

(5,5'-Dimethyl-2,2'-bipyridine- κ^2N,N')-(1-naphthylacetato- κO)(1-naphthylacetato- κ^2O,O')zinc hemihydrate

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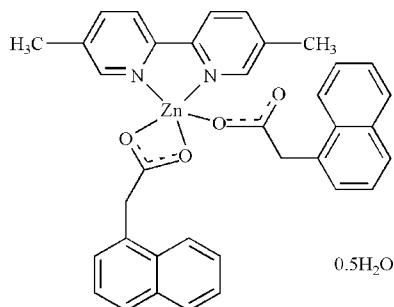
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.007$ Å; R factor = 0.044; wR factor = 0.106; data-to-parameter ratio = 13.5.

In the title compound, $[Zn(C_{12}H_9O_2)_2(C_{12}H_{12}N_2)] \cdot 0.5H_2O$, the water molecule lies on a twofold rotation axis. The Zn^{II} atom is coordinated by three O atoms from two 1-naphthylacetate ligands, one monodentate and the other asymmetric bidentate chelate, and two N atoms from a 5,5'-dimethyl-2,2'-bipyridine ligand, giving an irregular environment. In the crystal, the complex molecules are interlinked through the water molecule by $O-H \cdots O_{\text{carboxylate}}$ hydrogen bonds, together with weak $C-H \cdots O$ and bipyridine ring $\pi-\pi$ stacking interactions [ring centroid separation = $3.761(2)$ Å], giving a two-dimensional network structure.

Related literature

For background to self-assembly of supramolecular architectures based on naphthylcarboxylate ligands, see: Kong *et al.* (2009); Li *et al.* (2009). The $Zn-O$ distance in the second ligand [$2.417(3)$ Å] suggests a non-negligible (bidentate) interaction, see: Guilera & Steed (1999).



Experimental

Crystal data

$[Zn(C_{12}H_9O_2)_2(C_{12}H_{12}N_2)] \cdot 0.5H_2O$
 $M_r = 629.00$
 Monoclinic, $C2/c$
 $a = 32.212(7)$ Å
 $b = 8.2668(17)$ Å
 $c = 25.314(5)$ Å
 $\beta = 117.865(4)^\circ$
 $V = 5959(2)$ Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.87$ mm⁻¹
 $T = 296$ K
 $0.30 \times 0.28 \times 0.21$ mm

Data collection

Bruker APEXII area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.756$, $T_{\max} = 0.819$
 21468 measured reflections
 5325 independent reflections
 3566 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.106$
 $S = 0.99$
 5325 reflections
 395 parameters
 2 restraints
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.45$ e Å⁻³
 $\Delta\rho_{\min} = -0.30$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O5-H5 \cdots O1$	0.82	2.21	2.948 (3)	150
$C8-H8A \cdots O4^i$	0.93	2.59	3.515 (6)	171

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; 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: ZS2105).

References

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 Li, Y.-P., Sun, D.-J., Zang, H., Su, G.-F. & Li, Y.-L. (2009). *Acta Cryst.* **C65**, m340–m342.
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supplementary materials

Acta Cryst. (2011). E67, m606 [doi:10.1107/S1600536811013353]

(5,5'-Dimethyl-2,2'-bipyridine- κ^2N,N')(1-naphthylacetato- κO)(1-naphthylacetato- κ^2O,O')zinc hemihydrate

L.-L. Ji, J.-S. Liu and W.-D. Song

Comment

Self-assembly of supramolecular architectures based on naphthylcarboxylate ligands has attracted much attention during recent decades (Kong *et al.*, 2009; Li *et al.*, 2009). However, to our knowledge, 1-naphthylacetic acid has not been used as a potential building block in the construction of supramolecular architectures. Herein we report the structure of the title compound, the mixed ligand complex $[(C_{12}H_{12}N_2)(C_{12}H_9O_2)_2]_2 \cdot 0.5H_2O$ (I), from the reaction of zinc nitrate with 1-naphthylacetic acid and 5,5'-dimethyl-2,2'-bipyridine in a basic aqueous solution.

The asymmetric unit in (I) (Fig. 1) consists of one Zn^{II} complex unit and a water molecule which lies on a two-fold rotation axis (Fig. 1). The five-coordinate Zn centre comprises three O atoms from two 1-naphthylacetate ligands and two N atoms from a 5,5'-dimethyl-2,2'-bipyridine ligand. There are two coordination modes for the 1-naphthylacetate ligands in the structure: one monodentate the other asymmetric bidentate chelate. The Zn1-O4 distance in the second ligand [2.417 (3) Å] suggests a non-negligible (bidentate) interaction (Guilera & Steed, 1999) whereas the Zn1—O5 distance in the first ligand [2.587 (3)] is considered beyond the distance maximum for a bidentate interaction. In the crystal, the supramolecular network is stabilized by water O—H \cdots O_{carboxyl} hydrogen bonds together with weak intermolecular aromatic C8—H \cdots O_{carboxyl} interactions (Table 1), giving a two-dimensional network structure. In addition the inter-ring separation between the pyridine rings of two adjacent 5,5'-dimethyl-2,2'-bipyridine ligands is 3.761 (2) Å, indicating weak π - π stacking interactions (Fig. 2).

Experimental

A mixture of 1-naphthylacetic acid (0.110 g, 0.5 mmol), 5,5'-dimethyl-2,2'-bipyridine (0.092 g, 0.5 mmol), zinc nitrate hexahydrate (0.075 g, 0.25 mmol), NaOH (0.08 g, 0.2 mmol) and water (10 ml) was placed in a 23 ml Teflon-lined reactor, which was heated to 423 K for 3 days, and then cooled to room temperature at a rate of 10 K h⁻¹. The colorless crystals obtained were washed with water and dried in air (yield 47% based on zinc).

Refinement

All H atoms were located from difference maps, and were treated as riding atoms with O—H = 0.82 Å and C—H = 0.93, 0.96 and 0.97 Å, for aryl, methyl and methine groups respectively, and with $U_{iso}(H) = 1.5U_{eq}$ (methyl C-atoms) and $1.2U_{eq}$ (non-methyl C-atoms or water O-atom).

Figures

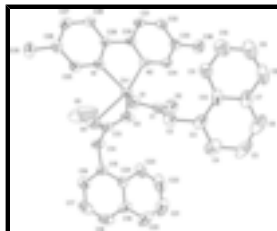


Fig. 1. The structure of the title compound, showing the atom numbering scheme. The water molecule of solvation (O5) lies on a twofold rotation axis. Non-H atoms are shown with 30% probability displacement ellipsoids and H atoms are omitted.

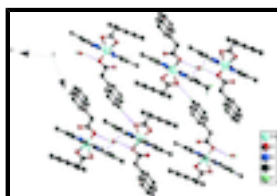


Fig. 2. A view of the three-dimensional network in (I) showing O—H...O, C—H...O and π - π stacking interactions as dashed lines.

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Crystal data

$[\text{Zn}(\text{C}_{12}\text{H}_9\text{O}_2)_2(\text{C}_{12}\text{H}_{12}\text{N}_2)] \cdot 0.5\text{H}_2\text{O}$

$M_r = 629.00$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 32.212\ (7)\ \text{\AA}$

$b = 8.2668\ (17)\ \text{\AA}$

$c = 25.314\ (5)\ \text{\AA}$

$\beta = 117.865\ (4)^\circ$

$V = 5959\ (2)\ \text{\AA}^3$

$Z = 8$

$F(000) = 2616$

$D_x = 1.402\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5837 reflections

$\theta = 2.8\text{--}27.9^\circ$

$\mu = 0.87\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Block, colorless

$0.30 \times 0.28 \times 0.21\ \text{mm}$

Data collection

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.756$, $T_{\max} = 0.819$

21468 measured reflections

5325 independent reflections

3566 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.049$

$\theta_{\max} = 25.2^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -38 \rightarrow 38$

$k = -9 \rightarrow 9$

$l = -30 \rightarrow 30$

Refinement

Refinement on F^2

Least-squares matrix: full

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$$R[F^2 > 2\sigma(F^2)] = 0.044$$

$$wR(F^2) = 0.106$$

$$S = 0.99$$

5325 reflections

395 parameters

2 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 11.176P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.020$$

$$\Delta\rho_{\max} = 0.45 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$$

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.

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 $F^2 > 2\sigma(F^2)$ 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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.120445 (14)	0.34832 (5)	0.280713 (17)	0.04660 (14)
O1	0.07142 (9)	0.4782 (3)	0.21694 (10)	0.0619 (6)
O2	0.12780 (10)	0.4724 (3)	0.19164 (11)	0.0687 (7)
O3	0.18066 (9)	0.4490 (3)	0.34162 (11)	0.0691 (7)
O4	0.12345 (12)	0.5188 (4)	0.35996 (13)	0.0879 (10)
N1	0.08321 (9)	0.1801 (3)	0.30436 (11)	0.0448 (7)
N2	0.14254 (9)	0.1318 (3)	0.26096 (11)	0.0442 (6)
C1	0.08888 (14)	0.5173 (4)	0.18284 (15)	0.0533 (9)
C2	0.05863 (14)	0.6281 (5)	0.13114 (16)	0.0660 (11)
H2A	0.0269	0.5856	0.1120	0.079*
H2B	0.0576	0.7335	0.1473	0.079*
C3	0.07433 (12)	0.6504 (5)	0.08408 (17)	0.0647 (11)
C4	0.09184 (16)	0.7942 (6)	0.0771 (2)	0.0952 (16)
H4A	0.0946	0.8806	0.1021	0.114*
C5	0.10634 (18)	0.8141 (8)	0.0303 (3)	0.107 (2)
H5A	0.1182	0.9118	0.0249	0.129*
C6	0.10167 (19)	0.6813 (9)	-0.0053 (3)	0.108 (2)
H6A	0.1106	0.6928	-0.0350	0.130*
C7	0.08495 (14)	0.5357 (7)	0.00033 (18)	0.0784 (12)
C8	0.08172 (16)	0.4032 (8)	-0.03669 (19)	0.0912 (16)
H8A	0.0905	0.4142	-0.0667	0.109*
C9	0.06576 (19)	0.2613 (9)	-0.0279 (2)	0.1072 (19)
H9A	0.0644	0.1735	-0.0516	0.129*
C10	0.05146 (17)	0.2409 (8)	0.0143 (2)	0.1002 (16)

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H10A	0.0402	0.1408	0.0187	0.120*
C11	0.05356 (14)	0.3666 (6)	0.05021 (18)	0.0737 (12)
H11A	0.0433	0.3512	0.0786	0.088*
C12	0.07062 (12)	0.5175 (6)	0.04549 (15)	0.0641 (11)
C13	0.16592 (17)	0.5149 (4)	0.37445 (16)	0.0638 (11)
C14	0.20119 (15)	0.5898 (5)	0.43349 (15)	0.0676 (12)
H14A	0.1916	0.5664	0.4638	0.081*
H14B	0.2317	0.5409	0.4460	0.081*
C15	0.20519 (12)	0.7702 (4)	0.42897 (13)	0.0492 (9)
C16	0.17724 (13)	0.8677 (6)	0.44192 (16)	0.0655 (11)
H16A	0.1560	0.8203	0.4525	0.079*
C17	0.17903 (17)	1.0338 (6)	0.44005 (19)	0.0818 (14)
H17A	0.1594	1.0964	0.4495	0.098*
C18	0.20899 (19)	1.1047 (5)	0.42461 (18)	0.0820 (14)
H18A	0.2097	1.2170	0.4230	0.098*
C19	0.23921 (14)	1.0145 (5)	0.41079 (15)	0.0629 (11)
C20	0.2712 (2)	1.0871 (8)	0.3958 (2)	0.1019 (19)
H20A	0.2722	1.1993	0.3938	0.122*
C21	0.3005 (2)	0.9985 (12)	0.3841 (2)	0.116 (2)
H21A	0.3211	1.0504	0.3734	0.140*
C22	0.30117 (18)	0.8311 (11)	0.3874 (2)	0.111 (2)
H22A	0.3229	0.7723	0.3807	0.133*
C23	0.26923 (15)	0.7514 (7)	0.40089 (16)	0.0795 (13)
H23A	0.2687	0.6390	0.4018	0.095*
C24	0.23771 (12)	0.8422 (5)	0.41318 (13)	0.0525 (9)
C25	0.05275 (12)	0.2135 (5)	0.32507 (14)	0.0537 (9)
H25A	0.0477	0.3213	0.3308	0.064*
C26	0.02851 (12)	0.0962 (5)	0.33832 (14)	0.0535 (9)
C27	0.03634 (12)	-0.0623 (5)	0.32856 (15)	0.0577 (10)
H27A	0.0202	-0.1448	0.3361	0.069*
C28	0.06785 (12)	-0.0999 (4)	0.30777 (15)	0.0514 (9)
H28A	0.0733	-0.2070	0.3015	0.062*
C29	0.09120 (11)	0.0246 (4)	0.29648 (13)	0.0412 (7)
C30	0.12614 (11)	-0.0026 (4)	0.27505 (13)	0.0401 (7)
C31	0.14199 (12)	-0.1536 (4)	0.26986 (14)	0.0496 (8)
H31A	0.1304	-0.2456	0.2795	0.060*
C32	0.17511 (12)	-0.1673 (5)	0.25029 (15)	0.0571 (9)
H32A	0.1859	-0.2690	0.2467	0.069*
C33	0.19239 (13)	-0.0319 (5)	0.23602 (16)	0.0575 (9)
C34	0.17446 (12)	0.1158 (4)	0.24173 (16)	0.0537 (9)
H34A	0.1853	0.2089	0.2316	0.064*
C35	-0.00465 (14)	0.1416 (6)	0.36237 (18)	0.0762 (12)
H35A	-0.0321	0.0742	0.3444	0.114*
H35B	-0.0137	0.2529	0.3532	0.114*
H35C	0.0106	0.1267	0.4049	0.114*
C36	0.22968 (16)	-0.0420 (6)	0.2159 (2)	0.0877 (14)
H36A	0.2215	-0.1249	0.1862	0.131*
H36B	0.2594	-0.0675	0.2495	0.131*
H36C	0.2319	0.0601	0.1993	0.131*

O5	0.0000	0.5928 (8)	0.2500	0.233 (5)
H5	0.0203	0.5336	0.2496	0.350*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0513 (2)	0.0329 (2)	0.0490 (2)	-0.0034 (2)	0.01794 (17)	-0.00328 (19)
O1	0.0735 (16)	0.0611 (17)	0.0491 (13)	0.0086 (12)	0.0271 (12)	0.0098 (11)
O2	0.0709 (18)	0.0643 (18)	0.0627 (16)	0.0214 (15)	0.0243 (14)	0.0167 (14)
O3	0.0811 (19)	0.0525 (17)	0.0566 (15)	-0.0065 (14)	0.0180 (15)	-0.0072 (13)
O4	0.087 (2)	0.093 (2)	0.0689 (18)	-0.030 (2)	0.0246 (17)	-0.0223 (17)
N1	0.0496 (16)	0.0399 (17)	0.0419 (14)	0.0014 (13)	0.0189 (13)	-0.0009 (12)
N2	0.0438 (15)	0.0358 (16)	0.0497 (15)	-0.0030 (13)	0.0191 (13)	-0.0008 (13)
C1	0.073 (3)	0.039 (2)	0.0403 (19)	0.0021 (19)	0.0200 (19)	-0.0002 (16)
C2	0.073 (3)	0.064 (3)	0.057 (2)	0.021 (2)	0.027 (2)	0.014 (2)
C3	0.052 (2)	0.067 (3)	0.064 (2)	0.014 (2)	0.0175 (19)	0.033 (2)
C4	0.088 (3)	0.080 (4)	0.097 (4)	0.015 (3)	0.027 (3)	0.035 (3)
C5	0.091 (4)	0.102 (5)	0.125 (5)	0.003 (3)	0.048 (4)	0.065 (4)
C6	0.085 (4)	0.127 (6)	0.109 (4)	0.017 (4)	0.043 (3)	0.064 (4)
C7	0.059 (3)	0.112 (4)	0.061 (3)	0.021 (3)	0.026 (2)	0.028 (2)
C8	0.071 (3)	0.152 (5)	0.050 (2)	0.031 (3)	0.028 (2)	0.014 (3)
C9	0.095 (4)	0.149 (6)	0.066 (3)	0.017 (4)	0.028 (3)	-0.002 (4)
C10	0.090 (4)	0.114 (5)	0.083 (3)	-0.006 (3)	0.029 (3)	-0.014 (3)
C11	0.067 (3)	0.090 (3)	0.061 (2)	0.002 (3)	0.028 (2)	0.000 (3)
C12	0.045 (2)	0.102 (4)	0.042 (2)	0.018 (2)	0.0176 (17)	0.022 (2)
C13	0.091 (3)	0.035 (2)	0.042 (2)	-0.013 (2)	0.011 (2)	0.0039 (17)
C14	0.089 (3)	0.047 (2)	0.0400 (19)	-0.020 (2)	0.0077 (19)	-0.0006 (16)
C15	0.052 (2)	0.046 (2)	0.0334 (17)	-0.0076 (17)	0.0067 (16)	-0.0008 (15)
C16	0.055 (2)	0.077 (3)	0.051 (2)	-0.002 (2)	0.0142 (18)	-0.008 (2)
C17	0.075 (3)	0.074 (3)	0.073 (3)	0.021 (3)	0.014 (2)	-0.011 (3)
C18	0.099 (4)	0.044 (2)	0.061 (3)	0.008 (3)	0.003 (3)	0.003 (2)
C19	0.064 (3)	0.059 (3)	0.044 (2)	-0.019 (2)	0.0076 (19)	0.0078 (18)
C20	0.092 (4)	0.118 (5)	0.067 (3)	-0.045 (4)	0.013 (3)	0.015 (3)
C21	0.076 (4)	0.185 (8)	0.075 (4)	-0.045 (5)	0.025 (3)	0.006 (5)
C22	0.065 (3)	0.198 (8)	0.064 (3)	0.002 (4)	0.025 (2)	-0.019 (4)
C23	0.070 (3)	0.109 (4)	0.050 (2)	0.004 (3)	0.020 (2)	-0.015 (2)
C24	0.0480 (19)	0.064 (2)	0.0318 (16)	-0.0043 (19)	0.0071 (15)	-0.0030 (17)
C25	0.058 (2)	0.050 (2)	0.050 (2)	0.0059 (18)	0.0224 (18)	-0.0012 (17)
C26	0.049 (2)	0.064 (3)	0.0421 (19)	0.0022 (18)	0.0167 (17)	0.0041 (17)
C27	0.053 (2)	0.062 (3)	0.053 (2)	-0.0085 (19)	0.0199 (18)	0.0090 (19)
C28	0.052 (2)	0.040 (2)	0.058 (2)	-0.0038 (16)	0.0228 (18)	0.0003 (16)
C29	0.0428 (19)	0.0373 (18)	0.0340 (16)	-0.0004 (15)	0.0101 (14)	0.0013 (14)
C30	0.0405 (18)	0.0328 (17)	0.0363 (16)	-0.0014 (14)	0.0091 (14)	-0.0019 (14)
C31	0.057 (2)	0.0340 (18)	0.0529 (19)	-0.0014 (17)	0.0214 (17)	0.0010 (17)
C32	0.062 (2)	0.044 (2)	0.065 (2)	0.0070 (19)	0.0292 (19)	-0.0030 (18)
C33	0.060 (2)	0.053 (2)	0.064 (2)	0.0037 (19)	0.032 (2)	-0.0004 (19)
C34	0.055 (2)	0.043 (2)	0.066 (2)	-0.0055 (17)	0.0298 (19)	0.0020 (17)
C35	0.070 (3)	0.095 (3)	0.076 (3)	0.014 (3)	0.045 (2)	0.010 (3)

supplementary materials

C36	0.098 (3)	0.076 (3)	0.122 (4)	0.015 (3)	0.079 (3)	0.010 (3)
O5	0.134 (5)	0.083 (5)	0.495 (15)	0.000	0.157 (8)	0.000

Geometric parameters (Å, °)

Zn1—O1	1.967 (2)	C16—C17	1.376 (6)
Zn1—O3	2.009 (3)	C16—H16A	0.9300
Zn1—N2	2.072 (3)	C17—C18	1.334 (6)
Zn1—N1	2.098 (3)	C17—H17A	0.9300
Zn1—O4	2.416 (3)	C18—C19	1.394 (6)
O1—C1	1.273 (4)	C18—H18A	0.9300
O2—C1	1.224 (4)	C19—C20	1.391 (6)
O3—C13	1.258 (5)	C19—C24	1.427 (5)
O4—C13	1.240 (5)	C20—C21	1.333 (8)
N1—C29	1.344 (4)	C20—H20A	0.9300
N1—C25	1.340 (4)	C21—C22	1.386 (9)
N2—C34	1.334 (4)	C21—H21A	0.9300
N2—C30	1.348 (4)	C22—C23	1.392 (7)
C1—C2	1.520 (5)	C22—H22A	0.9300
C2—C3	1.507 (5)	C23—C24	1.410 (5)
C2—H2A	0.9700	C23—H23A	0.9300
C2—H2B	0.9700	C25—C26	1.381 (5)
C3—C4	1.363 (6)	C25—H25A	0.9300
C3—C12	1.437 (6)	C26—C27	1.378 (5)
C4—C5	1.470 (7)	C26—C35	1.503 (5)
C4—H4A	0.9300	C27—C28	1.379 (5)
C5—C6	1.383 (8)	C27—H27A	0.9300
C5—H5A	0.9300	C28—C29	1.381 (4)
C6—C7	1.352 (7)	C28—H28A	0.9300
C6—H6A	0.9300	C29—C30	1.477 (4)
C7—C8	1.414 (7)	C30—C31	1.378 (4)
C7—C12	1.427 (5)	C31—C32	1.375 (5)
C8—C9	1.340 (8)	C31—H31A	0.9300
C8—H8A	0.9300	C32—C33	1.372 (5)
C9—C10	1.356 (7)	C32—H32A	0.9300
C9—H9A	0.9300	C33—C34	1.387 (5)
C10—C11	1.362 (6)	C33—C36	1.509 (5)
C10—H10A	0.9300	C34—H34A	0.9300
C11—C12	1.391 (6)	C35—H35A	0.9600
C11—H11A	0.9300	C35—H35B	0.9600
C13—C14	1.523 (5)	C35—H35C	0.9600
C14—C15	1.505 (5)	C36—H36A	0.9600
C14—H14A	0.9700	C36—H36B	0.9600
C14—H14B	0.9700	C36—H36C	0.9600
C15—C16	1.358 (5)	O5—H5	0.8199
C15—C24	1.415 (5)		
O1—Zn1—O3	121.37 (11)	C15—C16—C17	122.7 (4)
O1—Zn1—N2	120.53 (10)	C15—C16—H16A	118.6
O3—Zn1—N2	103.04 (11)	C17—C16—H16A	118.6

O1—Zn1—N1	104.43 (11)	C18—C17—C16	119.7 (5)
O3—Zn1—N1	122.09 (10)	C18—C17—H17A	120.1
N2—Zn1—N1	78.64 (11)	C16—C17—H17A	120.1
O1—Zn1—O4	93.91 (11)	C17—C18—C19	121.6 (4)
O3—Zn1—O4	58.10 (11)	C17—C18—H18A	119.2
N2—Zn1—O4	145.01 (11)	C19—C18—H18A	119.2
N1—Zn1—O4	87.49 (11)	C20—C19—C18	122.1 (5)
C1—O1—Zn1	104.8 (2)	C20—C19—C24	119.1 (5)
C13—O3—Zn1	99.2 (3)	C18—C19—C24	118.8 (4)
C13—O4—Zn1	80.9 (2)	C21—C20—C19	121.1 (6)
C29—N1—C25	118.7 (3)	C21—C20—H20A	119.5
C29—N1—Zn1	114.6 (2)	C19—C20—H20A	119.5
C25—N1—Zn1	126.6 (2)	C20—C21—C22	121.8 (6)
C34—N2—C30	118.6 (3)	C20—C21—H21A	119.1
C34—N2—Zn1	125.8 (2)	C22—C21—H21A	119.1
C30—N2—Zn1	115.3 (2)	C21—C22—C23	119.8 (6)
O2—C1—O1	122.7 (3)	C21—C22—H22A	120.1
O2—C1—C2	122.0 (3)	C23—C22—H22A	120.1
O1—C1—C2	115.4 (3)	C22—C23—C24	119.5 (5)
C3—C2—C1	115.9 (3)	C22—C23—H23A	120.2
C3—C2—H2A	108.3	C24—C23—H23A	120.2
C1—C2—H2A	108.3	C23—C24—C15	122.9 (4)
C3—C2—H2B	108.3	C23—C24—C19	118.7 (4)
C1—C2—H2B	108.3	C15—C24—C19	118.4 (4)
H2A—C2—H2B	107.4	N1—C25—C26	123.5 (3)
C4—C3—C12	119.1 (4)	N1—C25—H25A	118.3
C4—C3—C2	121.5 (5)	C26—C25—H25A	118.3
C12—C3—C2	119.4 (4)	C27—C26—C25	116.9 (3)
C3—C4—C5	120.6 (5)	C27—C26—C35	122.3 (4)
C3—C4—H4A	119.7	C25—C26—C35	120.8 (4)
C5—C4—H4A	119.7	C26—C27—C28	120.8 (4)
C6—C5—C4	117.2 (5)	C26—C27—H27A	119.6
C6—C5—H5A	121.4	C28—C27—H27A	119.6
C4—C5—H5A	121.4	C27—C28—C29	118.7 (3)
C7—C6—C5	124.4 (6)	C27—C28—H28A	120.7
C7—C6—H6A	117.8	C29—C28—H28A	120.7
C5—C6—H6A	117.8	N1—C29—C28	121.4 (3)
C6—C7—C8	122.0 (5)	N1—C29—C30	115.6 (3)
C6—C7—C12	118.1 (5)	C28—C29—C30	123.0 (3)
C8—C7—C12	119.9 (5)	N2—C30—C31	120.9 (3)
C9—C8—C7	118.9 (5)	N2—C30—C29	115.6 (3)
C9—C8—H8A	120.6	C31—C30—C29	123.5 (3)
C7—C8—H8A	120.6	C32—C31—C30	119.6 (3)
C8—C9—C10	122.6 (6)	C32—C31—H31A	120.2
C8—C9—H9A	118.7	C30—C31—H31A	120.2
C10—C9—H9A	118.7	C31—C32—C33	120.4 (4)
C9—C10—C11	120.1 (6)	C31—C32—H32A	119.8
C9—C10—H10A	120.0	C33—C32—H32A	119.8
C11—C10—H10A	120.0	C32—C33—C34	116.8 (3)

supplementary materials

C10—C11—C12	121.7 (5)	C32—C33—C36	121.9 (4)
C10—C11—H11A	119.1	C34—C33—C36	121.3 (4)
C12—C11—H11A	119.1	N2—C34—C33	123.8 (3)
C11—C12—C7	116.9 (5)	N2—C34—H34A	118.1
C11—C12—C3	122.5 (4)	C33—C34—H34A	118.1
C7—C12—C3	120.6 (4)	C26—C35—H35A	109.5
O4—C13—O3	121.4 (4)	C26—C35—H35B	109.5
O4—C13—C14	119.6 (4)	H35A—C35—H35B	109.5
O3—C13—C14	119.1 (4)	C26—C35—H35C	109.5
C15—C14—C13	112.3 (3)	H35A—C35—H35C	109.5
C15—C14—H14A	109.1	H35B—C35—H35C	109.5
C13—C14—H14A	109.1	C33—C36—H36A	109.5
C15—C14—H14B	109.1	C33—C36—H36B	109.5
C13—C14—H14B	109.1	H36A—C36—H36B	109.5
H14A—C14—H14B	107.9	C33—C36—H36C	109.5
C16—C15—C24	118.7 (4)	H36A—C36—H36C	109.5
C16—C15—C14	118.7 (4)	H36B—C36—H36C	109.5
C24—C15—C14	122.6 (4)		
O3—Zn1—O1—C1	69.3 (3)	Zn1—O3—C13—O4	-7.8 (4)
N2—Zn1—O1—C1	-62.5 (3)	Zn1—O3—C13—C14	171.6 (3)
N1—Zn1—O1—C1	-147.6 (2)	O4—C13—C14—C15	-81.9 (5)
O4—Zn1—O1—C1	124.0 (2)	O3—C13—C14—C15	98.7 (4)
O1—Zn1—O3—C13	77.4 (2)	C13—C14—C15—C16	91.5 (4)
N2—Zn1—O3—C13	-143.8 (2)	C13—C14—C15—C24	-90.0 (5)
N1—Zn1—O3—C13	-59.2 (3)	C24—C15—C16—C17	0.3 (5)
O4—Zn1—O3—C13	4.0 (2)	C14—C15—C16—C17	178.8 (3)
O1—Zn1—O4—C13	-128.9 (2)	C15—C16—C17—C18	0.5 (6)
O3—Zn1—O4—C13	-4.1 (2)	C16—C17—C18—C19	-0.7 (6)
N2—Zn1—O4—C13	60.8 (3)	C17—C18—C19—C20	-178.7 (4)
N1—Zn1—O4—C13	126.8 (2)	C17—C18—C19—C24	0.2 (6)
O1—Zn1—N1—C29	119.4 (2)	C18—C19—C20—C21	178.4 (4)
O3—Zn1—N1—C29	-97.9 (2)	C24—C19—C20—C21	-0.5 (6)
N2—Zn1—N1—C29	0.5 (2)	C19—C20—C21—C22	-1.2 (8)
O4—Zn1—N1—C29	-147.2 (2)	C20—C21—C22—C23	2.7 (8)
O1—Zn1—N1—C25	-59.6 (3)	C21—C22—C23—C24	-2.4 (7)
O3—Zn1—N1—C25	83.1 (3)	C22—C23—C24—C15	-178.1 (3)
N2—Zn1—N1—C25	-178.5 (3)	C22—C23—C24—C19	0.7 (5)
O4—Zn1—N1—C25	33.8 (3)	C16—C15—C24—C23	177.9 (3)
O1—Zn1—N2—C34	83.3 (3)	C14—C15—C24—C23	-0.5 (5)
O3—Zn1—N2—C34	-55.9 (3)	C16—C15—C24—C19	-0.8 (4)
N1—Zn1—N2—C34	-176.6 (3)	C14—C15—C24—C19	-179.3 (3)
O4—Zn1—N2—C34	-108.0 (3)	C20—C19—C24—C23	0.8 (5)
O1—Zn1—N2—C30	-103.9 (2)	C18—C19—C24—C23	-178.2 (3)
O3—Zn1—N2—C30	116.9 (2)	C20—C19—C24—C15	179.5 (3)
N1—Zn1—N2—C30	-3.7 (2)	C18—C19—C24—C15	0.6 (5)
O4—Zn1—N2—C30	64.9 (3)	C29—N1—C25—C26	-0.7 (5)
Zn1—O1—C1—O2	1.7 (4)	Zn1—N1—C25—C26	178.3 (2)
Zn1—O1—C1—C2	-176.5 (3)	N1—C25—C26—C27	-0.8 (5)
O2—C1—C2—C3	12.7 (6)	N1—C25—C26—C35	179.0 (3)

O1—C1—C2—C3	-169.0 (3)	C25—C26—C27—C28	1.4 (5)
C1—C2—C3—C4	-110.8 (4)	C35—C26—C27—C28	-178.5 (3)
C1—C2—C3—C12	69.5 (5)	C26—C27—C28—C29	-0.5 (5)
C12—C3—C4—C5	0.6 (6)	C25—N1—C29—C28	1.7 (4)
C2—C3—C4—C5	-179.2 (4)	Zn1—N1—C29—C28	-177.4 (2)
C3—C4—C5—C6	-0.4 (7)	C25—N1—C29—C30	-178.4 (3)
C4—C5—C6—C7	-0.3 (8)	Zn1—N1—C29—C30	2.5 (3)
C5—C6—C7—C8	-178.9 (5)	C27—C28—C29—N1	-1.1 (5)
C5—C6—C7—C12	0.7 (8)	C27—C28—C29—C30	179.0 (3)
C6—C7—C8—C9	178.6 (5)	C34—N2—C30—C31	0.1 (4)
C12—C7—C8—C9	-1.0 (7)	Zn1—N2—C30—C31	-173.3 (2)
C7—C8—C9—C10	1.7 (8)	C34—N2—C30—C29	179.5 (3)
C8—C9—C10—C11	-0.8 (8)	Zn1—N2—C30—C29	6.1 (3)
C9—C10—C11—C12	-0.7 (7)	N1—C29—C30—N2	-5.7 (4)
C10—C11—C12—C7	1.3 (6)	C28—C29—C30—N2	174.1 (3)
C10—C11—C12—C3	-178.2 (4)	N1—C29—C30—C31	173.7 (3)
C6—C7—C12—C11	180.0 (4)	C28—C29—C30—C31	-6.5 (5)
C8—C7—C12—C11	-0.4 (6)	N2—C30—C31—C32	0.3 (5)
C6—C7—C12—C3	-0.5 (6)	C29—C30—C31—C32	-179.1 (3)
C8—C7—C12—C3	179.1 (4)	C30—C31—C32—C33	0.0 (5)
C4—C3—C12—C11	179.4 (4)	C31—C32—C33—C34	-0.7 (5)
C2—C3—C12—C11	-0.9 (5)	C31—C32—C33—C36	178.4 (4)
C4—C3—C12—C7	-0.1 (6)	C30—N2—C34—C33	-0.8 (5)
C2—C3—C12—C7	179.6 (3)	Zn1—N2—C34—C33	171.8 (3)
Zn1—O4—C13—O3	6.5 (3)	C32—C33—C34—N2	1.1 (5)
Zn1—O4—C13—C14	-172.9 (3)	C36—C33—C34—N2	-177.9 (3)

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>
O5—H5 \cdots O1	0.82	2.21	2.948 (3)	150
C8—H8A \cdots O4 ⁱ	0.93	2.59	3.515 (6)	171

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

Fig. 1

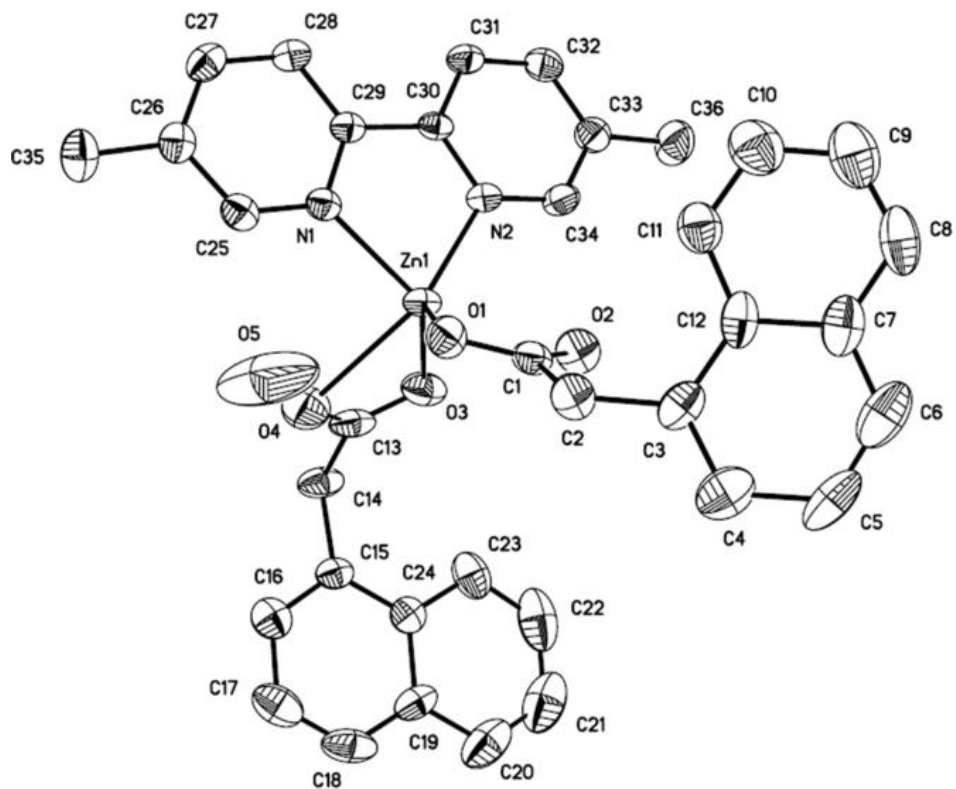


Fig. 2

