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Hexaaquazinc(II) naphthalene-1,5-disulfonate

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Key indicators

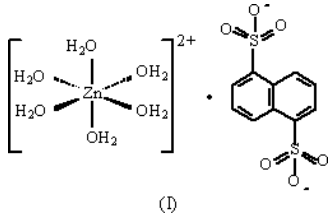
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.022
wR factor = 0.062
Data-to-parameter ratio = 14.7

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

The title complex, $[Zn(H_2O)_6](C_{10}H_6O_6S_2)$, consists of $[Zn(H_2O)_6]^{2+}$ cations and naphthalene-1,5-disulfonate anions. The Zn atom is coordinated by six water molecules to form an octahedral geometry [Zn—O = 2.0478 (12)–2.1322 (11) Å]. The cations and anions, which lie on different centers of symmetry, are linked by O—H···O hydrogen bonds into a three-dimensional supramolecular framework.

Comment

Naphthalene-1,5-disulfonic acid is known as a good candidate for the construction of supramolecular complexes, particularly as the sulfonate unit has a high propensity to form strong hydrogen bonds (Côté & Shimizu, 2003; Cai, 2004). To date, four transition metal complexes of the type $[M(H_2O)_6](1,5\text{-nds})$ (M = Co, Cu, Ni, Cd; 1,5-nds is the naphthalene-1,5-disulfonate dianion; An *et al.*, 2004; Cai *et al.*, 2001; Chen *et al.*, 2002) have been reported. In these, the metal ions are coordinated by six water molecules, whereas the sulfonate groups behave as counter-anions to form extensive hydrogen-bonding interactions with the aquametal cations. Recently, we synthesized the Zn^{II} analog under similar reaction conditions, and it is isostructural with the $[M(H_2O)_6](1,5\text{-nds})$ complexes, whose structures have been presented in detail.



(I)

Experimental

The title complex was the product of the reaction resulting from the addition of naphthalene-1,5-disulfonic acid (1 mmol) and disodium naphthalene-2,7-disulfonate (1 mmol) to an aqueous solution of $Zn(acetate)_2{\cdot}2H_2O$ (2 mmol). The mixed solution was allowed to evaporate slowly at room temperature; colorless plate-shaped crystals were isolated after about some days. Analysis calculated for $C_{10}H_{18}O_{12}S_2Zn$: C 26.13, H 3.95%; found: C 26.17, H 3.91%.

Crystal data

$[Zn(H_2O)_6](C_{10}H_6O_6S_2)$
M_r = 459.77
Monoclinic, $P2_1/c$
a = 13.237 (3) Å
b = 6.6598 (13) Å
c = 9.6849 (19) Å
β = 92.27 (3)°
V = 853.1 (3) Å^3
Z = 2
D_x = 1.790 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7302 reflections
θ = 3.1–27.4°
μ = 1.74 mm^{-1}
T = 295 (2) K
Plate, colorless
0.37 × 0.28 × 0.14 mm

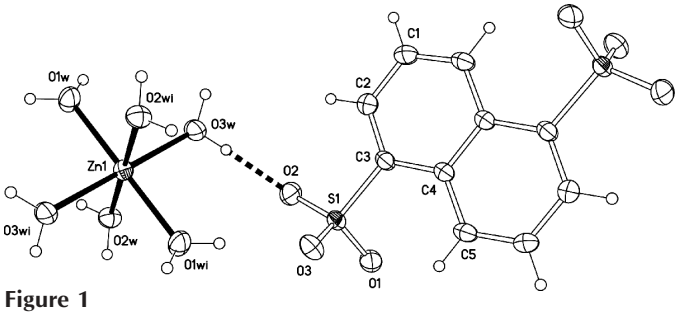


Figure 1
The molecular structure of the title compound, shown with 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.565, T_{max} = 0.792
8017 measured reflections
1957 independent reflections
1842 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 27.4°
$h = -17 \rightarrow 17$
$k = -8 \rightarrow 8$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.062
S = 1.03
1957 reflections
133 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.2395P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1*w*	2.0835 (11)	Zn1—O3*w*	2.0478 (12)
Zn1—O2*w*	2.1322 (11)		
O1*w*—Zn1—O1*w*^{i}	180	O2*w*—Zn1—O2*w*^{i}	180
O1*w*—Zn1—O2*w*	90.44 (5)	O2*w*—Zn1—O3*w*	87.31 (4)
O1*w*—Zn1—O2*w*^{i}	89.56 (5)	O2*w*—Zn1—O3*w*^{i}	92.69 (5)
O1*w*—Zn1—O3*w*	87.64 (5)	O3*w*—Zn1—O3*w*^{i}	180
O1*w*^{i}—Zn1—O2*w*	89.56 (5)		

Symmetry code: (i) $1-x, -y, 1-z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O2*w*^{ii}	0.841 (9)	2.058 (9)	2.8900 (17)	170.5 (18)
O1*w*—H1*w*2···O3^{i}	0.850 (9)	2.003 (9)	2.8518 (16)	177 (2)
O2*w*—H2*w*1···O3^{iii}	0.842 (9)	1.962 (9)	2.8019 (16)	175.3 (19)
O2*w*—H2*w*2···O2^{ii}	0.848 (9)	1.929 (9)	2.7710 (15)	172.3 (19)
O3*w*—H3*w*1···O1^{iv}	0.850 (9)	1.861 (9)	2.7043 (16)	172 (2)
O3*w*—H3*w*2···O2	0.848 (9)	1.868 (9)	2.7161 (16)	178.4 (19)

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

The carbon-bound H atoms were placed in calculated positions [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C)] and refined using the riding-model approximation. The H atoms of water molecules were located in a difference map and refined with O—H distance restraints of 0.85 (1) Å and U_{iso}(H) = 1.5U_{eq}(O).

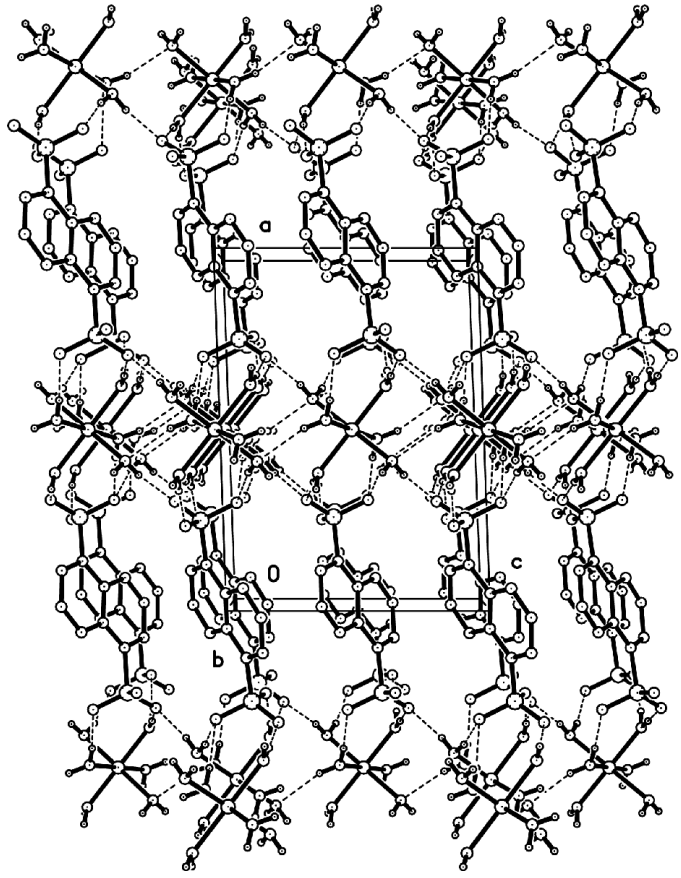


Figure 2
Packing diagram of the title complex, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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