Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[*cis*-diaqua(2,2′-bipyridine)zinc(II)]-μ-5-sulfonatosalicylato]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.083
Data-to-parameter ratio = 13.9

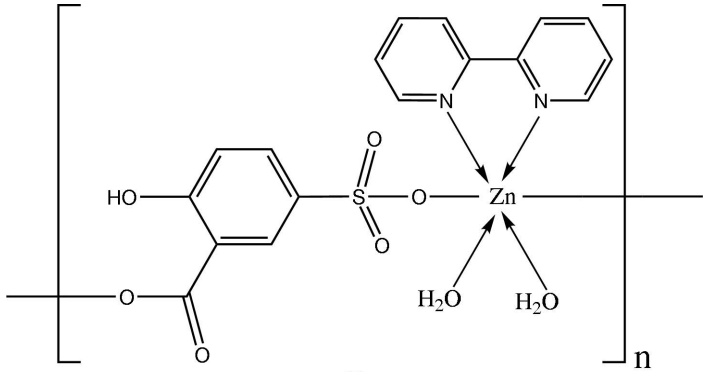
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 22 March 2005
Accepted 29 March 2005
Online 9 April 2005

In the title polymeric compound, $[Zn(C_7H_4O_6S)(C_{10}H_8N_2)(H_2O)_2]$, the octahedral coordination of the Zn atom comprises N-atom donors of 2,2′-bipyridine, O atoms of two water molecules, the carboxyl O atom of the 5-sulfosalicylate dianion and the sulfonyl O atom of a symmetry-related dianion. The water molecules with sulfonyl O atoms form hydrogen bonds between chains, giving rise to a two-dimensional network.

Comment

Recently metal complexes of 5-sulfosalicylic acid (H_3ssal) have been extensively explored in our laboratory (Fan & Zhu, 2005; Fan, Cai *et al.*, 2005; Fan, Xiao & Zhu, 2005; Fan *et al.*, 2005*a*,*b*,*c*,*d*). As part of our systematic studies on the H_3ssal metal complexes, the title zinc(II) compound, (I), was synthesized.



(I)

In the title compound, the Zn^{II} atom adopts an octahedral geometry defined by two N-atom donors from one 2,2′-bipyridine ligand, two O atoms from one sulfonyl and one carboxyl group of two $Hssal^{2-}$ ligands and two O atoms from two water molecules that are *cis* to each other (Fig. 1 and Table 1). The 5-sulfonatosalicylato dianion uses the carboxyl and the sulfonyl groups to bridge two Zn^{II} atoms, producing a chain structure (Fig. 2). Moreover, the water molecules and uncoordinated carboxyl O atoms are engaged in hydrogen bonding only within each chain, while water molecules and sulfonyl O atoms form hydrogen bonds between chains, generating a two-dimensional hydrogen-bonding network (Fig. 3 and Table 2).

Experimental

2,2′-Bipyridine (0.079 g, 0.51 mmol) dissolved in methanol (5 ml) was added slowly to an aqueous solution (15 ml) of zinc(II) acetate

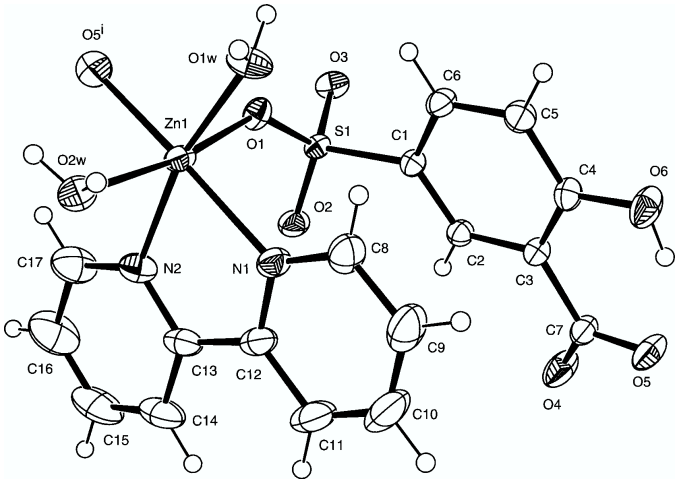


Figure 1
An *ORTEP* view (Farrugia, 1997) of a fragment of (I). Displacement ellipsoids are drawn at the 40% probability level. [Symmetry code (i): $x+\frac{1}{2}, \frac{3}{2}-y, z+\frac{1}{2}$.]

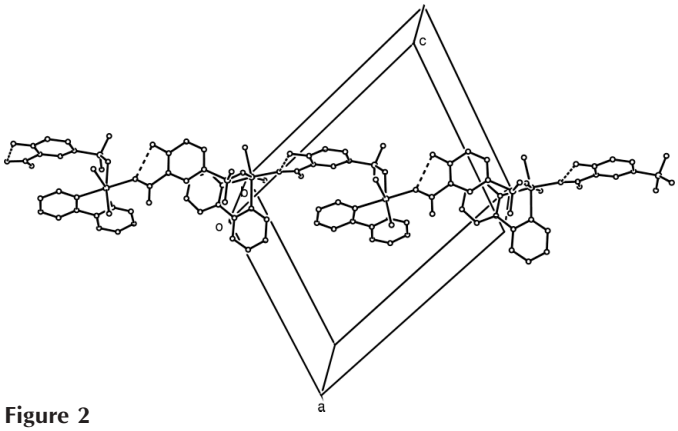


Figure 2
A view of the one-dimensional chain for (I). Hydrogen bonds are shown as dashed lines and H atoms have been omitted for clarity.

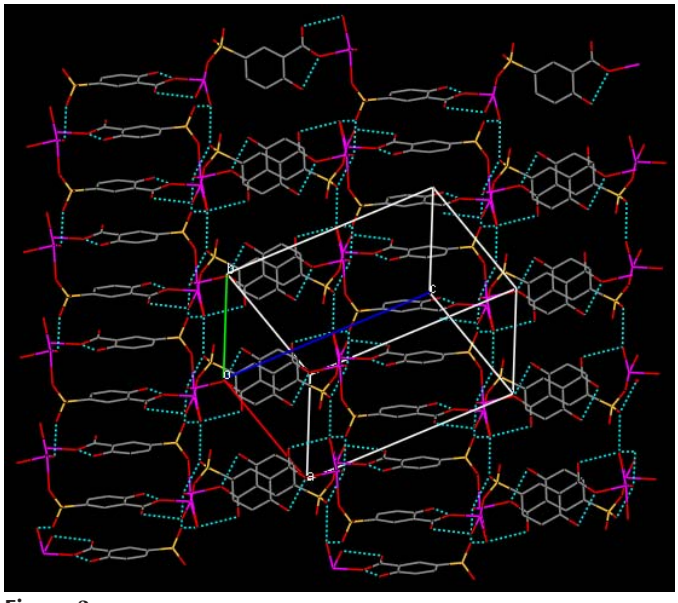


Figure 3
A view of the two-dimensional hydrogen-bonding (dashed lines) network for (I). The 2,2′-bipyridine ligands and H atoms have been omitted for clarity.

dihydrate (0.109 g, 0.5 mmol) and 5-sulfosalicylic acid dihydrate (0.127 g, 0.5 mmol). After 1 d, colorless block-shaped crystals of (I) had grown and these were separated by filtration.

Crystal data

$[Zn(C_7H_4O_6S)(C_{10}H_8N_2)(H_2O)_2]$	D_x = 1.696 Mg m^{-3}
M_r = 473.75	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 6964 reflections
a = 14.433 (2) Å	θ = 2.3–28.2°
b = 7.6395 (8) Å	μ = 1.49 mm^{-1}
c = 18.089 (2) Å	T = 295 (2) K
β = 111.527 (2)°	Block, colorless
V = 1855.4 (4) Å^3	0.44 × 0.34 × 0.31 mm
Z = 4	

Data collection

Bruker SMART APEX area-detector diffractometer	3847 independent reflections
	3586 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.019
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	θ_{max} = 26.5°
	$h = -18 \rightarrow 16$
T_{min} = 0.561, T_{max} = 0.636	$k = -7 \rightarrow 9$
10467 measured reflections	$l = -19 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.5177P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.030	
$wR(F^2)$ = 0.083	
S = 1.09	$(\Delta/\sigma)_{max}$ = 0.001
3847 reflections	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
277 parameters	$\Delta\rho_{min}$ = −0.69 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.187 (1)	Zn1—N2	2.114 (2)
Zn1—O5^{i}	2.036 (1)	Zn1—O1*W*	2.034 (1)
Zn1—N1	2.137 (2)	Zn1—O2*W*	2.179 (2)
O1*W*—Zn1—O5^{i}	94.30 (7)	N2—Zn1—O2*W*	89.70 (6)
O1*W*—Zn1—N2	167.15 (7)	N1—Zn1—O2*W*	93.00 (6)
O5^{i}—Zn1—N2	97.81 (7)	O1*W*—Zn1—O1	86.40 (5)
O1*W*—Zn1—N1	90.82 (7)	O5^{i}—Zn1—O1	80.20 (5)
O5^{i}—Zn1—N1	173.20 (6)	N2—Zn1—O1	91.42 (6)
N2—Zn1—N1	76.78 (7)	N1—Zn1—O1	95.68 (5)
O1*W*—Zn1—O2*W*	94.38 (6)	O2*W*—Zn1—O1	171.27 (5)
O5^{i}—Zn1—O2*W*	91.08 (5)		

Symmetry code: (i) $\frac{1}{2}+x, \frac{3}{2}-y, \frac{1}{2}+z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6O···O5	0.85 (1)	1.80 (2)	2.572 (2)	151 (2)
O1*W*—H1*W*1···O3^{ii}	0.85 (3)	1.88 (3)	2.722 (2)	172 (3)
O1*W*—H2*W*1···O3^{iii}	0.84 (1)	1.86 (1)	2.702 (2)	178 (3)
O2*W*—H1*W*2···O2^{iii}	0.84 (1)	2.00 (1)	2.820 (2)	164 (2)
O2*W*—H2*W*2···O4^{i}	0.85 (1)	1.90 (1)	2.714 (2)	159 (3)

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

The aromatic H atoms were positioned geometrically and were refined in the riding-model approximation [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C)]. The water and hydroxyl H atoms were located in a difference Fourier map and were refined with a distance restraint of O—H = 0.85 (1) Å and with fixed isotropic displacement parameters of U_{iso}(H) = 0.05 Å^2.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We thank the National Natural Science Foundation of China (No. 50073019).

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