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Bis(1*H*-imidazole-κN^3)[(2-oxidobenzylideneamino)methanesulfonato-$\kappa^2 N,O$]-zinc(II)

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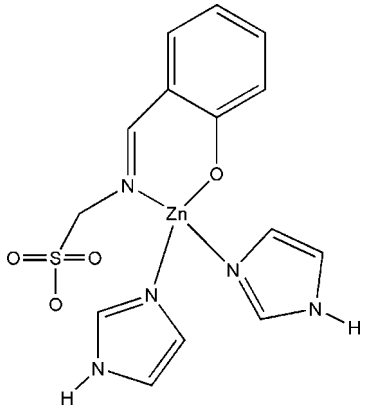
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.060; data-to-parameter ratio = 13.9.

The Zn^{II} ion in the title complex, $[Zn(C_9H_4NO_4S)(C_3H_4N_2)_2]$, is coordinated by an N atom and an O atom of a deprotonated tridentate Schiff base ligand, and two N atoms from two different imidazole ligands in a distorted tetrahedral geometry. In the crystal structure, molecules are connected *via* intermolecular N—H···O hydrogen bonds, forming extended one-dimensional chains along [111].

Related literature

For related literature, see: Deng *et al.* (2006); Jiang *et al.* (2006); Casella *et al.* (1981, 1986); Li *et al.* (2005).



Experimental

Crystal data

$[Zn(C_9H_4NO_4S)(C_3H_4N_2)_2]$
M_r = 414.74
Triclinic, $P\overline{1}$
a = 8.7931 (10) Å
b = 9.7881 (11) Å
c = 10.8602 (12) Å
α = 90.010 (1)°
β = 107.443 (1)°
γ = 100.798 (1)°
V = 874.36 (17) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.55 mm^{-1}
T = 293 (2) K
0.44 × 0.27 × 0.26 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.535, T_{max} = 0.689
6254 measured reflections
3151 independent reflections
2897 reflections with $I > 2\sigma(I)$
R_{int} = 0.011

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.060
S = 1.03
3151 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.9679 (14)	Zn1—N2	2.0039 (16)
Zn1—N4	1.9914 (15)	Zn1—N1	2.0212 (15)
O1—Zn1—N4	103.16 (6)	N2—Zn1—N1	122.81 (6)
O1—Zn1—N2	99.07 (7)	O1—Zn1—O4	167.00 (5)
N4—Zn1—N2	113.05 (7)	N4—Zn1—O4	87.41 (5)
O1—Zn1—N1	92.46 (6)	N2—Zn1—O4	83.35 (6)
N4—Zn1—N1	118.29 (6)	N1—Zn1—O4	75.70 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5D···O3^{i}	0.86	1.91	2.765 (2)	173
N3—H3D···O2^{ii}	0.86	2.08	2.860 (2)	151

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: LH2539).

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supplementary materials

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Bis(1*H*-imidazole-κN^3)[(2-oxidobenzylideneamino)methanesulfonato-$\kappa^2 N,O$]zinc(II)

K.-H. He, J.-M. Li and Y.-M. Jiang

Comment

There is considerable interest in the study of Schiff-base complexes containing sulfur and complexes of amino acid Schiff-bases (Deng *et al.*, 2006; Jiang *et al.*, 2006; Casella *et al.*, 1981,1986) due to their antiviral, anticancer and antibacterial activities. Herein, we report the synthesis and crystal structure of the title zinc(II) complex. The Zn^{II} cation is coordinated by one N atom and one O atom of a deprotonated tridentate schiff base ligand and two N atoms (Fig.1 and Table.1) from two different 1*H*-Imidazole ligands in a distorted tetrahedral geometry. In the crystal structure, molecules are connected *via* intermolecular N—H···O hydrogen bonds to form extended one-dimensional chains along [111].

Experimental

The potassium salt of the Schiff base ligand [(2-Hydroxy-benzylidene)-amino]-methanesulfonic acid, *L*, was synthesized according to the approach of Li *et al.* (2005). *L* (1.0 mmol) in 10 ml me thanol was added dropwise to a stirred solution of $ZnCl_2$ (1.0 mmol) in 5 ml me thanol and 5 ml water. To this mixed solution, a solution of 1*H*-Imidazole (2.0 mmol) in 5 ml me thanol was added slowly. The resulting yellow solution was filtered and left to stand for two weeks to evaporate slowly at room temperature to give yellow prism-shaped single crystals in yield of 55%.

Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H distances 0.93Å and N—H distances 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

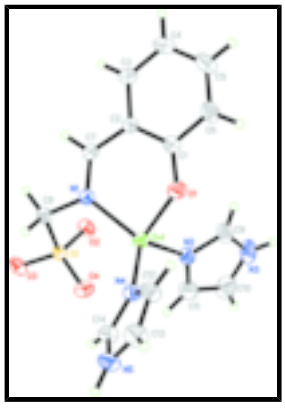

Fig. 1. The molecular structure with displacement ellipsoids at the 30% probability level.

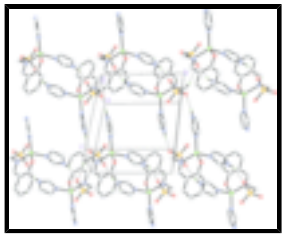

Fig. 2. Part of the crystal structure showing hydrogen bonds as dashed lines. Only H stoms involved in hydrogen bonds are included.

Bis(1*H*-imidazole-κ*N*^{3})[(2-oxidobenzylideneamino)methanesulfonato-\ κ$_2$N,*O*]zinc(II)

Crystal data

$[Zn(C_9H_4NO_4S)(C_3H_4N_2)_2]$	$Z = 2$
$M_r = 414.74$	$F_{000} = 424$
Triclinic, $P\bar{1}$	$D_x = 1.575$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.7931$ (10) Å	Cell parameters from 4316 reflections
$b = 9.7881$ (11) Å	$\theta = 2.5$–28.1º
$c = 10.8602$ (12) Å	$\mu = 1.55$ mm^{-1}
$\alpha = 90.010$ (1)º	$T = 293$ (2) K
$\beta = 107.443$ (1)º	Block, yellow
$\gamma = 100.798$ (1)º	0.44 × 0.27 × 0.26 mm
$V = 874.36$ (17) Å^3	

Data collection

Bruker SMART CCD diffractometer	3151 independent reflections
Radiation source: fine-focus sealed tube	2897 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.011$
$T = 293$(2) K	$\theta_{max} = 25.5$º
φ and ω scans	$\theta_{min} = 2.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.535$, $T_{max} = 0.689$	$k = -11 \rightarrow 11$
6254 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.023$	H-atom parameters constrained
$wR(F^2) = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.0287P)^2 + 0.3794P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$

3151 reflections	$\Delta\rho_{max} = 0.30$ e Å^{-3}
226 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.38626 (3)	0.74569 (2)	0.14640 (2)	0.03885 (8)
S1	0.13599 (5)	0.93736 (5)	0.20311 (4)	0.03197 (11)
O1	0.46352 (18)	0.68569 (16)	0.00677 (13)	0.0502 (4)
O2	−0.00090 (15)	0.84950 (14)	0.10831 (13)	0.0431 (3)
O3	0.08886 (16)	1.05113 (15)	0.26015 (13)	0.0466 (3)
O4	0.23487 (17)	0.85840 (15)	0.29732 (13)	0.0486 (3)
N1	0.31567 (17)	0.91200 (15)	0.05194 (14)	0.0315 (3)
N2	0.2293 (2)	0.57083 (16)	0.15324 (16)	0.0424 (4)
N3	0.0918 (2)	0.35836 (19)	0.0995 (2)	0.0645 (6)
H3D	0.0515	0.2790	0.0570	0.077*
N4	0.58586 (18)	0.77884 (16)	0.29863 (15)	0.0380 (3)
N5	0.7630 (2)	0.8389 (2)	0.48859 (17)	0.0518 (4)
H5D	0.8037	0.8681	0.5686	0.062*
C1	0.4071 (2)	0.71274 (19)	−0.11433 (18)	0.0366 (4)
C2	0.3259 (2)	0.82584 (18)	−0.15616 (17)	0.0319 (4)

C3	0.2756 (2)	0.8502 (2)	−0.28977 (18)	0.0404 (4)
H3	0.2248	0.9249	−0.3165	0.048*
C4	0.2998 (3)	0.7668 (3)	−0.3805 (2)	0.0535 (6)
H4	0.2661	0.7846	−0.4677	0.064*
C5	0.3761 (3)	0.6546 (3)	−0.3399 (2)	0.0595 (6)
H5	0.3922	0.5969	−0.4008	0.071*
C6	0.4275 (3)	0.6282 (2)	−0.2113 (2)	0.0515 (5)
H6	0.4774	0.5524	−0.1874	0.062*
C7	0.2925 (2)	0.92062 (18)	−0.07104 (17)	0.0318 (4)
H7	0.2496	0.9961	−0.1083	0.038*
C8	0.2696 (2)	1.01987 (18)	0.11775 (18)	0.0352 (4)
H8A	0.2154	1.0797	0.0552	0.042*
H8B	0.3656	1.0767	0.1777	0.042*
C9	0.1900 (3)	0.4635 (2)	0.0680 (2)	0.0524 (5)
H9	0.2262	0.4619	−0.0040	0.063*
C10	0.0660 (3)	0.3977 (3)	0.2098 (3)	0.0710 (7)
H10	0.0027	0.3446	0.2542	0.085*
C11	0.1507 (3)	0.5295 (2)	0.2425 (2)	0.0584 (6)
H11	0.1549	0.5837	0.3143	0.070*
C12	0.7353 (2)	0.7591 (2)	0.2954 (2)	0.0484 (5)
H12	0.7574	0.7256	0.2238	0.058*
C13	0.8448 (3)	0.7960 (3)	0.4130 (2)	0.0575 (6)
H13	0.9548	0.7927	0.4373	0.069*
C14	0.6084 (2)	0.8279 (2)	0.41716 (19)	0.0447 (5)
H14	0.5275	0.8516	0.4469	0.054*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03963 (13)	0.03755 (13)	0.03377 (13)	0.00707 (9)	0.00320 (9)	0.00622 (9)
S1	0.0283 (2)	0.0370 (2)	0.0294 (2)	0.00515 (18)	0.00793 (17)	−0.00237 (18)
O1	0.0591 (9)	0.0575 (9)	0.0392 (8)	0.0312 (7)	0.0107 (7)	0.0089 (7)
O2	0.0332 (7)	0.0474 (8)	0.0420 (8)	−0.0030 (6)	0.0080 (6)	−0.0078 (6)
O3	0.0415 (7)	0.0540 (8)	0.0458 (8)	0.0122 (6)	0.0137 (6)	−0.0137 (6)
O4	0.0477 (8)	0.0555 (9)	0.0404 (8)	0.0137 (7)	0.0079 (6)	0.0113 (7)
N1	0.0296 (7)	0.0332 (8)	0.0329 (8)	0.0062 (6)	0.0113 (6)	0.0015 (6)
N2	0.0434 (9)	0.0341 (8)	0.0414 (9)	0.0044 (7)	0.0022 (7)	−0.0023 (7)
N3	0.0509 (11)	0.0362 (10)	0.0857 (16)	0.0013 (8)	−0.0055 (10)	−0.0120 (10)
N4	0.0356 (8)	0.0416 (9)	0.0340 (8)	0.0070 (7)	0.0068 (6)	0.0021 (7)
N5	0.0479 (10)	0.0639 (12)	0.0346 (9)	0.0091 (9)	0.0002 (8)	−0.0052 (8)
C1	0.0316 (9)	0.0400 (10)	0.0383 (10)	0.0070 (8)	0.0107 (8)	0.0013 (8)
C2	0.0267 (8)	0.0359 (9)	0.0330 (9)	0.0031 (7)	0.0107 (7)	0.0028 (7)
C3	0.0366 (10)	0.0478 (11)	0.0361 (10)	0.0067 (8)	0.0112 (8)	0.0074 (8)
C4	0.0529 (13)	0.0749 (16)	0.0321 (10)	0.0108 (11)	0.0130 (9)	0.0001 (10)
C5	0.0618 (14)	0.0724 (16)	0.0473 (13)	0.0186 (12)	0.0176 (11)	−0.0147 (11)
C6	0.0509 (12)	0.0529 (12)	0.0530 (13)	0.0208 (10)	0.0131 (10)	−0.0061 (10)
C7	0.0257 (8)	0.0332 (9)	0.0364 (10)	0.0051 (7)	0.0097 (7)	0.0069 (7)
C8	0.0344 (9)	0.0317 (9)	0.0408 (10)	0.0044 (7)	0.0146 (8)	−0.0006 (8)

C9	0.0478 (12)	0.0448 (12)	0.0559 (13)	0.0118 (10)	0.0012 (10)	−0.0087 (10)
C10	0.0640 (16)	0.0527 (14)	0.0826 (19)	−0.0103 (12)	0.0151 (14)	0.0083 (13)
C11	0.0642 (15)	0.0490 (12)	0.0534 (14)	−0.0061 (11)	0.0157 (11)	0.0004 (10)
C12	0.0427 (11)	0.0582 (13)	0.0456 (12)	0.0140 (10)	0.0130 (9)	−0.0052 (10)
C13	0.0357 (11)	0.0732 (16)	0.0588 (14)	0.0152 (11)	0.0042 (10)	−0.0051 (12)
C14	0.0405 (11)	0.0548 (12)	0.0389 (11)	0.0097 (9)	0.0120 (9)	0.0017 (9)

Geometric parameters (Å, °)

Zn1—O1	1.9679 (14)	C1—C6	1.413 (3)
Zn1—N4	1.9914 (15)	C1—C2	1.429 (3)
Zn1—N2	2.0039 (16)	C2—C3	1.419 (3)
Zn1—N1	2.0212 (15)	C2—C7	1.438 (2)
Zn1—O4	2.7447 (15)	C3—C4	1.369 (3)
S1—O2	1.4551 (13)	C3—H3	0.9300
S1—O4	1.4557 (14)	C4—C5	1.396 (4)
S1—O3	1.4568 (14)	C4—H4	0.9300
S1—C8	1.7856 (18)	C5—C6	1.373 (3)
O1—C1	1.305 (2)	C5—H5	0.9300
N1—C7	1.295 (2)	C6—H6	0.9300
N1—C8	1.457 (2)	C7—H7	0.9300
N2—C9	1.323 (3)	C8—H8A	0.9700
N2—C11	1.371 (3)	C8—H8B	0.9700
N3—C9	1.329 (3)	C9—H9	0.9300
N3—C10	1.353 (4)	C10—C11	1.352 (3)
N3—H3D	0.8600	C10—H10	0.9300
N4—C14	1.318 (2)	C11—H11	0.9300
N4—C12	1.374 (3)	C12—C13	1.349 (3)
N5—C14	1.332 (3)	C12—H12	0.9300
N5—C13	1.355 (3)	C13—H13	0.9300
N5—H5D	0.8600	C14—H14	0.9300
O1—Zn1—N4	103.16 (6)	C4—C3—C2	121.92 (19)
O1—Zn1—N2	99.07 (7)	C4—C3—H3	119.0
N4—Zn1—N2	113.05 (7)	C2—C3—H3	119.0
O1—Zn1—N1	92.46 (6)	C3—C4—C5	118.7 (2)
N4—Zn1—N1	118.29 (6)	C3—C4—H4	120.6
N2—Zn1—N1	122.81 (6)	C5—C4—H4	120.6
O1—Zn1—O4	167.00 (5)	C6—C5—C4	121.1 (2)
N4—Zn1—O4	87.41 (5)	C6—C5—H5	119.5
N2—Zn1—O4	83.35 (6)	C4—C5—H5	119.5
N1—Zn1—O4	75.70 (5)	C5—C6—C1	122.0 (2)
O2—S1—O4	113.12 (9)	C5—C6—H6	119.0
O2—S1—O3	112.65 (8)	C1—C6—H6	119.0
O4—S1—O3	114.02 (9)	N1—C7—C2	126.90 (16)
O2—S1—C8	106.88 (8)	N1—C7—H7	116.5
O4—S1—C8	104.07 (9)	C2—C7—H7	116.5
O3—S1—C8	105.09 (9)	N1—C8—S1	108.39 (12)
C1—O1—Zn1	124.51 (12)	N1—C8—H8A	110.0
S1—O4—Zn1	100.45 (7)	S1—C8—H8A	110.0

C7—N1—C8	116.93 (15)	N1—C8—H8B	110.0
C7—N1—Zn1	122.22 (12)	S1—C8—H8B	110.0
C8—N1—Zn1	120.44 (11)	H8A—C8—H8B	108.4
C9—N2—C11	105.59 (19)	N2—C9—N3	110.7 (2)
C9—N2—Zn1	123.10 (16)	N2—C9—H9	124.6
C11—N2—Zn1	131.17 (14)	N3—C9—H9	124.6
C9—N3—C10	108.18 (19)	C11—C10—N3	106.2 (2)
C9—N3—H3D	125.9	C11—C10—H10	126.9
C10—N3—H3D	125.9	N3—C10—H10	126.9
C14—N4—C12	105.77 (17)	C10—C11—N2	109.2 (2)
C14—N4—Zn1	129.98 (14)	C10—C11—H11	125.4
C12—N4—Zn1	124.18 (13)	N2—C11—H11	125.4
C14—N5—C13	107.93 (18)	C13—C12—N4	109.04 (19)
C14—N5—H5D	126.0	C13—C12—H12	125.5
C13—N5—H5D	126.0	N4—C12—H12	125.5
O1—C1—C6	119.40 (18)	C12—C13—N5	106.47 (19)
O1—C1—C2	123.67 (17)	C12—C13—H13	126.8
C6—C1—C2	116.92 (18)	N5—C13—H13	126.8
C3—C2—C1	119.28 (17)	N4—C14—N5	110.79 (18)
C3—C2—C7	116.36 (16)	N4—C14—H14	124.6
C1—C2—C7	124.35 (16)	N5—C14—H14	124.6
N4—Zn1—O1—C1	−146.69 (15)	Zn1—O1—C1—C2	22.6 (3)
N2—Zn1—O1—C1	96.91 (16)	O1—C1—C2—C3	177.14 (17)
N1—Zn1—O1—C1	−26.88 (16)	C6—C1—C2—C3	−2.0 (3)
O4—Zn1—O1—C1	−2.9 (4)	O1—C1—C2—C7	−1.9 (3)
O2—S1—O4—Zn1	72.22 (8)	C6—C1—C2—C7	178.94 (17)
O3—S1—O4—Zn1	−157.33 (7)	C1—C2—C3—C4	1.2 (3)
C8—S1—O4—Zn1	−43.41 (8)	C7—C2—C3—C4	−179.65 (18)
O1—Zn1—O4—S1	−3.5 (3)	C2—C3—C4—C5	0.1 (3)
N4—Zn1—O4—S1	141.30 (8)	C3—C4—C5—C6	−0.6 (4)
N2—Zn1—O4—S1	−105.13 (8)	C4—C5—C6—C1	−0.3 (4)
N1—Zn1—O4—S1	21.23 (7)	O1—C1—C6—C5	−177.6 (2)
O1—Zn1—N1—C7	18.53 (14)	C2—C1—C6—C5	1.6 (3)
N4—Zn1—N1—C7	124.90 (13)	C8—N1—C7—C2	−178.97 (15)
N2—Zn1—N1—C7	−83.91 (15)	Zn1—N1—C7—C2	−6.3 (2)
O4—Zn1—N1—C7	−156.06 (14)	C3—C2—C7—N1	174.17 (16)
O1—Zn1—N1—C8	−169.04 (13)	C1—C2—C7—N1	−6.8 (3)
N4—Zn1—N1—C8	−62.67 (14)	C7—N1—C8—S1	126.47 (14)
N2—Zn1—N1—C8	88.51 (14)	Zn1—N1—C8—S1	−46.35 (15)
O4—Zn1—N1—C8	16.37 (12)	O2—S1—C8—N1	−57.15 (14)
O1—Zn1—N2—C9	−7.38 (17)	O4—S1—C8—N1	62.79 (14)
N4—Zn1—N2—C9	−115.96 (16)	O3—S1—C8—N1	−177.07 (12)
N1—Zn1—N2—C9	91.51 (17)	C11—N2—C9—N3	0.0 (2)
O4—Zn1—N2—C9	159.73 (17)	Zn1—N2—C9—N3	176.16 (14)
O1—Zn1—N2—C11	167.7 (2)	C10—N3—C9—N2	−0.3 (3)
N4—Zn1—N2—C11	59.2 (2)	C9—N3—C10—C11	0.5 (3)
N1—Zn1—N2—C11	−93.4 (2)	N3—C10—C11—N2	−0.5 (3)
O4—Zn1—N2—C11	−25.2 (2)	C9—N2—C11—C10	0.3 (3)
O1—Zn1—N4—C14	175.79 (17)	Zn1—N2—C11—C10	−175.43 (17)

N2—Zn1—N4—C14	−78.22 (19)	C14—N4—C12—C13	0.4 (3)
N1—Zn1—N4—C14	75.66 (19)	Zn1—N4—C12—C13	177.64 (16)
O4—Zn1—N4—C14	3.43 (18)	N4—C12—C13—N5	−0.1 (3)
O1—Zn1—N4—C12	−0.73 (17)	C14—N5—C13—C12	−0.2 (3)
N2—Zn1—N4—C12	105.26 (17)	C12—N4—C14—N5	−0.5 (2)
N1—Zn1—N4—C12	−100.86 (17)	Zn1—N4—C14—N5	−177.53 (14)
O4—Zn1—N4—C12	−173.09 (16)	C13—N5—C14—N4	0.4 (3)
Zn1—O1—C1—C6	−158.23 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5D···O3^{i}	0.86	1.91	2.765 (2)	173
N3—H3D···O2^{ii}	0.86	2.08	2.860 (2)	151

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

Fig. 1

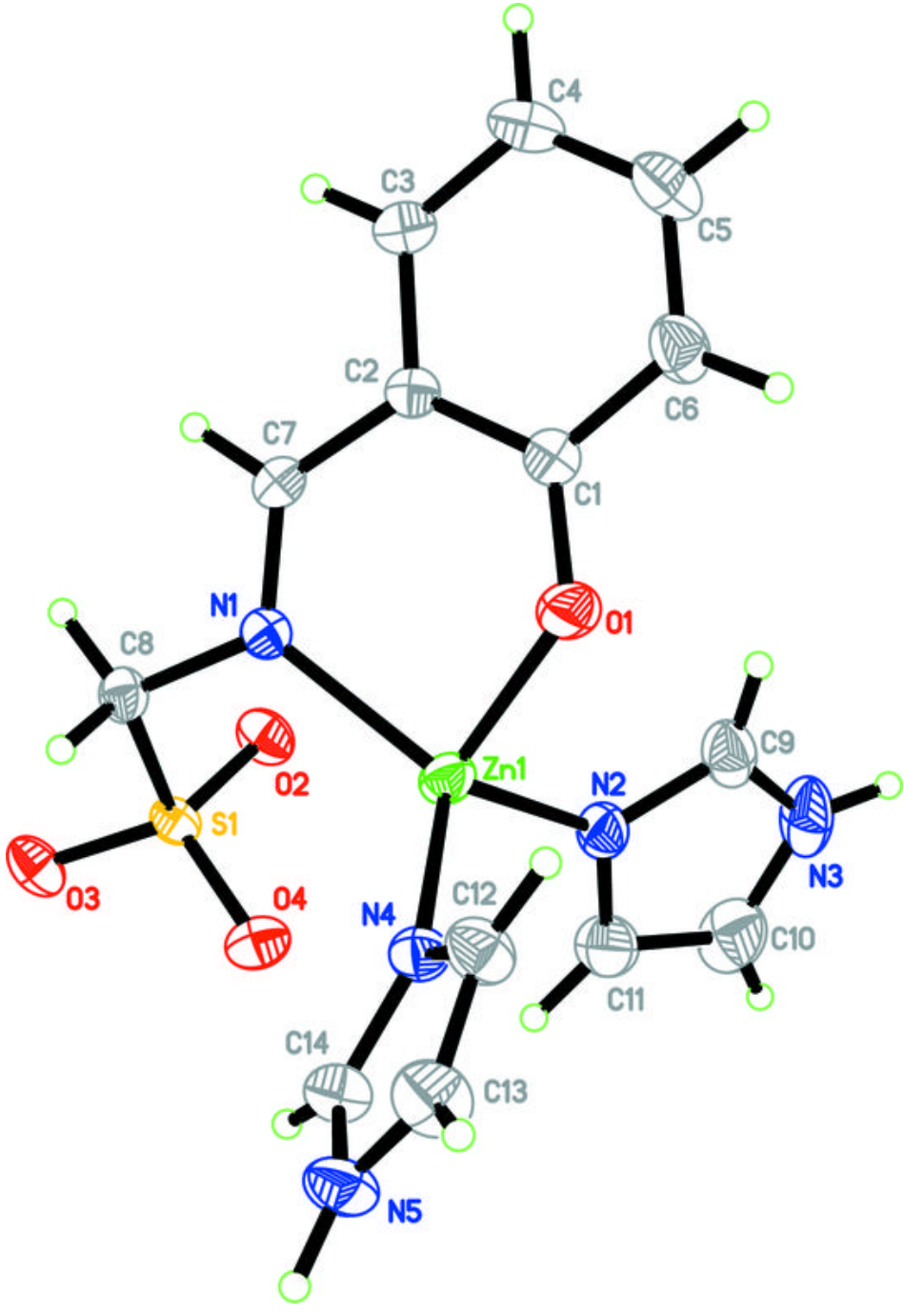
C4
C3
C5
C2
C6
C7
C1
N1
O1
C8
O2
Zn1
N2
C9
S1
N3
O3
O4
N4
C12
C10
C11
C14
C13
N5

Fig. 2