* 2016). We now report the chiral crystallization on a zinc(II) complex.



2. Structural commentary

In the title compound (Fig. 1), the Zn atom is coordinated by a pentadentate Schiff base ligand in distorted trigonal–bipyramidal [ONNNO] geometry. The equatorial plane is formed by the two phenolic O [Zn—O3 = 2.001 (2) Å; Zn—O2 = 1.975 (2) Å] and one amine N [Zn—N2 = 2.152 (3) Å]. The axial positions are occupied by amine N atoms [Zn—N1 = 2.094 (2) Å, Zn—N3; 2.107 (2) Å]. The trigonality index (τ) for the complex is calculated as $\tau = (\beta - \alpha)/60$ where α and β are the main opposing angles in the coordination polyhedron (Addison *et al.*, 1984). For perfect square-pyramidal and trigonal–bipyramidal coordination geometries, the values of τ are zero and unity, respectively. In the present complex, for Zn, β = O2—Zn—O3 = 122.87 (10)° and α = N1—Zn—N3 = 173.91 (12)° so the trigonality index is 0.85. According to this value, the coordination geometry around the zinc ion is best described as distorted trigonal–bipyramidal. An intramolecular O—H···O hydrogen bond is observed between the methoxy function and the oxygen atom in the six-membered ring (Table 1). This molecule has neither an asymmetric carbon nor a helical structure, so it is an achiral compound.

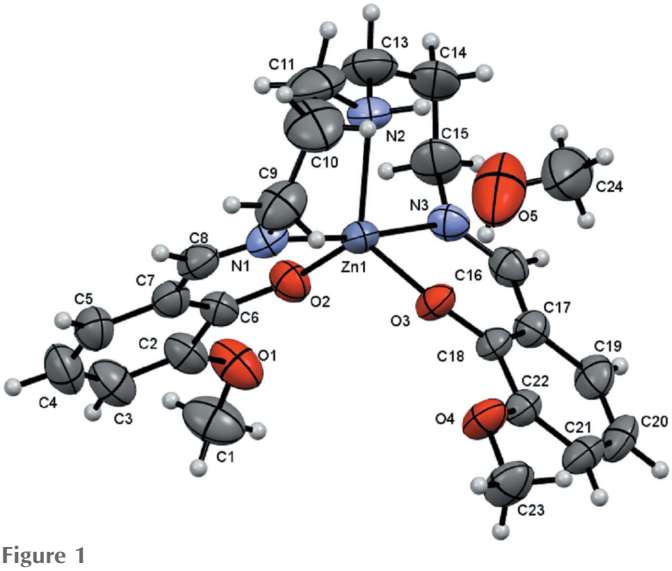


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13A···O2^{i}	0.97	2.58	3.549 (6)	172
C10—H10B···O5	0.97	2.50	3.340 (7)	144
O5—H5A···O3	0.82	2.01	2.722 (5)	144

Symmetry code: (i) $-x+1, -y+1, z+\frac{1}{2}$.

3. Supramolecular features

In the crystal, molecules are connected by O—H···O hydrogen bonds (Fig. 2, Table 1). In addition, weak supramolecular C—H···O interactions are found (Table 1 and Fig. 3).

4. Hirshfeld Surface analysis

In order to visualize the intermolecular interactions in the crystal of the title compound, a Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) was performed with *CrystalExplorer17.5* (Turner *et al.*, 2017). The fingerprint plot for this

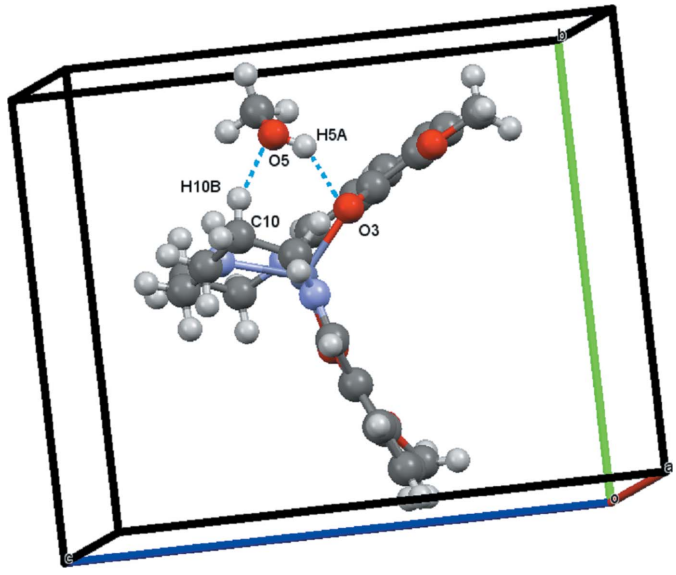


Figure 2
A view of the O5—H5A···O3 and C10—H10B···O5 interactions (dashed lines).

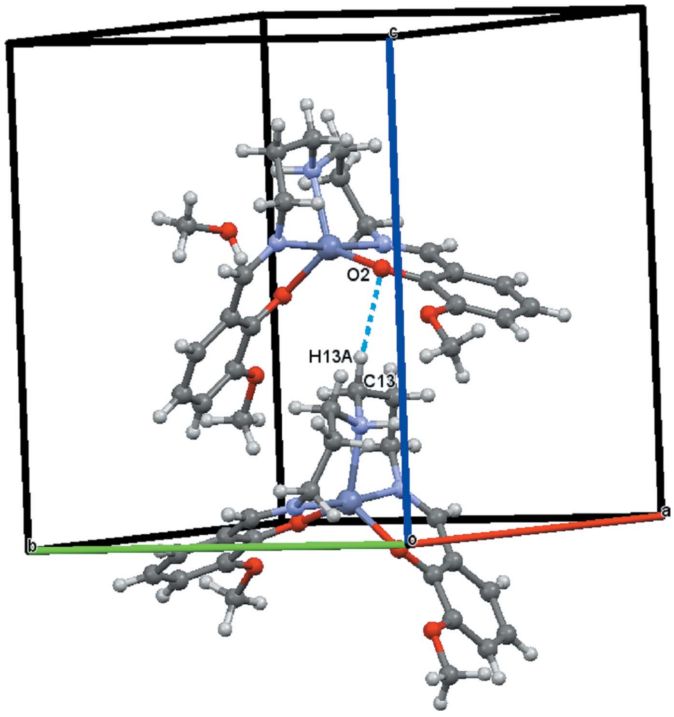


Figure 3
A view of the C13—H13*A*···O2 interaction (dashed lines).

structure shows typical 'wings' (Fig. 4i). The percentage contribution to the Hirshfeld surface area by close contacts with H atoms inside the surface and H atoms outside is 57.4% (Fig. 4ii), for O atoms inside the surface and H atoms outside it is 9.1% (Fig. 4iii), for H atoms inside the surface and O atoms outside it is 8.5% (Fig. 4iv), for C atoms inside the surface and H atoms outside it is 14.5% (Fig. 4v), and for H atoms inside the surface and C atoms outside it is 8.2% (Fig. 4vi). Hirshfeld surface analysis of the H···O interaction clearly shows the close intermolecular contact near methanol, (d_i is 1.1 Å and d_e is 0.75 Å).

5. Database survey

A search in the Cambridge Structural Database (CSD, Version 5.41, update November 2019; Groom *et al.*, 2016) for similar structures returned three relevant entries: (2,2′-bipyridine-κ^2N,N')[*N*-(2-oxido-1-naphthylidene)threoninato-κ^3O^1,N,O^2]-copper(II) (BIZGIB; Qiu *et al.*, 2008), diaqua(*N*-salicylidene-L-threoninato)copper(II) (SLCDCU; Korhonen & Hämäläinen, 1981) and [*N*-(3-methoxy-2-oxidobenzylidene-κO^2)-threoninato-κ^2O^1,N](1,10-phenanthroline-κ^2N,N')copper(II) hemihydrate (UQUYUB; Jing *et al.*, 2011). The metal atom in BIZGIB is five-coordinated by one N atom and two O atoms, and two N atoms from a distorted square-pyramidal 2,2-bipyridine ligand. In the crystal, a two-dimensional network is formed by a combination of intermolecular O—H···O and C—H···O hydrogen bonds. In SLCDCU, two molecules form square planes by two intermolecular hydrogen bonds. In UQUYUB, intermolecular O—H···O hydrogen bonds form a one-dimensional left-handed helical structure extending parallel to [001].

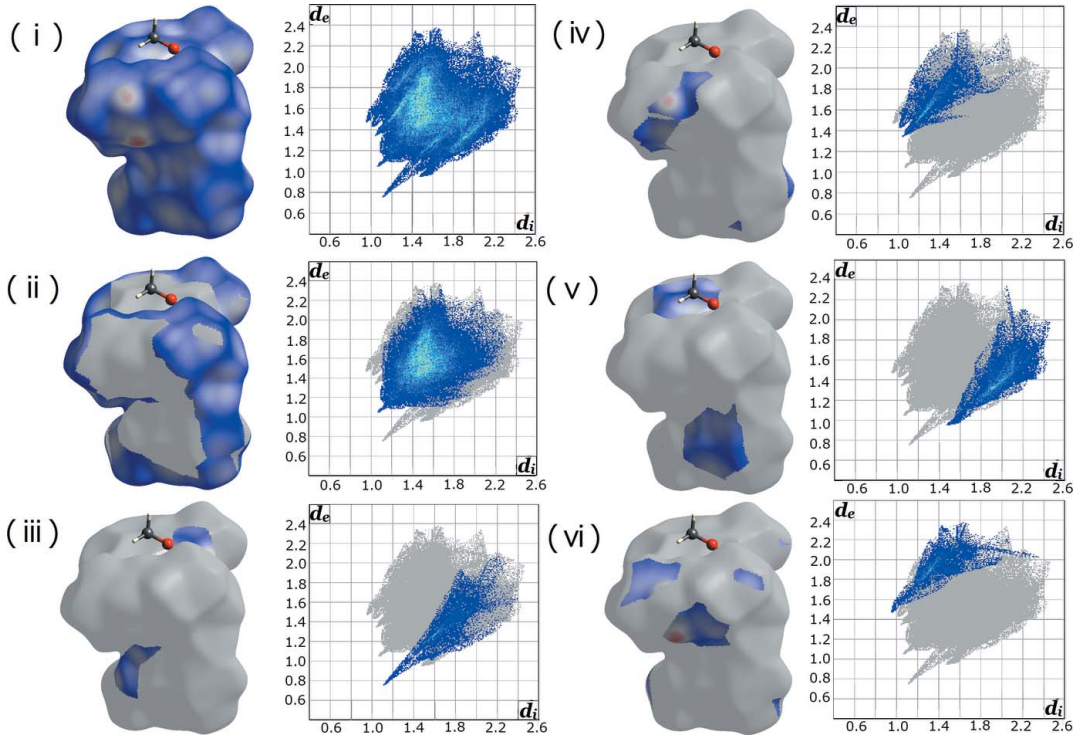


Figure 4
The three-dimensional Hirshfeld surface showing the intermolecular interactions plotted over d_{norm} and the two-dimensional fingerprint plots of the title compound, showing (i) all interactions, and delineated into (ii) H···H, (iii) O···H, (iv) H···O, (v) C···H and (vi) H···C interactions.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_{22}H_{27}N_3O_4)]\cdot CH_4O$
M_r	494.88
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	293
a, b, c (Å)	14.5937 (6), 11.4425 (5), 13.5794 (5)
V (Å^3)	2267.60 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.12
Crystal size (mm)	0.53 × 0.49 × 0.45
Data collection	
Diffractometer	Bruker APEXIII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2017)
T_{min}, T_{max}	0.53, 0.63
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28025, 6099, 4682
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.730
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.087, 1.04
No. of reflections	6099
No. of parameters	294
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.47
Absolute structure	Flack x determined using 1852 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.006 (5)

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *shelXle* (Hübschle *et al.*, 2011) and *SHELXTL* (Sheldrick, 2008).

6. Synthesis and crystallization

The Schiff base ligand H_2L was prepared according to a reported procedure (Matar *et al.*, 2015) by a condensation reaction between 3-methoxy-2-hydroxybenzaldehyde (10 mmol, 1.52 mg) and dipropylenetriamine (5.0 mmol, 0.641 mL) in ethanol solution (30 cm^3) under reflux conditions. After solvent removal, a yellow oil was obtained in 85% yield. ν(C═N) 1630 cm^{-1}.

The title compound was synthesized by the reaction of H_2L (1 mmol, 0.399 mg) with $Zn(OAc)_2\cdot 2H_2O$ (1 mmol, 0.18 mg) in MeOH:H_2O (v/v, 10:1) (50 cm^3) with a few drops of LiOH (1%). The reaction mixture was heated to 343 K for 1 h. The yellow solid obtained was filtered off and dried. ν(C═N) 1618 cm^{-1}. Single crystals suitable for X-ray crystallography were obtained several days after dissolving the solid in 40 cm^3 of hot methanol.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All C-bound H atoms were placed in geometrically calculated positions and refined using a riding model [C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms]. The O-bound H atom was located in a difference-Fourier map and refined using a riding model [O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O)].

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supporting information

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Computing details

Data collection: *APEX3* (Bruker, 2017); cell refinement: *APEX3* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015b); molecular graphics: *shelXle* (Hübschle *et al.*, 2011); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

{6,6′-Dimethoxy-2,2′-[(4-azaheptane-1,7-diyl)bis(nitrilomethanylidyne)]diphenolato}zinc(II) methanol monosolvate

Crystal data

$[Zn(C_{22}H_{27}N_3O_4)]\cdot CH_4O$
M_r = 494.88
Orthorhombic, $Pna2_1$
a = 14.5937 (6) Å
b = 11.4425 (5) Å
c = 13.5794 (5) Å
V = 2267.60 (16) Å^3
Z = 4
$F(000)$ = 1040
D_x = 1.450 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3270 reflections
θ = 2.2–23.9°
μ = 1.12 mm^{-1}
T = 293 K
Prism, yellow
0.53 × 0.49 × 0.45 mm

Data collection

Bruker APEXIII CCD diffractometer
Detector resolution: 7.3910 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.53, T_{max} = 0.63
28025 measured reflections
6099 independent reflections
4682 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 31.2°, θ_{min} = 2.3°
h = −21→20
k = −16→16
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.087
S = 1.04
6099 reflections
294 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick 2015b)

Extinction coefficient: 0.0091 (12)

Absolute structure: Flack *x* determined using 1852 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.006 (5)

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.

Refinement. Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.
_reflns_Friedel_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.52170 (2)	0.52816 (3)	0.56294 (4)	0.04284 (12)
O1	0.40493 (18)	0.1936 (2)	0.4333 (2)	0.0724 (8)
N1	0.65984 (15)	0.4787 (2)	0.5612 (3)	0.0493 (5)
C1	0.3627 (3)	0.1110 (5)	0.3702 (4)	0.0857 (13)
H1A	0.396883	0.10538	0.310017	0.129*
H1B	0.301217	0.135516	0.355979	0.129*
H1C	0.361408	0.036045	0.401999	0.129*
O2	0.48708 (13)	0.3687 (2)	0.52144 (19)	0.0520 (5)
N2	0.5413 (2)	0.5782 (3)	0.7143 (2)	0.0650 (8)
H2	0.529572	0.662482	0.715739	0.078*
C2	0.4980 (2)	0.1835 (3)	0.4463 (3)	0.0549 (8)
O3	0.53164 (12)	0.6620 (2)	0.46866 (16)	0.0457 (5)
N3	0.38225 (17)	0.5711 (2)	0.58014 (19)	0.0486 (6)
C3	0.5487 (3)	0.0903 (3)	0.4162 (3)	0.0693 (10)
H3	0.520034	0.028129	0.38465	0.083*
C4	0.6437 (3)	0.0868 (3)	0.4321 (3)	0.0720 (10)
H4	0.677466	0.021275	0.414127	0.086*
O4	0.58178 (14)	0.7754 (2)	0.30994 (16)	0.0545 (5)
C5	0.6856 (2)	0.1802 (3)	0.4741 (3)	0.0610 (8)
H5	0.74875	0.179029	0.483288	0.073*
O5	0.5841 (3)	0.8341 (4)	0.5950 (4)	0.140 (2)
H5A	0.581512	0.801846	0.541104	0.21*
C6	0.5391 (2)	0.2829 (3)	0.4930 (2)	0.0453 (6)
C7	0.6353 (2)	0.2785 (3)	0.5037 (2)	0.0479 (6)
C8	0.68830 (19)	0.3763 (3)	0.54147 (19)	0.0502 (7)
H8	0.750228	0.362278	0.552506	0.06*
C9	0.7273 (3)	0.5641 (4)	0.5954 (3)	0.0735 (11)
H9A	0.731688	0.625957	0.54678	0.088*
H9B	0.786656	0.526017	0.59861	0.088*
C10	0.7079 (3)	0.6176 (5)	0.6924 (4)	0.0995 (17)
H10A	0.763926	0.615887	0.730831	0.119*

H10B	0.692303	0.698978	0.681751	0.119*
C11	0.6358 (4)	0.5649 (5)	0.7506 (3)	0.0890 (14)
H11A	0.638748	0.597758	0.816366	0.107*
H11B	0.648732	0.48201	0.756321	0.107*
C13	0.4737 (4)	0.5284 (4)	0.7786 (4)	0.0809 (15)
H13A	0.488874	0.551024	0.845482	0.097*
H13B	0.47908	0.444052	0.774871	0.097*
C14	0.3754 (4)	0.5598 (5)	0.7606 (3)	0.0848 (14)
H14A	0.369652	0.644202	0.763231	0.102*
H14B	0.338813	0.527906	0.81384	0.102*
C15	0.3349 (3)	0.5172 (4)	0.6626 (3)	0.0708 (11)
H15A	0.340711	0.432901	0.658309	0.085*
H15B	0.270299	0.536678	0.659841	0.085*
C16	0.33585 (19)	0.6329 (3)	0.5196 (2)	0.0491 (7)
H16	0.273212	0.638729	0.531279	0.059*
C17	0.37116 (18)	0.6945 (3)	0.4351 (2)	0.0444 (6)
C18	0.46571 (18)	0.7052 (3)	0.4135 (2)	0.0395 (6)
C19	0.3057 (2)	0.7452 (3)	0.3712 (3)	0.0560 (8)
H19	0.243749	0.739602	0.386674	0.067*
C20	0.3314 (2)	0.8021 (3)	0.2878 (3)	0.0606 (8)
H20	0.287289	0.833751	0.246236	0.073*
C21	0.4235 (2)	0.8127 (3)	0.2647 (2)	0.0536 (8)
H21	0.440955	0.850523	0.207094	0.064*
C22	0.4898 (2)	0.7674 (3)	0.3267 (2)	0.0432 (6)
C23	0.6092 (3)	0.8324 (4)	0.2225 (3)	0.0684 (10)
H23A	0.585095	0.791083	0.166649	0.103*
H23B	0.674874	0.833728	0.218869	0.103*
H23C	0.586221	0.910978	0.222502	0.103*
C24	0.5060 (6)	0.8915 (6)	0.6115 (6)	0.123 (2)
H24A	0.519332	0.971869	0.626096	0.185*
H24B	0.47469	0.856789	0.666377	0.185*
H24C	0.467835	0.887306	0.554073	0.185*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.04857 (18)	0.04890 (19)	0.03106 (16)	0.00482 (12)	−0.00223 (18)	0.00193 (18)
O1	0.0517 (13)	0.0781 (16)	0.0876 (19)	−0.0119 (13)	0.0060 (13)	−0.0318 (16)
N1	0.0489 (10)	0.0563 (13)	0.0427 (11)	−0.0010 (10)	−0.0077 (17)	0.0044 (15)
C1	0.075 (3)	0.101 (3)	0.081 (3)	−0.025 (2)	0.002 (2)	−0.032 (3)
O2	0.0430 (9)	0.0563 (12)	0.0568 (13)	0.0031 (9)	0.0028 (9)	−0.0092 (11)
N2	0.0852 (19)	0.073 (2)	0.0362 (14)	0.0177 (17)	−0.0110 (14)	−0.0066 (15)
C2	0.0546 (15)	0.057 (2)	0.0533 (19)	−0.0019 (15)	0.0102 (15)	−0.0081 (17)
O3	0.0393 (9)	0.0580 (13)	0.0399 (10)	0.0031 (9)	−0.0055 (8)	0.0109 (10)
N3	0.0498 (12)	0.0543 (13)	0.0416 (15)	0.0015 (11)	0.0116 (11)	0.0017 (11)
C3	0.078 (2)	0.056 (2)	0.073 (2)	−0.0023 (18)	0.011 (2)	−0.0154 (19)
C4	0.075 (2)	0.058 (2)	0.083 (3)	0.0167 (18)	0.013 (2)	−0.010 (2)
O4	0.0462 (10)	0.0713 (14)	0.0459 (11)	−0.0025 (10)	−0.0006 (9)	0.0192 (11)

C5	0.0577 (17)	0.065 (2)	0.0597 (19)	0.0159 (16)	0.0042 (15)	0.0035 (17)
O5	0.152 (4)	0.088 (2)	0.181 (5)	0.016 (2)	−0.098 (4)	−0.033 (3)
C6	0.0496 (14)	0.0481 (16)	0.0383 (14)	0.0045 (13)	0.0059 (12)	−0.0011 (13)
C7	0.0490 (14)	0.0536 (16)	0.0411 (15)	0.0061 (14)	0.0025 (13)	0.0063 (13)
C8	0.0425 (12)	0.0681 (18)	0.0399 (18)	0.0039 (13)	−0.0036 (11)	0.0076 (13)
C9	0.068 (2)	0.072 (2)	0.080 (3)	−0.0142 (19)	−0.0219 (19)	0.007 (2)
C10	0.085 (3)	0.116 (4)	0.097 (4)	−0.006 (3)	−0.036 (3)	−0.028 (3)
C11	0.111 (4)	0.109 (3)	0.047 (2)	−0.009 (3)	−0.029 (2)	−0.002 (2)
C13	0.115 (4)	0.088 (4)	0.041 (2)	0.000 (2)	0.009 (2)	0.0057 (19)
C14	0.108 (3)	0.099 (3)	0.047 (2)	0.027 (3)	0.028 (2)	0.010 (2)
C15	0.074 (2)	0.075 (2)	0.063 (2)	−0.0035 (19)	0.026 (2)	0.0137 (19)
C16	0.0394 (12)	0.0556 (16)	0.0522 (15)	0.0033 (13)	0.0045 (13)	−0.0066 (15)
C17	0.0406 (13)	0.0490 (14)	0.0436 (14)	0.0035 (12)	−0.0033 (12)	−0.0017 (13)
C18	0.0405 (12)	0.0432 (14)	0.0347 (13)	0.0033 (11)	−0.0082 (10)	0.0015 (11)
C19	0.0407 (14)	0.0634 (19)	0.064 (2)	0.0070 (14)	−0.0124 (15)	−0.0038 (17)
C20	0.0544 (16)	0.0613 (19)	0.066 (2)	0.0089 (15)	−0.0237 (16)	0.0129 (17)
C21	0.0617 (18)	0.0544 (17)	0.0446 (16)	−0.0014 (15)	−0.0120 (15)	0.0125 (14)
C22	0.0459 (14)	0.0437 (15)	0.0401 (15)	−0.0009 (12)	−0.0065 (12)	0.0036 (13)
C23	0.064 (2)	0.083 (3)	0.058 (2)	−0.002 (2)	0.0065 (18)	0.026 (2)
C24	0.189 (6)	0.083 (4)	0.097 (4)	0.033 (4)	−0.034 (4)	−0.016 (3)

Geometric parameters (Å, º)

Zn1—O2	1.975 (2)	C9—C10	1.480 (7)
Zn1—O3	2.001 (2)	C9—H9A	0.97
Zn1—N1	2.094 (2)	C9—H9B	0.97
Zn1—N3	2.107 (2)	C10—C11	1.448 (7)
Zn1—N2	2.152 (3)	C10—H10A	0.97
O1—C2	1.375 (4)	C10—H10B	0.97
O1—C1	1.416 (5)	C11—H11A	0.97
N1—C8	1.273 (4)	C11—H11B	0.97
N1—C9	1.462 (5)	C13—C14	1.499 (7)
C1—H1A	0.96	C13—H13A	0.97
C1—H1B	0.96	C13—H13B	0.97
C1—H1C	0.96	C14—C15	1.535 (7)
O2—C6	1.300 (4)	C14—H14A	0.97
N2—C13	1.435 (6)	C14—H14B	0.97
N2—C11	1.473 (6)	C15—H15A	0.97
N2—H2	0.98	C15—H15B	0.97
C2—C3	1.361 (5)	C16—C17	1.443 (4)
C2—C6	1.432 (5)	C16—H16	0.93
O3—C18	1.316 (3)	C17—C19	1.415 (4)
N3—C16	1.278 (4)	C17—C18	1.416 (4)
N3—C15	1.453 (4)	C18—C22	1.421 (4)
C3—C4	1.403 (6)	C19—C20	1.359 (5)
C3—H3	0.93	C19—H19	0.93
C4—C5	1.357 (6)	C20—C21	1.386 (5)
C4—H4	0.93	C20—H20	0.93

O4—C22	1.365 (4)	C21—C22	1.382 (4)
O4—C23	1.413 (4)	C21—H21	0.93
C5—C7	1.402 (4)	C23—H23A	0.96
C5—H5	0.93	C23—H23B	0.96
O5—C24	1.334 (8)	C23—H23C	0.96
O5—H5A	0.82	C24—H24A	0.96
C6—C7	1.413 (4)	C24—H24B	0.96
C7—C8	1.453 (5)	C24—H24C	0.96
C8—H8	0.93		

O2—Zn1—O3	122.87 (10)	C9—C10—H10A	108.1
O2—Zn1—N1	89.63 (9)	C11—C10—H10B	108.1
O3—Zn1—N1	97.45 (10)	C9—C10—H10B	108.1
O2—Zn1—N3	90.01 (9)	H10A—C10—H10B	107.3
O3—Zn1—N3	87.84 (9)	C10—C11—N2	117.1 (4)
N1—Zn1—N3	173.91 (12)	C10—C11—H11A	108.0
O2—Zn1—N2	123.50 (13)	N2—C11—H11A	108.0
O3—Zn1—N2	113.44 (12)	C10—C11—H11B	108.0
N1—Zn1—N2	87.40 (13)	N2—C11—H11B	108.0
N3—Zn1—N2	87.73 (11)	H11A—C11—H11B	107.3
C2—O1—C1	116.9 (3)	N2—C13—C14	117.6 (4)
C8—N1—C9	117.5 (3)	N2—C13—H13A	107.9
C8—N1—Zn1	124.4 (2)	C14—C13—H13A	107.9
C9—N1—Zn1	117.7 (2)	N2—C13—H13B	107.9
O1—C1—H1A	109.5	C14—C13—H13B	107.9
O1—C1—H1B	109.5	H13A—C13—H13B	107.2
H1A—C1—H1B	109.5	C13—C14—C15	115.7 (4)
O1—C1—H1C	109.5	C13—C14—H14A	108.4
H1A—C1—H1C	109.5	C15—C14—H14A	108.4
H1B—C1—H1C	109.5	C13—C14—H14B	108.4
C6—O2—Zn1	129.32 (19)	C15—C14—H14B	108.4
C13—N2—C11	113.5 (4)	H14A—C14—H14B	107.4
C13—N2—Zn1	112.6 (3)	N3—C15—C14	110.5 (3)
C11—N2—Zn1	114.6 (3)	N3—C15—H15A	109.5
C13—N2—H2	105.0	C14—C15—H15A	109.5
C11—N2—H2	105.0	N3—C15—H15B	109.5
Zn1—N2—H2	105.0	C14—C15—H15B	109.5
C3—C2—O1	124.3 (4)	H15A—C15—H15B	108.1
C3—C2—C6	121.8 (3)	N3—C16—C17	126.3 (3)
O1—C2—C6	113.8 (3)	N3—C16—H16	116.8
C18—O3—Zn1	126.77 (18)	C17—C16—H16	116.8
C16—N3—C15	118.6 (3)	C19—C17—C18	119.8 (3)
C16—N3—Zn1	124.7 (2)	C19—C17—C16	116.5 (3)
C15—N3—Zn1	116.4 (2)	C18—C17—C16	123.7 (3)
C2—C3—C4	120.9 (4)	O3—C18—C17	124.3 (3)
C2—C3—H3	119.6	O3—C18—C22	118.7 (2)
C4—C3—H3	119.6	C17—C18—C22	117.1 (2)
C5—C4—C3	119.2 (3)	C20—C19—C17	121.3 (3)

C5—C4—H4	120.4	C20—C19—H19	119.3
C3—C4—H4	120.4	C17—C19—H19	119.3
C22—O4—C23	116.7 (2)	C19—C20—C21	119.9 (3)
C4—C5—C7	121.1 (3)	C19—C20—H20	120.0
C4—C5—H5	119.5	C21—C20—H20	120.0
C7—C5—H5	119.5	C22—C21—C20	120.5 (3)
C24—O5—H5A	109.5	C22—C21—H21	119.7
O2—C6—C7	125.2 (3)	C20—C21—H21	119.7
O2—C6—C2	119.2 (3)	O4—C22—C21	124.1 (3)
C7—C6—C2	115.7 (3)	O4—C22—C18	114.5 (2)
C5—C7—C6	121.3 (3)	C21—C22—C18	121.4 (3)
C5—C7—C8	116.1 (3)	O4—C23—H23A	109.5
C6—C7—C8	122.6 (3)	O4—C23—H23B	109.5
N1—C8—C7	127.6 (3)	H23A—C23—H23B	109.5
N1—C8—H8	116.2	O4—C23—H23C	109.5
C7—C8—H8	116.2	H23A—C23—H23C	109.5
N1—C9—C10	115.4 (4)	H23B—C23—H23C	109.5
N1—C9—H9A	108.4	O5—C24—H24A	109.5
C10—C9—H9A	108.4	O5—C24—H24B	109.5
N1—C9—H9B	108.4	H24A—C24—H24B	109.5
C10—C9—H9B	108.4	O5—C24—H24C	109.5
H9A—C9—H9B	107.5	H24A—C24—H24C	109.5
C11—C10—C9	116.9 (4)	H24B—C24—H24C	109.5
C11—C10—H10A	108.1		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*A*···O2^{i}	0.97	2.58	3.549 (6)	172
C10—H10*B*···O5	0.97	2.50	3.340 (7)	144
O5—H5*A*···O3	0.82	2.01	2.722 (5)	144

Symmetry code: (i) −*x*+1, −*y*+1, *z*+1/2.