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Tetraaquabis[2-(4-pyridyl)ethanesulfonato-*N*]zinc(II)

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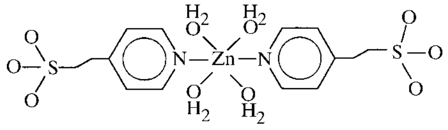
The title compound, $[Zn(C_7H_8NO_3S)_2(H_2O)_4]$, has an octahedral coordination around the central Zn atom composed of two axial N atoms from the pyridine ligands and four equatorial O atoms of water molecules, forming a monomeric centrosymmetric complex. The two Zn—N bond distances are 2.102 (3) Å, while the four Zn—O bond distances range from 2.114 (2) to 2.167 (2) Å. Packing is determined by hydrogen bonds formed by the water molecules. The sulfonate group does not take part in coordination to the Zn atom.

Comment

There has been considerable interest in pyridylethanesulfonic acid as a bifunctional ligand of new ternary radiopharmaceutical complexes (Costanzo *et al.*, 1997; Edwards & Shuang, 1997; Shuang *et al.*, 1998), but we have not found any reports about the crystal structures of complexes it can form with metal ions. Recently, one of us has prepared a number of complexes having two-dimensional square grids by hydrothermal synthesis (Xiong *et al.*, 1998, 1999; Lin *et al.*, 1998; Owen, Wang *et al.*, 1999; Owen, Xiong *et al.*, 1999), and tried to synthesize new complexes formed by 2-(4-pyridyl)ethanesulfonic acid (PES).

In this paper, we report on the crystal structure of the title compound, (I), which represents the first example of a metal complex with PES. The X-ray crystal structure determination shows that the N atom of the pyridine ring of PES coordinates to the Zn atom, but the sulfonate group of PES is not involved in coordination to the metal, so a centrosymmetric monomer is formed with four water molecules equatorially coordinating in a plane while two N atoms occupy the axial positions, instead of constructing two- and three-dimensional supramolecular networks (Fig. 1). The environment around the central Zn atom is an almost perfect octahedron with an N—Zn—N bond angle of 180° and an N—Zn—O bond angle of almost 90°, similar to that of tetraaquabis(*N*-isonicotinato)zinc(II) (Biagini *et al.*, 1971), in which two carboxylate ligands are not involved in coordination to zinc. The Zn1—O2 and Zn1—O3 distances are 2.167 (2) and 2.114 (2) Å, respectively, while the Zn1—N1 bond distance is 2.102 (3) Å. The C—C, C═C, S—O and N═C bond distances are unexceptional.



(I)

The complex molecules are packed in the crystal by a hydrogen-bonding system involving the water molecules, whose relevant geometric parameters are quoted in Table 1. The complex molecules are piled up in turn as layers through strong intermolecular O2*W*—H1···O2, O1*W*—H3···O1 and O1*W*—H4···O3 hydrogen bonds. These layers are linked through strong O2*W*—H2···O3 hydrogen bonds and weak C4—H4*A*···O2 ones to form a three-dimensional network structure. Further work will focus on solvothermal synthesis to eliminate the coordinated water and have the sulfonate group connecting metal centres to construct one-, two- and three-dimensional supramolecular frameworks.

Experimental

2-(4-Pyridyl)ethanesulfonic acid (0.1 g) and $Zn(ClO_4)_2 \cdot 2H_2O$ (0.1 g) were added to water (10 ml) and pyridine (0.12 ml). The resulting solution was evaporated at room temperature for a few days. Colorless block-shaped crystals were obtained. The IR spectrum displayed a strong absorption band at 3350 cm^{-1}.

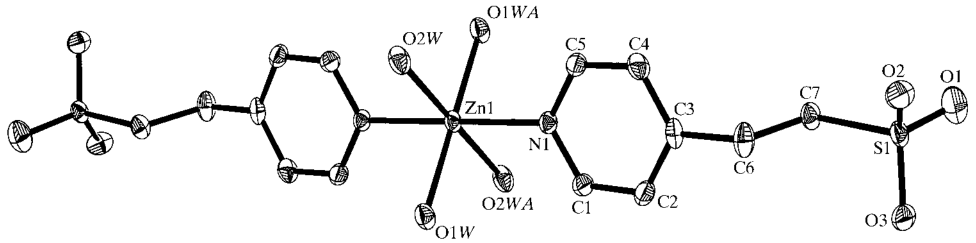


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are shown at the 35% probability level.

Crystal data

$[Zn(C_7H_8NO_3S)_2(H_2O)_4]$
$M_r = 509.84$
Monoclinic, $P2_1/c$
$a = 9.0967\ (14)$ Å
$b = 8.8122\ (13)$ Å
$c = 12.5396\ (14)$ Å
$\beta = 94.910\ (10)^\circ$
$V = 1001.5\ (2)$ Å^3
$Z = 2$
$D_x = 1.691$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 45 reflections
$\theta = 5.16$–11.78°
$\mu = 1.491$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
$0.60 \times 0.40 \times 0.15$ mm

Data collection

Bruker *P*4 diffractometer
$2\theta/\omega$ scans
Absorption correction: empirical (North *et al.*, 1968)
$T_{\min} = 0.618$, $T_{\max} = 0.800$
2411 measured reflections
1765 independent reflections
1429 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\max} = 25^\circ$
$h = -1 \rightarrow 10$
$k = -1 \rightarrow 10$
$l = -14 \rightarrow 14$
3 standard reflections every 97 reflections intensity decay: 6.11%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.092$
$S = 1.041$
1765 reflections
134 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 1.0422P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.76$ e Å^{-3}
$\Delta\rho_{\min} = -0.56$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 1997)
Extinction coefficient: 0.0129 (17)

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2W—H1···O2$^{\rm i}$	0.85 (5)	1.97 (4)	2.814 (4)	167 (2)
O2W—H2···O3$^{\rm ii}$	0.85 (3)	1.95 (1)	2.795 (3)	170 (1)
O1W—H3···O1$^{\rm iii}$	0.85 (4)	1.93 (6)	2.788 (4)	175 (1)
O1W—H4···O3$^{\rm i}$	0.85 (6)	1.89 (6)	2.743 (4)	170 (1)
C4—H4A···O2$^{\rm iv}$	0.93 (1)	2.58 (8)	3.379 (4)	143 (1)

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

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

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1464). Services for accessing these data are described at the back of the journal.

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