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Aquabis(5-chlorosalicylato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)zinc(II)

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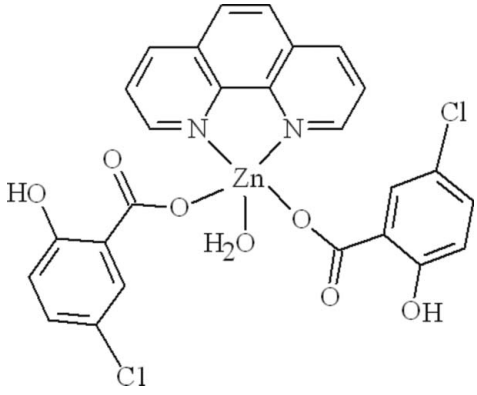
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.084; data-to-parameter ratio = 15.6.

In the title complex, $[Zn(C_7H_4ClO_3)_2(C_{12}H_8N_2)(H_2O)]$, the Zn atom is coordinated by two 5-chlorosalicylate anions, one 1,10-phenanthroline molecule and one water molecule, displaying a distorted trigonal–bipyramidal geometry. The crystal structure is stabilized by intra- and intermolecular O—H···O hydrogen bonds.

Related literature

For related literature, see: Brownless *et al.* (1999); Lemoine *et al.* (2002, 2004); Melnik *et al.* (2001); Sun *et al.* (2001); Wen *et al.* (2007*a*,*b*,*c*); Yin *et al.* (2004); Zhu *et al.* (2003).



Experimental

Crystal data

$[Zn(C_7H_4ClO_3)_2(C_{12}H_8N_2)(H_2O)]$
M_r = 606.69
Triclinic, $P\overline{1}$
a = 8.681 (4) Å
b = 11.777 (6) Å
c = 12.982 (9) Å
α = 72.06 (2)°
β = 76.98 (2)°
γ = 81.592 (19)°
V = 1225.9 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.27 mm^{-1}
T = 293 (2) K
0.28 × 0.26 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID Weissenberg IP diffractometer
Absorption correction: none
12131 measured reflections
5553 independent reflections
4462 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.084
S = 1.04
5553 reflections
355 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.9706 (18)	Zn1—O7	2.1154 (17)
Zn1—O4	2.0094 (17)	Zn1—N2	2.1599 (18)
Zn1—N1	2.099 (2)		
O1—Zn1—O4	123.68 (8)	N1—Zn1—O7	89.25 (7)
O1—Zn1—N1	98.46 (8)	O1—Zn1—N2	96.73 (8)
O4—Zn1—N1	137.84 (7)	O4—Zn1—N2	94.37 (7)
O1—Zn1—O7	94.31 (8)	N1—Zn1—N2	78.09 (8)
O4—Zn1—O7	88.75 (7)	O7—Zn1—N2	164.28 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2	0.85 (1)	1.78 (2)	2.552 (3)	151 (2)
O6—H6A···O5	0.85 (1)	1.80 (2)	2.577 (3)	150 (2)
O7—H7A···O4^{i}	0.85 (1)	1.97 (1)	2.785 (3)	162 (3)
O7—H7B···O2^{i}	0.84 (1)	1.84 (1)	2.672 (3)	171 (2)

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

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); 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: OM2150).

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supplementary materials

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Aquabis(5-chlorosalicylato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)zinc(II)

D. Wen and S. Ying

Comment

A lot of attention has been paid to the metal salicylate owing to their intriguing structural features (Brownless *et al.*, 1999; Lemoine *et al.*, 2002; Zhu *et al.*, 2003; Yin *et al.*, 2004; Wen *et al.*, 2007*a*,b,c) and biological applications (Lemoine *et al.*, 2004). We report here the structure of a Zn (II) complex with 5-chloroosalicylate ligand (Melnik *et al.*, 2001). The title complex, $Zn(C_7H_4ClO_3)_2(C_{12}H_8N_2)(H_2O)$ was synthesized under hydrothermal conditions. The Zn atom is coordinated in a distorted trigonal bipyramid geometry by two O atoms from two 5-chlorosalicylate ligands, two N atoms from one 1,10-phenanthroline and one water O atom (Fig. 1). One Zn—N bond is significantly shorter than the other (Zn1—N1 = 2.099 (2) Å, Zn1—N2 = 2.160 (2) Å). These distances are comparable to the Zn—N bond lengths (Zn—N1 = 2.109 (3) Å, Zn—N2 = 2.178 (3) Å) in $[Zn(ta)(phen)(H_2O)]_n$ (Sun *et al.*, 2001). The complex has rich hydrogen bonds formed by the coordinated water molecule, hydroxy and carboxyl O atoms (Fig. 2). The crystal structure is stabilized by intra- and intermolecular O—H···O hydrogen bonds interactions (Fig. 3).

Experimental

A mixture of $Zn(NO_3)_2{\cdot}6H_2O$ (0.1 mmol), phen (0.1 mmol), 5-chlorosalicylic acid (0.2 mmol) and distilled water (10 ml) was put into a Teflon-lined autoclave (20 ml) and then heated at 413 K for 72 h. Colorless block-like crystals suitable for X-ray analysis were collected from the reaction mixture.

Refinement

The aromatic H atoms were positioned geometrically and were included in the refinement in the riding-model approximation [C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C)]. The water H atoms were found in a difference Fourier map and were refined with distance restraints of O—H = 0.85 (1)Å and U_{iso}(H) = 1.2 U_{eq}(O).

Figures

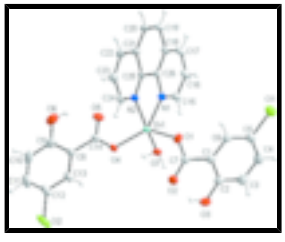

Fig. 1. Molecular structure of the title complex with 30% probability ellipsoids.

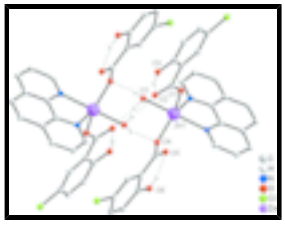

Fig. 2. Representation of hydrogen bonds (dashed lines) observed in the title compound.

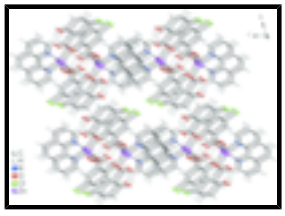

Fig. 3. Packing diagram of the title compound viewed down the *a* axis. Hydrogen bonds are represented by dashed lines.

Aquabis(5-chlorosalicylato-κ*O*)(1,10-phenanthroline-κ^2*N*,*N*')zinc(II)

Crystal data

$[Zn(C_7H_4ClO_3)_2(C_{12}H_8N_2)(H_2O)]$	$Z = 2$
$M_r = 606.69$	$F_{000} = 616$
Triclinic, $P\overline{1}$	$D_x = 1.644$ Mg m^{-3}
$a = 8.681$ (4) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 11.777$ (6) Å	Cell parameters from 5553 reflections
$c = 12.982$ (9) Å	$\theta = 3.2$–27.5º
$\alpha = 72.06$ (2)º	$\mu = 1.27$ mm^{-1}
$\beta = 76.98$ (2)º	$T = 293$ (2) K
$\gamma = 81.592$ (19)º	Block, colourless
$V = 1225.9$ (12) Å^3	0.28 × 0.26 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID Weissenberg IP diffractometer	4462 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.049$
Monochromator: graphite	$\theta_{max} = 27.5$º
$T = 293$(2) K	$\theta_{min} = 3.2$º
ω scans	$h = -11 \rightarrow 9$
Absorption correction: none	$k = -15 \rightarrow 14$
12131 measured reflections	$l = -16 \rightarrow 16$
5553 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of

	independent and constrained refinement
$wR(F^2) = 0.084$	$w = 1/[\sigma^2(F_o^2) + (0.0162P)^2 + 0.2964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.002$
5553 reflections	$\Delta\rho_{max} = 0.54$ e Å^{-3}
355 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.64074 (3)	0.98442 (2)	0.813250 (19)	0.03415 (9)
N1	0.5901 (2)	1.07549 (15)	0.65649 (14)	0.0353 (4)
N2	0.8038 (2)	0.88896 (14)	0.71017 (14)	0.0333 (4)
O1	0.7926 (2)	1.09096 (14)	0.81791 (15)	0.0494 (4)
O2	0.7919 (2)	1.05973 (15)	0.99631 (15)	0.0510 (4)
O3	0.9882 (2)	1.15930 (17)	1.05330 (15)	0.0578 (5)
H3A	0.917 (2)	1.115 (2)	1.058 (3)	0.069*
O4	0.57974 (18)	0.83560 (12)	0.93499 (11)	0.0373 (3)
O5	0.4509 (2)	0.80266 (16)	0.81983 (14)	0.0563 (5)
O6	0.2744 (3)	0.6264 (2)	0.8834 (2)	0.0726 (6)
H6A	0.317 (4)	0.6903 (18)	0.843 (3)	0.087*
C1	0.9516 (2)	1.20453 (18)	0.86614 (18)	0.0348 (5)
C2	1.0224 (3)	1.2225 (2)	0.9464 (2)	0.0418 (5)
C3	1.1299 (3)	1.3083 (2)	0.9158 (2)	0.0527 (6)
H3	1.1788	1.3186	0.9688	0.063*
C4	1.1657 (3)	1.3782 (2)	0.8093 (3)	0.0540 (7)
H4	1.2380	1.4358	0.7900	0.065*
C5	1.0934 (3)	1.3625 (2)	0.7307 (2)	0.0423 (5)
C6	0.9881 (3)	1.27671 (19)	0.75859 (19)	0.0385 (5)
H6	0.9407	1.2669	0.7047	0.046*
C7	0.8372 (2)	1.11091 (19)	0.8966 (2)	0.0380 (5)
C8	0.4146 (2)	0.67431 (18)	1.00260 (18)	0.0359 (5)
C9	0.3112 (3)	0.6059 (2)	0.9838 (2)	0.0502 (6)

C10	0.2413 (3)	0.5146 (2)	1.0708 (3)	0.0643 (8)
H10	0.1718	0.4693	1.0586	0.077*
C11	0.2734 (3)	0.4907 (2)	1.1739 (3)	0.0660 (9)
H11	0.2261	0.4293	1.2315	0.079*
C12	0.3758 (3)	0.5577 (2)	1.1922 (2)	0.0522 (7)
C13	0.4467 (3)	0.64840 (19)	1.10822 (18)	0.0400 (5)
H13	0.5164	0.6926	1.1218	0.048*
C14	0.4861 (2)	0.77654 (18)	0.91259 (17)	0.0356 (5)
C15	0.4887 (3)	1.1706 (2)	0.63063 (19)	0.0463 (6)
H15	0.4287	1.2009	0.6868	0.056*
C16	0.4683 (3)	1.2270 (2)	0.5230 (2)	0.0529 (6)
H16	0.3968	1.2942	0.5080	0.064*
C17	0.5538 (3)	1.1834 (2)	0.4396 (2)	0.0501 (6)
H17	0.5398	1.2196	0.3674	0.060*
C18	0.6633 (3)	1.0831 (2)	0.46356 (18)	0.0400 (5)
C19	0.7607 (3)	1.0325 (2)	0.38123 (19)	0.0489 (6)
H19	0.7508	1.0655	0.3078	0.059*
C20	0.8664 (3)	0.9377 (2)	0.40863 (19)	0.0497 (6)
H20	0.9288	0.9068	0.3536	0.060*
C21	0.8846 (3)	0.8841 (2)	0.52007 (18)	0.0403 (5)
C22	0.9915 (3)	0.7849 (2)	0.5542 (2)	0.0495 (6)
H22	1.0534	0.7483	0.5030	0.059*
C23	1.0045 (3)	0.7421 (2)	0.6625 (2)	0.0481 (6)
H23	1.0762	0.6771	0.6854	0.058*
C24	0.9086 (3)	0.79723 (19)	0.73877 (19)	0.0408 (5)
H24	0.9190	0.7683	0.8123	0.049*
C25	0.7908 (2)	0.93152 (17)	0.60344 (17)	0.0324 (4)
C26	0.6781 (2)	1.03261 (18)	0.57349 (17)	0.0331 (4)
Cl1	1.13591 (10)	1.45253 (6)	0.59530 (6)	0.0686 (2)
Cl2	0.41211 (12)	0.52968 (9)	1.32473 (7)	0.0937 (3)
O7	0.4401 (2)	1.07947 (14)	0.88416 (13)	0.0429 (4)
H7B	0.364 (2)	1.0363 (18)	0.915 (2)	0.051*
H7A	0.455 (3)	1.108 (2)	0.9330 (17)	0.051*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.04762 (15)	0.03512 (13)	0.01979 (12)	−0.01181 (11)	−0.00212 (10)	−0.00721 (9)
N1	0.0421 (9)	0.0392 (9)	0.0238 (9)	−0.0076 (9)	−0.0023 (7)	−0.0088 (7)
N2	0.0397 (9)	0.0355 (9)	0.0251 (9)	−0.0125 (8)	−0.0022 (7)	−0.0080 (7)
O1	0.0595 (10)	0.0475 (9)	0.0518 (11)	−0.0156 (8)	−0.0167 (8)	−0.0198 (8)
O2	0.0553 (10)	0.0515 (9)	0.0451 (11)	−0.0131 (8)	0.0009 (8)	−0.0158 (8)
O3	0.0748 (13)	0.0657 (11)	0.0397 (10)	−0.0093 (10)	−0.0192 (9)	−0.0176 (9)
O4	0.0483 (8)	0.0349 (7)	0.0252 (8)	−0.0110 (7)	−0.0010 (6)	−0.0045 (6)
O5	0.0710 (11)	0.0678 (11)	0.0312 (9)	−0.0140 (10)	−0.0138 (8)	−0.0091 (8)
O6	0.0778 (14)	0.0823 (14)	0.0773 (17)	−0.0227 (12)	−0.0165 (12)	−0.0426 (13)
C1	0.0333 (10)	0.0362 (10)	0.0398 (12)	0.0021 (10)	−0.0085 (9)	−0.0189 (9)
C2	0.0433 (12)	0.0470 (12)	0.0422 (13)	0.0039 (11)	−0.0148 (10)	−0.0214 (10)

C3	0.0488 (13)	0.0626 (15)	0.0601 (18)	−0.0070 (13)	−0.0238 (13)	−0.0262 (13)
C4	0.0394 (12)	0.0540 (15)	0.075 (2)	−0.0095 (12)	−0.0121 (13)	−0.0238 (14)
C5	0.0390 (11)	0.0421 (11)	0.0443 (14)	−0.0016 (11)	−0.0036 (10)	−0.0140 (10)
C6	0.0407 (11)	0.0408 (11)	0.0390 (13)	0.0030 (10)	−0.0111 (10)	−0.0191 (9)
C7	0.0369 (11)	0.0359 (11)	0.0447 (13)	0.0020 (10)	−0.0072 (10)	−0.0193 (10)
C8	0.0355 (10)	0.0312 (10)	0.0383 (12)	−0.0037 (9)	0.0003 (9)	−0.0108 (9)
C9	0.0462 (13)	0.0470 (13)	0.0644 (18)	−0.0048 (12)	−0.0034 (12)	−0.0308 (12)
C10	0.0592 (16)	0.0442 (14)	0.092 (2)	−0.0211 (13)	0.0075 (16)	−0.0305 (15)
C11	0.0615 (17)	0.0361 (12)	0.080 (2)	−0.0152 (13)	0.0175 (16)	−0.0048 (13)
C12	0.0478 (13)	0.0418 (12)	0.0498 (16)	−0.0025 (12)	0.0020 (12)	0.0030 (11)
C13	0.0378 (11)	0.0344 (10)	0.0391 (13)	−0.0056 (10)	−0.0013 (10)	−0.0010 (9)
C14	0.0403 (11)	0.0352 (10)	0.0278 (11)	−0.0007 (10)	0.0006 (9)	−0.0101 (8)
C15	0.0538 (14)	0.0479 (13)	0.0333 (13)	−0.0008 (12)	−0.0040 (11)	−0.0106 (10)
C16	0.0602 (15)	0.0522 (13)	0.0382 (14)	0.0050 (13)	−0.0103 (12)	−0.0049 (11)
C17	0.0609 (15)	0.0576 (14)	0.0280 (12)	−0.0115 (13)	−0.0120 (11)	−0.0013 (10)
C18	0.0502 (12)	0.0466 (12)	0.0243 (11)	−0.0162 (11)	−0.0030 (9)	−0.0090 (9)
C19	0.0664 (15)	0.0598 (14)	0.0225 (11)	−0.0184 (14)	−0.0031 (11)	−0.0123 (10)
C20	0.0644 (15)	0.0596 (14)	0.0286 (12)	−0.0140 (14)	0.0037 (11)	−0.0228 (11)
C21	0.0490 (12)	0.0443 (12)	0.0314 (12)	−0.0130 (11)	0.0007 (10)	−0.0179 (9)
C22	0.0536 (14)	0.0497 (13)	0.0484 (15)	−0.0070 (12)	0.0026 (12)	−0.0265 (11)
C23	0.0503 (13)	0.0420 (12)	0.0535 (16)	−0.0020 (12)	−0.0094 (12)	−0.0170 (11)
C24	0.0477 (12)	0.0376 (11)	0.0373 (13)	−0.0105 (11)	−0.0076 (10)	−0.0081 (9)
C25	0.0376 (10)	0.0357 (10)	0.0261 (10)	−0.0160 (9)	0.0004 (8)	−0.0110 (8)
C26	0.0401 (11)	0.0382 (10)	0.0228 (10)	−0.0163 (10)	−0.0012 (8)	−0.0089 (8)
Cl1	0.0842 (5)	0.0558 (4)	0.0535 (4)	−0.0097 (4)	0.0007 (4)	−0.0062 (3)
Cl2	0.1015 (6)	0.1024 (6)	0.0450 (4)	−0.0271 (5)	−0.0060 (4)	0.0281 (4)
O7	0.0572 (10)	0.0429 (8)	0.0263 (8)	−0.0089 (8)	0.0018 (7)	−0.0116 (6)

Geometric parameters (Å, °)

Zn1—O1	1.9706 (18)	C9—C10	1.390 (4)
Zn1—O4	2.0094 (17)	C10—C11	1.364 (5)
Zn1—N1	2.099 (2)	C10—H10	0.9300
Zn1—O7	2.1154 (17)	C11—C12	1.373 (4)
Zn1—N2	2.1599 (18)	C11—H11	0.9300
N1—C15	1.325 (3)	C12—C13	1.372 (3)
N1—C26	1.361 (3)	C12—Cl2	1.741 (3)
N2—C24	1.323 (3)	C13—H13	0.9300
N2—C25	1.345 (3)	C15—C16	1.389 (3)
O1—C7	1.265 (3)	C15—H15	0.9300
O2—C7	1.247 (3)	C16—C17	1.363 (3)
O3—C2	1.346 (3)	C16—H16	0.9300
O3—H3A	0.847 (10)	C17—C18	1.404 (3)
O4—C14	1.275 (3)	C17—H17	0.9300
O5—C14	1.244 (3)	C18—C26	1.395 (3)
O6—C9	1.354 (4)	C18—C19	1.432 (3)
O6—H6A	0.854 (10)	C19—C20	1.348 (3)
C1—C6	1.386 (3)	C19—H19	0.9300
C1—C2	1.404 (3)	C20—C21	1.424 (3)

C1—C7	1.494 (3)	C20—H20	0.9300
C2—C3	1.383 (4)	C21—C22	1.404 (3)
C3—C4	1.366 (4)	C21—C25	1.410 (3)
C3—H3	0.9300	C22—C23	1.365 (4)
C4—C5	1.382 (4)	C22—H22	0.9300
C4—H4	0.9300	C23—C24	1.400 (3)
C5—C6	1.372 (3)	C23—H23	0.9300
C5—Cl1	1.738 (3)	C24—H24	0.9300
C6—H6	0.9300	C25—C26	1.439 (3)
C8—C13	1.393 (3)	O7—H7B	0.844 (10)
C8—C9	1.395 (3)	O7—H7A	0.847 (10)
C8—C14	1.492 (3)		
O1—Zn1—O4	123.68 (8)	C10—C11—H11	120.2
O1—Zn1—N1	98.46 (8)	C12—C11—H11	120.2
O4—Zn1—N1	137.84 (7)	C13—C12—C11	121.0 (3)
O1—Zn1—O7	94.31 (8)	C13—C12—Cl2	119.5 (2)
O4—Zn1—O7	88.75 (7)	C11—C12—Cl2	119.5 (2)
N1—Zn1—O7	89.25 (7)	C12—C13—C8	120.1 (2)
O1—Zn1—N2	96.73 (8)	C12—C13—H13	120.0
O4—Zn1—N2	94.37 (7)	C8—C13—H13	120.0
N1—Zn1—N2	78.09 (8)	O5—C14—O4	122.4 (2)
O7—Zn1—N2	164.28 (7)	O5—C14—C8	119.6 (2)
C15—N1—C26	118.14 (19)	O4—C14—C8	117.99 (19)
C15—N1—Zn1	127.30 (15)	N1—C15—C16	122.7 (2)
C26—N1—Zn1	114.49 (14)	N1—C15—H15	118.6
C24—N2—C25	118.49 (18)	C16—C15—H15	118.6
C24—N2—Zn1	128.86 (15)	C17—C16—C15	119.6 (2)
C25—N2—Zn1	112.65 (13)	C17—C16—H16	120.2
C7—O1—Zn1	132.72 (17)	C15—C16—H16	120.2
C2—O3—H3A	106 (2)	C16—C17—C18	119.4 (2)
C14—O4—Zn1	113.35 (13)	C16—C17—H17	120.3
C9—O6—H6A	106 (3)	C18—C17—H17	120.3
C6—C1—C2	118.6 (2)	C26—C18—C17	117.4 (2)
C6—C1—C7	120.8 (2)	C26—C18—C19	119.1 (2)
C2—C1—C7	120.6 (2)	C17—C18—C19	123.4 (2)
O3—C2—C3	118.3 (2)	C20—C19—C18	120.9 (2)
O3—C2—C1	122.1 (2)	C20—C19—H19	119.5
C3—C2—C1	119.5 (2)	C18—C19—H19	119.5
C4—C3—C2	121.2 (2)	C19—C20—C21	121.4 (2)
C4—C3—H3	119.4	C19—C20—H20	119.3
C2—C3—H3	119.4	C21—C20—H20	119.3
C3—C4—C5	119.3 (3)	C22—C21—C25	116.4 (2)
C3—C4—H4	120.3	C22—C21—C20	124.2 (2)
C5—C4—H4	120.3	C25—C21—C20	119.3 (2)
C6—C5—C4	120.5 (2)	C23—C22—C21	120.1 (2)
C6—C5—Cl1	119.76 (19)	C23—C22—H22	120.0
C4—C5—Cl1	119.7 (2)	C21—C22—H22	120.0
C5—C6—C1	120.8 (2)	C22—C23—C24	119.2 (2)
C5—C6—H6	119.6	C22—C23—H23	120.4

C1—C6—H6	119.6	C24—C23—H23	120.4
O2—C7—O1	125.1 (2)	N2—C24—C23	122.5 (2)
O2—C7—C1	118.2 (2)	N2—C24—H24	118.7
O1—C7—C1	116.7 (2)	C23—C24—H24	118.7
C13—C8—C9	119.0 (2)	N2—C25—C21	123.3 (2)
C13—C8—C14	120.0 (2)	N2—C25—C26	117.74 (17)
C9—C8—C14	121.0 (2)	C21—C25—C26	118.9 (2)
O6—C9—C10	118.5 (3)	N1—C26—C18	122.7 (2)
O6—C9—C8	122.1 (2)	N1—C26—C25	116.99 (19)
C10—C9—C8	119.4 (3)	C18—C26—C25	120.32 (18)
C11—C10—C9	120.9 (3)	Zn1—O7—H7B	112.3 (16)
C11—C10—H10	119.6	Zn1—O7—H7A	115.6 (17)
C9—C10—H10	119.6	H7B—O7—H7A	105 (3)
C10—C11—C12	119.6 (3)		
O1—Zn1—N1—C15	−81.8 (2)	C10—C11—C12—C13	−0.1 (4)
O4—Zn1—N1—C15	99.7 (2)	C10—C11—C12—Cl2	178.2 (2)
O7—Zn1—N1—C15	12.4 (2)	C11—C12—C13—C8	0.4 (3)
N2—Zn1—N1—C15	−177.0 (2)	Cl2—C12—C13—C8	−177.89 (16)
O1—Zn1—N1—C26	95.23 (15)	C9—C8—C13—C12	−0.8 (3)
O4—Zn1—N1—C26	−83.21 (17)	C14—C8—C13—C12	177.21 (19)
O7—Zn1—N1—C26	−170.52 (15)	Zn1—O4—C14—O5	7.2 (2)
N2—Zn1—N1—C26	0.08 (14)	Zn1—O4—C14—C8	−171.40 (13)
O1—Zn1—N2—C24	82.48 (19)	C13—C8—C14—O5	−176.59 (19)
O4—Zn1—N2—C24	−42.21 (19)	C9—C8—C14—O5	1.3 (3)
N1—Zn1—N2—C24	179.75 (19)	C13—C8—C14—O4	2.1 (3)
O7—Zn1—N2—C24	−143.2 (2)	C9—C8—C14—O4	−179.99 (17)
O1—Zn1—N2—C25	−98.22 (15)	C26—N1—C15—C16	0.5 (4)
O4—Zn1—N2—C25	137.10 (14)	Zn1—N1—C15—C16	177.5 (2)
N1—Zn1—N2—C25	−0.95 (14)	N1—C15—C16—C17	0.7 (4)
O7—Zn1—N2—C25	36.1 (3)	C15—C16—C17—C18	−1.1 (4)
O4—Zn1—O1—C7	−24.4 (2)	C16—C17—C18—C26	0.3 (4)
N1—Zn1—O1—C7	156.85 (18)	C16—C17—C18—C19	−178.7 (2)
O7—Zn1—O1—C7	66.96 (19)	C26—C18—C19—C20	−0.4 (4)
N2—Zn1—O1—C7	−124.25 (19)	C17—C18—C19—C20	178.5 (2)
O1—Zn1—O4—C14	−176.53 (12)	C18—C19—C20—C21	0.4 (4)
N1—Zn1—O4—C14	1.62 (17)	C19—C20—C21—C22	179.5 (2)
O7—Zn1—O4—C14	89.13 (14)	C19—C20—C21—C25	−0.4 (4)
N2—Zn1—O4—C14	−75.44 (14)	C25—C21—C22—C23	−2.3 (3)
C6—C1—C2—O3	177.31 (19)	C20—C21—C22—C23	177.7 (2)
C7—C1—C2—O3	−1.7 (3)	C21—C22—C23—C24	0.9 (4)
C6—C1—C2—C3	−2.1 (3)	C25—N2—C24—C23	−0.9 (3)
C7—C1—C2—C3	178.89 (19)	Zn1—N2—C24—C23	178.34 (17)
O3—C2—C3—C4	−177.8 (2)	C22—C23—C24—N2	0.8 (4)
C1—C2—C3—C4	1.7 (3)	C24—N2—C25—C21	−0.7 (3)
C2—C3—C4—C5	−0.2 (4)	Zn1—N2—C25—C21	179.95 (16)
C3—C4—C5—C6	−0.7 (3)	C24—N2—C25—C26	−178.95 (18)
C3—C4—C5—Cl1	179.04 (18)	Zn1—N2—C25—C26	1.7 (2)
C4—C5—C6—C1	0.3 (3)	C22—C21—C25—N2	2.3 (3)
Cl1—C5—C6—C1	−179.52 (15)	C20—C21—C25—N2	−177.8 (2)

C2—C1—C6—C5	1.2 (3)	C22—C21—C25—C26	−179.5 (2)
C7—C1—C6—C5	−179.84 (17)	C20—C21—C25—C26	0.5 (3)
Zn1—O1—C7—O2	2.0 (3)	C15—N1—C26—C18	−1.4 (3)
Zn1—O1—C7—C1	−177.15 (13)	Zn1—N1—C26—C18	−178.73 (17)
C6—C1—C7—O2	−170.38 (18)	C15—N1—C26—C25	178.12 (19)
C2—C1—C7—O2	8.6 (3)	Zn1—N1—C26—C25	0.8 (2)
C6—C1—C7—O1	8.9 (3)	C17—C18—C26—N1	1.0 (3)
C2—C1—C7—O1	−172.16 (18)	C19—C18—C26—N1	180.0 (2)
C13—C8—C9—O6	179.8 (2)	C17—C18—C26—C25	−178.5 (2)
C14—C8—C9—O6	1.9 (3)	C19—C18—C26—C25	0.5 (3)
C13—C8—C9—C10	0.8 (3)	N2—C25—C26—N1	−1.7 (3)
C14—C8—C9—C10	−177.2 (2)	C21—C25—C26—N1	179.96 (19)
O6—C9—C10—C11	−179.5 (2)	N2—C25—C26—C18	177.8 (2)
C8—C9—C10—C11	−0.5 (4)	C21—C25—C26—C18	−0.5 (3)
C9—C10—C11—C12	0.1 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···O2	0.85 (1)	1.78 (2)	2.552 (3)	151 (2)
O6—H6A···O5	0.85 (1)	1.80 (2)	2.577 (3)	150 (2)
O7—H7A···O4^{i}	0.85 (1)	1.97 (1)	2.785 (3)	162 (3)
O7—H7B···O2^{i}	0.84 (1)	1.84 (1)	2.672 (3)	171 (2)

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

Fig. 1

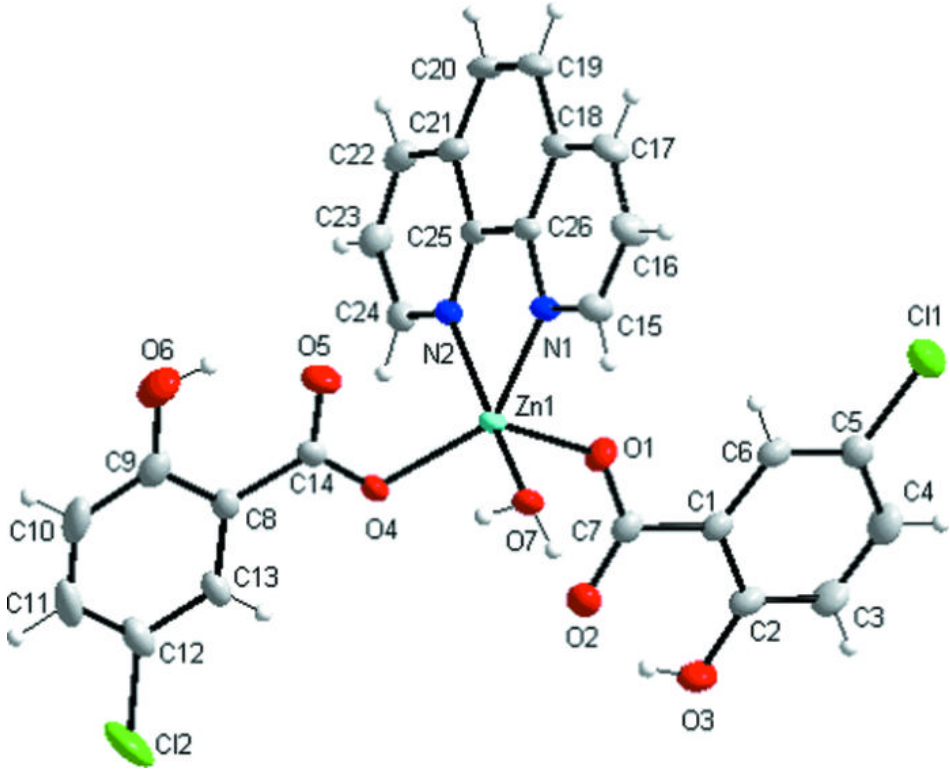
C20
C19
C21
C18
C17
C22
C23
C25
C26
C16
C24
N2
N1
C15
Cl1
O6
O5
Zn1
C9
C14
O1
C6
C5
C1
C4
C10
C8
O4
O7
C7
C13
C11
O2
C2
C3
C12
O3
Cl2

Fig. 2

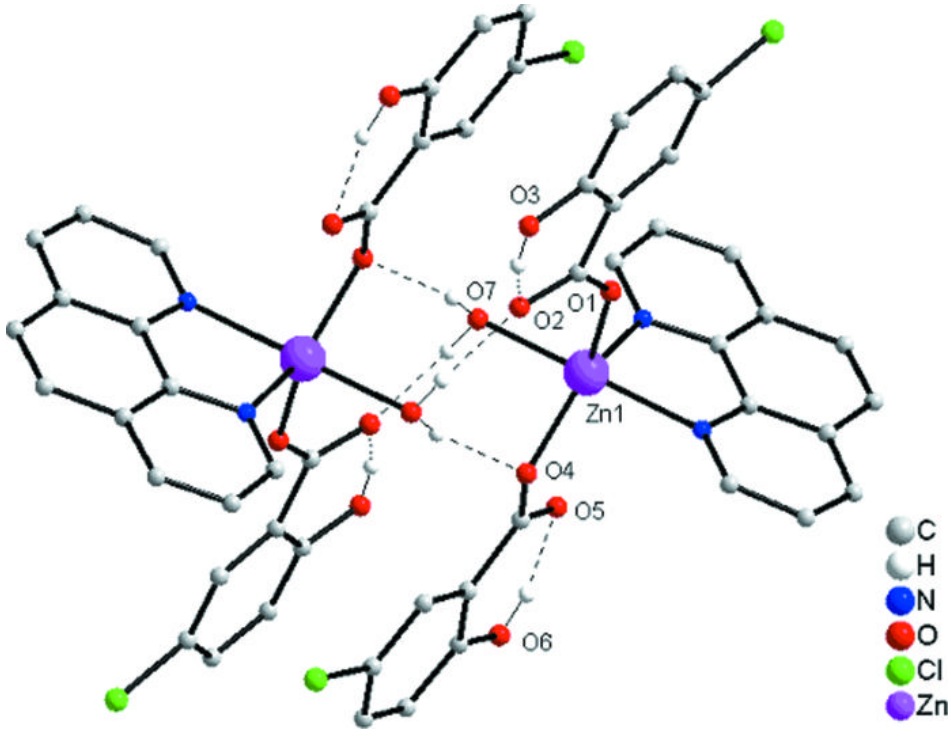

Fig. 3