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Crystallographic report

Diaquabis(1,10-phenanthroline)zinc(II) 4,5-dihydroxy-1,3-benzenedisulfonate trihydrate

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The zinc atom has a distorted octahedral geometry defined by two 1,10-phenanthroline and two *cis* water molecules. A three-dimensional network structure arises owing to extensive hydrogen bonds involving all the components of $[Zn(phen)_2(H_2O)_2][C_6H_2(OH)_2(SO_3)_2]\cdot 3H_2O$. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc; 1,10-phenanthroline; hydrogen bond

COMMENT

In $[Zn(H_2O)_2(phen)_2][C_6H_2(OH)_2(SO_3)_2]\cdot 3H_2O$, Fig. 1, the bidentate 1,10-phenanthroline ligands and two *cis* water molecules coordinate to the zinc atom in a distorted octahedral geometry. The Zn–Ow (average 2.111(3) Å) and Zn–N distances (average 2.162(4) Å) fall within the ranges usually observed in aqua complexes of zinc(II) containing phen ligands.[1–3] The components of the crystal are held together by extensive hydrogen bonds (O···O distances: 2.678(6)–2.971(8) Å), yielding a three-dimensional network.

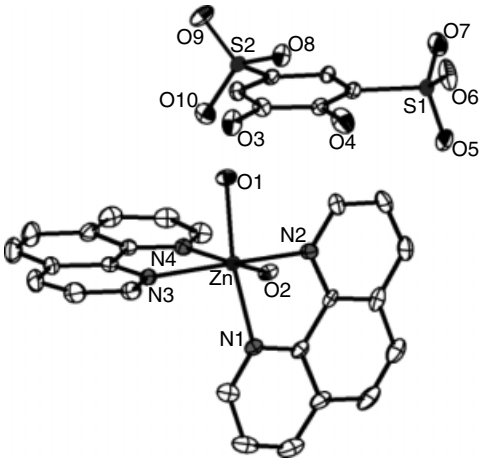

Figure 1. Molecular structure of $[Zn(phen)_2(H_2O)_2][C_6H_2(OH)_2(SO_3)_2]\cdot 3H_2O$; water molecules and hydrogen atoms omitted for clarity. Key geometric parameters: Zn–O1 2.132(3), Zn–O2 2.090(3), Zn–N1 2.155(3), Zn–N2 2.140(3), Zn–N3 2.169(3), Zn–N4 2.182(3) Å; O1–Zn–O2 84.99(13), N1–Zn–N2 78.32-(12), N3–Zn–N4 76.83(12)°.

EXPERIMENTAL

4,5-Dihydroxy-1,3-benzenedisulfonate monohydrate (0.332 g, 1 mmol) was added to a solution of $Zn(NO_3)_2\cdot 6H_2O$ (0.297 g, 1 mmol) in H_2O (20 ml). The colorless solution was mixed with a methanol (5 ml) solution of phen (0.396 g, 2 mmol). Upon standing and slow evaporation, light-yellow crystals were obtained. Main IR features (cm^{-1}, KBr): 1519(s), 1429(sh), 1178(vs), 1039(s), 725(s). Data were collected at 295 K on a Siemens-Smart CCD diffractometer using Mo Kα radiation on a crystal $0.08 \times 0.12 \times 0.18$ mm^3. Crystal data: $C_{30}H_{30}N_4O_{13}S_2Zn$, $M = 784.07$, triclinic, space group $P\bar{1}$, $a = 9.6968(4)$, $b = 12.7392(5)$, $c = 14.4411(6)$ Å, $\alpha = 98.224(1)$, $\beta = 97.920(1)$, $\gamma = 106.409(1)°$, $V = 1663.54(12)$ $Å^3$, $Z = 2$, $R = 0.048$ (3784 data $I \geq 2\sigma(I)$), $wR = 0.106$ (all 5017 data; $\theta_{max} = 25.0°$). Programs used: SAINT. SHELXL97 and ORTEP. CCDC deposition number: 243759.

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