Polymeric diaqua-8-hydroxyquinolinyl-5-sulfonatozinc(II)

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The crystal structure of polymeric diaqua-8-hydroxy-quinolinyl-5-sulfonatozinc(II) consists of a centrosymmetric $(C_9H_5NO_4S)_2(H_2O)_2Zn_2$ entity which is linked into a network structure by intermolecular sulfonyl bridges. The network is further consolidated by hydrogen bonds involving the coordinated water molecules.

Key indicators

Single-crystal X-ray study

T = 298 K

Mean σ(C–C) = 0.004 Å

R factor = 0.032

wR factor = 0.085

Data-to-parameter ratio = 13.1

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

Comment

The deprotonated 8-hydroxyquinoline anion chelates to a bewildering variety of metal systems. With a sulfonato substituent in the aromatic system, bridging through this group is possible and this is observed in the silver salt, C_9H_6NO–SO_3Ag. In fact, the three sulfonato O atoms are involved in bridging to three Ag atoms, and the compound is a rare example of Ag in a five-coordinate geometry (Xie *et al.*, 1992). Few metal 8-hydroxyquinolinyl-5-sulfonates have been crystallographically authenticated; other than the Ag complex, only Cu complexes have been reported (Ammor *et al.*, 1992; Petit, Ammor *et al.*, 1993; Petit, Coquerel *et al.*, 1993). The structure of a hydrated sodium salt is also known (Viossat *et al.*, 1982).

(I)
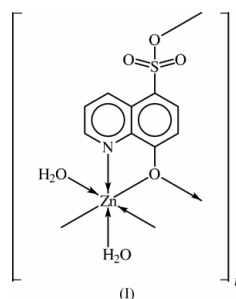
The structure of the diaqua zinc derivative, (I), consists of a centrosymmetric $(C_9H_5NO_4S)_2(H_2O)_2Zn_2$ entity in which the 8-hydroxyquinolinyl portion of the ligand chelates to the Zn atom [Zn1—O1 2.075 (2) Å and Zn1 ← N1 2.097 (2) Å]. The O atom also interacts with the other Zn atom [Zn1^i—O1 2.035 (2) Å; symmetry code (i) = 1 − x, 1 − y, 1 − z], the bridging interaction being somewhat stronger than a covalent bond. The N1, O1, O1^i and O2w atoms comprise a plane of the octahedron around the Zn atom, and the other two sites are occupied by a second water molecule and one sulfonato O atom of an adjacent entity (Fig. 1), giving rise to a network structure. The other two sulfonato O atoms are each involved in the formation of two hydrogen bonds (Table 2), the four hydrogen bonds further consolidating the structure.

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Experimental

8-Hydroxyquinolinyl-5-sulfonic acid (0.13 g, 0.5 mmol) was dissolved in water (5 ml) and aqueous sodium hydroxide was added to raise the pH to 6. Zinc nitrate hexahydrate (0.15 g, 0.5 mmol) in water (5 ml) was added to the solution and the mixture heated to 323 K. After the mixture was stirred for 30 min., the solution was filtered and the filtered solution set aside for the compound to crystallize.

Crystal data

$[Zn(C_9H_5NO_4)(H_2O)_2]$	Mo $K\alpha$ radiation
$M_r = 324.60$	Cell parameters from 5070
Orthorhombic, $Pbca$	reflections
$a = 9.2974\ (5)$ Å	$\theta = 2.5–28.0°$
$b = 15.2169\ (8)$ Å	$\mu = 2.36$ mm^{-1}
$c = 16.1024\ (8)$ Å	$T = 298\ (2)$ K
$V = 2278.1\ (2)$ Å^3	Block, gold
$Z = 8$	$0.30 \times 0.16 \times 0.12$ mm
$D_x = 1.893$ Mg m^{-3}	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2597 independent reflections
	2197 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.033$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{max} = 27.5°$
	$h = -11 \rightarrow 12$
$T_{min} = 0.482$, $T_{max} = 0.754$	$k = -19 \rightarrow 19$
12660 measured reflections	$l = -16 \rightarrow 20$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2]$
$wR(F^2) = 0.085$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
2597 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.075 (2)	Zn1—O1w	2.140 (2)
Zn1—O1^i	2.035 (2)	Zn1—O2w	2.032 (2)
Zn1—O2^{ii}	2.223 (2)	Zn1—N1	2.097 (2)
O1—Zn1—O1^i	76.1 (1)	O1^i—Zn1—N1	154.5 (1)
O1—Zn1—O2^{ii}	94.7 (1)	O2^{ii}—Zn1—O1w	169.2 (1)
O1—Zn1—O1w	95.7 (1)	O2^{ii}—Zn1—O2w	80.4 (1)
O1—Zn1—O2w	173.8 (1)	O2^{ii}—Zn1—N1	94.5 (1)
O1—Zn1—N1	78.7 (1)	O1w—Zn1—O2w	89.5 (1)
O1^i—Zn1—O2^{ii}	91.4 (1)	O1w—Zn1—N1	90.3 (1)
O1^i—Zn1—O1w	88.4 (1)	O2w—Zn1—N1	97.8 (1)
O1^i—Zn1—O2w	107.7 (1)		

Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $x - \frac{1}{2}, y, \frac{3}{2} - z$.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1w—H1w1⋯O3^{iii}	0.85 (1)	1.98 (1)	2.816 (3)	169 (2)
O1w—H1w2⋯O4^{iv}	0.84 (1)	1.99 (1)	2.800 (2)	165 (3)
O2w—H2w2⋯O3^v	0.84 (1)	1.97 (2)	2.760 (3)	156 (3)
O2w—H2w1⋯O4^{iii}	0.84 (1)	1.86 (1)	2.699 (2)	175 (3)

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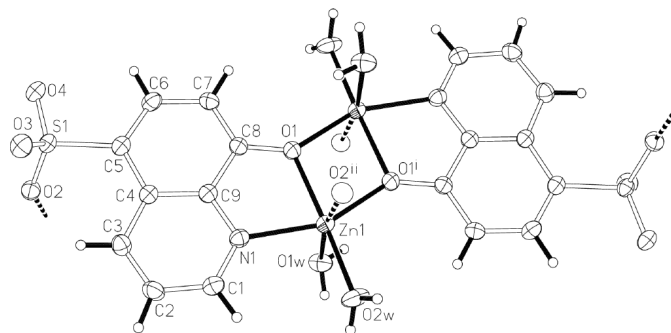

Figure 1
ORTEP (Johnson, 1976) plot of a fragment of diaqua-8-hydroxy-quinolinyl-5-sulfonatozinc(II); displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $x - \frac{1}{2}, y, \frac{3}{2} - z$.]

The room-temperature diffraction measurements were of a sufficiently high quality to enable the H atoms to be located and refined with O—H 0.85 (1) and C—H 0.95 (1) Å distance restraints.

Data collection: SMART (Bruker, 2001); cell refinement: SMART; data reduction: SAINT (Bruker, 2001); 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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