研究简报

有机二磺酸二邻菲咯啉二水合锌配合物

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关键词: 晶体结构; 2,2′-二甲氧基-1,1′-二萘-6,6′-二磺酸; 锌

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[Bis(1,10-phenanthroline)-diauqa-Zn(Ⅱ)] [(*R*,*S*)-2,2′-dimethoxy-1,1′-binaphthylene-6,6′-disulfonate]

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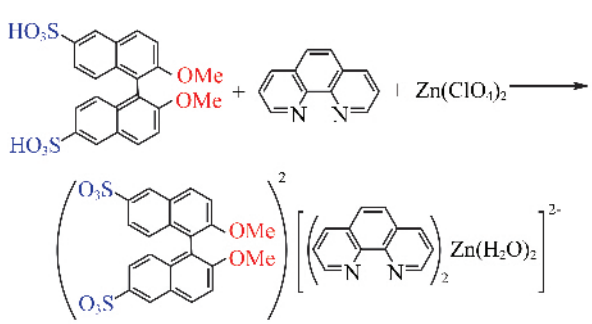
Abstract: The crystal structure of $[Zn(H_2O)_2(phen)_2][DBDA]$ (**1**) (DBDA=2,2′-dimethoxy-1,1′-binaphthylene-6,6′-disulfonate, phen=1,10-phenanthroline) involves the anion part (2,2′-dimethoxy-1,1′-binaphthylene-6,6′-disulfonate) and the cation part which compose of a octahedron coordinated zinc center surrounded by two water and four nitrogen atoms from two phen rings, the 3D packing structure was formed through the strong H-bonding interaction between sulfonate and water. CCDC: 277923.

Key words: crystal structure; 2,2′-dimethoxy-1,1′-binaphthylene-6,6′-disulfonic acid; Zinc(Ⅱ)

Compound **1** was achieved by hydrothermal treatment of 2,2′-dimethoxy-1,1′-binaphthylene-6,6′-disulfonic acid (H_2DBDA), 1.10-phenanthroline (phen) and Zn $(ClO_4)_2\cdot 6H_2O$. X-ray crystallographic analysis of **1** clearly shows that its structure consists of $[Zn(H_2O)_2(phen)_2]$ moiety and the uncoordinated DBDA as shown in Fig.1[1-5]. The zinc atom coordinates to four nitrogen atoms from two different phen ligands and two oxygen atoms from water to lead to the formation of a slightly distorted octahedron. Thus, the DBDA ligand fails to coordinate to zinc atom and just loses its two protons of sulfonate group to balance the electron charge, while the dihedral angle between two naphthalene rings has 97.3°, closely perpendicular to each other. The presence of strong H-bond between sulfonate group and water results in the formation of the 3D network. To this end, the bond distances of C-N, C-C, C-S, S-O, C-O, Zn-N and Zn-O are unexceptional.



Scheme 1

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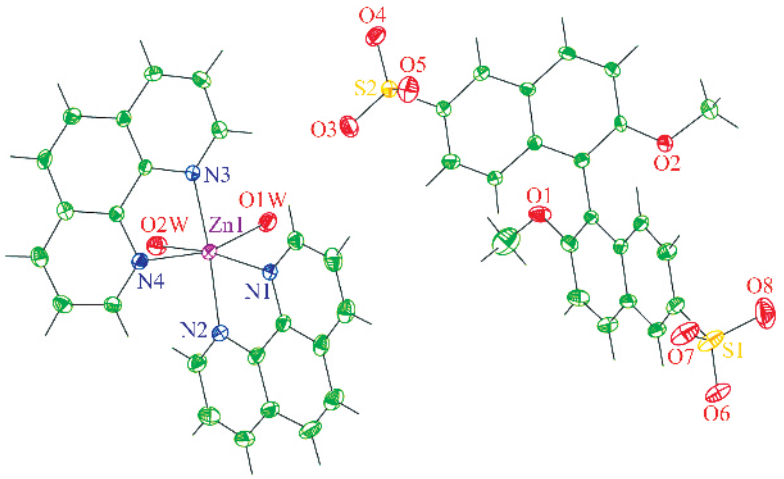

Fig.1 ORTEP diagram (30% probability ellipsoids) showing the solid-state structure and atom numbering scheme for **1**
Selected bond lengths (nm) and (°):
Zn(1)-O(2W) 0.210 5(5), Zn(1)-N(1) 0.210 8(5), Zn(1)-N(2) 0.213 3(5), Zn(1)-N(3) 0.214 3(5), Zn(1)-O(1W) 0.214 7(5), Zn(1)-N(4) 0.217 3(5)
O(2W)-Zn(1)-N(1) 166.37(19) O(2W)-Zn(1)-N(2) 90.30(19) N(1)-Zn(1)-N(2) 77.9(2), O(2W)-Zn(1)-N(3) 91.53(19), N(1)-Zn(1)-N(3) 101.0(2), N(2)-Zn(1)-N(3) 172.9(2), O(2W)-Zn(1)-O(1W) 85.82(19) N(1)-Zn(1)-O(1W) 88.97(19), N(2)-Zn(1)-O(1W) 97.71(19),N(3)-Zn(1)-O(1W) 89.32(19), O(2W)-Zn(1)-N(4) 85.93(19), N(1)-Zn(1)-N(4) 101.94(19), N(2)-Zn(1)-N(4) 96.1(2), N(3)-Zn(1)-N(4) 77.2(2), O(1W)-Zn(1)-N(4) 163.96(17)

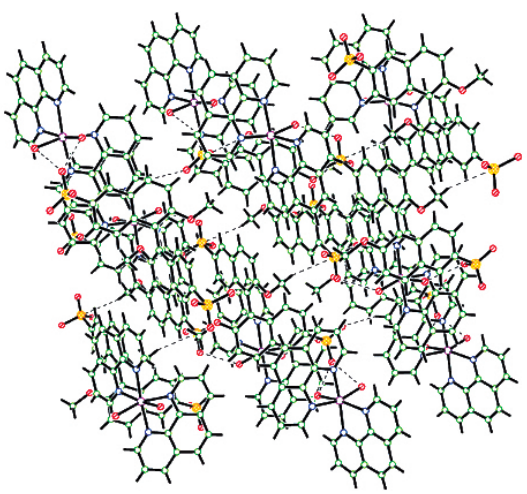

Fig.2 A crystal-packing view of **1** showing 3D-network structure through hydrogen bond

Experiment

Hydrothermal treatment of $Zn(ClO_4)_2 \cdot 6H_2O$ (0.3 mmol), 2,2′-dimethoxy-1,1′-binaphthylene-6,6′-disulfonic acid (0.6 mmol), 1,10-phenanthroline(phen) (1.2 mol), water (1.0 mL) and alcohol (1.0 mL) over two days at 120 ℃ yielded colorless block crystals[6-9]. The yield was about 50% based on acid (H_2DBDA). Intensity data were collected at 296(2) K on a Bruker AXS SMART CCD for a colorless block 0.05 mm × 0.10 mm × 0.20 mm. $C_{46}H_{36}ZnN_4O_{10}S_2$, M=934.28, triclinic, $P\bar{1}$, a=1.044 9(12) nm, b=1.227 3(12) nm, c=1.756 3(7) nm, α=69.661(3)°, β=72.962(4)°, γ=77.770(3)°, V=1.979 2(4) nm^3, Z=2, 7 691 unique data (θ_{max}=26.0°), R=0.087 1 (4 304 [$I \geqslant 2\sigma(I)$] reflections), wR=0.222 (all data), ρ_{max}=1 220 e·nm^{-3}; water-H were not located. Programs used: SAINT, SADABS, SHELX-97, ORTEP.

CCDC: 277923.

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