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Bis(salicylhydrazide-κ^2N,O)-sulfatozinc(II) monohydrate

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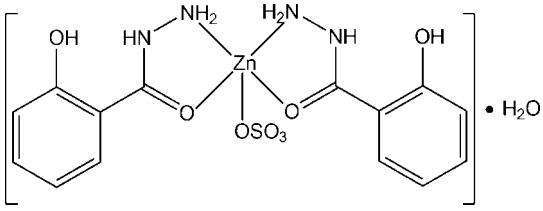
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.048; wR factor = 0.101; data-to-parameter ratio = 14.3.

The title complex, $[Zn(SO_4)(C_7H_8N_2O_2)_2]\cdot H_2O$, contains neutral molecules of a mononuclear Zn^{II} complex, in which the salicylhydrazide ligand is *N,O*-chelated to the Zn^{II} ion. The Zn^{II} ion is coordinated, in a tetragonal–pyramidal environment, by two O atoms and two N atoms from two salicylhydrazide ligands forming a basal plane, and one O atom from the sulfate anion occupying the apical position. The water molecule is disordered over two positions; the site occupancy factors are *ca* 0.6 and 0.4.

Related literature

For related literature, see: Tao *et al.* (2000).



Experimental

Crystal data

$[Zn(SO_4)(C_7H_8N_2O_2)_2]\cdot H_2O$
M_r = 483.75
Triclinic, $P\overline{1}$
a = 7.2028 (6) Å
b = 8.8006 (7) Å
c = 15.6983 (13) Å
α = 101.930 (1)°
β = 95.491 (2)°
γ = 104.210 (1)°
V = 932.50 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.49 mm^{-1}
T = 293 (2) K
0.20 × 0.15 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
8372 measured reflections
3978 independent reflections
2757 reflections with $I > 2\sigma(I)$
R_{int} = 0.078

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.101
S = 0.92
3978 reflections
278 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2	0.86	1.95	2.613 (2)	133
N2—H2A···O7^{i}	0.90	2.14	3.026 (3)	169
N2—H2B···O8^{ii}	0.90	2.00	2.898 (3)	175
N3—H3B···O4	0.86	2.01	2.655 (2)	131
N3—H3B···O9′^{iii}	0.86	2.54	3.085 (4)	122
N3—H3B···O9^{iii}	0.86	2.63	3.158 (6)	120
N4—H4B···O6^{ii}	0.90	2.33	3.053 (3)	137
N4—H4C···O8^{i}	0.90	2.24	2.817 (2)	121
N4—H4C···O7	0.90	2.49	3.056 (3)	121
O2—H2C···O6^{iv}	0.82	1.79	2.606 (2)	177
O4—H4D···O5^{v}	0.82	1.91	2.727 (2)	175
O9′—H9A···O7	0.82 (1)	2.02 (1)	2.833 (4)	173 (2)
O9′—H9B···O4	0.82 (1)	2.33 (1)	3.144 (4)	169 (2)
O9—H9C···O7	0.82 (1)	2.36 (1)	2.912 (5)	125 (1)
O9—H9C···O2^{vi}	0.82 (1)	2.61 (1)	3.333 (6)	147 (1)
O9—H9D···O9^{vii}	0.82 (1)	1.39 (2)	2.130 (11)	147 (3)

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x+1, y, z$; (iii) $-x, -y+1, -z+1$; (iv) $x+1, y+1, z$; (v) $x, y-1, z$; (vi) $x-1, y-1, z$; (vii) $-x-1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2063).

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supplementary materials

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Bis(salicylhydrazide-κ^2N,O)sulfatozinc(II) monohydrate

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Comment

The molecular self-assembly of supramolecular architectures has received much attention during recent decades (Tao *et al.*, 2000). The structures and properties of such systems depend on the coordination and geometric preferences of both the central metal ions and the bridging building blocks, as well as on the influence of weaker non-covalent interactions, such as hydrogen bonds and π-π stacking interactions. In this paper, we report the synthesis and crystal structure of the title compound, (I), $[ZnSO_4(C_7H_8N_2O_2)_2]\cdot H_2O$, (Fig.1) a novel Zn^{II} complex formed by the ligand salicylhydrazide. The Zn^{II} ion is situated in a tetragonal-pyramidal enviroment consisting of two O atoms and two N atoms from two ligands in the basal plane,and an O atom from the sulfate anion in the apical position. Intermolecular O—H···O hydrogen bonds (Table 1) result in a two-dimensional network.

Experimental

Salicylhydrazide (15.2 mg, 0.1 mmol) was dissolved in a mixed solvent (20 ml) of DMF and methanol (1:1), then $ZnSO_4\cdot 7H_2O$ (28.7 mg, 0.1 mmol) was added, stired for 10 min and filtered. Colourless single crystals suitable for X-ray diffraction analysis were obtained by slow diffusion of the filtrate for one week,.

Refinement

Except the water H atoms, all the H atoms were located at the ideal positions with C–H = 0.93 Å (aromatic), N–H = 0.86 Å (imine) and 0.90 Å (amine), O–H = 0.82 Å(phenol); and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, U_{iso}(H) = 1.2U_{eq}(N) for H atoms bonded to N atoms and U_{iso}(H) = 1.2U_{eq}(O) for hydroxyl H atoms. The water H atoms were located from the difference maps and refined with the constraints of O–H = 0.82 (1) Å, H–H = 1.35 (1) Å, and the U_{iso} values of these two H atoms were set 1.5 times of U_{eq} value of water O9 atom. The water O atom was disordered over two positions with occupancies of 0.589 (3):0.411 (3).

Figures

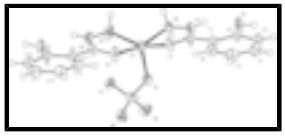

Fig. 1. Molecular structure of (I), showing the atom-numbering scheme.

Fig. 2. Part of the crystal structure of (I), showing the formation of the two-dimensional network.

Bis(salicylhydrazide-κ^2*N*,*O*)sulfatozinc(II) monohydrate

Crystal data

$[Zn(SO_4)(C_7H_8N_2O_2)_2]\cdot H_2O$	$Z = 2$
$M_r = 483.75$	$F_{000} = 496$
Triclinic, $P\overline{1}$	$D_x = 1.723$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.2028$ (6) Å	Cell parameters from 2048 reflections
$b = 8.8006$ (7) Å	$\theta = 2.5$–25.1º
$c = 15.6983$ (13) Å	$\mu = 1.49$ mm^{-1}
$\alpha = 101.9300$ (10)º	$T = 293$ (2) K
$\beta = 95.491$ (2)º	Plate, colourless
$\gamma = 104.2100$ (10)º	0.20 × 0.15 × 0.08 mm
$V = 932.50$ (13) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2757 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.078$
Monochromator: graphite	$\theta_{max} = 27.0$º
$T = 298$(2) K	$\theta_{min} = 2.5$º
0.3° wide ω exposures scans	$h = -9\rightarrow9$
Absorption correction: none	$k = -11\rightarrow11$
8372 measured reflections	$l = -18\rightarrow19$
3978 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
$R[F^2 > 2\sigma(F^2)] = 0.048$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.92$	$(\Delta/\sigma)_{max} = 0.012$
3978 reflections	$\Delta\rho_{max} = 0.58$ e Å^{-3}
278 parameters	$\Delta\rho_{min} = -0.51$ e Å^{-3}
6 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}	Occ. (<1)
Zn1	0.13536 (4)	0.88473 (3)	0.314727 (19)	0.03306 (9)	
C1	0.3139 (4)	1.2506 (3)	0.18144 (15)	0.0286 (6)	
C2	0.4106 (4)	1.4158 (3)	0.20697 (16)	0.0298 (6)	
C3	0.4111 (4)	1.5095 (3)	0.14579 (17)	0.0436 (8)	
H3A	0.4734	1.6194	0.1627	0.052*	
C4	0.3203 (4)	1.4411 (3)	0.06052 (18)	0.0466 (8)	
H4A	0.3225	1.5050	0.0201	0.056*	
C5	0.2259 (4)	1.2786 (3)	0.03429 (18)	0.0452 (8)	
H5A	0.1641	1.2327	−0.0234	0.054*	
C6	0.2246 (4)	1.1852 (3)	0.09485 (16)	0.0374 (7)	
H6A	0.1621	1.0754	0.0771	0.045*	
C7	0.2938 (4)	1.1418 (3)	0.24223 (15)	0.0284 (6)	
C8	−0.1049 (4)	0.3849 (3)	0.21322 (16)	0.0293 (6)	
C9	−0.1469 (4)	0.2470 (3)	0.24732 (16)	0.0316 (7)	
C10	−0.2507 (4)	0.1002 (3)	0.19232 (18)	0.0404 (8)	
H10A	−0.2821	0.0095	0.2154	0.049*	
C11	−0.3077 (4)	0.0858 (3)	0.10502 (19)	0.0434 (8)	
H11A	−0.3756	−0.0142	0.0689	0.052*	
C12	−0.2645 (4)	0.2206 (3)	0.06998 (18)	0.0452 (8)	
H12A	−0.3025	0.2117	0.0104	0.054*	
C13	−0.1651 (4)	0.3667 (3)	0.12426 (17)	0.0386 (7)	
H13A	−0.1370	0.4569	0.1007	0.046*	
C14	0.0002 (4)	0.5478 (2)	0.26454 (15)	0.0281 (6)	
N1	0.3799 (3)	1.1983 (2)	0.32565 (12)	0.0316 (6)	
H1A	0.4540	1.2952	0.3437	0.038*	
N2	0.3466 (3)	1.0954 (2)	0.38360 (12)	0.0299 (5)	
H2A	0.3047	1.1433	0.4316	0.036*	
H2B	0.4567	1.0719	0.4011	0.036*	
N3	0.0868 (3)	0.5710 (2)	0.34653 (13)	0.0361 (6)	
H3B	0.0820	0.4914	0.3709	0.043*	
N4	0.1867 (3)	0.7301 (2)	0.39233 (14)	0.0371 (6)	
H4B	0.3146	0.7397	0.4030	0.044*	
H4C	0.1446	0.7549	0.4442	0.044*	

O1	0.1941 (3)	0.99810 (18)	0.21592 (10)	0.0369 (5)	
O2	0.5027 (3)	1.48017 (18)	0.29031 (11)	0.0441 (6)	
H2C	0.5256	1.5787	0.3009	0.066*	
O3	0.0069 (3)	0.66568 (18)	0.23094 (11)	0.0434 (5)	
O4	−0.0854 (3)	0.26218 (19)	0.33444 (11)	0.0471 (6)	
H4D	−0.0849	0.1733	0.3428	0.071*	
O5	−0.0905 (3)	0.95954 (19)	0.35224 (11)	0.0407 (5)	
O6	−0.4187 (3)	0.7940 (2)	0.33021 (12)	0.0438 (5)	
O7	−0.1873 (3)	0.78945 (19)	0.45077 (11)	0.0414 (5)	
O8	−0.3047 (2)	1.02338 (19)	0.45151 (11)	0.0403 (5)	
S1	−0.25252 (9)	0.88909 (6)	0.39720 (4)	0.02728 (16)	
O9'	−0.2612 (6)	0.4713 (4)	0.4754 (2)	0.0685 (12)	0.589 (3)
H9A	−0.235 (3)	0.5609 (9)	0.4650 (14)	0.103*	0.589 (3)
H9B	−0.2009 (19)	0.4211 (16)	0.4438 (14)	0.103*	0.589 (3)
O9	−0.3556 (8)	0.4900 (6)	0.5003 (3)	0.0685 (12)	0.411 (3)
H9C	−0.359 (3)	0.5274 (19)	0.4567 (8)	0.103*	0.411 (3)
H9D	−0.4656 (14)	0.478 (4)	0.5129 (13)	0.103*	0.411 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03925 (18)	0.01937 (13)	0.04079 (17)	0.00402 (12)	0.00967 (14)	0.01088 (12)
C1	0.0320 (14)	0.0254 (11)	0.0308 (13)	0.0077 (10)	0.0100 (11)	0.0096 (10)
C2	0.0326 (14)	0.0254 (11)	0.0325 (13)	0.0060 (10)	0.0080 (11)	0.0101 (10)
C3	0.0506 (18)	0.0314 (12)	0.0536 (16)	0.0083 (12)	0.0144 (14)	0.0211 (12)
C4	0.0535 (18)	0.0486 (14)	0.0452 (15)	0.0132 (13)	0.0067 (14)	0.0290 (12)
C5	0.0493 (17)	0.0499 (15)	0.0371 (15)	0.0132 (14)	0.0041 (14)	0.0131 (13)
C6	0.0407 (16)	0.0332 (12)	0.0384 (14)	0.0078 (12)	0.0085 (13)	0.0102 (11)
C7	0.0285 (13)	0.0235 (11)	0.0334 (13)	0.0058 (10)	0.0089 (11)	0.0072 (10)
C8	0.0269 (13)	0.0216 (11)	0.0383 (14)	0.0058 (10)	0.0042 (11)	0.0058 (10)
C9	0.0333 (14)	0.0225 (11)	0.0375 (14)	0.0072 (11)	0.0006 (12)	0.0064 (10)
C10	0.0390 (16)	0.0250 (12)	0.0528 (16)	0.0033 (12)	0.0002 (14)	0.0091 (12)
C11	0.0413 (16)	0.0254 (13)	0.0523 (17)	0.0062 (12)	−0.0048 (14)	−0.0063 (13)
C12	0.0490 (18)	0.0399 (14)	0.0398 (16)	0.0083 (14)	−0.0060 (14)	0.0045 (13)
C13	0.0451 (17)	0.0301 (12)	0.0384 (15)	0.0070 (12)	0.0000 (13)	0.0103 (11)
C14	0.0314 (13)	0.0191 (10)	0.0344 (13)	0.0061 (10)	0.0075 (11)	0.0076 (10)
N1	0.0387 (12)	0.0190 (9)	0.0330 (11)	−0.0013 (9)	0.0033 (10)	0.0094 (8)
N2	0.0347 (11)	0.0276 (9)	0.0311 (10)	0.0079 (9)	0.0082 (9)	0.0144 (8)
N3	0.0470 (13)	0.0181 (9)	0.0401 (12)	0.0059 (9)	−0.0039 (11)	0.0083 (9)
N4	0.0423 (13)	0.0186 (9)	0.0418 (12)	0.0058 (9)	−0.0080 (11)	−0.0020 (9)
O1	0.0485 (11)	0.0223 (8)	0.0329 (9)	−0.0027 (8)	0.0042 (9)	0.0069 (7)
O2	0.0637 (13)	0.0206 (8)	0.0398 (10)	−0.0020 (9)	0.0017 (10)	0.0083 (8)
O3	0.0654 (13)	0.0218 (8)	0.0363 (10)	0.0002 (9)	−0.0027 (9)	0.0108 (7)
O4	0.0676 (13)	0.0212 (8)	0.0474 (11)	0.0032 (9)	−0.0051 (10)	0.0141 (8)
O5	0.0403 (10)	0.0380 (8)	0.0565 (10)	0.0153 (8)	0.0240 (9)	0.0259 (8)
O6	0.0394 (11)	0.0298 (9)	0.0507 (11)	0.0004 (8)	−0.0059 (9)	0.0009 (9)
O7	0.0475 (11)	0.0395 (8)	0.0477 (10)	0.0167 (8)	0.0143 (9)	0.0244 (8)
O8	0.0418 (10)	0.0385 (9)	0.0399 (10)	0.0200 (8)	0.0024 (9)	−0.0013 (8)

S1	0.0293 (3)	0.0204 (3)	0.0324 (3)	0.0048 (2)	0.0054 (3)	0.0090 (2)
O9'	0.089 (3)	0.0608 (14)	0.0756 (19)	0.0311 (19)	0.029 (2)	0.0403 (14)
O9	0.089 (3)	0.0608 (14)	0.0756 (19)	0.0311 (19)	0.029 (2)	0.0403 (14)

Geometric parameters (Å, °)

Zn1—O5	1.9937 (19)	C11—H11A	0.9300
Zn1—O1	2.0343 (16)	C12—C13	1.367 (3)
Zn1—O3	2.0361 (15)	C12—H12A	0.9300
Zn1—N4	2.079 (2)	C13—H13A	0.9300
Zn1—N2	2.0962 (17)	C14—O3	1.250 (3)
C1—C6	1.386 (3)	C14—N3	1.328 (3)
C1—C2	1.403 (3)	N1—N2	1.407 (2)
C1—C7	1.478 (3)	N1—H1A	0.8600
C2—O2	1.348 (3)	N2—H2A	0.9000
C2—C3	1.389 (3)	N2—H2B	0.9000
C3—C4	1.374 (3)	N3—N4	1.409 (2)
C3—H3A	0.9300	N3—H3B	0.8600
C4—C5	1.380 (3)	N4—H4B	0.9000
C4—H4A	0.9300	N4—H4C	0.9000
C5—C6	1.379 (4)	O2—H2C	0.8200
C5—H5A	0.9300	O4—H4D	0.8200
C6—H6A	0.9300	O5—S1	1.4928 (18)
C7—O1	1.252 (2)	O6—S1	1.4634 (17)
C7—N1	1.331 (3)	O7—S1	1.4588 (17)
C8—C13	1.386 (3)	O8—S1	1.4585 (17)
C8—C9	1.404 (3)	O9'—H9A	0.819 (9)
C8—C14	1.466 (3)	O9'—H9B	0.821 (9)
C9—O4	1.365 (3)	O9'—H9C	1.011 (18)
C9—C10	1.384 (3)	O9—H9A	1.191 (19)
C10—C11	1.363 (4)	O9—H9C	0.819 (9)
C10—H10A	0.9300	O9—H9D	0.822 (9)
C11—C12	1.388 (4)		
O5—Zn1—O1	101.24 (7)	C13—C12—H12A	120.5
O5—Zn1—O3	102.77 (8)	C11—C12—H12A	120.5
O1—Zn1—O3	93.86 (6)	C12—C13—C8	122.3 (2)
O5—Zn1—N4	107.05 (8)	C12—C13—H13A	118.9
O1—Zn1—N4	151.69 (9)	C8—C13—H13A	118.9
O3—Zn1—N4	78.90 (7)	O3—C14—N3	119.87 (19)
O5—Zn1—N2	95.68 (7)	O3—C14—C8	119.7 (2)
O1—Zn1—N2	79.12 (7)	N3—C14—C8	120.5 (2)
O3—Zn1—N2	161.25 (8)	C7—N1—N2	118.25 (17)
N4—Zn1—N2	99.01 (7)	C7—N1—H1A	120.9
C6—C1—C2	118.6 (2)	N2—N1—H1A	120.9
C6—C1—C7	117.3 (2)	N1—N2—Zn1	107.10 (12)
C2—C1—C7	124.0 (2)	N1—N2—H2A	110.3
O2—C2—C3	121.3 (2)	Zn1—N2—H2A	110.3
O2—C2—C1	119.2 (2)	N1—N2—H2B	110.3
C3—C2—C1	119.5 (2)	Zn1—N2—H2B	110.3

C4—C3—C2	120.5 (2)	H2A—N2—H2B	108.6
C4—C3—H3A	119.7	C14—N3—N4	117.91 (18)
C2—C3—H3A	119.7	C14—N3—H3B	121.0
C3—C4—C5	120.7 (2)	N4—N3—H3B	121.0
C3—C4—H4A	119.7	N3—N4—Zn1	108.09 (14)
C5—C4—H4A	119.7	N3—N4—H4B	110.1
C6—C5—C4	119.0 (2)	Zn1—N4—H4B	110.1
C6—C5—H5A	120.5	N3—N4—H4C	110.1
C4—C5—H5A	120.5	Zn1—N4—H4C	110.1
C5—C6—C1	121.7 (2)	H4B—N4—H4C	108.4
C5—C6—H6A	119.1	C7—O1—Zn1	113.80 (15)
C1—C6—H6A	119.1	C2—O2—H2C	109.5
O1—C7—N1	120.1 (2)	C14—O3—Zn1	114.63 (14)
O1—C7—C1	120.3 (2)	C9—O4—H4D	109.5
N1—C7—C1	119.53 (19)	S1—O5—Zn1	132.28 (10)
C13—C8—C9	118.0 (2)	O8—S1—O7	111.27 (10)
C13—C8—C14	117.1 (2)	O8—S1—O6	109.20 (11)
C9—C8—C14	124.9 (2)	O7—S1—O6	111.30 (10)
O4—C9—C10	121.8 (2)	O8—S1—O5	107.26 (10)
O4—C9—C8	118.82 (19)	O7—S1—O5	108.94 (11)
C10—C9—C8	119.4 (2)	O6—S1—O5	108.75 (11)
C11—C10—C9	121.3 (2)	H9A—O9'—H9B	104.5 (15)
C11—C10—H10A	119.4	H9A—O9'—H9C	54.7 (17)
C9—C10—H10A	119.4	H9B—O9'—H9C	127.7 (18)
C10—C11—C12	120.0 (2)	H9A—O9—H9C	46.1 (16)
C10—C11—H11A	120.0	H9A—O9—H9D	146 (2)
C12—C11—H11A	120.0	H9C—O9—H9D	104.3 (15)
C13—C12—C11	119.0 (2)		
C6—C1—C2—O2	−178.1 (2)	C7—N1—N2—Zn1	−6.3 (3)
C7—C1—C2—O2	4.5 (4)	O5—Zn1—N2—N1	−91.44 (15)
C6—C1—C2—C3	1.3 (4)	O1—Zn1—N2—N1	8.95 (14)
C7—C1—C2—C3	−176.1 (2)	O3—Zn1—N2—N1	78.3 (3)
O2—C2—C3—C4	178.4 (3)	N4—Zn1—N2—N1	160.26 (15)
C1—C2—C3—C4	−1.0 (4)	O3—C14—N3—N4	−1.0 (4)
C2—C3—C4—C5	0.5 (5)	C8—C14—N3—N4	179.5 (2)
C3—C4—C5—C6	−0.3 (5)	C14—N3—N4—Zn1	6.2 (3)
C4—C5—C6—C1	0.6 (4)	O5—Zn1—N4—N3	93.69 (16)
C2—C1—C6—C5	−1.1 (4)	O1—Zn1—N4—N3	−83.7 (2)
C7—C1—C6—C5	176.4 (3)	O3—Zn1—N4—N3	−6.42 (15)
C6—C1—C7—O1	−2.4 (4)	N2—Zn1—N4—N3	−167.49 (16)
C2—C1—C7—O1	175.1 (2)	N1—C7—O1—Zn1	11.9 (3)
C6—C1—C7—N1	178.8 (2)	C1—C7—O1—Zn1	−166.91 (18)
C2—C1—C7—N1	−3.8 (4)	O5—Zn1—O1—C7	82.16 (18)
C13—C8—C9—O4	178.8 (2)	O3—Zn1—O1—C7	−173.99 (18)
C14—C8—C9—O4	−0.6 (4)	N4—Zn1—O1—C7	−100.4 (2)
C13—C8—C9—C10	−1.9 (4)	N2—Zn1—O1—C7	−11.53 (18)
C14—C8—C9—C10	178.7 (3)	N3—C14—O3—Zn1	−5.2 (3)
O4—C9—C10—C11	−178.6 (3)	C8—C14—O3—Zn1	174.31 (18)
C8—C9—C10—C11	2.1 (4)	O5—Zn1—O3—C14	−98.63 (19)

C9—C10—C11—C12	−1.0 (4)	O1—Zn1—O3—C14	158.93 (19)
C10—C11—C12—C13	−0.2 (4)	N4—Zn1—O3—C14	6.55 (19)
C11—C12—C13—C8	0.4 (4)	N2—Zn1—O3—C14	91.9 (3)
C9—C8—C13—C12	0.7 (4)	O1—Zn1—O5—S1	155.47 (13)
C14—C8—C13—C12	−179.9 (3)	O3—Zn1—O5—S1	58.85 (15)
C13—C8—C14—O3	10.4 (4)	N4—Zn1—O5—S1	−23.28 (16)
C9—C8—C14—O3	−170.2 (2)	N2—Zn1—O5—S1	−124.53 (14)
C13—C8—C14—N3	−170.1 (2)	Zn1—O5—S1—O8	147.72 (13)
C9—C8—C14—N3	9.3 (4)	Zn1—O5—S1—O7	27.17 (17)
O1—C7—N1—N2	−3.5 (4)	Zn1—O5—S1—O6	−94.30 (15)
C1—C7—N1—N2	175.4 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2	0.86	1.95	2.613 (2)	133
N2—H2A···O7^{i}	0.90	2.14	3.026 (3)	169
N2—H2B···O8^{ii}	0.90	2.00	2.898 (3)	175
N3—H3B···O4	0.86	2.01	2.655 (2)	131
N3—H3B···O9'^{iii}	0.86	2.54	3.085 (4)	122
N3—H3B···O9^{iii}	0.86	2.63	3.158 (6)	120
N4—H4B···O6^{ii}	0.90	2.33	3.053 (3)	137
N4—H4C···O8^{i}	0.90	2.24	2.817 (2)	121
N4—H4C···O7	0.90	2.49	3.056 (3)	121
O2—H2C···O6^{iv}	0.82	1.79	2.606 (2)	177
O4—H4D···O5^{v}	0.82	1.91	2.727 (2)	175
O9'—H9A···O7	0.819 (9)	2.018 (8)	2.833 (4)	173 (2)
O9'—H9B···O4	0.821 (9)	2.334 (11)	3.144 (4)	168.8 (18)
O9—H9C···O7	0.819 (9)	2.360 (14)	2.912 (5)	125.3 (13)
O9—H9C···O2^{vi}	0.819 (9)	2.614 (11)	3.333 (6)	147.3 (14)
O9—H9D···O9^{vii}	0.822 (9)	1.39 (2)	2.130 (11)	147 (3)

Symmetry codes: (i) −*x*, −*y*+2, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) −*x*, −*y*+1, −*z*+1; (iv) *x*+1, *y*+1, *z*; (v) *x*, *y*−1, *z*; (vi) *x*−1, *y*−1, *z*; (vii) −*x*−1, −*y*+1, −*z*+1.

Fig. 1

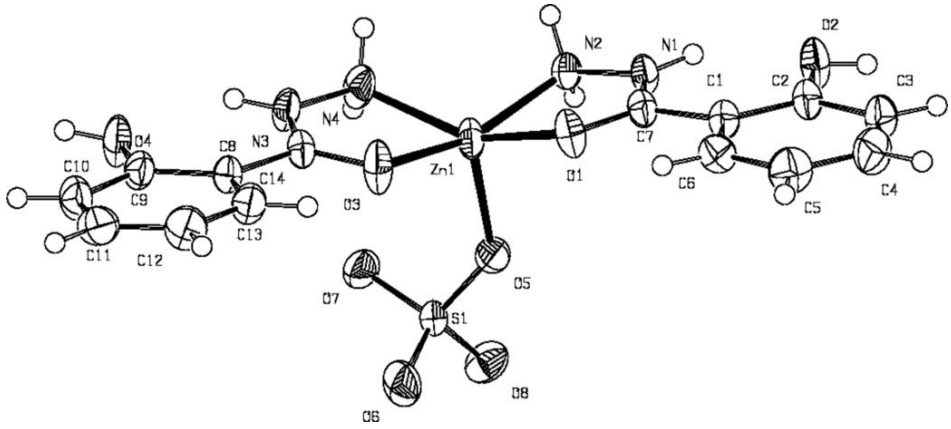
O2
N2
N1
C1
C2
C3
N4
O4
C8
N3
C7
C10
C14
Zn1
O1
C6
C4
C9
O3
C5
C11
C12
C13
O7
O5
S1
O8
O6

Fig. 2