

catena-Poly[[dimethyl sulfoxide- κO)-zinc(II)]- μ -(E)-2-[(2-oxido-1-naphthyl)-methyleneamino]propanoato- $\kappa^4 O^2,N,O^1:O^1]$]

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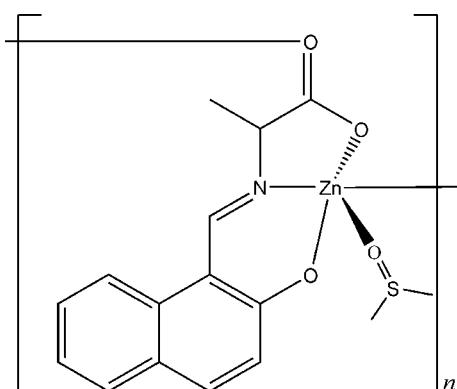
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Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(C-C) = 0.003$ Å;
 R factor = 0.024; wR factor = 0.056; data-to-parameter ratio = 17.7.

In the title coordination polymer, $[Zn(C_{14}H_{11}NO_3)(C_2H_6OS)]_n$, each Zn^{II} ion is five-coordinated in a slightly distorted trigonal-bipyramidal coordination environment, formed by three O atoms from two 2-[(2-oxido-1-naphthyl)-methyleneamino]propanoate ligands, one O atom from a dimethyl sulfoxide molecule and the N atom from the aminopropanoate ligand. The propanoate ligands bridge Zn^{II} ions, forming a zigzag chain parallel to [010].

Related literature

For the synthesis of (E)-2-[(2-hydroxynaphthalen-1-yl)-methyleneamino]propanoic acid, see: Audriceth *et al.* (1954).



Experimental

Crystal data

$[Zn(C_{14}H_{11}NO_3)(C_2H_6OS)]$	$V = 832.6$ (7) Å ³
$M_r = 384.74$	$Z = 2$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 9.676$ (4) Å	$\mu = 1.62$ mm ⁻¹
$b = 7.651$ (4) Å	$T = 291$ (2) K
$c = 11.715$ (5) Å	$0.31 \times 0.28 \times 0.24$ mm
$\beta = 106.256$ (15)°	

Data collection

Rigaku R-AXIS RAPID diffractometer	8191 measured reflections
Absorption correction: multi-scan (<i>ABSCOR</i> ; Higashi, 1995)	3729 independent reflections
$T_{min} = 0.633$, $T_{max} = 0.697$	3533 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$	H-atom parameters constrained
$wR(F^2) = 0.056$	$\Delta\rho_{\text{max}} = 0.25$ e Å ⁻³
$S = 1.06$	$\Delta\rho_{\text{min}} = -0.19$ e Å ⁻³
3729 reflections	Absolute structure: Flack (1983), 1675 Friedel pairs
211 parameters	Flack parameter: 0.006 (8)
1 restraint	

Table 1
Selected geometric parameters (Å, °).

N1–Zn1	2.0119 (18)	O3–Zn1 ⁱ	1.9560 (15)
O1–Zn1	2.0040 (15)	O4–Zn1	2.0520 (17)
O2–Zn1	2.1891 (16)		
O3 ⁱⁱ –Zn1–O1	98.54 (7)	N1–Zn1–O4	118.82 (7)
O3 ⁱⁱ –Zn1–N1	138.57 (7)	O3 ⁱⁱ –Zn1–O2	93.89 (7)
O1–Zn1–N1	88.32 (7)	O1–Zn1–O2	166.10 (6)
O3 ⁱⁱ –Zn1–O4	101.12 (7)	N1–Zn1–O2	78.22 (6)
O1–Zn1–O4	96.09 (7)	O4–Zn1–O2	87.52 (7)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2495).

References

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supplementary materials

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Comment

The continuous interest in designing and making novel Schiff base ligand and transition-metal complexes have persisted because of their impressive catalytic property. In this paper, we report the new title compound, (I), synthesized by the reaction of (E)-2-((2-hydroxynaphthalen-1-yl)methyleneamino)propanoic acid ligands and Zn(OAc)₂ in an aqueous solution.

As shown in Fig. 1, Zn^{II} ion is five-coordinate in a slightly distorted trigonal-bipyramidal coordination environment, formed by four O atoms and one N atom. Each quadridentate Schiff base ligand bridge two different Cu^{II} ions, resulting in a one-dimensional polymeric structure chain (Fig. 2).

Experimental

(E)-2-((2-Hydroxynaphthalen-1-yl)methyleneamino)propanoic acid was prepared of *L*-alanine acid and 2-hydroxy-1-naphthaldehyde in aqueous solution (Audriceth *et al.*, 1954). (E)-2-((2-Hydroxynaphthalen-1-yl)methyleneamino)propanoic acid (0.243 g, 1 mmol) and Zn(OAc)₂ (0.190 g, 1 mmol) dissolved in hot aqueous solution (20 ml) then refluxed for 1 h. After cooling to room temperature the solution was filtered, the residue was recrystaled in DMSO and methanol (10/1, V/V) solution, several days latter, a suitable for X-ray diffraction yellow crystal was obtained.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (Caromatic); C—H = 0.96 Å (methyl); C—H = 0.98 ° Å (methine), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

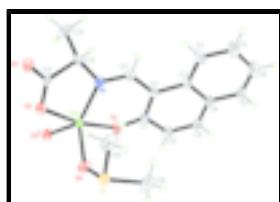


Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 30% probability level for non-H atoms. [Symmetry code: (I) $-x + 1, 1/2 + y, -z + 1$].

supplementary materials

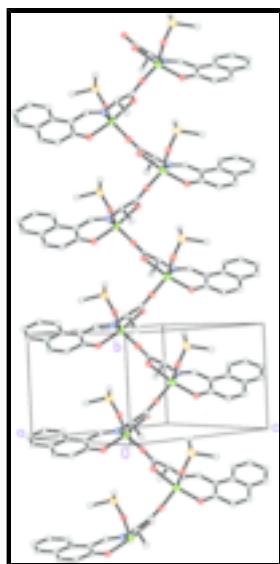


Fig. 2. A partial packing view, showing the one-dimensional chain structure. H atoms have been omitted for clarity.

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Crystal data

[Zn(C ₁₄ H ₁₁ NO ₃)(C ₂ H ₆ OS)]	$F_{000} = 396$
$M_r = 384.74$	$D_x = 1.535 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
Hall symbol: P 2yb	$\lambda = 0.71073 \text{ \AA}$
$a = 9.676 (4) \text{ \AA}$	Cell parameters from 7870 reflections
$b = 7.651 (4) \text{ \AA}$	$\theta = 3.2\text{--}27.5^\circ$
$c = 11.715 (5) \text{ \AA}$	$\mu = 1.62 \text{ mm}^{-1}$
$\beta = 106.256 (15)^\circ$	$T = 291 (2) \text{ K}$
$V = 832.6 (7) \text{ \AA}^3$	Block, yellow
$Z = 2$	$0.31 \times 0.28 \times 0.24 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID diffractometer	3729 independent reflections
Radiation source: fine-focus sealed tube	3533 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.020$
$T = 291(2) \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
ω scans	$\theta_{\text{min}} = 3.2^\circ$
Absorption correction: Multi-scan (ABSCOR; Higashi, 1995)	$h = -11 \rightarrow 12$
$T_{\text{min}} = 0.633$, $T_{\text{max}} = 0.697$	$k = -9 \rightarrow 9$
8191 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.024$	$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.056$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.06$	$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$
3729 reflections	$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$
211 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1675 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.006 (8)
Secondary atom site location: difference Fourier map	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7743 (2)	-0.1178 (3)	0.23967 (18)	0.0288 (4)
C2	0.66925 (19)	-0.0224 (3)	0.15494 (15)	0.0272 (4)
C3	0.6855 (2)	0.0055 (4)	0.03564 (15)	0.0304 (4)
C4	0.5858 (3)	0.0965 (3)	-0.0557 (2)	0.0429 (6)
H4	0.5020	0.1392	-0.0416	0.051*
C5	0.6085 (3)	0.1243 (4)	-0.1655 (2)	0.0477 (6)
H5	0.5400	0.1837	-0.2243	0.057*
C6	0.7336 (3)	0.0636 (3)	-0.1883 (2)	0.0483 (6)
H6	0.7504	0.0859	-0.2613	0.058*
C7	0.8305 (3)	-0.0276 (4)	-0.10433 (19)	0.0445 (6)
H7	0.9131	-0.0694	-0.1209	0.053*
C8	0.8094 (2)	-0.0613 (3)	0.00897 (19)	0.0340 (5)
C9	0.9098 (2)	-0.1605 (4)	0.0950 (2)	0.0418 (5)
H9	0.9890	-0.2075	0.0756	0.050*
C10	0.8947 (2)	-0.1897 (3)	0.2055 (2)	0.0382 (5)
H10	0.9628	-0.2568	0.2595	0.046*

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C11	0.5465 (2)	0.0524 (3)	0.18248 (18)	0.0292 (4)
H11	0.4778	0.1043	0.1198	0.035*
C12	0.3897 (2)	0.1430 (3)	0.29272 (17)	0.0307 (4)
H12	0.3676	0.2387	0.2349	0.037*
C13	0.2635 (2)	0.0163 (5)	0.2663 (3)	0.0612 (9)
H13A	0.2422	-0.0219	0.1851	0.092*
H13B	0.1808	0.0738	0.2788	0.092*
H13C	0.2879	-0.0829	0.3182	0.092*
C14	0.4141 (2)	0.2180 (3)	0.41799 (18)	0.0274 (4)
C15	0.7228 (3)	0.4372 (3)	0.3802 (3)	0.0555 (7)
H15A	0.6852	0.3618	0.3132	0.083*
H15B	0.7508	0.5467	0.3534	0.083*
H15C	0.6501	0.4571	0.4202	0.083*
C16	0.9720 (3)	0.2924 (4)	0.3760 (3)	0.0566 (7)
H16A	1.0605	0.2349	0.4161	0.085*
H16B	0.9930	0.3998	0.3418	0.085*
H16C	0.9161	0.2180	0.3143	0.085*
N1	0.52124 (17)	0.0554 (2)	0.28544 (14)	0.0268 (3)
O1	0.77231 (16)	-0.1464 (2)	0.34856 (12)	0.0355 (3)
O2	0.51906 (16)	0.1680 (2)	0.49919 (13)	0.0372 (4)
O3	0.32074 (15)	0.3268 (2)	0.42825 (13)	0.0354 (3)
O4	0.82733 (16)	0.1620 (2)	0.51567 (15)	0.0422 (4)
S1	0.87374 (6)	0.33792 (8)	0.47907 (5)	0.03915 (13)
Zn1	0.66361 (2)	-0.00892 (3)	0.440772 (16)	0.02749 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0313 (10)	0.0256 (11)	0.0325 (9)	-0.0010 (8)	0.0141 (9)	-0.0017 (8)
C2	0.0308 (8)	0.0236 (10)	0.0288 (8)	0.0005 (10)	0.0113 (7)	-0.0007 (10)
C3	0.0376 (9)	0.0261 (11)	0.0303 (8)	-0.0042 (11)	0.0141 (8)	-0.0031 (10)
C4	0.0557 (15)	0.0403 (14)	0.0372 (11)	0.0075 (12)	0.0204 (12)	0.0064 (10)
C5	0.0727 (17)	0.0373 (14)	0.0331 (11)	-0.0006 (13)	0.0146 (12)	0.0055 (10)
C6	0.0787 (18)	0.0388 (13)	0.0374 (11)	-0.0155 (13)	0.0323 (14)	-0.0064 (10)
C7	0.0566 (13)	0.0462 (16)	0.0411 (10)	-0.0114 (14)	0.0308 (11)	-0.0094 (12)
C8	0.0387 (11)	0.0339 (13)	0.0330 (10)	-0.0073 (9)	0.0162 (9)	-0.0070 (8)
C9	0.0357 (11)	0.0521 (15)	0.0441 (12)	0.0053 (11)	0.0221 (11)	-0.0068 (11)
C10	0.0345 (11)	0.0424 (14)	0.0392 (11)	0.0104 (10)	0.0130 (10)	-0.0003 (10)
C11	0.0311 (10)	0.0269 (10)	0.0291 (9)	0.0025 (8)	0.0076 (9)	0.0001 (7)
C12	0.0280 (10)	0.0330 (12)	0.0319 (10)	0.0043 (9)	0.0096 (9)	-0.0071 (9)
C13	0.0308 (11)	0.073 (2)	0.0840 (18)	-0.0102 (14)	0.0225 (12)	-0.0487 (19)
C14	0.0279 (10)	0.0267 (10)	0.0333 (10)	-0.0044 (8)	0.0181 (9)	-0.0043 (8)
C15	0.0493 (14)	0.0333 (14)	0.088 (2)	0.0012 (11)	0.0255 (15)	0.0115 (12)
C16	0.0464 (15)	0.0558 (19)	0.0764 (19)	-0.0036 (13)	0.0319 (15)	-0.0019 (15)
N1	0.0266 (8)	0.0274 (9)	0.0284 (7)	0.0022 (6)	0.0106 (7)	-0.0035 (6)
O1	0.0414 (8)	0.0361 (9)	0.0325 (7)	0.0111 (7)	0.0161 (7)	0.0074 (6)
O2	0.0369 (8)	0.0455 (10)	0.0309 (7)	0.0056 (7)	0.0121 (7)	-0.0044 (7)
O3	0.0358 (8)	0.0372 (9)	0.0365 (7)	0.0056 (7)	0.0156 (7)	-0.0104 (7)

O4	0.0371 (8)	0.0357 (9)	0.0520 (9)	-0.0084 (7)	0.0094 (7)	0.0051 (8)
S1	0.0388 (3)	0.0311 (3)	0.0503 (3)	-0.0096 (2)	0.0169 (3)	-0.0059 (2)
Zn1	0.02884 (11)	0.02883 (11)	0.02707 (10)	0.00032 (12)	0.01157 (8)	0.00374 (11)

Geometric parameters (\AA , $^{\circ}$)

C1—O1	1.300 (2)	C12—C14	1.531 (3)
C1—C2	1.410 (3)	C12—H12	0.9800
C1—C10	1.443 (3)	C13—H13A	0.9600
C2—C11	1.434 (3)	C13—H13B	0.9600
C2—C3	1.465 (2)	C13—H13C	0.9600
C3—C4	1.408 (3)	C14—O2	1.242 (3)
C3—C8	1.416 (3)	C14—O3	1.259 (3)
C4—C5	1.381 (3)	C15—S1	1.762 (3)
C4—H4	0.9300	C15—H15A	0.9600
C5—C6	1.391 (4)	C15—H15B	0.9600
C5—H5	0.9300	C15—H15C	0.9600
C6—C7	1.348 (4)	C16—S1	1.768 (3)
C6—H6	0.9300	C16—H16A	0.9600
C7—C8	1.422 (3)	C16—H16B	0.9600
C7—H7	0.9300	C16—H16C	0.9600
C8—C9	1.409 (3)	N1—Zn1	2.0119 (18)
C9—C10	1.361 (3)	O1—Zn1	2.0040 (15)
C9—H9	0.9300	O2—Zn1	2.1891 (16)
C10—H10	0.9300	O3—Zn1 ⁱ	1.9560 (15)
C11—N1	1.296 (2)	O4—S1	1.5184 (18)
C11—H11	0.9300	O4—Zn1	2.0520 (17)
C12—N1	1.462 (2)	Zn1—O3 ⁱⁱ	1.9560 (15)
C12—C13	1.521 (3)		
O1—C1—C2	124.91 (17)	C12—C13—H13B	109.5
O1—C1—C10	116.32 (19)	H13A—C13—H13B	109.5
C2—C1—C10	118.77 (17)	C12—C13—H13C	109.5
C1—C2—C11	121.86 (16)	H13A—C13—H13C	109.5
C1—C2—C3	119.89 (17)	H13B—C13—H13C	109.5
C11—C2—C3	118.24 (18)	O2—C14—O3	125.85 (18)
C4—C3—C8	116.96 (17)	O2—C14—C12	119.49 (17)
C4—C3—C2	124.27 (18)	O3—C14—C12	114.66 (19)
C8—C3—C2	118.77 (19)	S1—C15—H15A	109.5
C5—C4—C3	122.0 (2)	S1—C15—H15B	109.5
C5—C4—H4	119.0	H15A—C15—H15B	109.5
C3—C4—H4	119.0	S1—C15—H15C	109.5
C4—C5—C6	120.1 (2)	H15A—C15—H15C	109.5
C4—C5—H5	120.0	H15B—C15—H15C	109.5
C6—C5—H5	120.0	S1—C16—H16A	109.5
C7—C6—C5	119.9 (2)	S1—C16—H16B	109.5
C7—C6—H6	120.1	H16A—C16—H16B	109.5
C5—C6—H6	120.1	S1—C16—H16C	109.5
C6—C7—C8	121.5 (2)	H16A—C16—H16C	109.5

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C6—C7—H7	119.2	H16B—C16—H16C	109.5
C8—C7—H7	119.2	C11—N1—C12	117.15 (17)
C9—C8—C3	119.56 (17)	C11—N1—Zn1	125.29 (13)
C9—C8—C7	120.97 (19)	C12—N1—Zn1	116.50 (12)
C3—C8—C7	119.5 (2)	C1—O1—Zn1	126.51 (14)
C10—C9—C8	122.14 (19)	C14—O2—Zn1	114.09 (12)
C10—C9—H9	118.9	C14—O3—Zn1 ⁱ	126.85 (14)
C8—C9—H9	118.9	S1—O4—Zn1	134.27 (11)
C9—C10—C1	120.8 (2)	O4—S1—C15	108.15 (11)
C9—C10—H10	119.6	O4—S1—C16	106.05 (12)
C1—C10—H10	119.6	C15—S1—C16	98.14 (15)
N1—C11—C2	126.87 (19)	O3 ⁱⁱ —Zn1—O1	98.54 (7)
N1—C11—H11	116.6	O3 ⁱⁱ —Zn1—N1	138.57 (7)
C2—C11—H11	116.6	O1—Zn1—N1	88.32 (7)
N1—C12—C13	111.01 (19)	O3 ⁱⁱ —Zn1—O4	101.12 (7)
N1—C12—C14	108.94 (16)	O1—Zn1—O4	96.09 (7)
C13—C12—C14	109.48 (17)	N1—Zn1—O4	118.82 (7)
N1—C12—H12	109.1	O3 ⁱⁱ —Zn1—O2	93.89 (7)
C13—C12—H12	109.1	O1—Zn1—O2	166.10 (6)
C14—C12—H12	109.1	N1—Zn1—O2	78.22 (6)
C12—C13—H13A	109.5	O4—Zn1—O2	87.52 (7)
O1—C1—C2—C11	−0.5 (4)	C13—C12—N1—C11	89.0 (2)
C10—C1—C2—C11	179.8 (2)	C14—C12—N1—C11	−150.37 (18)
O1—C1—C2—C3	178.2 (2)	C13—C12—N1—Zn1	−102.1 (2)
C10—C1—C2—C3	−1.4 (3)	C14—C12—N1—Zn1	18.5 (2)
C1—C2—C3—C4	179.0 (2)	C2—C1—O1—Zn1	−20.7 (3)
C11—C2—C3—C4	−2.2 (4)	C10—C1—O1—Zn1	158.98 (16)
C1—C2—C3—C8	−1.5 (3)	O3—C14—O2—Zn1	−175.97 (16)
C11—C2—C3—C8	177.3 (2)	C12—C14—O2—Zn1	4.9 (2)
C8—C3—C4—C5	−1.7 (4)	O2—C14—O3—Zn1 ⁱ	16.7 (3)
C2—C3—C4—C5	177.8 (3)	C12—C14—O3—Zn1 ⁱ	−164.18 (13)
C3—C4—C5—C6	−0.8 (4)	Zn1—O4—S1—C15	23.79 (18)
C4—C5—C6—C7	2.2 (4)	Zn1—O4—S1—C16	−80.64 (17)
C5—C6—C7—C8	−1.1 (4)	C1—O1—Zn1—O3 ⁱⁱ	165.79 (17)
C4—C3—C8—C9	−177.1 (2)	C1—O1—Zn1—N1	26.85 (17)
C2—C3—C8—C9	3.4 (3)	C1—O1—Zn1—O4	−91.96 (18)
C4—C3—C8—C7	2.8 (3)	C1—O1—Zn1—O2	12.5 (4)
C2—C3—C8—C7	−176.7 (2)	C11—N1—Zn1—O3 ⁱⁱ	−122.75 (17)
C6—C7—C8—C9	178.4 (2)	C12—N1—Zn1—O3 ⁱⁱ	69.40 (17)
C6—C7—C8—C3	−1.4 (4)	C11—N1—Zn1—O1	−21.72 (17)
C3—C8—C9—C10	−2.4 (4)	C12—N1—Zn1—O1	170.43 (14)
C7—C8—C9—C10	177.7 (2)	C11—N1—Zn1—O4	74.31 (18)
C8—C9—C10—C1	−0.6 (4)	C12—N1—Zn1—O4	−93.54 (15)
O1—C1—C10—C9	−177.2 (2)	C11—N1—Zn1—O2	154.80 (18)
C2—C1—C10—C9	2.5 (3)	C12—N1—Zn1—O2	−13.05 (14)
C1—C2—C11—N1	5.6 (4)	S1—O4—Zn1—O3 ⁱⁱ	−170.20 (14)

supplementary materials

C3—C2—C11—N1	−173.2 (2)	S1—O4—Zn1—O1	89.82 (14)
N1—C12—C14—O2	−15.1 (3)	S1—O4—Zn1—N1	−1.61 (17)
C13—C12—C14—O2	106.5 (2)	S1—O4—Zn1—O2	−76.72 (14)
N1—C12—C14—O3	165.76 (17)	C14—O2—Zn1—O3 ⁱⁱ	−134.50 (15)
C13—C12—C14—O3	−72.7 (3)	C14—O2—Zn1—O1	19.0 (4)
C2—C11—N1—C12	178.6 (2)	C14—O2—Zn1—N1	4.39 (14)
C2—C11—N1—Zn1	10.9 (3)	C14—O2—Zn1—O4	124.51 (15)

Symmetry codes: (i) $-x+1, y+1/2, -z+1$; (ii) $-x+1, y-1/2, -z+1$.

supplementary materials

Fig. 1

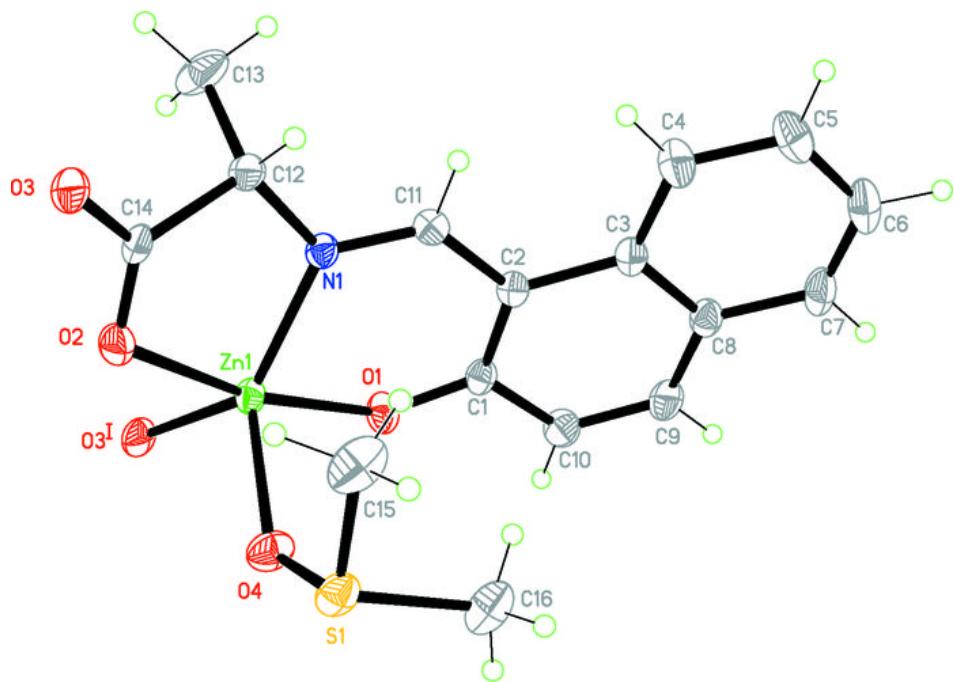


Fig. 2

