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Hexaaquazinc(II) 3-ammonionaphthalene-1,5-disulfonate tetrahydrate

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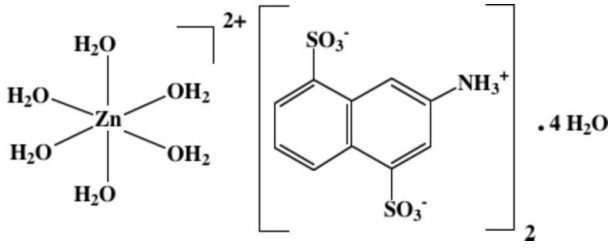
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.002 Å; H-atom completeness 89%; disorder in solvent or counterion; R factor = 0.038; wR factor = 0.107; data-to-parameter ratio = 22.2.

The title compound, $[Zn(H_2O)_6][H_3NC_{10}H_5(SO_3)_2]_2\cdot 4H_2O$ (Zn site symmetry $\overline{1}$), is isostructural with its nickel(II) and cobalt(II) analogues. An extensive network of N—H···O and O—H···O hydrogen bonds involving the ammonio group, water molecules, and sulfonate O atoms helps to establish the packing. One of the uncoordinated water molecules is disordered over at least two sites (modelled over two positions with site occupancy ratio *ca* 2:1).

Related literature

Compound (I) is isostructural with its nickel(II) (Gunderman, Kabell *et al.*, 1997) and cobalt(II) (Genther *et al.*, 2007) analogues. For background, see: Chen *et al.* (2002); Gunderman, Dubey & Squattrito (1997); Huo *et al.* (2005).



Experimental

Crystal data

$[Zn(H_2O)_6](C_{10}H_8NO_6S_2)_2\cdot 4H_2O$
M_r = 850.12
Triclinic, $P\overline{1}$
a = 5.4294 (2) Å
b = 12.7411 (5) Å
c = 12.9537 (6) Å
α = 114.497 (1)°
β = 101.563 (1)°
γ = 90.889 (1)°
V = 793.97 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 273 (2) K
0.25 × 0.22 × 0.10 mm

Data collection

Bruker SMART 6000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.757, T_{max} = 0.890
17231 measured reflections
6235 independent reflections
5724 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.107
S = 0.94
6235 reflections
281 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.21 e Å^{-3}
$\Delta\rho_{min}$ = −1.03 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O9	2.0605 (12)	Zn1—O8	2.1244 (12)
Zn1—O7	2.0925 (11)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H9···O1^{i}	0.823 (17)	1.824 (17)	2.6360 (16)	169 (3)
O7—H10···O5^{ii}	0.794 (17)	1.868 (18)	2.6452 (16)	166 (3)
O8—H11···O1^{iii}	0.816 (17)	1.928 (17)	2.7439 (16)	177 (3)
O8—H12···O2	0.811 (17)	1.971 (18)	2.7662 (17)	166 (3)
O9—H13···O7^{iv}	0.814 (17)	1.994 (18)	2.8015 (17)	172 (3)
O9—H14···O4^{ii}	0.812 (17)	1.865 (18)	2.6660 (17)	169 (3)
N1—H6···O6^{iv}	0.80 (3)	2.01 (3)	2.7966 (19)	166 (3)
N1—H7···O3^{v}	0.86 (3)	1.97 (3)	2.8107 (18)	166 (2)
N1—H8···O11*A*	0.82 (3)	2.08 (3)	2.863 (6)	160 (3)
O10—H15···O6^{ii}	0.93 (4)	1.95 (2)	2.876 (2)	171 (4)
O10—H16···O8	0.92 (3)	2.24 (3)	3.036 (3)	144 (4)

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2484).

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supplementary materials

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Hexaaquazinc(II) 3-ammonionaphthalene-1,5-disulfonate tetrahydrate

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Comment

As part of our ongoing studies of salts of 3-aminonaphthalene-1,5-sulfonate with divalent transition metals, we now report the structure of the title compound, (I), which is isostructural with its nickel(II) (Gunderman, Kabell *et al.*, 1997) and cobalt(II) analogues (Genther *et al.*, 2007). Compound (I) consists of centrosymmetic hexaaquazinc(II) cations, 3-ammonionaphthalene-1,5-disulfonate anions, and water molecules of crystallization (Fig. 1). Owing to the protonation of the amine group, each anion carries a single negative charge and the salt has the same 1:2 stoichiometry as would be observed with a monosulfonate anion. The cations reside on centers of inversion and display very regular octahedral geometry with maximum deviation from ideal 90° bond angles of just under 5°. This feature is very similar to what is found in the zinc naphthalene-1,5-disulfonate compound without the amine functionality (Huo *et al.*, 2005).

The crystal packing (Fig. 2) is typical for transition metal arene- and naphthalenesulfonates (Chen *et al.*, 2002; Gunderman, Dubey & Squattrito, 1997), consisting of alternating layers of hexaaquametal cations and sulfonate anions parallel to the *ac* plane, with the anions positioned so that the charged groups (*i.e.*, NH_3^+ and SO_3–) line the surface of the layer. The anions are positioned so that all the rings are parallel with contacts between adjacent rings of *ca* 3.7 Å. Neighboring rows of anions running along the *a* axis have the ammonio groups inverted. The water molecules of crystallization are located in between the cations in close association with the charged groups and coordinated water molecules so as to participate in hydrogen bonding interactions. One of the two crystallographically independent water molecules is disordered over at least two positions.

The layers are held together by a series of strong O—H···O and N—H···O hydrogen bonds involving water and ammonio donors and sulfonate and water acceptors (Table 2).

Experimental

The title compound was prepared by direct reaction of $Zn(NO_3)_2{\cdot}6H_2O$ and disodium 3-aminonaphthalene-1,5-disulfonate (1:2 stoichiometry) in aqueous solution. Following approximately one hour of heating, during which most of the reactants dissolved, the resulting solution was gravity filtered and set out in open air. Upon evaporation of the water, many small colorless, needles of (I) were recovered.

Refinement

The O11 atom, corresponding to one water of crystallization, was found to be disordered and was refined on split positions *ca* 0.5 Å apart with occupancy factors constrained to sum to 1. Final occupancies were roughly 63% (O11A) and 37% (O11B). The B site has a significantly prolate displacement ellipsoid, but further splitting of the position could not be successfully modeled. The H atoms attached to the disordered water molecule could not be located. All other H atoms were located in

difference maps and positionally refined either freely or with distance restraints of O—H = 0.82 (2) Å, and with U_{iso}(H) = 1.2U_{eq}(N,*C*) or U_{iso}(H) = 1.5U_{eq}(O).

Figures

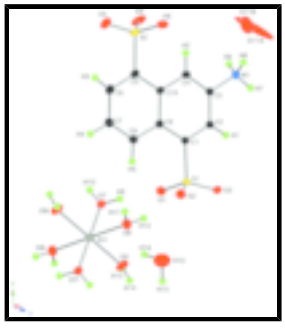

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms. Symmetry-equivalent water molecules (marked 'i') are included to show the full coordination sphere of the zinc cation. [symmetry operation (i): −*x*, −*y*, −*z*]

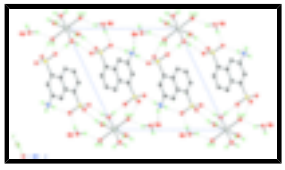

Fig. 2. The packing of (I), viewed down the *a* axis, showing layers connected by O—H···O and N—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

Hexaaquazinc(II) 3-ammonionaphthalene-1,5-disulfonate tetrahydrate

Crystal data

$[Zn_1(H_2O_1)_6](C_{10}H_8N_1O_6S_2)_2{\cdot}4H_2O$	$Z = 1$
$M_r = 850.12$	$F_{000} = 440$
Triclinic, $P\overline{1}$	$D_x = 1.778$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.4294$ (2) Å	Cell parameters from 6586 reflections
$b = 12.7411$ (5) Å	$\theta = 3.0$–34.4º
$c = 12.9537$ (6) Å	$\mu = 1.13$ mm^{-1}
$\alpha = 114.497$ (1)º	$T = 273$ (2) K
$\beta = 101.563$ (1)º	Pyramidal, colourless
$\gamma = 90.889$ (1)º	0.25 × 0.22 × 0.10 mm
$V = 793.97$ (6) Å^3	

Data collection

Bruker SMART 6000 CCD area-detector diffractometer	6235 independent reflections
Radiation source: fine-focus sealed tube	5724 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 273$(2) K	$\theta_{max} = 34.5$º
ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -8 \rightarrow 8$

T_{min} = 0.757, T_{max} = 0.890
17231 measured reflections

k = −20→19
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.107
S = 0.94
6235 reflections
281 parameters
8 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0664P)^2 + 0.8611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 1.21 e Å^{-3}
$\Delta\rho_{min}$ = −1.03 e Å^{-3}
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 $F^2 > 2$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	0.0000	0.0000	0.0000	0.01329 (6)	
O7	−0.2667 (2)	−0.12300 (10)	−0.00440 (10)	0.01655 (19)	
H9	−0.347 (5)	−0.168 (2)	−0.0698 (16)	0.025*	
H10	−0.227 (5)	−0.154 (2)	0.037 (2)	0.025*	
O8	−0.0542 (2)	0.10549 (11)	0.16894 (10)	0.0191 (2)	
H11	−0.166 (4)	0.148 (2)	0.181 (2)	0.029*	
H12	0.062 (4)	0.148 (2)	0.220 (2)	0.029*	
O9	0.3033 (2)	−0.05209 (12)	0.08378 (12)	0.0214 (2)	
H13	0.433 (4)	−0.066 (2)	0.060 (2)	0.032*	
H14	0.275 (6)	−0.090 (2)	0.119 (2)	0.032*	
S1	0.53398 (6)	0.32440 (3)	0.32236 (3)	0.01257 (7)	
O1	0.5772 (2)	0.25319 (10)	0.20550 (10)	0.0174 (2)	
O2	0.3014 (2)	0.28147 (10)	0.33812 (10)	0.0182 (2)	
O3	0.7536 (2)	0.34056 (10)	0.41396 (11)	0.0197 (2)	
S2	0.01825 (7)	0.76440 (3)	0.20463 (3)	0.01679 (8)	

O4	0.2443 (2)	0.80350 (13)	0.18042 (14)	0.0272 (3)	
O5	−0.2114 (2)	0.75525 (12)	0.12018 (12)	0.0237 (2)	
O6	0.0005 (3)	0.83525 (11)	0.32527 (11)	0.0236 (2)	
N1	0.8696 (3)	0.75553 (12)	0.48044 (12)	0.0181 (2)	
H6	0.931 (5)	0.779 (2)	0.441 (2)	0.022*	
H7	0.975 (5)	0.731 (2)	0.523 (2)	0.022*	
H8	0.810 (5)	0.811 (2)	0.524 (2)	0.022*	
C1	0.4944 (3)	0.46453 (12)	0.32637 (12)	0.0129 (2)	
C2	0.6842 (3)	0.55153 (12)	0.39906 (12)	0.0140 (2)	
H1	0.823 (5)	0.537 (2)	0.442 (2)	0.017*	
C3	0.6666 (3)	0.66315 (12)	0.40379 (12)	0.0143 (2)	
C4	0.4673 (3)	0.68879 (12)	0.33900 (13)	0.0150 (2)	
H2	0.453 (5)	0.762 (2)	0.342 (2)	0.018*	
C5	0.0526 (3)	0.62251 (13)	0.19425 (13)	0.0149 (2)	
C6	−0.1367 (3)	0.53564 (14)	0.12033 (14)	0.0182 (3)	
H3	−0.266 (5)	0.556 (2)	0.080 (2)	0.022*	
C7	−0.1215 (3)	0.42251 (14)	0.11220 (14)	0.0185 (3)	
H4	−0.257 (5)	0.358 (2)	0.055 (2)	0.022*	
C8	0.0801 (3)	0.39811 (13)	0.17860 (13)	0.0159 (2)	
H5	0.083 (5)	0.321 (2)	0.171 (2)	0.019*	
C9	0.2798 (3)	0.48562 (12)	0.25578 (12)	0.0129 (2)	
C10	0.2676 (3)	0.60071 (12)	0.26362 (12)	0.0133 (2)	
O10	−0.2280 (5)	0.04341 (18)	0.3472 (2)	0.0540 (5)	
H15	−0.171 (8)	−0.028 (2)	0.338 (4)	0.081*	
H16	−0.233 (9)	0.036 (4)	0.273 (2)	0.081*	
O11A	0.5941 (15)	0.9487 (4)	0.5787 (5)	0.091 (3)	0.628 (15)
O11B	0.687 (2)	0.9475 (6)	0.5944 (16)	0.136 (7)	0.372 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01269 (10)	0.01336 (11)	0.01533 (11)	0.00281 (7)	0.00337 (8)	0.00746 (8)
O7	0.0166 (5)	0.0175 (5)	0.0169 (5)	0.0004 (4)	0.0012 (4)	0.0099 (4)
O8	0.0162 (5)	0.0202 (5)	0.0175 (5)	0.0044 (4)	0.0030 (4)	0.0050 (4)
O9	0.0170 (5)	0.0293 (6)	0.0305 (6)	0.0088 (4)	0.0090 (4)	0.0230 (5)
S1	0.01214 (13)	0.01096 (13)	0.01408 (14)	0.00084 (10)	0.00037 (10)	0.00599 (11)
O1	0.0180 (5)	0.0148 (5)	0.0174 (5)	0.0041 (4)	0.0042 (4)	0.0047 (4)
O2	0.0168 (5)	0.0185 (5)	0.0206 (5)	−0.0025 (4)	0.0037 (4)	0.0100 (4)
O3	0.0171 (5)	0.0174 (5)	0.0226 (5)	−0.0008 (4)	−0.0061 (4)	0.0115 (4)
S2	0.01698 (15)	0.01829 (16)	0.02169 (16)	0.00366 (12)	0.00445 (12)	0.01480 (13)
O4	0.0202 (5)	0.0358 (7)	0.0423 (7)	0.0043 (5)	0.0094 (5)	0.0318 (6)
O5	0.0200 (5)	0.0283 (6)	0.0302 (6)	0.0056 (4)	0.0014 (5)	0.0215 (5)
O6	0.0353 (7)	0.0156 (5)	0.0235 (5)	0.0048 (5)	0.0084 (5)	0.0111 (4)
N1	0.0224 (6)	0.0141 (5)	0.0156 (5)	−0.0039 (4)	−0.0032 (4)	0.0079 (4)
C1	0.0130 (5)	0.0115 (5)	0.0139 (5)	0.0017 (4)	0.0019 (4)	0.0057 (4)
C2	0.0143 (5)	0.0123 (5)	0.0145 (5)	−0.0003 (4)	0.0000 (4)	0.0065 (4)
C3	0.0164 (6)	0.0120 (5)	0.0133 (5)	−0.0010 (4)	0.0005 (4)	0.0057 (4)
C4	0.0175 (6)	0.0120 (5)	0.0158 (6)	0.0008 (4)	0.0019 (5)	0.0072 (4)

C5	0.0148 (6)	0.0163 (6)	0.0164 (6)	0.0034 (4)	0.0029 (5)	0.0099 (5)
C6	0.0156 (6)	0.0206 (6)	0.0197 (6)	0.0019 (5)	0.0002 (5)	0.0116 (5)
C7	0.0160 (6)	0.0178 (6)	0.0197 (6)	0.0003 (5)	−0.0010 (5)	0.0083 (5)
C8	0.0139 (5)	0.0143 (6)	0.0184 (6)	0.0010 (4)	0.0008 (5)	0.0072 (5)
C9	0.0129 (5)	0.0127 (5)	0.0135 (5)	0.0022 (4)	0.0024 (4)	0.0061 (4)
C10	0.0141 (5)	0.0133 (5)	0.0138 (5)	0.0021 (4)	0.0025 (4)	0.0074 (4)
O10	0.0723 (15)	0.0376 (10)	0.0527 (12)	0.0136 (9)	0.0136 (11)	0.0199 (9)
O11A	0.117 (5)	0.042 (2)	0.057 (3)	0.039 (3)	−0.040 (3)	−0.0083 (18)
O11B	0.103 (7)	0.018 (3)	0.253 (15)	−0.019 (3)	0.150 (9)	−0.023 (5)

Geometric parameters (Å, °)

Zn1—O9	2.0605 (12)	N1—H7	0.86 (3)
Zn1—O9^{i}	2.0605 (12)	N1—H8	0.82 (3)
Zn1—O7	2.0925 (11)	C1—C2	1.3739 (19)
Zn1—O7^{i}	2.0926 (11)	C1—C9	1.4328 (19)
Zn1—O8	2.1244 (12)	C2—C3	1.404 (2)
Zn1—O8^{i}	2.1244 (12)	C2—H1	0.91 (2)
O7—H9	0.823 (17)	C3—C4	1.363 (2)
O7—H10	0.794 (17)	C4—C10	1.420 (2)
O8—H11	0.817 (17)	C4—H2	0.92 (2)
O8—H12	0.811 (17)	C5—C6	1.375 (2)
O9—H13	0.814 (17)	C5—C10	1.4297 (19)
O9—H14	0.812 (17)	C6—C7	1.406 (2)
S1—O3	1.4471 (11)	C6—H3	0.89 (3)
S1—O2	1.4526 (12)	C7—C8	1.375 (2)
S1—O1	1.4764 (12)	C7—H4	1.01 (3)
S1—C1	1.7820 (14)	C8—C9	1.422 (2)
S2—O5	1.4520 (13)	C8—H5	0.94 (2)
S2—O4	1.4554 (13)	C9—C10	1.431 (2)
S2—O6	1.4694 (14)	O10—H15	0.93 (4)
S2—C5	1.7721 (15)	O10—H16	0.92 (3)
N1—C3	1.4621 (19)	O11A—O11B	0.510 (15)
N1—H6	0.80 (3)		
O9—Zn1—O9^{i}	180.0	C3—N1—H7	110.0 (17)
O9—Zn1—O7	94.77 (5)	H6—N1—H7	115 (3)
O9^{i}—Zn1—O7	85.24 (5)	C3—N1—H8	109.7 (18)
O9—Zn1—O7^{i}	85.24 (5)	H6—N1—H8	106 (3)
O9^{i}—Zn1—O7^{i}	94.76 (5)	H7—N1—H8	108 (2)
O7—Zn1—O7^{i}	180.0	C2—C1—C9	121.35 (13)
O9—Zn1—O8^{i}	93.93 (5)	C2—C1—S1	116.45 (10)
O9^{i}—Zn1—O8^{i}	86.07 (5)	C9—C1—S1	122.18 (10)
O7—Zn1—O8^{i}	93.91 (5)	C1—C2—C3	119.06 (13)
O7^{i}—Zn1—O8^{i}	86.09 (5)	C1—C2—H1	121.1 (15)
O9—Zn1—O8	86.07 (5)	C3—C2—H1	119.8 (15)
O9^{i}—Zn1—O8	93.93 (5)	C4—C3—C2	122.40 (13)

O7—Zn1—O8	86.08 (5)	C4—C3—N1	118.54 (13)
O7^{i}—Zn1—O8	93.92 (5)	C2—C3—N1	119.06 (13)
O8^{i}—Zn1—O8	180.0	C3—C4—C10	119.75 (13)
Zn1—O7—H9	115.4 (19)	C3—C4—H2	123.3 (15)
Zn1—O7—H10	118 (2)	C10—C4—H2	116.9 (15)
H9—O7—H10	113 (3)	C6—C5—C10	121.47 (13)
Zn1—O8—H11	124 (2)	C6—C5—S2	117.93 (11)
Zn1—O8—H12	121 (2)	C10—C5—S2	120.57 (11)
H11—O8—H12	99 (3)	C5—C6—C7	119.90 (14)
Zn1—O9—H13	122 (2)	C5—C6—H3	116.4 (17)
Zn1—O9—H14	118 (2)	C7—C6—H3	123.7 (17)
H13—O9—H14	113 (3)	C8—C7—C6	120.54 (14)
O3—S1—O2	114.10 (7)	C8—C7—H4	119.9 (15)
O3—S1—O1	112.15 (7)	C6—C7—H4	119.6 (15)
O2—S1—O1	111.45 (7)	C7—C8—C9	121.15 (14)
O3—S1—C1	105.83 (7)	C7—C8—H5	118.2 (15)
O2—S1—C1	107.51 (7)	C9—C8—H5	120.7 (15)
O1—S1—C1	105.11 (7)	C8—C9—C10	118.74 (13)
O5—S2—O4	113.19 (8)	C8—C9—C1	123.30 (13)
O5—S2—O6	112.69 (8)	C10—C9—C1	117.96 (12)
O4—S2—O6	111.13 (9)	C4—C10—C5	122.34 (13)
O5—S2—C5	106.45 (7)	C4—C10—C9	119.47 (13)
O4—S2—C5	107.12 (8)	C5—C10—C9	118.19 (13)
O6—S2—C5	105.70 (7)	H15—O10—H16	97 (4)
C3—N1—H6	108.6 (19)		
O3—S1—C1—C2	7.97 (13)	S2—C5—C6—C7	−177.90 (12)
O2—S1—C1—C2	130.29 (12)	C5—C6—C7—C8	0.7 (2)
O1—S1—C1—C2	−110.88 (12)	C6—C7—C8—C9	−0.9 (2)
O3—S1—C1—C9	−173.49 (12)	C7—C8—C9—C10	0.1 (2)
O2—S1—C1—C9	−51.18 (13)	C7—C8—C9—C1	−179.69 (14)
O1—S1—C1—C9	67.66 (13)	C2—C1—C9—C8	179.43 (14)
C9—C1—C2—C3	−0.1 (2)	S1—C1—C9—C8	1.0 (2)
S1—C1—C2—C3	178.47 (11)	C2—C1—C9—C10	−0.4 (2)
C1—C2—C3—C4	0.2 (2)	S1—C1—C9—C10	−178.83 (11)
C1—C2—C3—N1	−179.51 (13)	C3—C4—C10—C5	179.46 (14)
C2—C3—C4—C10	0.2 (2)	C3—C4—C10—C9	−0.7 (2)
N1—C3—C4—C10	179.88 (14)	C6—C5—C10—C4	178.88 (15)
O5—S2—C5—C6	−4.21 (15)	S2—C5—C10—C4	−3.0 (2)
O4—S2—C5—C6	−125.58 (13)	C6—C5—C10—C9	−1.0 (2)
O6—S2—C5—C6	115.84 (13)	S2—C5—C10—C9	177.09 (11)
O5—S2—C5—C10	177.62 (12)	C8—C9—C10—C4	−179.08 (13)
O4—S2—C5—C10	56.25 (14)	C1—C9—C10—C4	0.7 (2)
O6—S2—C5—C10	−62.33 (13)	C8—C9—C10—C5	0.8 (2)
C10—C5—C6—C7	0.3 (2)	C1—C9—C10—C5	−179.38 (12)

Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H9···O1^{i}	0.823 (17)	1.824 (17)	2.6360 (16)	169 (3)
O7—H10···O5^{ii}	0.794 (17)	1.868 (18)	2.6452 (16)	166 (3)
O8—H11···O1^{iii}	0.816 (17)	1.928 (17)	2.7439 (16)	177 (3)
O8—H12···O2	0.811 (17)	1.971 (18)	2.7662 (17)	166 (3)
O9—H13···O7^{iv}	0.814 (17)	1.994 (18)	2.8015 (17)	172 (3)
O9—H14···O4^{ii}	0.812 (17)	1.865 (18)	2.6660 (17)	169 (3)
N1—H6···O6^{iv}	0.80 (3)	2.01 (3)	2.7966 (19)	166 (3)
N1—H7···O3^{v}	0.86 (3)	1.97 (3)	2.8107 (18)	166 (2)
N1—H8···O11A	0.82 (3)	2.08 (3)	2.863 (6)	160 (3)
O10—H15···O6^{ii}	0.93 (4)	1.95 (2)	2.876 (2)	171 (4)
O10—H16···O8	0.92 (3)	2.24 (3)	3.036 (3)	144 (4)

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

Fig. 1

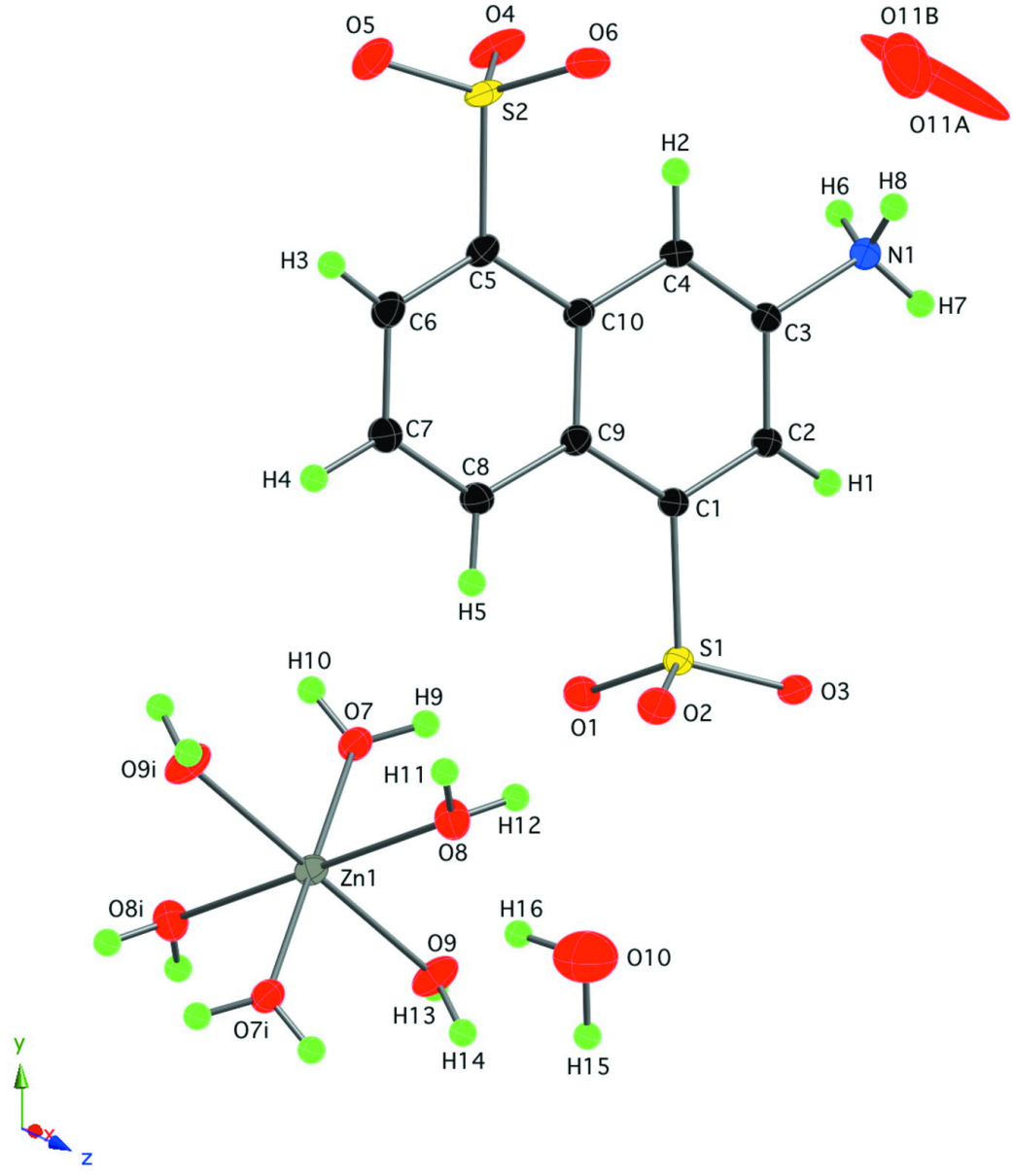
O5
O4
O6
S2
O11B
O11A
H2
H6
H8
N1
H7
H3
C5
C4
C6
C10
C3
C7
C9
C2
H4
C8
H1
C1
H5
S1
H10
O7
H9
O3
O1
O2
O9i
H11
H12
O8
Zn1
O8i
H16
O9
O10
O7i
H13
H14
H15
y
x
z

Fig. 2