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Diaquabis(ethylenediamine-κ^2N,N')-zinc(II) bis(4-aminonaphthalene-1-sulfonate) dihydrate

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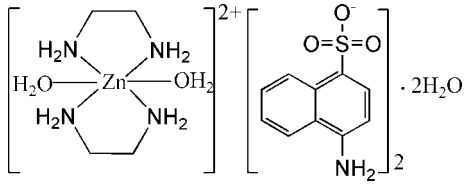
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.086; data-to-parameter ratio = 14.2.

In the title compound, $[Zn(C_2H_8N_2)_2(H_2O)_2](C_{10}H_8NO_3S)_2\cdot 2H_2O$, the Zn^{II} cation lies on an inversion centre and has a distorted octahedral coordination geometry, defined by four N atoms from two ethylenediamine ligands and two water O atoms. In the crystal structure, pairs of 4-aminonaphthalene-1-sulfonate anions are connected *via* N—H···O hydrogen bonds to form centrosymmetric $R_2^2(16)$ rings. Cations, anions and water molecules are further connected by N—H···O, O—H···O and O—H···N hydrogen bonds and π–π stacking interactions [with a centroid-to-centroid distance of 3.5099 (13) Å] to form a three-dimensional network.

Related literature

The isostructural Ni^{II}, Cu^{II} and Cd^{II} analogues have been reported previously (Li *et al.*, 2005*a*,*b*, 2006).

For related literature, see: Gunderman *et al.* (1997); Işık *et al.* (2005); Kosnic *et al.* (1992); Shubnell *et al.* (1994).



Experimental

Crystal data

$[Zn(C_2H_8N_2)_2(H_2O)_2]\cdot(C_{10}H_8NO_3S)_2\cdot 2H_2O$
M_r = 702.11
Monoclinic, $P2_1/c$
a = 12.425 (3) Å
b = 9.6851 (19) Å
c = 12.305 (3) Å
β = 90.50 (3)°
V = 1480.7 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 292 (2) K
0.46 × 0.36 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.647, T_{max} = 0.820
9734 measured reflections
3354 independent reflections
2729 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.086
S = 0.98
3354 reflections
236 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O4^{i}	0.86 (2)	2.41 (2)	3.170 (2)	147 (2)
N1—H1A···O2^{ii}	0.836 (18)	2.570 (19)	3.337 (3)	153 (2)
N2—H2A···O2^{iii}	0.87 (2)	2.28 (2)	3.109 (2)	159 (2)
N2—H2B···O5	0.915 (18)	2.113 (19)	2.992 (3)	161 (2)
N3—H3A···O2^{iv}	0.782 (19)	2.67 (2)	3.451 (2)	176 (2)
N3—H3B···O3^{v}	0.836 (19)	2.246 (19)	3.076 (3)	171.6 (18)
O1—H1E···O5	0.79 (2)	2.08 (2)	2.834 (3)	158 (2)
O5—H5B···N3^{vi}	0.87 (2)	2.02 (2)	2.882 (3)	173 (3)
O5—H5A···O4^{vii}	0.77 (2)	2.15 (2)	2.918 (3)	172 (3)
O1—H1F···O4^{i}	0.75 (2)	2.11 (2)	2.818 (2)	159 (3)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x, -y+1, -z+1$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x+1, -y+2, -z$; (vi) $-x+1, -y+1, -z+1$; (vii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2390).

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supplementary materials

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Diaquabis(ethylenediamine-κ^2N,N')zinc(II) bis(4-aminonaphthalene-1-sulfonate) dihydrate

M.-T. Li, X.-C. Fu, X.-Y. Wang and C.-G. Wang

Comment

Due to the weak coordination strength of sulfonate anions with transition metals, the sulfonates usually act as the counter-balance of the charge (Kosnic *et al.*, 1992; Shubnell *et al.*, 1994; Gunderman *et al.*, 1997). Herein, we report the crystal structure of such a novel compound, $[Cu(en)_2(H_2O)_2](ans)_2\ 2H_2O$, (I), (en = diethylenediamine; ans = 4-aminonaphthalene-1-sulfonate). The molecular structure of (I) is shown in Fig.1. The Zn atom lies on an inversion center and has has a distorted octahedral geometry, coordinated by four N atoms from two diethylenediamine ligands, which lie in the equatorial plane, and by two water O atoms occupying the axial sites. The average Zn—N bond length of 2.1278 (16) Å, is longer than the Zn—N bond distances in $[Zn(en)_2(H_2O)_2](sap)_2 3H_2O$ (sap = 2-sulfanilamidopyrimidine; Zn—N 1.996 (2)–2.016 (2) Å) (Isik *et al.*, 2005). The Zn—O bond distance of 2.2386 (17) Å, is significantly shorter than the Zn—O distances in $[Zn(en)_2(H_2O)_2](sap)_2$ (Zn—O 2.49 (2) Å and 2.68 (2) Å)(Isik *et al.*, 2005). The naphthalene ring is essentially planar (r.m.s. deviation 0.002 Å), with the greatest deviation from planarity being 0.0258 (18)Å for C6. The S and N atoms deviate by 0.1632 (5) Å and 0.0035 (19) Å from the naphthalene plane, respectively. As shown in Fig.2, an organic cation layer is linked to an inorganic anionic layer through a series of N—H···O, O—H···O and O—H···N hydrogen bonds, and adjacent 4-aminonaphthalene-1-sulfonate anions are antiparallel, showing significant π-π interactions interactions. The plane-to-plane distances and displacement angles of $Cg1\cdots Cg2^{i}$ are 3.378, 3.367 Å and 1.04, 16.37 °, respectively [*Cg*1 and *Cg*2 are C3—C7/C12 and C7—C12 ring centroids; symmetry code: (i) $1-x, 2-y, -z$]). These interactions together with the hydrogen bonds stabilize the crystal structure.

Experimental

Ethylenediamine (0.06 g, 1 mmol) was added to an aqueous solution (20 mL) of $Zn(OAc)_2{\cdot}2H_2O$(0.110 g, 0.5 mmol). After the mixture was stirred for 2 h at the room temperature, the solution was then treated with 4-aminonaphthalene-1-sulfonic acid sodium salt tetrahydrate (0.32 g, 1 mmol) in 10 ml e thanol. After filtration, the colorless solutions were allowed to stand at room temperature. The well shaped colorless block crystals of the title complex were obtained by slow evaporation of solvent about one week.

Refinement

The water H atoms and amine H atoms were located in a difference Fourier map and refined with the restraints O—H = 0.75 (2)–0.87 (2) Å and N—H = 0.782 (19)–0.915 (2) Å, and U_{iso}(H) = 1.5U_{eq}(carrier). H atoms on C atoms were placed in geometrically idealized positions and refined in riding mode, with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

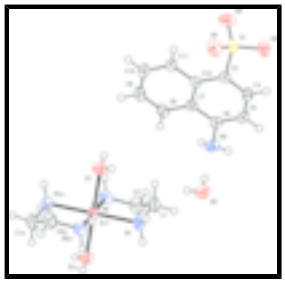

Fig. 1. The molecular structure of (I), showing ellipsoids at the 50% probability level [symmetry code: $-x$, $-y$, $1-z$].

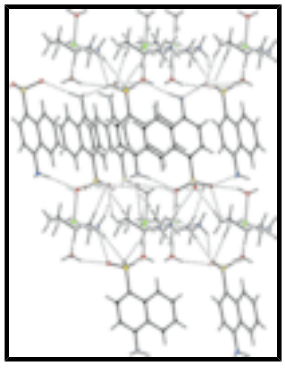

Fig. 2. Part of the crystal structure of (I), with hydrogen bonds shown as dashed lines.

[Diaquabis(ethylenediamine-κ^2*N*,*N*')zinc(II)] [bis(4-aminonaphthalene-1-sulfonate)] dihydrate

Crystal data

$[Zn(C_2H_8N_2)_2(H_2O)_2](C_{10}H_8NO_3S)_2\cdot 2H_2O$	F_{000} = 736
M_r = 702.11	D_x = 1.575 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3865 reflections
a = 12.425 (3) Å	θ = 2.7–28.1º
b = 9.6851 (19) Å	μ = 1.04 mm^{-1}
c = 12.305 (3) Å	T = 292 (2) K
β = 90.50 (3)º	Block, colourless
V = 1480.7 (5) Å^3	0.46 × 0.36 × 0.20 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	3354 independent reflections
Radiation source: fine-focus sealed tube	2729 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
T = 292(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	h = −12→16

T_{min} = 0.647, T_{max} = 0.820	k = −12→12
9734 measured reflections	l = −10→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.086	$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.98	$(\Delta/\sigma)_{max} < 0.001$
3354 reflections	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
236 parameters	$\Delta\rho_{min}$ = −0.66 e Å^{-3}
10 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}
Zn1	0.0000	0.0000	0.5000	0.02820 (11)
N1	0.00131 (16)	0.16231 (19)	0.38096 (15)	0.0372 (4)
N2	−0.01612 (14)	0.16750 (18)	0.60803 (15)	0.0338 (4)
O1	0.17965 (13)	0.00886 (17)	0.51362 (15)	0.0394 (4)
C1	0.02957 (17)	0.2888 (2)	0.4403 (2)	0.0461 (6)
H1C	0.0134	0.3690	0.3959	0.055*
H1D	0.1060	0.2894	0.4572	0.055*
C2	−0.03471 (18)	0.2943 (2)	0.54452 (19)	0.0466 (6)
H2C	−0.0131	0.3742	0.5870	0.056*
H2D	−0.1107	0.3032	0.5273	0.056*
C3	0.38445 (13)	0.94913 (18)	0.18557 (14)	0.0241 (4)
C4	0.44306 (15)	1.0471 (2)	0.24009 (15)	0.0296 (4)
H4	0.4095	1.1022	0.2916	0.036*
C5	0.55247 (15)	1.06581 (19)	0.21962 (16)	0.0310 (4)

H5	0.5904	1.1337	0.2573	0.037*
C6	0.60475 (15)	0.98605 (17)	0.14515 (15)	0.0266 (4)
C7	0.54778 (14)	0.87878 (17)	0.08887 (14)	0.0235 (4)
C8	0.59937 (15)	0.79072 (19)	0.01412 (15)	0.0303 (4)
H8	0.6727	0.8010	0.0020	0.036*
C9	0.54368 (16)	0.6911 (2)	−0.04046 (16)	0.0354 (5)
H9	0.5788	0.6347	−0.0900	0.043*
C10	0.43368 (16)	0.67369 (19)	−0.02191 (15)	0.0337 (4)
H10	0.3962	0.6051	−0.0591	0.040*
C11	0.38054 (14)	0.75566 (17)	0.04986 (14)	0.0274 (4)
H11	0.3073	0.7426	0.0606	0.033*
C12	0.43560 (14)	0.86090 (16)	0.10847 (14)	0.0228 (4)
N3	0.71563 (14)	1.00495 (19)	0.12848 (16)	0.0339 (4)
O2	0.21294 (11)	0.80591 (14)	0.23913 (12)	0.0429 (4)
O3	0.19412 (12)	0.98569 (15)	0.10337 (13)	0.0431 (4)
O4	0.22193 (11)	1.04667 (15)	0.29095 (12)	0.0408 (4)
O5	0.20692 (14)	0.1749 (2)	0.70145 (14)	0.0477 (4)
S1	0.24345 (4)	0.94473 (5)	0.20564 (4)	0.02944 (13)
H1E	0.2027 (19)	0.060 (2)	0.558 (2)	0.056 (9)*
H1F	0.206 (2)	0.023 (3)	0.4602 (19)	0.055 (9)*
H3A	0.7328 (17)	1.075 (2)	0.1555 (19)	0.045 (7)*
H3B	0.7366 (17)	0.9997 (19)	0.0642 (16)	0.030 (6)*
H5A	0.215 (2)	0.250 (2)	0.720 (2)	0.077 (11)*
H5B	0.226 (2)	0.124 (3)	0.757 (2)	0.067 (9)*
H2A	−0.0723 (18)	0.151 (2)	0.6477 (19)	0.062 (8)*
H1A	−0.0590 (15)	0.169 (2)	0.3507 (18)	0.048 (7)*
H1B	0.0491 (19)	0.146 (3)	0.332 (2)	0.072 (9)*
H2B	0.0438 (16)	0.175 (2)	0.6514 (18)	0.049 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03346 (19)	0.02544 (17)	0.02576 (18)	0.00102 (12)	0.00379 (13)	0.00048 (12)
N1	0.0362 (11)	0.0407 (10)	0.0347 (10)	0.0026 (8)	0.0058 (9)	0.0084 (8)
N2	0.0300 (9)	0.0361 (9)	0.0354 (10)	0.0002 (7)	0.0058 (8)	−0.0064 (8)
O1	0.0314 (8)	0.0494 (10)	0.0373 (9)	−0.0016 (7)	0.0041 (7)	−0.0020 (8)
C1	0.0479 (13)	0.0299 (10)	0.0605 (15)	−0.0024 (9)	0.0058 (11)	0.0109 (10)
C2	0.0516 (13)	0.0294 (10)	0.0589 (15)	0.0065 (10)	0.0076 (12)	−0.0037 (10)
C3	0.0252 (9)	0.0256 (8)	0.0215 (9)	−0.0002 (7)	0.0032 (7)	0.0040 (7)
C4	0.0349 (10)	0.0307 (9)	0.0233 (9)	0.0012 (8)	0.0042 (8)	−0.0034 (8)
C5	0.0355 (10)	0.0289 (9)	0.0284 (10)	−0.0056 (8)	−0.0025 (8)	−0.0042 (8)
C6	0.0270 (9)	0.0283 (9)	0.0244 (9)	−0.0026 (7)	−0.0012 (8)	0.0067 (7)
C7	0.0272 (9)	0.0231 (8)	0.0203 (9)	0.0014 (7)	0.0011 (7)	0.0045 (7)
C8	0.0297 (10)	0.0325 (10)	0.0288 (10)	0.0050 (8)	0.0061 (8)	0.0029 (8)
C9	0.0432 (11)	0.0315 (10)	0.0317 (11)	0.0056 (9)	0.0081 (9)	−0.0054 (8)
C10	0.0443 (12)	0.0267 (9)	0.0301 (11)	−0.0049 (8)	0.0004 (9)	−0.0042 (8)
C11	0.0284 (9)	0.0273 (9)	0.0267 (10)	−0.0034 (7)	0.0010 (8)	0.0013 (8)
C12	0.0278 (9)	0.0221 (8)	0.0186 (8)	0.0007 (7)	0.0026 (7)	0.0034 (7)

N3	0.0279 (9)	0.0405 (10)	0.0332 (10)	−0.0067 (7)	0.0001 (8)	0.0006 (8)
O2	0.0391 (8)	0.0380 (8)	0.0518 (10)	−0.0064 (6)	0.0161 (7)	0.0035 (7)
O3	0.0302 (8)	0.0623 (10)	0.0370 (9)	0.0054 (6)	0.0007 (7)	0.0058 (7)
O4	0.0390 (8)	0.0435 (8)	0.0400 (9)	0.0044 (7)	0.0145 (7)	−0.0087 (7)
O5	0.0522 (10)	0.0440 (10)	0.0466 (10)	−0.0010 (8)	−0.0133 (8)	0.0002 (8)
S1	0.0265 (2)	0.0334 (3)	0.0286 (3)	0.00020 (19)	0.00845 (19)	−0.0001 (2)

Geometric parameters (Å, °)

Zn1—N2	2.1080 (17)	C4—H4	0.9300
Zn1—N2^{i}	2.1080 (17)	C5—C6	1.367 (3)
Zn1—N1^{i}	2.1488 (18)	C5—H5	0.9300
Zn1—N1	2.1488 (18)	C6—N3	1.407 (3)
Zn1—O1^{i}	2.2386 (17)	C6—C7	1.432 (2)
Zn1—O1	2.2386 (17)	C7—C8	1.412 (2)
N1—C1	1.468 (3)	C7—C12	1.427 (2)
N1—H1A	0.836 (18)	C8—C9	1.361 (3)
N1—H1B	0.86 (2)	C8—H8	0.9300
N2—C2	1.473 (3)	C9—C10	1.398 (3)
N2—H2A	0.87 (2)	C9—H9	0.9300
N2—H2B	0.915 (18)	C10—C11	1.362 (2)
O1—H1E	0.79 (2)	C10—H10	0.9300
O1—H1F	0.75 (2)	C11—C12	1.421 (2)
C1—C2	1.517 (3)	C11—H11	0.9300
C1—H1C	0.9700	N3—H3A	0.782 (19)
C1—H1D	0.9700	N3—H3B	0.836 (19)
C2—H2C	0.9700	O2—S1	1.4573 (15)
C2—H2D	0.9700	O3—S1	1.4504 (16)
C3—C4	1.369 (3)	O4—S1	1.4674 (15)
C3—C12	1.430 (2)	O5—H5A	0.77 (2)
C3—S1	1.7719 (17)	O5—H5B	0.87 (2)
C4—C5	1.397 (3)		
N2—Zn1—N2^{i}	180.0	H2C—C2—H2D	108.2
N2—Zn1—N1^{i}	97.57 (8)	C4—C3—C12	120.14 (16)
N2^{i}—Zn1—N1^{i}	82.43 (8)	C4—C3—S1	118.09 (14)
N2—Zn1—N1	82.43 (8)	C12—C3—S1	121.59 (13)
N2^{i}—Zn1—N1	97.57 (8)	C3—C4—C5	121.07 (17)
N1^{i}—Zn1—N1	180.0	C3—C4—H4	119.5
N2—Zn1—O1^{i}	88.66 (7)	C5—C4—H4	119.5
N2^{i}—Zn1—O1^{i}	91.34 (7)	C6—C5—C4	121.12 (17)
N1^{i}—Zn1—O1^{i}	90.55 (7)	C6—C5—H5	119.4
N1—Zn1—O1^{i}	89.45 (7)	C4—C5—H5	119.4
N2—Zn1—O1	91.34 (7)	C5—C6—N3	119.74 (17)
N2^{i}—Zn1—O1	88.66 (7)	C5—C6—C7	119.88 (17)
N1^{i}—Zn1—O1	89.45 (7)	N3—C6—C7	120.29 (17)
N1—Zn1—O1	90.55 (7)	C8—C7—C12	119.09 (16)

O1^{i}—Zn1—O1	180.0	C8—C7—C6	121.85 (16)
C1—N1—Zn1	105.95 (13)	C12—C7—C6	119.05 (16)
C1—N1—H1A	111.5 (16)	C9—C8—C7	121.18 (17)
Zn1—N1—H1A	110.4 (16)	C9—C8—H8	119.4
C1—N1—H1B	109.7 (17)	C7—C8—H8	119.4
Zn1—N1—H1B	110.5 (17)	C8—C9—C10	119.90 (17)
H1A—N1—H1B	109 (2)	C8—C9—H9	120.0
C2—N2—Zn1	108.81 (13)	C10—C9—H9	120.0
C2—N2—H2A	109.1 (16)	C11—C10—C9	121.03 (17)
Zn1—N2—H2A	107.2 (16)	C11—C10—H10	119.5
C2—N2—H2B	111.5 (15)	C9—C10—H10	119.5
Zn1—N2—H2B	110.3 (15)	C10—C11—C12	120.88 (16)
H2A—N2—H2B	110 (2)	C10—C11—H11	119.6
Zn1—O1—H1E	115.4 (18)	C12—C11—H11	119.6
Zn1—O1—H1F	113 (2)	C11—C12—C7	117.90 (15)
H1E—O1—H1F	110 (3)	C11—C12—C3	123.41 (16)
N1—C1—C2	108.92 (17)	C7—C12—C3	118.69 (15)
N1—C1—H1C	109.9	C6—N3—H3A	108.4 (17)
C2—C1—H1C	109.9	C6—N3—H3B	116.3 (15)
N1—C1—H1D	109.9	H3A—N3—H3B	112 (2)
C2—C1—H1D	109.9	H5A—O5—H5B	106 (3)
H1C—C1—H1D	108.3	O3—S1—O2	112.87 (9)
N2—C2—C1	109.75 (16)	O3—S1—O4	111.00 (9)
N2—C2—H2C	109.7	O2—S1—O4	111.66 (9)
C1—C2—H2C	109.7	O3—S1—C3	106.46 (9)
N2—C2—H2D	109.7	O2—S1—C3	108.76 (8)
C1—C2—H2D	109.7	O4—S1—C3	105.67 (9)
N2—Zn1—N1—C1	19.84 (14)	C6—C7—C8—C9	−178.60 (17)
N2^{i}—Zn1—N1—C1	−160.16 (14)	C7—C8—C9—C10	−0.7 (3)
O1^{i}—Zn1—N1—C1	108.55 (14)	C8—C9—C10—C11	0.4 (3)
O1—Zn1—N1—C1	−71.45 (14)	C9—C10—C11—C12	−0.3 (3)
N1^{i}—Zn1—N2—C2	−171.14 (14)	C10—C11—C12—C7	0.7 (3)
N1—Zn1—N2—C2	8.86 (14)	C10—C11—C12—C3	−179.36 (17)
O1^{i}—Zn1—N2—C2	−80.76 (14)	C8—C7—C12—C11	−1.0 (2)
O1—Zn1—N2—C2	99.24 (14)	C6—C7—C12—C11	178.68 (15)
Zn1—N1—C1—C2	−44.7 (2)	C8—C7—C12—C3	179.03 (16)
Zn1—N2—C2—C1	−35.8 (2)	C6—C7—C12—C3	−1.3 (2)
N1—C1—C2—N2	55.4 (3)	C4—C3—C12—C11	179.11 (17)
C12—C3—C4—C5	1.9 (3)	S1—C3—C12—C11	−5.9 (2)
S1—C3—C4—C5	−173.30 (14)	C4—C3—C12—C7	−0.9 (3)
C3—C4—C5—C6	−0.6 (3)	S1—C3—C12—C7	174.10 (12)
C4—C5—C6—N3	−178.31 (17)	C4—C3—S1—O3	112.32 (16)
C4—C5—C6—C7	−1.7 (3)	C12—C3—S1—O3	−62.78 (16)
C5—C6—C7—C8	−177.73 (17)	C4—C3—S1—O2	−125.78 (16)
N3—C6—C7—C8	−1.2 (3)	C12—C3—S1—O2	59.12 (16)
C5—C6—C7—C12	2.6 (2)	C4—C3—S1—O4	−5.78 (17)
N3—C6—C7—C12	179.19 (16)	C12—C3—S1—O4	179.12 (14)
C12—C7—C8—C9	1.1 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1B···O4^{ii}	0.86 (2)	2.41 (2)	3.170 (2)	147 (2)
N1—H1A···O2^{iii}	0.836 (18)	2.570 (19)	3.337 (3)	153 (2)
N2—H2A···O2^{iv}	0.87 (2)	2.28 (2)	3.109 (2)	159 (2)
N2—H2B···O5	0.915 (18)	2.113 (19)	2.992 (3)	161 (2)
N3—H3A···O2^{v}	0.782 (19)	2.67 (2)	3.451 (2)	176 (2)
N3—H3B···O3^{vi}	0.836 (19)	2.246 (19)	3.076 (3)	171.6 (18)
O1—H1E···O5	0.79 (2)	2.08 (2)	2.834 (3)	158 (2)
O5—H5B···N3^{vii}	0.87 (2)	2.02 (2)	2.882 (3)	173 (3)
O5—H5A···O4^{viii}	0.77 (2)	2.15 (2)	2.918 (3)	172 (3)
O1—H1F···O4^{ii}	0.75 (2)	2.11 (2)	2.818 (2)	159 (3)

Symmetry codes: (ii) *x*, *y*−1, *z*; (iii) −*x*, *y*−1/2, −*z*+1/2; (iv) −*x*, −*y*+1, −*z*+1; (v) −*x*+1, *y*+1/2, −*z*+1/2; (vi) −*x*+1, −*y*+2, −*z*; (vii) −*x*+1, −*y*+1, −*z*+1; (viii) *x*, −*y*+3/2, *z*+1/2.

Fig. 1

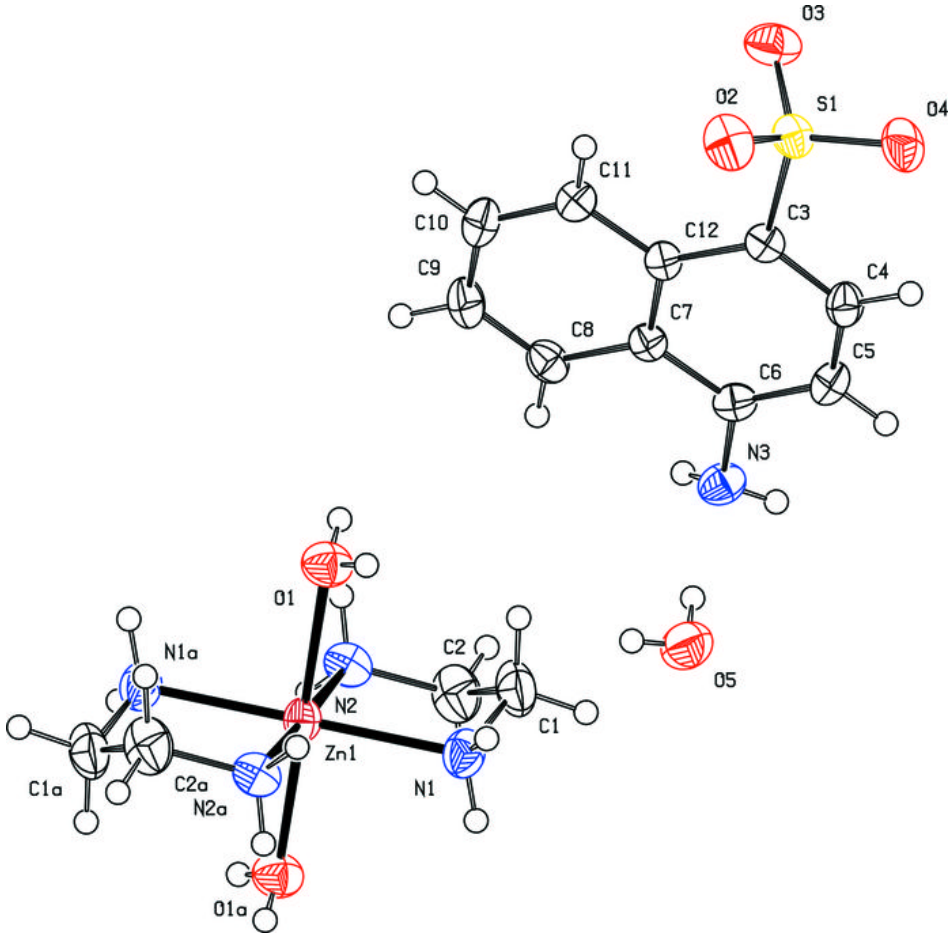
O3
O2
S1
O4
C11
C10
C12
C3
C9
C4
C7
C8
C5
C6
N3
O1
N1a
C2
N2
C1
Zn1
C1a
C2a
N2a
N1
O1a
O5

Fig. 2