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(Ethanol-κO){4,4′,6,6′-tetra-*tert*-butyl-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato-$\kappa^4 O,O',N,N'$}zinc(II) ethanol solvate

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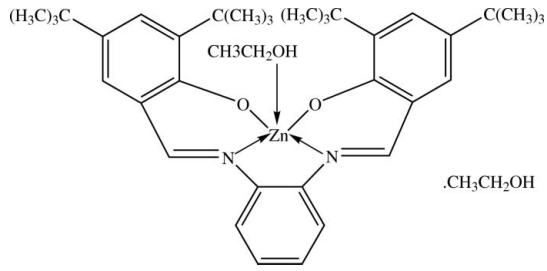
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.133; data-to-parameter ratio = 19.3.

The title compound, $[Zn(C_{36}H_{46}N_2O_2)(C_2H_6O)]\cdot C_2H_5OH$, adopts a square-pyramidal Zn^{II} coordination, with the N_2O_2 tetradentate Schiff base ligand bound in the basal plane and the coordinated ethanol molecule occupying the apical site. Inversion-related Zn^{II} complex molecules are linked *via* O—H···O hydrogen bonding involving the coordinated and uncoordinated ethanol molecules, forming dimers which are stacked along the c axis. Intramolecular C—H···O and C—H···π interactions are observed in the Zn^{II} complex.

Related literature

For bond-length data, see: Allen *et al.* (1987). For general background on Schiff base–Zn^{II} coordination complexes, see: Pal *et al.* (2005); Collinson & Fenton (1996); Assaf & Chung (1984); Berg & Shi (1996); Tarafder *et al.* (2002). For related structures, see: Eltayeb, Teoh, Chantrapromma *et al.* (2007*a*, 2007*b*); Eltayeb, Teoh, Fun *et al.* (2007); Eltayeb, Teoh, Ng *et al.* (2007); Eltayeb, Teoh, Teh *et al.* (2007).



Experimental

Crystal data

$[Zn(C_{36}H_{46}N_2O_2)(C_2H_6O)]\cdot C_2H_6O$
M_r = 696.25
Monoclinic, $P2_1/c$
a = 13.0909 (3) Å
b = 24.8935 (6) Å
c = 11.6289 (3) Å
β = 92.303 (1)°
V = 3786.55 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 100.0 (1) K
0.40 × 0.34 × 0.30 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.770, T_{max} = 0.822
32064 measured reflections
8595 independent reflections
6701 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.133
S = 1.08
8595 reflections
445 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C8–C13 and C15–C20 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1O3···O4^{i}	0.75 (4)	1.97 (4)	2.684 (3)	160 (4)
O4—H1O4···O3	0.83 (3)	2.20 (3)	2.975 (3)	156 (4)
C22—H22*B*···O1	0.96	2.28	2.933 (3)	124
C24—H24*B*···O1	0.96	2.34	2.968 (3)	123
C34—H34*A*···O2	0.96	2.35	3.000 (3)	124
C36—H36*A*···O2	0.96	2.37	3.004 (3)	124
C39—H39*A*···*Cg*1	0.97	2.79	3.641 (5)	146
C26—H26*A*···*Cg*2^{ii}	0.96	2.73	3.534 (3)	142

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2400).

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supplementary materials

Acta Cryst. (2007). E**63**, m2024-m2025 [**doi:10.1107/S1600536807030863**]

(Ethanol-κO){4,4',6,6'-tetra-*tert*-butyl-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato-$\kappa^4 O,O',N,N'$}zinc(II) ethanol solvate

N. E. Eltayeb, S. G. Teoh, S. Chantrapromma, H.-K. Fun and K. Ibrahim

Comment

Zinc, an element of strong interest in biology, medicine, materials, and catalysis, plays important roles in various biological systems such as neurotransmission, signal transduction and gene expression (Assaf & Chung, 1984; Berg & Shi, 1996). It is well known that Schiff base ligands have played an important role in the development of coordination chemistry as they readily form stable complexes with most transition metal ions (Pal *et al.*, 2005). Zinc complexes with Schiff-bases are importance in biological systems and coordination chemistry (Collinson & Fenton, 1996; Tarafder *et al.*, 2002). Recently, we have reported crystal structures of Zn^{II} complexes with Schiff base ligands. As a continuation of our research on Schiff base complexes, we report here the crystal structure of the title compound, (I).

The Zn^{II} complex is characterized by an approximately square-pyramidal Zn^{II} coordination, with the N_2O_2 tetradentate Schiff-base ligand in the basal plane and an ethanol molecule in the apical site (Fig. 1). The Zn^{II} atom is displaced 0.025 (5) Å out of the mean N1/N2/O1/O2 basal plane towards the axial atom, O4, of ethanol molecule. The cyclic skeleton of the tetradentate Schiff-base ligand is essentially planar. The dihedral angles between the central benzene ring (C8—C13) and the other two benzene rings (C1—C6 and C15—C20) are 2.96 (11)° and 9.35 (11)°, respectively. Bond lengths and angles observed in the structure are in normal ranges (Allen *et al.*, 1987) and comparable with the related structures (Eltayeb *et al.*, 2007*a*; 2007*b*; Eltayeb, Teoh, Fun *et al.*, 2007; Eltayeb, Teoh, Ng *et al.*, 2007; Eltayeb, Teoh, Teh *et al.*, 2007).

Intramolecular C—H···O interactions (Table 1), and C—H···π interactions involving the C8—C13 (centroid *Cg*1) ring are observed in the complex molecule. Inversion-related Zn^{II} complex molecules are linked *via* O—H···O hydrogen bonding (Table 1) involving the coordinated and two free ethanol molecules, forming dimers which are stacked along the *c* axis (Fig.2). Molecules in the adjacent stacks are linked *via* C—H···π interactions involving the C15—C20 ring (centroid *Cg*2).

Experimental

The title compound (I) was synthesized by adding 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde (0.936 g, 4 mmol) to a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol 95% (20 ml). The mixture was refluxed with stirring for half an hour. Zinc chloride (0.272 g, 2 mmol) in ethanol (10 ml) was then added, followed by triethylamine (0.5 ml, 3.6 mmol). The mixture was stirred at room temperature for 2 h. A yellow-orange solution was obtained and it was filtered. Orange crystals suitable for X-ray diffraction were formed after 4 d of slow evaporation of the ethanol at room temperature.

Refinement

Hydroxyl H atoms were located in a difference map and refined with a O4-H1O4 distance restraint of 0.82 Å. The remainning H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H

atoms. A rotating group model was used for the methyl groups. The highest residual peak is located 0.91 Å from H39B and the deepest hole is located 0.45 Å from C38.

Figures

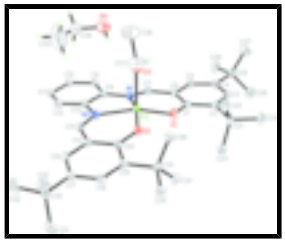

Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering. C-bound H atoms of the Zn^{II} complex have been omitted for clarity.

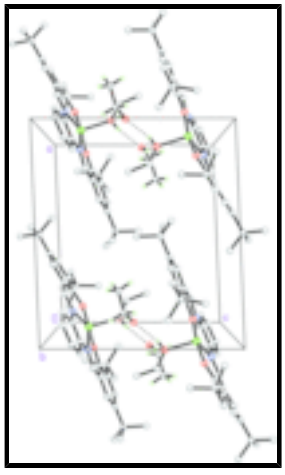

Fig. 2. The crystal packing of (I), viewed along the *b* axis. C-bound H atoms of the Zn^{II} complex have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

(Ethanol-κ*O*){4,4',6,6'-tetra-*tert*-butyl-2,2'-[1,2- phenylenebis(nitrilomethylidyne)]diphenolato-κ^4*O*,*O*',*N*,*N*'}zinc(II) ethanol solvate

Crystal data

$[Zn(C_{36}H_{46}N_2O_2)(C_2H_6O)]\cdot C_2H_6O$	F_{000} = 1496
M_r = 696.25	D_x = 1.221 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8959 reflections
a = 13.0909 (3) Å	θ = 1.6–27.5º
b = 24.8935 (6) Å	μ = 0.69 mm^{-1}
c = 11.6289 (3) Å	*T* = 100.0 (1) K
β = 92.303 (1)º	Block, orange
V = 3786.55 (16) Å^3	0.40 × 0.34 × 0.30 mm
Z = 4	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	8595 independent reflections

Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 8.33 pixels mm^{-1}
T = 100.0(1) K
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2005)
T_{min} = 0.770, T_{max} = 0.822
32064 measured reflections

6701 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5º
θ_{min} = 1.6º
h = −17→15
k = −32→32
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.133
S = 1.08
8595 reflections
445 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 3.4587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}
Extinction correction: none

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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	0.97460 (2)	0.576492 (10)	0.80021 (2)	0.01646 (9)
O1	1.08663 (13)	0.62577 (7)	0.78053 (17)	0.0225 (4)
O2	0.87455 (13)	0.63224 (7)	0.83442 (16)	0.0202 (4)
O3	0.92767 (16)	0.55880 (8)	0.62450 (18)	0.0261 (4)
H1O3	0.971 (3)	0.5634 (13)	0.586 (3)	0.031 (10)*
O4	0.9358 (2)	0.44593 (10)	0.5413 (2)	0.0513 (6)

H1O4	0.917 (3)	0.4741 (11)	0.572 (4)	0.077*
N1	1.07893 (15)	0.51318 (8)	0.80696 (18)	0.0165 (4)
N2	0.89009 (15)	0.51947 (8)	0.88074 (18)	0.0173 (4)
C1	1.17831 (18)	0.61734 (9)	0.7472 (2)	0.0178 (5)
C2	1.23835 (18)	0.66228 (9)	0.7098 (2)	0.0169 (5)
C3	1.33454 (18)	0.65251 (9)	0.6715 (2)	0.0190 (5)
H3A	1.3711	0.6816	0.6441	0.023*
C4	1.38200 (18)	0.60149 (10)	0.6706 (2)	0.0187 (5)
C5	1.32620 (18)	0.55910 (10)	0.7100 (2)	0.0194 (5)
H5A	1.3558	0.5251	0.7125	0.023*
C6	1.22513 (18)	0.56528 (9)	0.7471 (2)	0.0173 (5)
C7	1.17450 (18)	0.51729 (9)	0.7821 (2)	0.0181 (5)
H7A	1.2137	0.4862	0.7875	0.022*
C8	1.03533 (18)	0.46422 (9)	0.8427 (2)	0.0171 (5)
C9	1.08428 (19)	0.41423 (9)	0.8405 (2)	0.0196 (5)
H9A	1.1491	0.4114	0.8112	0.024*
C10	1.03601 (19)	0.36891 (9)	0.8821 (2)	0.0203 (5)
H10A	1.0686	0.3358	0.8801	0.024*
C11	0.9397 (2)	0.37277 (10)	0.9264 (2)	0.0225 (5)
H11A	0.9089	0.3424	0.9561	0.027*
C12	0.8891 (2)	0.42147 (10)	0.9268 (2)	0.0218 (5)
H12A	0.8240	0.4235	0.9557	0.026*
C13	0.93529 (18)	0.46790 (9)	0.8839 (2)	0.0172 (5)
C14	0.80138 (18)	0.52882 (9)	0.9231 (2)	0.0179 (5)
H14A	0.7669	0.4992	0.9512	0.022*
C15	0.75093 (18)	0.57960 (9)	0.9315 (2)	0.0170 (5)
C16	0.65790 (18)	0.57868 (9)	0.9900 (2)	0.0186 (5)
H16A	0.6323	0.5458	1.0134	0.022*
C17	0.60436 (18)	0.62436 (10)	1.0133 (2)	0.0185 (5)
C18	0.64779 (18)	0.67355 (10)	0.9770 (2)	0.0180 (5)
H18A	0.6140	0.7052	0.9948	0.022*
C19	0.73647 (18)	0.67789 (9)	0.9171 (2)	0.0172 (5)
C20	0.79118 (18)	0.62952 (9)	0.8911 (2)	0.0169 (5)
C21	1.19322 (18)	0.71917 (9)	0.7153 (2)	0.0191 (5)
C22	1.09384 (19)	0.72357 (10)	0.6404 (2)	0.0245 (6)
H22A	1.0654	0.7589	0.6483	0.037*
H22B	1.0457	0.6973	0.6650	0.037*
H22C	1.1085	0.7173	0.5613	0.037*
C23	1.2677 (2)	0.76128 (10)	0.6729 (3)	0.0261 (6)
H23A	1.3302	0.7597	0.7189	0.039*
H23B	1.2379	0.7963	0.6792	0.039*
H23C	1.2818	0.7542	0.5939	0.039*
C24	1.1715 (2)	0.73315 (10)	0.8407 (2)	0.0260 (6)
H24A	1.2339	0.7312	0.8868	0.039*
H24B	1.1229	0.7081	0.8694	0.039*
H24C	1.1443	0.7689	0.8442	0.039*
C25	1.48993 (19)	0.59658 (10)	0.6245 (2)	0.0225 (5)
C26	1.5621 (2)	0.63712 (12)	0.6854 (3)	0.0311 (6)
H26A	1.5654	0.6299	0.7666	0.047*

H26B	1.5369	0.6729	0.6720	0.047*
H26C	1.6292	0.6339	0.6556	0.047*
C27	1.4859 (2)	0.60832 (13)	0.4953 (3)	0.0354 (7)
H27A	1.4429	0.5824	0.4561	0.053*
H27B	1.5536	0.6063	0.4668	0.053*
H27C	1.4587	0.6437	0.4818	0.053*
C28	1.5348 (2)	0.54038 (11)	0.6454 (3)	0.0345 (7)
H28A	1.4914	0.5141	0.6079	0.052*
H28B	1.5395	0.5332	0.7266	0.052*
H28C	1.6018	0.5386	0.6148	0.052*
C29	0.50307 (19)	0.62484 (10)	1.0739 (2)	0.0213 (5)
C30	0.4188 (2)	0.64933 (12)	0.9945 (2)	0.0290 (6)
H30A	0.4369	0.6855	0.9754	0.043*
H30B	0.3554	0.6494	1.0332	0.043*
H30C	0.4114	0.6284	0.9254	0.043*
C31	0.5145 (2)	0.65778 (12)	1.1846 (2)	0.0304 (6)
H31A	0.5307	0.6943	1.1660	0.046*
H31B	0.5684	0.6429	1.2331	0.046*
H31C	0.4516	0.6568	1.2242	0.046*
C32	0.4692 (2)	0.56795 (12)	1.1064 (4)	0.0420 (8)
H32A	0.4587	0.5468	1.0379	0.063*
H32B	0.4066	0.5699	1.1465	0.063*
H32C	0.5212	0.5515	1.1553	0.063*
C33	0.77535 (18)	0.73289 (9)	0.8761 (2)	0.0184 (5)
C34	0.88318 (19)	0.74462 (10)	0.9275 (2)	0.0218 (5)
H34A	0.9285	0.7160	0.9080	0.033*
H34B	0.8807	0.7473	1.0097	0.033*
H34C	0.9076	0.7778	0.8969	0.033*
C35	0.7060 (2)	0.77923 (10)	0.9124 (2)	0.0231 (5)
H35A	0.6377	0.7732	0.8821	0.035*
H35B	0.7313	0.8125	0.8828	0.035*
H35C	0.7059	0.7810	0.9948	0.035*
C36	0.7769 (2)	0.73394 (10)	0.7447 (2)	0.0228 (5)
H36A	0.8215	0.7062	0.7189	0.034*
H36B	0.8012	0.7683	0.7199	0.034*
H36C	0.7091	0.7280	0.7129	0.034*
C37	0.8406 (3)	0.58757 (15)	0.5761 (3)	0.0432 (8)
H37A	0.8594	0.6249	0.5656	0.052*
H37B	0.7860	0.5865	0.6301	0.052*
C38	0.8021 (3)	0.56542 (16)	0.4642 (3)	0.0540 (10)
H38A	0.7447	0.5863	0.4359	0.081*
H38B	0.7811	0.5288	0.4744	0.081*
H38C	0.8553	0.5668	0.4099	0.081*
C39	0.8839 (4)	0.40238 (17)	0.5901 (4)	0.0609 (11)
H39A	0.9213	0.3911	0.6596	0.073*
H39B	0.8832	0.3725	0.5365	0.073*
C40	0.7779 (4)	0.4149 (3)	0.6186 (6)	0.121 (3)
H40A	0.7463	0.3834	0.6487	0.181*
H40B	0.7404	0.4266	0.5505	0.181*

H40C	0.7780	0.4430	0.6752	0.181*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01590 (15)	0.01228 (14)	0.02151 (17)	−0.00033 (10)	0.00465 (10)	0.00128 (11)
O1	0.0173 (8)	0.0144 (8)	0.0365 (11)	−0.0007 (6)	0.0084 (7)	0.0024 (7)
O2	0.0183 (8)	0.0145 (8)	0.0283 (10)	0.0009 (6)	0.0084 (7)	0.0015 (7)
O3	0.0229 (10)	0.0326 (11)	0.0231 (11)	0.0059 (8)	0.0041 (8)	0.0004 (8)
O4	0.0597 (16)	0.0464 (15)	0.0491 (16)	−0.0047 (12)	0.0191 (13)	−0.0107 (12)
N1	0.0181 (10)	0.0125 (9)	0.0191 (11)	−0.0015 (7)	0.0027 (8)	0.0003 (8)
N2	0.0185 (10)	0.0120 (9)	0.0214 (11)	0.0007 (7)	0.0028 (8)	0.0002 (8)
C1	0.0168 (11)	0.0162 (11)	0.0206 (12)	−0.0015 (9)	0.0018 (9)	−0.0009 (9)
C2	0.0180 (11)	0.0158 (11)	0.0167 (12)	−0.0019 (9)	−0.0001 (9)	0.0008 (9)
C3	0.0205 (12)	0.0173 (12)	0.0195 (13)	−0.0049 (9)	0.0023 (10)	0.0004 (9)
C4	0.0175 (12)	0.0204 (12)	0.0182 (12)	−0.0001 (9)	0.0017 (9)	−0.0020 (9)
C5	0.0191 (12)	0.0159 (11)	0.0231 (13)	0.0013 (9)	0.0017 (10)	−0.0028 (10)
C6	0.0182 (11)	0.0157 (11)	0.0183 (12)	−0.0019 (9)	0.0031 (9)	0.0008 (9)
C7	0.0191 (12)	0.0139 (11)	0.0215 (13)	0.0014 (9)	0.0014 (9)	−0.0010 (9)
C8	0.0196 (11)	0.0125 (11)	0.0191 (12)	0.0007 (9)	0.0012 (9)	0.0003 (9)
C9	0.0197 (12)	0.0157 (12)	0.0236 (14)	0.0014 (9)	0.0034 (10)	−0.0001 (9)
C10	0.0254 (13)	0.0115 (11)	0.0240 (13)	0.0017 (9)	0.0025 (10)	0.0012 (9)
C11	0.0316 (14)	0.0132 (11)	0.0232 (13)	−0.0036 (10)	0.0058 (11)	0.0023 (10)
C12	0.0228 (12)	0.0183 (12)	0.0248 (14)	−0.0006 (9)	0.0087 (10)	0.0007 (10)
C13	0.0206 (12)	0.0133 (11)	0.0178 (12)	0.0001 (9)	0.0024 (9)	0.0002 (9)
C14	0.0175 (11)	0.0134 (11)	0.0232 (13)	−0.0014 (9)	0.0041 (9)	0.0016 (9)
C15	0.0172 (11)	0.0148 (11)	0.0190 (12)	−0.0010 (9)	0.0021 (9)	−0.0005 (9)
C16	0.0163 (11)	0.0152 (11)	0.0245 (13)	−0.0018 (9)	0.0046 (9)	0.0028 (9)
C17	0.0163 (11)	0.0205 (12)	0.0188 (12)	−0.0006 (9)	0.0021 (9)	0.0017 (9)
C18	0.0187 (11)	0.0174 (11)	0.0180 (12)	0.0037 (9)	0.0021 (9)	−0.0015 (9)
C19	0.0175 (11)	0.0153 (11)	0.0185 (12)	0.0009 (9)	−0.0010 (9)	0.0019 (9)
C20	0.0162 (11)	0.0170 (11)	0.0174 (12)	−0.0005 (9)	0.0016 (9)	0.0001 (9)
C21	0.0198 (12)	0.0140 (11)	0.0233 (13)	−0.0014 (9)	0.0011 (10)	0.0024 (9)
C22	0.0225 (13)	0.0194 (12)	0.0316 (15)	0.0008 (10)	0.0014 (11)	0.0049 (11)
C23	0.0258 (13)	0.0163 (12)	0.0366 (16)	−0.0029 (10)	0.0049 (11)	0.0034 (11)
C24	0.0298 (14)	0.0182 (12)	0.0303 (15)	−0.0010 (10)	0.0067 (11)	−0.0022 (11)
C25	0.0184 (12)	0.0205 (12)	0.0292 (15)	−0.0011 (9)	0.0078 (10)	−0.0016 (10)
C26	0.0190 (13)	0.0313 (15)	0.0433 (18)	−0.0038 (11)	0.0070 (12)	−0.0066 (13)
C27	0.0338 (16)	0.0441 (18)	0.0292 (16)	0.0015 (13)	0.0128 (12)	−0.0008 (13)
C28	0.0241 (14)	0.0263 (14)	0.054 (2)	0.0032 (11)	0.0137 (13)	0.0019 (14)
C29	0.0186 (12)	0.0190 (12)	0.0269 (14)	0.0014 (9)	0.0093 (10)	0.0001 (10)
C30	0.0207 (13)	0.0380 (16)	0.0284 (15)	0.0039 (11)	0.0036 (11)	−0.0069 (12)
C31	0.0264 (14)	0.0390 (16)	0.0261 (15)	0.0023 (11)	0.0065 (11)	−0.0011 (12)
C32	0.0304 (16)	0.0258 (15)	0.072 (2)	0.0002 (12)	0.0278 (16)	0.0049 (15)
C33	0.0220 (12)	0.0132 (11)	0.0200 (13)	−0.0002 (9)	0.0034 (10)	0.0002 (9)
C34	0.0218 (12)	0.0175 (12)	0.0260 (14)	−0.0023 (9)	−0.0003 (10)	0.0006 (10)
C35	0.0278 (13)	0.0151 (12)	0.0268 (14)	0.0026 (10)	0.0044 (11)	0.0023 (10)
C36	0.0300 (14)	0.0169 (12)	0.0217 (13)	−0.0025 (10)	0.0043 (10)	0.0026 (10)

C37	0.0395 (18)	0.051 (2)	0.0380 (19)	0.0229 (15)	−0.0091 (15)	−0.0118 (15)
C38	0.057 (2)	0.058 (2)	0.047 (2)	0.0122 (18)	−0.0054 (18)	−0.0036 (18)
C39	0.082 (3)	0.059 (2)	0.043 (2)	−0.029 (2)	0.011 (2)	−0.0090 (19)
C40	0.060 (3)	0.186 (7)	0.112 (5)	−0.047 (4)	−0.039 (3)	0.067 (5)

Geometric parameters (Å, °)

Zn1—O1	1.9326 (17)	C23—H23A	0.96
Zn1—O2	1.9600 (17)	C23—H23B	0.96
Zn1—N2	2.049 (2)	C23—H23C	0.96
Zn1—N1	2.0850 (19)	C24—H24A	0.96
Zn1—O3	2.155 (2)	C24—H24B	0.96
O1—C1	1.293 (3)	C24—H24C	0.96
O2—C20	1.299 (3)	C25—C27	1.530 (4)
O3—C37	1.442 (3)	C25—C28	1.533 (4)
O3—H1O3	0.74 (4)	C25—C26	1.536 (4)
O4—C39	1.411 (5)	C26—H26A	0.96
O4—H1O4	0.83 (3)	C26—H26B	0.96
N1—C7	1.299 (3)	C26—H26C	0.96
N1—C8	1.415 (3)	C27—H27A	0.96
N2—C14	1.301 (3)	C27—H27B	0.96
N2—C13	1.413 (3)	C27—H27C	0.96
C1—C6	1.434 (3)	C28—H28A	0.96
C1—C2	1.444 (3)	C28—H28B	0.96
C2—C3	1.374 (3)	C28—H28C	0.96
C2—C21	1.537 (3)	C29—C31	1.529 (4)
C3—C4	1.414 (3)	C29—C32	1.536 (4)
C3—H3A	0.93	C29—C30	1.536 (4)
C4—C5	1.373 (3)	C30—H30A	0.96
C4—C25	1.536 (3)	C30—H30B	0.96
C5—C6	1.416 (3)	C30—H30C	0.96
C5—H5A	0.93	C31—H31A	0.96
C6—C7	1.433 (3)	C31—H31B	0.96
C7—H7A	0.93	C31—H31C	0.96
C8—C9	1.400 (3)	C32—H32A	0.96
C8—C13	1.415 (3)	C32—H32B	0.96
C9—C10	1.389 (3)	C32—H32C	0.96
C9—H9A	0.93	C33—C36	1.529 (4)
C10—C11	1.384 (4)	C33—C35	1.537 (3)
C10—H10A	0.93	C33—C34	1.539 (3)
C11—C12	1.381 (3)	C34—H34A	0.96
C11—H11A	0.93	C34—H34B	0.96
C12—C13	1.405 (3)	C34—H34C	0.96
C12—H12A	0.93	C35—H35A	0.96
C14—C15	1.431 (3)	C35—H35B	0.96
C14—H14A	0.93	C35—H35C	0.96
C15—C16	1.419 (3)	C36—H36A	0.96
C15—C20	1.436 (3)	C36—H36B	0.96
C16—C17	1.369 (3)	C36—H36C	0.96

C16—H16A	0.93	C37—C38	1.483 (5)
C17—C18	1.422 (3)	C37—H37A	0.97
C17—C29	1.526 (3)	C37—H37B	0.97
C18—C19	1.382 (3)	C38—H38A	0.96
C18—H18A	0.93	C38—H38B	0.96
C19—C20	1.439 (3)	C38—H38C	0.96
C19—C33	1.543 (3)	C39—C40	1.473 (7)
C21—C23	1.527 (3)	C39—H39A	0.97
C21—C24	1.536 (4)	C39—H39B	0.97
C21—C22	1.540 (3)	C40—H40A	0.96
C22—H22A	0.96	C40—H40B	0.96
C22—H22B	0.96	C40—H40C	0.96
C22—H22C	0.96		
O1—Zn1—O2	95.22 (7)	C21—C24—H24B	109.5
O1—Zn1—N2	156.93 (8)	H24A—C24—H24B	109.5
O2—Zn1—N2	91.17 (8)	C21—C24—H24C	109.5
O1—Zn1—N1	89.15 (7)	H24A—C24—H24C	109.5
O2—Zn1—N1	165.86 (8)	H24B—C24—H24C	109.5
N2—Zn1—N1	79.86 (8)	C27—C25—C28	109.1 (2)
O1—Zn1—O3	101.90 (8)	C27—C25—C26	108.9 (2)
O2—Zn1—O3	99.78 (8)	C28—C25—C26	107.6 (2)
N2—Zn1—O3	98.81 (8)	C27—C25—C4	109.4 (2)
N1—Zn1—O3	92.44 (8)	C28—C25—C4	111.7 (2)
C1—O1—Zn1	130.57 (15)	C26—C25—C4	110.2 (2)
C20—O2—Zn1	130.38 (15)	C25—C26—H26A	109.5
C37—O3—Zn1	117.34 (18)	C25—C26—H26B	109.5
C37—O3—H1O3	107 (3)	H26A—C26—H26B	109.5
Zn1—O3—H1O3	110 (3)	C25—C26—H26C	109.5
C39—O4—H1O4	109 (3)	H26A—C26—H26C	109.5
C7—N1—C8	122.4 (2)	H26B—C26—H26C	109.5
C7—N1—Zn1	124.55 (16)	C25—C27—H27A	109.5
C8—N1—Zn1	113.00 (15)	C25—C27—H27B	109.5
C14—N2—C13	122.1 (2)	H27A—C27—H27B	109.5
C14—N2—Zn1	123.76 (16)	C25—C27—H27C	109.5
C13—N2—Zn1	114.07 (15)	H27A—C27—H27C	109.5
O1—C1—C6	123.3 (2)	H27B—C27—H27C	109.5
O1—C1—C2	119.2 (2)	C25—C28—H28A	109.5
C6—C1—C2	117.5 (2)	C25—C28—H28B	109.5
C3—C2—C1	118.5 (2)	H28A—C28—H28B	109.5
C3—C2—C21	122.4 (2)	C25—C28—H28C	109.5
C1—C2—C21	119.1 (2)	H28A—C28—H28C	109.5
C2—C3—C4	124.7 (2)	H28B—C28—H28C	109.5
C2—C3—H3A	117.6	C17—C29—C31	109.6 (2)
C4—C3—H3A	117.6	C17—C29—C32	111.8 (2)
C5—C4—C3	116.6 (2)	C31—C29—C32	107.9 (3)
C5—C4—C25	124.4 (2)	C17—C29—C30	110.0 (2)
C3—C4—C25	119.0 (2)	C31—C29—C30	109.7 (2)
C4—C5—C6	122.3 (2)	C32—C29—C30	107.9 (2)
C4—C5—H5A	118.8	C29—C30—H30A	109.5

C6—C5—H5A	118.8	C29—C30—H30B	109.5
C5—C6—C7	116.4 (2)	H30A—C30—H30B	109.5
C5—C6—C1	120.2 (2)	C29—C30—H30C	109.5
C7—C6—C1	123.4 (2)	H30A—C30—H30C	109.5
N1—C7—C6	126.1 (2)	H30B—C30—H30C	109.5
N1—C7—H7A	116.9	C29—C31—H31A	109.5
C6—C7—H7A	116.9	C29—C31—H31B	109.5
C9—C8—N1	124.7 (2)	H31A—C31—H31B	109.5
C9—C8—C13	119.6 (2)	C29—C31—H31C	109.5
N1—C8—C13	115.7 (2)	H31A—C31—H31C	109.5
C10—C9—C8	120.0 (2)	H31B—C31—H31C	109.5
C10—C9—H9A	120.0	C29—C32—H32A	109.5
C8—C9—H9A	120.0	C29—C32—H32B	109.5
C11—C10—C9	120.5 (2)	H32A—C32—H32B	109.5
C11—C10—H10A	119.8	C29—C32—H32C	109.5
C9—C10—H10A	119.8	H32A—C32—H32C	109.5
C12—C11—C10	120.4 (2)	H32B—C32—H32C	109.5
C12—C11—H11A	119.8	C36—C33—C35	107.0 (2)
C10—C11—H11A	119.8	C36—C33—C34	109.6 (2)
C11—C12—C13	120.5 (2)	C35—C33—C34	107.1 (2)
C11—C12—H12A	119.7	C36—C33—C19	110.0 (2)
C13—C12—H12A	119.7	C35—C33—C19	112.1 (2)
C12—C13—N2	124.8 (2)	C34—C33—C19	110.93 (19)
C12—C13—C8	118.9 (2)	C33—C34—H34A	109.5
N2—C13—C8	116.2 (2)	C33—C34—H34B	109.5
N2—C14—C15	127.2 (2)	H34A—C34—H34B	109.5
N2—C14—H14A	116.4	C33—C34—H34C	109.5
C15—C14—H14A	116.4	H34A—C34—H34C	109.5
C16—C15—C14	115.2 (2)	H34B—C34—H34C	109.5
C16—C15—C20	120.3 (2)	C33—C35—H35A	109.5
C14—C15—C20	124.5 (2)	C33—C35—H35B	109.5
C17—C16—C15	122.5 (2)	H35A—C35—H35B	109.5
C17—C16—H16A	118.7	C33—C35—H35C	109.5
C15—C16—H16A	118.7	H35A—C35—H35C	109.5
C16—C17—C18	116.3 (2)	H35B—C35—H35C	109.5
C16—C17—C29	124.0 (2)	C33—C36—H36A	109.5
C18—C17—C29	119.7 (2)	C33—C36—H36B	109.5
C19—C18—C17	124.8 (2)	H36A—C36—H36B	109.5
C19—C18—H18A	117.6	C33—C36—H36C	109.5
C17—C18—H18A	117.6	H36A—C36—H36C	109.5
C18—C19—C20	118.4 (2)	H36B—C36—H36C	109.5
C18—C19—C33	121.3 (2)	O3—C37—C38	113.2 (3)
C20—C19—C33	120.3 (2)	O3—C37—H37A	108.9
O2—C20—C15	122.5 (2)	C38—C37—H37A	108.9
O2—C20—C19	119.9 (2)	O3—C37—H37B	108.9
C15—C20—C19	117.6 (2)	C38—C37—H37B	108.9
C23—C21—C24	107.2 (2)	H37A—C37—H37B	107.8
C23—C21—C2	111.6 (2)	C37—C38—H38A	109.5
C24—C21—C2	109.5 (2)	C37—C38—H38B	109.5

C23—C21—C22	107.7 (2)	H38A—C38—H38B	109.5
C24—C21—C22	109.7 (2)	C37—C38—H38C	109.5
C2—C21—C22	111.1 (2)	H38A—C38—H38C	109.5
C21—C22—H22A	109.5	H38B—C38—H38C	109.5
C21—C22—H22B	109.5	O4—C39—C40	113.6 (4)
H22A—C22—H22B	109.5	O4—C39—H39A	108.8
C21—C22—H22C	109.5	C40—C39—H39A	108.8
H22A—C22—H22C	109.5	O4—C39—H39B	108.8
H22B—C22—H22C	109.5	C40—C39—H39B	108.8
C21—C23—H23A	109.5	H39A—C39—H39B	107.7
C21—C23—H23B	109.5	C39—C40—H40A	109.5
H23A—C23—H23B	109.5	C39—C40—H40B	109.5
C21—C23—H23C	109.5	H40A—C40—H40B	109.5
H23A—C23—H23C	109.5	C39—C40—H40C	109.5
H23B—C23—H23C	109.5	H40A—C40—H40C	109.5
C21—C24—H24A	109.5	H40B—C40—H40C	109.5
O2—Zn1—O1—C1	−174.0 (2)	C10—C11—C12—C13	−1.0 (4)
N2—Zn1—O1—C1	80.5 (3)	C11—C12—C13—N2	−179.9 (2)
N1—Zn1—O1—C1	19.4 (2)	C11—C12—C13—C8	−1.4 (4)
O3—Zn1—O1—C1	−72.9 (2)	C14—N2—C13—C12	3.1 (4)
O1—Zn1—O2—C20	−155.7 (2)	Zn1—N2—C13—C12	−175.2 (2)
N2—Zn1—O2—C20	2.2 (2)	C14—N2—C13—C8	−175.3 (2)
N1—Zn1—O2—C20	−48.1 (4)	Zn1—N2—C13—C8	6.3 (3)
O3—Zn1—O2—C20	101.3 (2)	C9—C8—C13—C12	3.0 (4)
O1—Zn1—O3—C37	−99.0 (2)	N1—C8—C13—C12	−176.5 (2)
O2—Zn1—O3—C37	−1.5 (2)	C9—C8—C13—N2	−178.5 (2)
N2—Zn1—O3—C37	91.3 (2)	N1—C8—C13—N2	2.0 (3)
N1—Zn1—O3—C37	171.4 (2)	C13—N2—C14—C15	175.8 (2)
O1—Zn1—N1—C7	−10.4 (2)	Zn1—N2—C14—C15	−6.0 (4)
O2—Zn1—N1—C7	−118.7 (3)	N2—C14—C15—C16	−175.2 (2)
N2—Zn1—N1—C7	−170.0 (2)	N2—C14—C15—C20	1.2 (4)
O3—Zn1—N1—C7	91.5 (2)	C14—C15—C16—C17	174.7 (2)
O1—Zn1—N1—C8	169.21 (16)	C20—C15—C16—C17	−1.8 (4)
O2—Zn1—N1—C8	60.9 (4)	C15—C16—C17—C18	−0.8 (4)
N2—Zn1—N1—C8	9.60 (16)	C15—C16—C17—C29	178.7 (2)
O3—Zn1—N1—C8	−88.92 (17)	C16—C17—C18—C19	2.6 (4)
O1—Zn1—N2—C14	110.3 (2)	C29—C17—C18—C19	−177.0 (2)
O2—Zn1—N2—C14	4.1 (2)	C17—C18—C19—C20	−1.5 (4)
N1—Zn1—N2—C14	173.1 (2)	C17—C18—C19—C33	177.1 (2)
O3—Zn1—N2—C14	−96.0 (2)	Zn1—O2—C20—C15	−6.8 (3)
O1—Zn1—N2—C13	−71.3 (3)	Zn1—O2—C20—C19	172.24 (16)
O2—Zn1—N2—C13	−177.59 (16)	C16—C15—C20—O2	−178.1 (2)
N1—Zn1—N2—C13	−8.59 (16)	C14—C15—C20—O2	5.7 (4)
O3—Zn1—N2—C13	82.33 (17)	C16—C15—C20—C19	2.9 (3)
Zn1—O1—C1—C6	−17.9 (4)	C14—C15—C20—C19	−173.4 (2)
Zn1—O1—C1—C2	163.24 (17)	C18—C19—C20—O2	179.7 (2)
O1—C1—C2—C3	−178.1 (2)	C33—C19—C20—O2	1.1 (3)
C6—C1—C2—C3	2.9 (3)	C18—C19—C20—C15	−1.3 (3)
O1—C1—C2—C21	2.5 (3)	C33—C19—C20—C15	−179.9 (2)

C6—C1—C2—C21	−176.5 (2)	C3—C2—C21—C23	0.4 (3)
C1—C2—C3—C4	−3.1 (4)	C1—C2—C21—C23	179.8 (2)
C21—C2—C3—C4	176.3 (2)	C3—C2—C21—C24	−118.1 (3)
C2—C3—C4—C5	0.8 (4)	C1—C2—C21—C24	61.2 (3)
C2—C3—C4—C25	179.7 (2)	C3—C2—C21—C22	120.6 (3)
C3—C4—C5—C6	1.6 (4)	C1—C2—C21—C22	−60.0 (3)
C25—C4—C5—C6	−177.2 (2)	C5—C4—C25—C27	111.9 (3)
C4—C5—C6—C7	177.7 (2)	C3—C4—C25—C27	−67.0 (3)
C4—C5—C6—C1	−1.6 (4)	C5—C4—C25—C28	−9.1 (4)
O1—C1—C6—C5	−179.6 (2)	C3—C4—C25—C28	172.1 (2)
C2—C1—C6—C5	−0.7 (3)	C5—C4—C25—C26	−128.5 (3)
O1—C1—C6—C7	1.1 (4)	C3—C4—C25—C26	52.7 (3)
C2—C1—C6—C7	180.0 (2)	C16—C17—C29—C31	120.1 (3)
C8—N1—C7—C6	−179.0 (2)	C18—C17—C29—C31	−60.4 (3)
Zn1—N1—C7—C6	0.6 (4)	C16—C17—C29—C32	0.6 (4)
C5—C6—C7—N1	−172.1 (2)	C18—C17—C29—C32	−179.9 (3)
C1—C6—C7—N1	7.2 (4)	C16—C17—C29—C30	−119.2 (3)
C7—N1—C8—C9	−9.0 (4)	C18—C17—C29—C30	60.3 (3)
Zn1—N1—C8—C9	171.4 (2)	C18—C19—C33—C36	−117.6 (3)
C7—N1—C8—C13	170.4 (2)	C20—C19—C33—C36	60.9 (3)
Zn1—N1—C8—C13	−9.2 (3)	C18—C19—C33—C35	1.3 (3)
N1—C8—C9—C10	177.3 (2)	C20—C19—C33—C35	179.8 (2)
C13—C8—C9—C10	−2.1 (4)	C18—C19—C33—C34	120.9 (2)
C8—C9—C10—C11	−0.3 (4)	C20—C19—C33—C34	−60.6 (3)
C9—C10—C11—C12	1.9 (4)	Zn1—O3—C37—C38	−168.8 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1O3···O4^{i}	0.75 (4)	1.97 (4)	2.684 (3)	160 (4)
O4—H1O4···O3	0.83 (3)	2.20 (3)	2.975 (3)	156 (4)
C22—H22B···O1	0.96	2.28	2.933 (3)	124
C24—H24B···O1	0.96	2.34	2.968 (3)	123
C34—H34A···O2	0.96	2.35	3.000 (3)	124
C36—H36A···O2	0.96	2.37	3.004 (3)	124
C39—H39A···Cg1	0.97	2.79	3.641 (5)	146
C26—H26A···Cg2^{ii}	0.96	2.73	3.534 (3)	142

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

Fig. 1

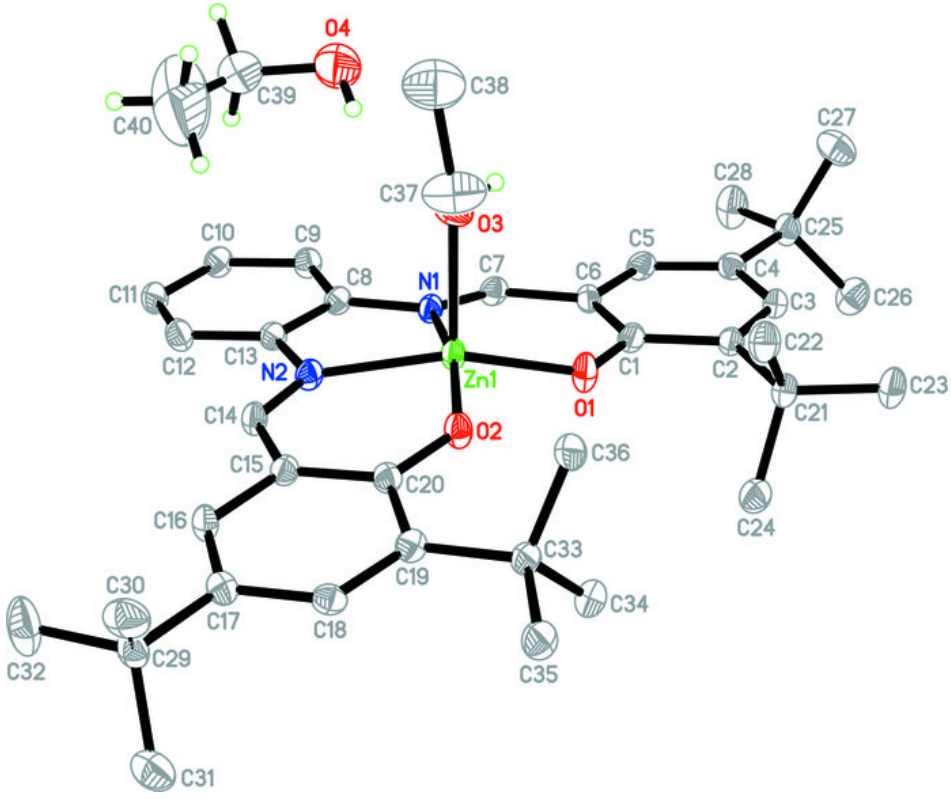
O4
C38
C39
C40
C37
O3
C27
C28
C25
C10
C9
C5
C8
N1
C7
C6
C4
C11
C3
C26
C12
C13
N2
Zn1
C1
C2
C22
C23
O1
C21
C14
O2
C36
C15
C20
C24
C16
C33
C19
C30
C34
C17
C18
C32
C29
C35
C31

Fig. 2