

Aqua(2,2'-bipyridine- κ^2N,N')bis(5-chlorosalicylato- κO)zinc(II)

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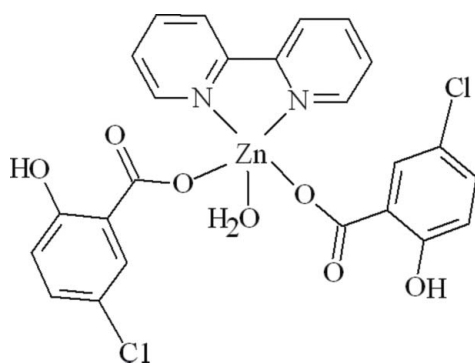
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.031; wR factor = 0.094; data-to-parameter ratio = 14.4.

In the title complex, $[Zn(C_7H_4ClO_3)_2(C_{10}H_8N_2)(H_2O)]$, the Zn^{II} atom is coordinated by two 5-chlorosalicylate ligands, one 2,2'-bipyridine ligand and one water molecule, displaying a distorted trigonal-bipyramidal geometry. The crystal structure is stabilized by intra- and intermolecular $O-H\cdots O$ and intermolecular $C-H\cdots Cl$ hydrogen bonds.

Related literature

For related literature, see: Brownless *et al.* (1999); Lemoine, Bendada & Viossat (2004); Lemoine, Viossat *et al.* (2004); Melnik *et al.* (2001); Wang *et al.* (2004); Wen *et al.* (2007a,b).



Experimental

Crystal data

$[Zn(C_7H_4ClO_3)_2(C_{10}H_8N_2)(H_2O)]$

$M_r = 582.67$

Triclinic, $P\bar{1}$

$a = 10.114$ (5) Å

$b = 11.141$ (6) Å

$c = 11.553$ (6) Å

$\alpha = 112.72$ (2)°

$\beta = 93.208$ (19)°

$\gamma = 97.93$ (2)°

$V = 1180.8$ (11) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 1.32$ mm⁻¹

$T = 293$ (2) K

$0.52 \times 0.50 \times 0.47$ mm

Data collection

Rigaku R-Axis RAPID

diffractometer

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.511$, $T_{\max} = 0.541$

10689 measured reflections

4865 independent reflections

4269 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.094$

$S = 1.11$

4865 reflections

337 parameters

4 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.28$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.63$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—O4	1.9863 (17)	Zn1—N2	2.104 (2)
Zn1—O7	2.0507 (17)	Zn1—N1	2.1514 (19)
Zn1—O1	2.0715 (17)		
O4—Zn1—O7	113.87 (7)	O1—Zn1—N2	89.69 (7)
O4—Zn1—O1	96.40 (7)	O4—Zn1—N1	103.25 (8)
O7—Zn1—O1	88.52 (7)	O7—Zn1—N1	90.52 (7)
O4—Zn1—N2	109.12 (7)	O1—Zn1—N1	158.89 (7)
O7—Zn1—N2	136.91 (7)	N2—Zn1—N1	76.73 (7)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H7B \cdots O2	0.82 (1)	1.85 (1)	2.640 (2)	160 (2)
O7—H7A \cdots O6 ⁱ	0.82 (1)	1.98 (1)	2.786 (3)	171 (2)
O3—H3B \cdots O2	0.82 (3)	1.78 (2)	2.516 (3)	148 (3)
O6—H6B \cdots O5	0.82 (3)	1.74 (2)	2.498 (3)	152 (2)
C16—H16A \cdots Cl2 ⁱⁱ	0.93	2.79	3.552 (3)	140

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); 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: HY2079).

References

- Brownless, N. J., Edwards, D. A. & Mahon, M. F. (1999). *Inorg. Chim. Acta*, **287**, 89–94.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Lemoine, P., Bendada, K. & Viossat, B. (2004). *Acta Cryst.* **C60**, m489–m491.
- Lemoine, P., Viossat, B., Dung, N. H., Tomas, A., Morgant, G., Greenaway, F. T. & Sorenson, J. R. J. (2004). *J. Inorg. Biochem.* **98**, 1734–1749.
- Melnik, M., Koman, M., Moncol, J. & Glowiak, T. (2001). *J. Coord. Chem.* **53**, 173–177.
- Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.

Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Wang, Y., Odoko, M. & Okabe, N. (2004). *Acta Cryst.* **C60**, m479–m481.
Wen, D.-C., Liu, S.-X. & Ribas, J. (2007a). *Inorg. Chem. Commun.* **10**, 661–665.
Wen, D.-C., Liu, S.-X. & Ribas, J. (2007b). *Polyhedron*, **26**, 3849–3856.

supplementary materials

Acta Cryst. (2007). E63, m2446-m2447 [doi:10.1107/S1600536807042316]

Aqua(2,2'-bipyridine- κ^2N,N')bis(5-chlorosalicylato- κO)zinc(II)

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Comment

Metal salicylate complexes are of current interest owing to their intriguing structural features and biological applications (Brownless *et al.*, 1999; Lemoine, Bendada & Viossat, 2004; Lemoine, Viossat *et al.*, 2004; Wang *et al.*, 2004; Wen *et al.*, 2007a,b). We report here the structure of a zinc(II) complex with 5-chlorosalicylate ligand (Melnik *et al.*, 2001).

The title complex was synthesized under hydrothermal conditions. The Zn^{II} atom is coordinated in a distorted trigonal bipyramidal geometry by two O atoms from two 5-chlorosalicylate ligands, two N atoms from a 2,2'-bipyridine ligand and one water O atom (Fig. 1 and Table 1). The water molecule, hydroxyl groups and the uncoordinated carboxylate oxygen atoms form intra- and intermolecular O—H \cdots O hydrogen bonds while the 2,2'-bipyridine ligand forms an intermolecular C—H \cdots Cl hydrogen bond with the Cl atom of a 5-chlorosalicylate ligand (Table 2), generating an extended chain architecture along the *a* axis (Fig. 2). The crystal structure is stabilized by the O—H \cdots O and C—H \cdots Cl hydrogen bonds.

Experimental

A mixture of Zn(NO₃)₂·6H₂O (0.030 g, 0.1 mmol), 2,2'-bipyridine (0.016 g, 0.1 mmol), 5-chlorosalicylic acid (0.035 g, 0.2 mmol) and distilled water (10 ml) was put into a 20 ml Teflon-lined autoclave and then heated at 413 K for 48 h. Yellow block-like crystals of the title compound suitable for X-ray analysis were collected from the reaction mixture.

Refinement

H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of water molecule and hydroxyl groups were found in a difference Fourier map and refined with a distance restraint of O—H = 0.82 (1)Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

Figures

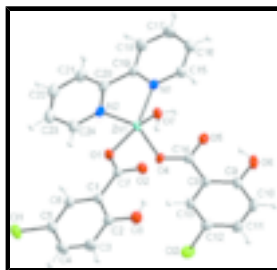


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

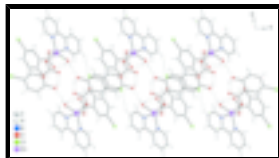


Fig. 2. A view of the extended hydrogen-bonding (dashed lines) chain along the *a* axis.

Aquabis(5-chlorosalicylato- κ O)(2,2'-bipyridine- κ^2 N,N')zinc(II)

Crystal data

$[\text{Zn}(\text{C}_7\text{H}_4\text{ClO}_3)_2(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$	$Z = 2$
$M_r = 582.67$	$F_{000} = 592$
Triclinic, $P\bar{1}$	$D_x = 1.639 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 10.114 (5) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 11.141 (6) \text{ \AA}$	Cell parameters from 4865 reflections
$c = 11.553 (6) \text{ \AA}$	$\theta = 3.1\text{--}26.5^\circ$
$\alpha = 112.72 (2)^\circ$	$\mu = 1.32 \text{ mm}^{-1}$
$\beta = 93.208 (19)^\circ$	$T = 293 (2) \text{ K}$
$\gamma = 97.93 (2)^\circ$	Block, yellow
$V = 1180.8 (11) \text{ \AA}^3$	$0.52 \times 0.50 \times 0.47 \text{ mm}$

Data collection

Rigaku R-Axis RAPID diffractometer	4865 independent reflections
Radiation source: rotation anode	4269 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.023$
$T = 293(2) \text{ K}$	$\theta_{\text{max}} = 26.5^\circ$
ω scans	$\theta_{\text{min}} = 3.1^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.511$, $T_{\text{max}} = 0.541$	$k = -13 \rightarrow 13$
10689 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.094$	$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 0.1147P]$
$S = 1.11$	where $P = (F_o^2 + 2F_c^2)/3$
4865 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
	$\Delta\rho_{\text{max}} = 0.28 \text{ e \AA}^{-3}$

337 parameters

$$\Delta\rho_{\min} = -0.63 \text{ e } \text{\AA}^{-3}$$

4 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.93725 (2)	0.88977 (2)	0.26799 (2)	0.03437 (9)
N1	1.07977 (17)	0.94611 (18)	0.15880 (17)	0.0397 (4)
N2	0.92448 (17)	1.08927 (17)	0.31238 (16)	0.0377 (4)
O1	0.84114 (15)	0.89774 (15)	0.42384 (14)	0.0427 (3)
O2	0.86926 (16)	0.70100 (16)	0.41829 (16)	0.0491 (4)
O3	0.7135 (2)	0.58124 (18)	0.51632 (19)	0.0605 (5)
H3B	0.781 (2)	0.599 (3)	0.486 (3)	0.073*
O4	0.78536 (14)	0.77602 (14)	0.13849 (13)	0.0398 (3)
O5	0.92178 (15)	0.63737 (17)	0.04523 (16)	0.0528 (4)
O6	0.83933 (18)	0.4330 (2)	-0.14905 (18)	0.0645 (5)
H6B	0.889 (3)	0.489 (3)	-0.088 (2)	0.077*
O7	1.06808 (15)	0.78652 (16)	0.31565 (14)	0.0431 (3)
H7B	1.019 (2)	0.749 (2)	0.351 (2)	0.052*
H7A	1.098 (2)	0.7280 (19)	0.2633 (18)	0.052*
C1	0.70639 (19)	0.8041 (2)	0.53918 (18)	0.0356 (4)
C2	0.6614 (2)	0.6930 (2)	0.5648 (2)	0.0424 (5)
C3	0.5595 (3)	0.6961 (3)	0.6410 (2)	0.0548 (6)
H3A	0.5278	0.6216	0.6560	0.066*
C4	0.5055 (3)	0.8082 (3)	0.6941 (2)	0.0558 (6)
H4A	0.4387	0.8105	0.7466	0.067*
C5	0.5500 (2)	0.9180 (2)	0.6698 (2)	0.0466 (5)
C6	0.6491 (2)	0.9165 (2)	0.59318 (19)	0.0404 (4)
H6A	0.6782	0.9910	0.5773	0.049*
C7	0.81292 (19)	0.8010 (2)	0.45482 (18)	0.0360 (4)
C8	0.6974 (2)	0.58857 (19)	-0.04858 (18)	0.0341 (4)
C9	0.7182 (2)	0.4718 (2)	-0.1443 (2)	0.0428 (5)
C10	0.6134 (3)	0.3919 (2)	-0.2364 (2)	0.0532 (6)
H10A	0.6279	0.3143	-0.3000	0.064*
C11	0.4887 (2)	0.4273 (2)	-0.2335 (2)	0.0496 (5)
H11A	0.4180	0.3732	-0.2942	0.060*
C12	0.4687 (2)	0.5434 (2)	-0.1404 (2)	0.0398 (5)
C13	0.5701 (2)	0.6234 (2)	-0.04767 (18)	0.0355 (4)
H13A	0.5541	0.7005	0.0156	0.043*
C14	0.8089 (2)	0.6724 (2)	0.05218 (19)	0.0364 (4)
C15	1.1575 (2)	0.8696 (2)	0.0834 (2)	0.0483 (5)
H15A	1.1523	0.7833	0.0771	0.058*
C16	1.2435 (3)	0.9120 (3)	0.0157 (2)	0.0550 (6)
H16A	1.2951	0.8554	-0.0364	0.066*
C17	1.2532 (3)	1.0403 (3)	0.0252 (3)	0.0587 (6)
H17A	1.3111	1.0720	-0.0203	0.070*

supplementary materials

C18	1.1753 (3)	1.1200 (3)	0.1037 (2)	0.0540 (6)
H18A	1.1808	1.2072	0.1126	0.065*
C19	1.0892 (2)	1.0712 (2)	0.16902 (19)	0.0376 (4)
C20	1.0020 (2)	1.1516 (2)	0.25444 (19)	0.0386 (4)
C21	0.9986 (3)	1.2815 (2)	0.2744 (2)	0.0517 (6)
H21A	1.0529	1.3231	0.2336	0.062*
C22	0.9138 (3)	1.3490 (2)	0.3554 (3)	0.0565 (6)
H22A	0.9101	1.4364	0.3695	0.068*
C23	0.8360 (3)	1.2871 (3)	0.4143 (2)	0.0553 (6)
H23A	0.7785	1.3315	0.4693	0.066*
C24	0.8430 (2)	1.1564 (2)	0.3917 (2)	0.0471 (5)
H24A	0.7898	1.1142	0.4326	0.057*
Cl1	0.47871 (7)	1.05894 (8)	0.73805 (8)	0.0718 (2)
Cl2	0.31025 (6)	0.58675 (7)	-0.14145 (7)	0.06070 (18)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03880 (14)	0.02641 (14)	0.03341 (14)	0.00365 (9)	0.00601 (9)	0.00750 (10)
N1	0.0443 (9)	0.0303 (9)	0.0408 (9)	0.0028 (7)	0.0071 (8)	0.0112 (8)
N2	0.0434 (9)	0.0299 (9)	0.0340 (8)	0.0064 (7)	-0.0002 (7)	0.0073 (7)
O1	0.0515 (8)	0.0353 (8)	0.0426 (8)	0.0099 (7)	0.0167 (7)	0.0146 (7)
O2	0.0550 (9)	0.0390 (9)	0.0560 (9)	0.0161 (7)	0.0201 (8)	0.0174 (8)
O3	0.0731 (11)	0.0379 (9)	0.0780 (13)	0.0130 (9)	0.0271 (10)	0.0275 (9)
O4	0.0433 (7)	0.0306 (8)	0.0355 (7)	0.0023 (6)	0.0017 (6)	0.0041 (6)
O5	0.0399 (8)	0.0440 (9)	0.0578 (10)	0.0066 (7)	0.0012 (7)	0.0034 (8)
O6	0.0549 (10)	0.0540 (12)	0.0600 (11)	0.0229 (9)	0.0037 (8)	-0.0077 (9)
O7	0.0492 (8)	0.0423 (9)	0.0363 (8)	0.0156 (7)	0.0107 (6)	0.0106 (7)
C1	0.0369 (9)	0.0338 (11)	0.0293 (9)	0.0018 (8)	0.0026 (8)	0.0069 (8)
C2	0.0481 (11)	0.0356 (12)	0.0407 (11)	0.0017 (9)	0.0040 (9)	0.0142 (10)
C3	0.0602 (14)	0.0522 (15)	0.0551 (14)	-0.0001 (12)	0.0142 (12)	0.0269 (13)
C4	0.0524 (13)	0.0661 (17)	0.0497 (13)	0.0079 (12)	0.0203 (11)	0.0227 (13)
C5	0.0452 (11)	0.0474 (13)	0.0413 (11)	0.0094 (10)	0.0110 (9)	0.0101 (10)
C6	0.0444 (10)	0.0355 (11)	0.0377 (10)	0.0043 (9)	0.0054 (9)	0.0114 (9)
C7	0.0387 (9)	0.0312 (10)	0.0306 (9)	0.0034 (8)	0.0010 (8)	0.0054 (8)
C8	0.0419 (10)	0.0263 (10)	0.0310 (9)	0.0020 (8)	0.0050 (8)	0.0093 (8)
C9	0.0495 (11)	0.0350 (11)	0.0381 (11)	0.0103 (9)	0.0053 (9)	0.0073 (9)
C10	0.0682 (15)	0.0366 (12)	0.0392 (12)	0.0078 (11)	0.0000 (11)	-0.0004 (10)
C11	0.0575 (13)	0.0400 (13)	0.0406 (11)	-0.0027 (10)	-0.0085 (10)	0.0101 (10)
C12	0.0426 (10)	0.0389 (12)	0.0409 (11)	0.0030 (9)	0.0002 (9)	0.0212 (10)
C13	0.0468 (10)	0.0267 (10)	0.0335 (9)	0.0056 (8)	0.0059 (8)	0.0125 (8)
C14	0.0409 (10)	0.0293 (10)	0.0365 (10)	0.0013 (8)	0.0037 (8)	0.0123 (9)
C15	0.0535 (12)	0.0359 (12)	0.0534 (13)	0.0081 (10)	0.0164 (11)	0.0142 (11)
C16	0.0569 (13)	0.0534 (16)	0.0537 (14)	0.0105 (12)	0.0177 (11)	0.0183 (12)
C17	0.0669 (15)	0.0567 (16)	0.0599 (15)	0.0043 (13)	0.0217 (13)	0.0313 (14)
C18	0.0712 (16)	0.0422 (13)	0.0548 (14)	0.0070 (12)	0.0135 (12)	0.0260 (12)
C19	0.0429 (10)	0.0323 (10)	0.0335 (10)	0.0011 (8)	-0.0015 (8)	0.0114 (9)
C20	0.0451 (10)	0.0309 (10)	0.0351 (10)	0.0042 (8)	-0.0050 (8)	0.0100 (9)

C21	0.0657 (14)	0.0351 (12)	0.0545 (13)	0.0076 (10)	0.0021 (12)	0.0193 (11)
C22	0.0676 (15)	0.0347 (12)	0.0640 (16)	0.0169 (11)	-0.0013 (13)	0.0146 (12)
C23	0.0587 (13)	0.0440 (14)	0.0558 (14)	0.0225 (11)	0.0017 (12)	0.0080 (12)
C24	0.0494 (12)	0.0400 (13)	0.0459 (12)	0.0118 (10)	0.0050 (10)	0.0095 (10)
Cl1	0.0735 (4)	0.0640 (4)	0.0754 (5)	0.0299 (4)	0.0333 (4)	0.0159 (4)
Cl2	0.0481 (3)	0.0614 (4)	0.0732 (4)	0.0105 (3)	-0.0080 (3)	0.0291 (3)

Geometric parameters (Å, °)

Zn1—O4	1.9863 (17)	C6—H6A	0.9300
Zn1—O7	2.0507 (17)	C8—C13	1.394 (3)
Zn1—O1	2.0715 (17)	C8—C9	1.396 (3)
Zn1—N2	2.104 (2)	C8—C14	1.490 (3)
Zn1—N1	2.1514 (19)	C9—C10	1.389 (3)
N1—C15	1.339 (3)	C10—C11	1.371 (4)
N1—C19	1.342 (3)	C10—H10A	0.9300
N2—C24	1.342 (3)	C11—C12	1.376 (3)
N2—C20	1.346 (3)	C11—H11A	0.9300
O1—C7	1.263 (3)	C12—C13	1.371 (3)
O2—C7	1.258 (2)	C12—Cl2	1.736 (2)
O3—C2	1.348 (3)	C13—H13A	0.9300
O3—H3B	0.82 (3)	C15—C16	1.356 (3)
O4—C14	1.264 (3)	C15—H15A	0.9300
O5—C14	1.254 (2)	C16—C17	1.380 (4)
O6—C9	1.351 (3)	C16—H16A	0.9300
O6—H6B	0.82 (3)	C17—C18	1.372 (4)
O7—H7B	0.826 (10)	C17—H17A	0.9300
O7—H7A	0.810 (10)	C18—C19	1.372 (3)
C1—C6	1.389 (3)	C18—H18A	0.9300
C1—C2	1.403 (3)	C19—C20	1.479 (3)
C1—C7	1.488 (3)	C20—C21	1.380 (3)
C2—C3	1.389 (3)	C21—C22	1.379 (4)
C3—C4	1.367 (4)	C21—H21A	0.9300
C3—H3A	0.9300	C22—C23	1.352 (4)
C4—C5	1.380 (4)	C22—H22A	0.9300
C4—H4A	0.9300	C23—C24	1.389 (3)
C5—C6	1.372 (3)	C23—H23A	0.9300
C5—Cl1	1.740 (2)	C24—H24A	0.9300
O4—Zn1—O7	113.87 (7)	O6—C9—C8	121.2 (2)
O4—Zn1—O1	96.40 (7)	C10—C9—C8	120.3 (2)
O7—Zn1—O1	88.52 (7)	C11—C10—C9	120.0 (2)
O4—Zn1—N2	109.12 (7)	C11—C10—H10A	120.0
O7—Zn1—N2	136.91 (7)	C9—C10—H10A	120.0
O1—Zn1—N2	89.69 (7)	C10—C11—C12	119.7 (2)
O4—Zn1—N1	103.25 (8)	C10—C11—H11A	120.2
O7—Zn1—N1	90.52 (7)	C12—C11—H11A	120.2
O1—Zn1—N1	158.89 (7)	C13—C12—C11	121.4 (2)
N2—Zn1—N1	76.73 (7)	C13—C12—Cl2	120.20 (17)
C15—N1—C19	118.18 (19)	C11—C12—Cl2	118.42 (17)

supplementary materials

C15—N1—Zn1	126.70 (15)	C12—C13—C8	119.75 (19)
C19—N1—Zn1	115.13 (14)	C12—C13—H13A	120.1
C24—N2—C20	118.58 (19)	C8—C13—H13A	120.1
C24—N2—Zn1	124.50 (16)	O5—C14—O4	123.54 (19)
C20—N2—Zn1	116.90 (14)	O5—C14—C8	118.04 (18)
C7—O1—Zn1	124.19 (13)	O4—C14—C8	118.40 (17)
C2—O3—H3B	106 (2)	N1—C15—C16	123.1 (2)
C14—O4—Zn1	117.68 (13)	N1—C15—H15A	118.4
C9—O6—H6B	106 (2)	C16—C15—H15A	118.4
Zn1—O7—H7B	100.3 (17)	C15—C16—C17	119.0 (2)
Zn1—O7—H7A	122.6 (18)	C15—C16—H16A	120.5
H7B—O7—H7A	105 (3)	C17—C16—H16A	120.5
C6—C1—C2	118.89 (19)	C18—C17—C16	118.3 (2)
C6—C1—C7	120.63 (19)	C18—C17—H17A	120.9
C2—C1—C7	120.48 (19)	C16—C17—H17A	120.9
O3—C2—C3	118.2 (2)	C19—C18—C17	120.1 (2)
O3—C2—C1	121.9 (2)	C19—C18—H18A	120.0
C3—C2—C1	119.9 (2)	C17—C18—H18A	120.0
C4—C3—C2	120.2 (2)	N1—C19—C18	121.3 (2)
C4—C3—H3A	119.9	N1—C19—C20	115.92 (18)
C2—C3—H3A	119.9	C18—C19—C20	122.8 (2)
C3—C4—C5	120.1 (2)	N2—C20—C21	121.5 (2)
C3—C4—H4A	119.9	N2—C20—C19	115.30 (18)
C5—C4—H4A	119.9	C21—C20—C19	123.2 (2)
C6—C5—C4	120.6 (2)	C22—C21—C20	119.3 (2)
C6—C5—C11	120.34 (19)	C22—C21—H21A	120.4
C4—C5—C11	119.05 (18)	C20—C21—H21A	120.4
C5—C6—C1	120.3 (2)	C23—C22—C21	119.5 (2)
C5—C6—H6A	119.9	C23—C22—H22A	120.2
C1—C6—H6A	119.9	C21—C22—H22A	120.2
O2—C7—O1	123.97 (19)	C22—C23—C24	119.2 (2)
O2—C7—C1	117.45 (19)	C22—C23—H23A	120.4
O1—C7—C1	118.57 (18)	C24—C23—H23A	120.4
C13—C8—C9	118.82 (19)	N2—C24—C23	121.9 (2)
C13—C8—C14	120.88 (18)	N2—C24—H24A	119.1
C9—C8—C14	120.28 (18)	C23—C24—H24A	119.1
O6—C9—C10	118.4 (2)		
O4—Zn1—N1—C15	-74.08 (19)	C14—C8—C9—O6	-0.9 (3)
O7—Zn1—N1—C15	40.62 (19)	C13—C8—C9—C10	-0.3 (3)
O1—Zn1—N1—C15	127.8 (2)	C14—C8—C9—C10	178.3 (2)
N2—Zn1—N1—C15	179.06 (19)	O6—C9—C10—C11	179.2 (2)
O4—Zn1—N1—C19	105.74 (15)	C8—C9—C10—C11	-0.1 (4)
O7—Zn1—N1—C19	-139.56 (15)	C9—C10—C11—C12	1.1 (4)
O1—Zn1—N1—C19	-52.3 (2)	C10—C11—C12—C13	-1.8 (4)
N2—Zn1—N1—C19	-1.13 (14)	C10—C11—C12—C12	178.80 (19)
O4—Zn1—N2—C24	80.39 (18)	C11—C12—C13—C8	1.4 (3)
O7—Zn1—N2—C24	-103.76 (18)	C12—C12—C13—C8	-179.18 (15)
O1—Zn1—N2—C24	-16.27 (17)	C9—C8—C13—C12	-0.4 (3)
N1—Zn1—N2—C24	-179.96 (18)	C14—C8—C13—C12	-178.97 (18)

O4—Zn1—N2—C20	-98.18 (15)	Zn1—O4—C14—O5	0.9 (3)
O7—Zn1—N2—C20	77.67 (17)	Zn1—O4—C14—C8	-177.68 (13)
O1—Zn1—N2—C20	165.16 (14)	C13—C8—C14—O5	-178.77 (19)
N1—Zn1—N2—C20	1.47 (14)	C9—C8—C14—O5	2.7 (3)
O4—Zn1—O1—C7	69.96 (17)	C13—C8—C14—O4	-0.1 (3)
O7—Zn1—O1—C7	-43.90 (17)	C9—C8—C14—O4	-178.68 (19)
N2—Zn1—O1—C7	179.16 (16)	C19—N1—C15—C16	-1.0 (3)
N1—Zn1—O1—C7	-131.49 (19)	Zn1—N1—C15—C16	178.78 (19)
O7—Zn1—O4—C14	-35.97 (16)	N1—C15—C16—C17	0.7 (4)
O1—Zn1—O4—C14	-127.18 (15)	C15—C16—C17—C18	0.2 (4)
N2—Zn1—O4—C14	140.92 (14)	C16—C17—C18—C19	-0.8 (4)
N1—Zn1—O4—C14	60.59 (16)	C15—N1—C19—C18	0.4 (3)
C6—C1—C2—O3	-179.4 (2)	Zn1—N1—C19—C18	-179.41 (17)
C7—C1—C2—O3	1.0 (3)	C15—N1—C19—C20	-179.48 (18)
C6—C1—C2—C3	1.3 (3)	Zn1—N1—C19—C20	0.7 (2)
C7—C1—C2—C3	-178.3 (2)	C17—C18—C19—N1	0.5 (4)
O3—C2—C3—C4	178.8 (2)	C17—C18—C19—C20	-179.6 (2)
C1—C2—C3—C4	-1.9 (4)	C24—N2—C20—C21	-0.4 (3)
C2—C3—C4—C5	1.5 (4)	Zn1—N2—C20—C21	178.29 (16)
C3—C4—C5—C6	-0.4 (4)	C24—N2—C20—C19	179.77 (18)
C3—C4—C5—C11	179.7 (2)	Zn1—N2—C20—C19	-1.6 (2)
C4—C5—C6—C1	-0.2 (3)	N1—C19—C20—N2	0.6 (3)
C11—C5—C6—C1	179.72 (16)	C18—C19—C20—N2	-179.3 (2)
C2—C1—C6—C5	-0.2 (3)	N1—C19—C20—C21	-179.3 (2)
C7—C1—C6—C5	179.32 (19)	C18—C19—C20—C21	0.8 (3)
Zn1—O1—C7—O2	20.1 (3)	N2—C20—C21—C22	-0.1 (3)
Zn1—O1—C7—C1	-159.64 (13)	C19—C20—C21—C22	179.8 (2)
C6—C1—C7—O2	173.64 (19)	C20—C21—C22—C23	0.3 (4)
C2—C1—C7—O2	-6.8 (3)	C21—C22—C23—C24	-0.1 (4)
C6—C1—C7—O1	-6.6 (3)	C20—N2—C24—C23	0.6 (3)
C2—C1—C7—O1	172.97 (19)	Zn1—N2—C24—C23	-177.97 (17)
C13—C8—C9—O6	-179.5 (2)	C22—C23—C24—N2	-0.3 (4)

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O7—H7B \cdots O2	0.82 (1)	1.85 (1)	2.640 (2)	160 (2)
O7—H7A \cdots O6 ⁱ	0.82 (1)	1.98 (1)	2.786 (3)	171 (2)
O3—H3B \cdots O2	0.82 (3)	1.78 (2)	2.516 (3)	148 (3)
O6—H6B \cdots O5	0.82 (3)	1.74 (2)	2.498 (3)	152 (2)
C16—H16A \cdots Cl2 ⁱⁱ	0.93	2.79	3.552 (3)	140

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

Fig. 1

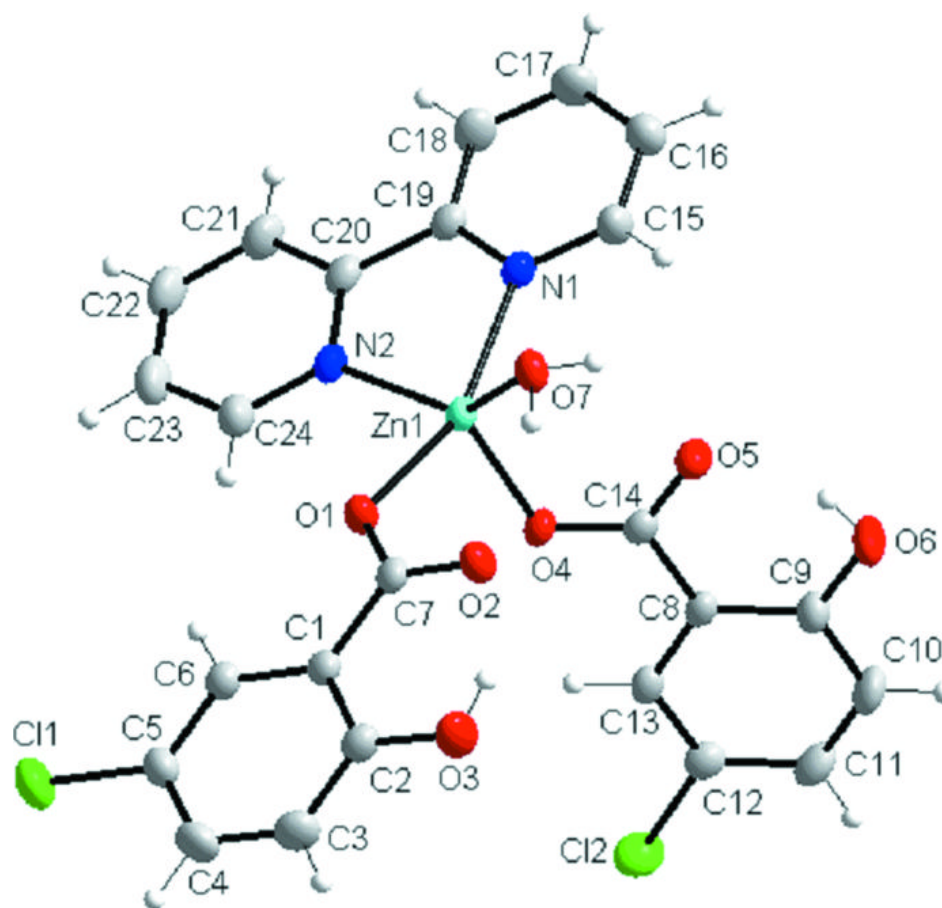


Fig. 2

