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trans-Diaquabis[2-(2-pyridyl)ethanol-$\kappa^2 N,O$]zinc(II) disaccharinate

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In the title complex, $[Zn(C_7H_{11}NO_2)_2](C_7H_4NO_3S)_2$, the Zn^{II} ion lies on a crystallographic inversion centre and possesses an octahedral geometry with two neutral 2-pyridylethanol (pyet) ligands and two coordinated water molecules. Pyet acts as an *N*,*O*-bidentate ligand, giving rise to a six-membered chelate ring. H atoms of the water molecules and the hydroxy group of pyet are involved in hydrogen bonding with amine-N, sulfonyl-O and carbonyl-O atoms of neighbouring saccharinate ions, creating a three-dimensional network.

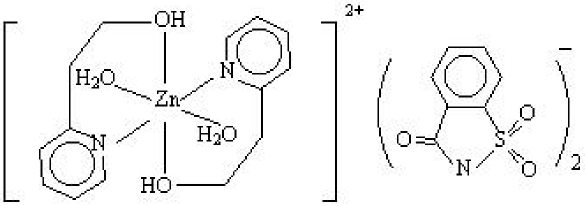
Key indicators

Single-crystal X-ray study
T = 133 K
Mean σ(C–C) = 0.002 Å
R factor = 0.024
wR factor = 0.069
Data-to-parameter ratio = 19.7

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

Comment

This work is part of our study on the synthesis and structural characterization of metal complexes with the saccharinate ion $(C_7H_4NO_3S)^-$ (sac), chemically known as *o*-sulfobenzimide, and co-ligands containing hydroxymethyl and hydroxyethyl groups, such as monoethanolamine (Andac *et al.*, 2000; Yilmaz, Andac *et al.*, 2001; Yilmaz, Topcu *et al.*, 2001), monoethanolethylenediamine (Yilmaz *et al.*, 2002), diethanolamine (Yilmaz, Topcu *et al.*, 2001), triethanolamine (Topcu *et al.*, 2001) and dimethanolpyridine (Andac *et al.*, 2002). We report here the crystal and molecular structure of the complex, (I), of zinc(II) saccharinate with 2-pyridylethanol (pyet) as an extension of this investigation to the 2B metals.



(I)

The structure of (I) consists of a complex cation, $[Zn(H_2O)_2(pyet)_2]^{2+}$, and two sac anions. In the cation, the Zn^{II} ion lies on an inversion centre and is octahedrally coordinated by two pyet ligands and two water molecules (Fig. 1). Each pyet ligand behaves as a bidentate ligand, coordinating through the N and hydroxyl O atoms, forming six-membered chelate rings with the Zn^{II} ion. The two pyet ligands form the equatorial plane of the coordination octahedron, while water molecules occupy the axial positions with a *trans* configuration. Some distortion of regular octahedral geometry is apparent as shown in Table 1, especially in the $O_{water}—Zn—N_{pyet}$ angles.

Both the sac (C11–C16/C21/N1/S1) and pyet (C31–C35/N2) moieties are essentially planar, with an r.m.s. deviation of *ca* 0.01 (1) Å, but the OH group significantly deviates from the pyet plane by 1.00 (1) Å. The bond geometry of the sac ion is

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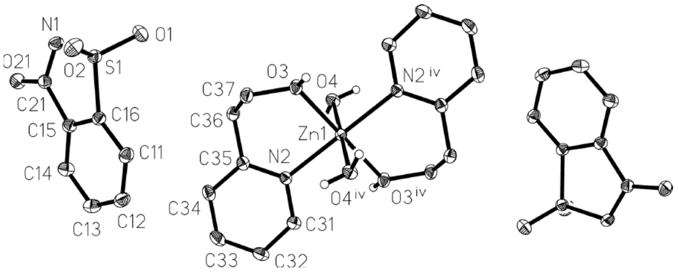

Figure 1
A view of the molecular structure of the title compound (50% displacement ellipsoids). H atoms attached to C atoms have been omitted for clarity. [Symmetry code: (iv) 1−*x*, −*y*, −*z*.]

similar to that of the Zn^{II}–triethanolamine complex containing sac as the counter-ion (Topcu *et al.*, 2001). The packing of (I) exhibits parallel stacking of pairs of sac ions, as shown in Fig. 2. The phenyl rings roughly superimpose on each other and, therefore, the π–π interactions between the sac ions are very weak (distances between centroids > 4.0 Å). The crystal structure exhibits three different hydrogen bonds. The H atom of the hydroxyl group of the pyet ligand forms a hydrogen bond with the carbonyl-O atom of the sac ions [O3···O21^{iii}; symmetry code: (iii) $x - \frac{1}{2}, -y - \frac{1}{2}, z - \frac{1}{2}$], while the water H atoms are involved in intermolecular hydrogen bonding with the sulfonyl-O atoms of the sac ions [O4···O2^{i}; symmetry code: (i) $x + \frac{1}{2}, -y - \frac{1}{2}, z - \frac{1}{2}$] and the N atoms of the py ring [O4···N1^{ii}; symmetry code: (ii) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$]. The overall hydrogen-bond scheme can be described as a three-dimensional network formed by the pyet ligands, water molecules and sac anions.

Experimental

Previously prepared [Zn(sac)$_2$(H$_2$O)$_4$].2H$_2$O (0.54 g, 1.0 mmol) was dissolved in 30 ml of methanol at 303 K with stirring. Then pyet (0.25 g, 2.0 mmol) was added to the solution dropwise. The resulting solution was left to stand at room temperature and allowed to evaporate slowly. The colourless crystals obtained after a week were collected by suction filtration, washed with acetone and dried in air.

Crystal data

$[Zn(C_7H_{11}NO_2)_2](C_7H_4NO_3S)_2$
$M_r = 712.05$
Monoclinic, $P2_1/n$
$a = 8.8270$ (6) Å
$b = 8.7748$ (6) Å
$c = 19.1473$ (10) Å
$\beta = 100.833$ (3)°
$V = 1456.63$ (16) Å^3
$Z = 2$
$D_x = 1.623$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 6687 reflections
$\theta = 2.4$–30.5°
$\mu = 1.05$ mm^{-1}
$T = 133$ (2) K
Prism, colourless
0.50 × 0.40 × 0.35 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.583$, $T_{max} = 0.692$
28712 measured reflections
4267 independent reflections
3997 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 30.0°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -26 \rightarrow 26$

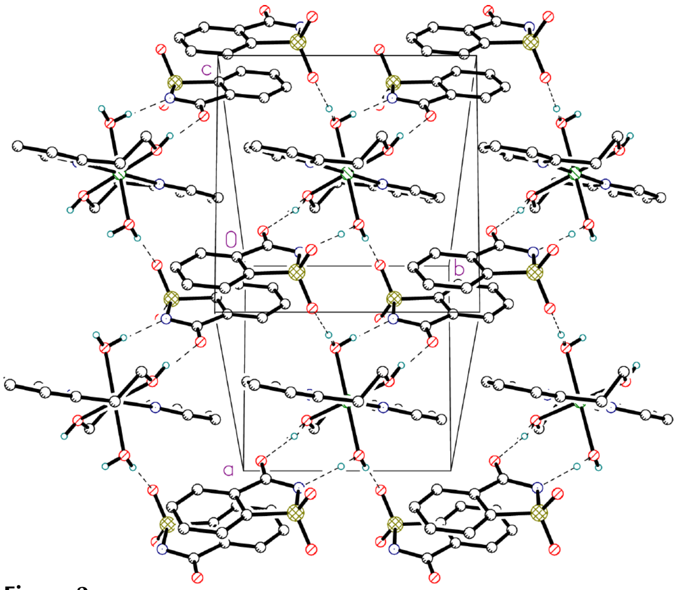

Figure 2
A packing diagram of the title compound, showing the hydrogen-bonding scheme.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.069$
$S = 1.04$
4267 reflections
217 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 0.4412P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N2	2.1093 (9)	Zn1—O4	2.1417 (8)
Zn1—O3	2.1233 (8)		
N2—Zn1—O3	89.99 (3)	O3—Zn1—O4	91.44 (3)
N2—Zn1—O4	93.11 (3)	N2—Zn1—O4^{iv}	86.89 (3)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H41···O2^{i}	0.835 (19)	2.002 (19)	2.8317 (12)	173 (2)
O4—H42···N1^{ii}	0.83 (2)	1.90 (2)	2.7355 (12)	174 (2)
O3—H3···O21^{iii}	0.84 (2)	1.82 (2)	2.6437 (11)	165 (2)

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

H atoms of the hydroxyl group and water molecules were refined freely, while H atoms bonded to C atoms were included using a riding model, starting from calculated positions.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

m370 Sevim Hamamci *et al.* • $[Zn(C_7H_{11}NO_2)_2](C_7H_4NO_3S)_2$ *Acta Cryst.* (2002). E**58**, m369–m371

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