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Bis(triethylaminium) hexaaquazinc(II) bis(naphthalene-1,6-disulfonate)

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Key indicators

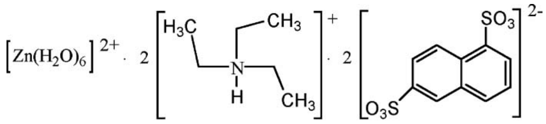
Single-crystal X-ray study
T = 289 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.106
Data-to-parameter ratio = 14.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title complex, $(C_6H_{16}N)_2[Zn(H_2O)_6](C_{10}H_6O_6S_2)_2$, is formed by aggregation of one hexahydrated zinc(II) cation, two triethylaminium cations and two naphthalene-1,6-disulfonate dianions. The Zn^{II} cation is six-coordinate and located at an inversion center. The coordination around the metal ion is octahedral, with tetragonal elongation.

Comment

Organic sulfoacids and their derivatives are widely used in the synthesis of surface active agents, dyes, medicines and so on. So far, a few crystallographic studies on naphthalenesulfonate complexes have been reported (Gunderman *et al.*, 1997; Alvarez *et al.*, 1998; Cai, Chen, Feng *et al.*, 2001; Cai, Chen, Liao *et al.*, 2001; Chen *et al.*, 2002; Chandrasekhar *et al.*, 2003; Chen *et al.*, 2004; Sharma *et al.*, 2005). Recently, the title complex, (I), was synthesized in our laboratory and its crystal structure is discussed here.



(I)

Owing to the weak coordination strength of sulfonate toward transition metal ions, most of the reported transition metal sulfonates prepared in aqueous solution were formed by aggregation of aquametal complex cations and sulfonate anions (Kosnic *et al.*, 1992; Shubnell *et al.*, 1994; Gunderman *et al.*, 1997). The same situation appears in (I), with the triclinic unit cell containing one hexahydrated zinc(II) cation, two triethylaminium cations and two naphthalene-1,6-disulfonate (1,6-nds) dianions (Fig. 1). The Zn^{II} ion is located at an inversion center and the coordination around the metal ion is

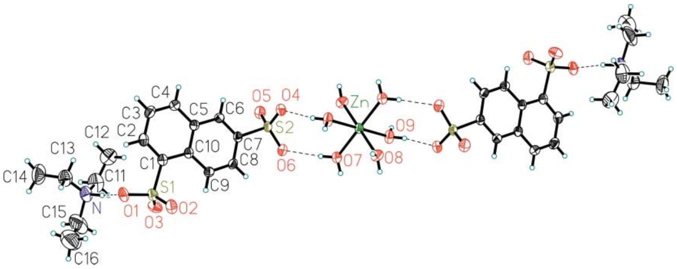


Figure 1
The structure of (I), showing 40% probability displacement ellipsoids and the atom-labeling scheme for the contents of the asymmetric unit. Unlabeled atoms are generated by the symmetry code $-x$, $-y$, $-z$. Dashed lines represent hydrogen bonds.

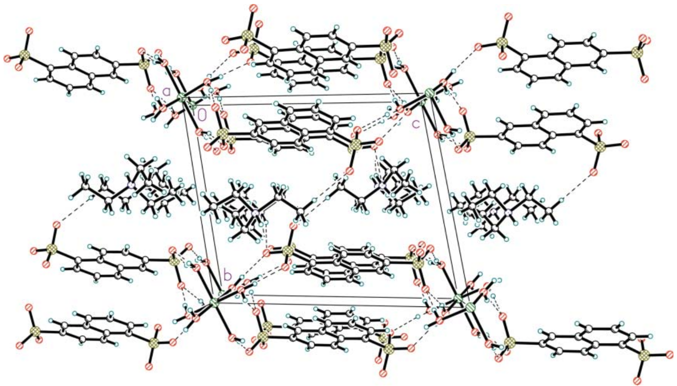


Figure 2
Packing diagram of (I), viewed along the *a* axis. Dashed lines represent hydrogen bonds.

octahedral, with tetragonal elongation. The Zn—O distances range from 2.049 (2) to 2.130 (2) Å.

Two intramolecular C—H···O hydrogen bonds (Steiner & Desiraju, 1998) are observed in the 1,6-nds dianions. In the crystal structure, the 1,6-nds dianions are linked to the hexhydrated Zn^{II} cations through O—H···O hydrogen bonds and connected to the triethylaminium cations by N—H···O and C—H···O hydrogen bonds (Table 2 and Fig. 2).

Experimental

Triethylamine, $ZnCl_2$ and naphthalene-1,6-disulfonate in a molar ratio of 2:1:2 were mixed and dissolved in sufficient water by heating to a temperature at which a clear solution resulted. Crystals of (I) were formed by slow evaporation of water over a period of three weeks at 293 K.

Crystal data

$(C_6H_{16}N)_2[Zn(H_2O)_6](C_{10}H_6O_6S_2)_2$
$M_r = 950.46$
Triclinic, $P\overline{1}$
$a = 7.078$ (1) Å
$b = 11.597$ (2) Å
$c = 13.924$ (2) Å
$\alpha = 77.89$ (1)°
$\beta = 75.41$ (1)°
$\gamma = 79.35$ (1)°
$V = 1070.9$ (3) Å^3
$Z = 1$
$D_x = 1.474$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 31 reflections
$\theta = 3.9$–15.2°
$\mu = 0.84$ mm^{-1}
$T = 289$ (2) K
Block, colorless
0.46 × 0.34 × 0.34 mm

Data collection

Siemens P4 diffractometer
ω scans
Absorption correction: ψ scan (*XSCANS*; Siemens, 1994)
$T_{min} = 0.716$, $T_{max} = 0.751$
4420 measured reflections
4067 independent reflections
3227 reflections with $I > 2\sigma(I)$
$R_{int} = 0.011$
$\theta_{max} = 25.8°$
$h = 0 \rightarrow 8$
$k = -13 \rightarrow 14$
$l = -16 \rightarrow 17$
3 standard reflections every 97 reflections intensity decay: 3.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.106$
$S = 1.10$
4067 reflections
291 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.1823P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0132 (18)

Table 1
Selected geometric parameters (Å, °).

Zn—O8	2.049 (2)	Zn—O7	2.130 (2)
Zn—O9	2.078 (2)		
O8—Zn—O8^i	180.00 (12)	O9—Zn—O7	87.79 (9)
O8—Zn—O9^i	93.85 (8)	O8—Zn—O7^i	86.55 (9)
O8—Zn—O9	86.15 (8)	O9—Zn—O7^i	92.21 (9)
O9^i—Zn—O9	180.00 (14)	O7—Zn—O7^i	180.00 (13)
O8—Zn—O7	93.45 (9)		

Symmetry code: (i) $-x, -y, -z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0N···O1	0.94 (4)	1.97 (4)	2.842 (4)	154 (3)
O7—H7*A*···O6	0.84 (1)	2.03 (1)	2.832 (4)	159 (3)
O7—H7*B*···O5^{ii}	0.84 (1)	2.00 (1)	2.827 (3)	169 (2)
O8—H8*A*···O1^{iii}	0.83 (1)	1.90 (1)	2.716 (3)	168 (2)
O8—H8*B*···O4^{ii}	0.84 (1)	1.91 (1)	2.727 (3)	166 (2)
O9—H9*A*···O2^{iv}	0.85 (1)	1.92 (1)	2.761 (4)	173 (2)
O9—H9*B*···O4^i	0.84 (1)	1.88 (1)	2.719 (4)	172 (3)
C2—H2···O1	0.93	2.41	2.827 (3)	107
C8—H8···O6	0.93	2.54	2.913 (4)	105
C12—H12*C*···O3^v	0.96	2.49	3.445 (4)	179

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

H atoms attached to the N atom and the H atoms of water molecules were located in a difference Fourier map and refined isotropically, with the O—H and H···H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively. The other H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H distances of 0.93 (aromatic), 0.96 (methyl) and 0.97 Å (methylene), and with $U_{iso}(H) = 1.2U_{eq}(C)$. The C—C bond lengths in the triethylaminium cation were restrained to be equal within 0.03 Å.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

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