

含轴手性磺酸配体的镉配合物

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关键词: 晶体结构; 6,6'-二溴-2,2'-二甲氧基-1,1'-二萘-4,4'-二磺酸; 镉

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Cd(II) Complex with Disulfonate Atropisomeric Ligand

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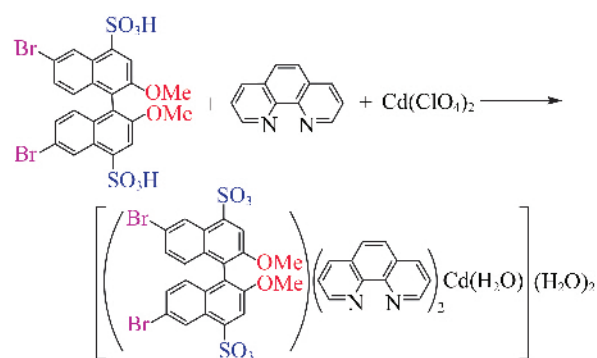
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Abstract: The crystal structure of $[\text{Cd}(\text{BDA})(\text{phen})_2(\text{H}_2\text{O})](\text{H}_2\text{O})_2$ (**1**) (BDA=6,6'-dibromo-2,2'-dimethoxy-1,1'-binaphthylene-4,4'-disulfonate, phen=1,10-phenanthroline) consists of a cadmium center whose coordination environment can be best described as a slightly distorted octahedron defined four nitrogen atoms from two phen ligands and two oxygen atoms differently from BDA ligand and water. There are strong hydrogen-bonding interactions between water and sulfonate group of BDA ligands to construct the 3D network. CCDC: 277921.

Key words: crystal structure; 6,6'-dibromo-2,2'-dimethoxy-1,1'-binaphthylene-4,4'-disulfonic acid; cadmium

Reaction of racemic 6,6'-dibromo-2,2'-dimethoxy-1,1'-binaphthylene-4,4'-disulfonic acid (H_2BDA) and $\text{Cd}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ through adding auxiliary ligand, 1,10-phenanthroline (phen) under hydrothermal treatment gives monomeric cadmium coordination compound **1**^[1-5]. The Cd center can be best described as a slightly distorted octahedron consisting of four nitrogen atoms from two phen ligands and two oxygen atoms from water and sulfonate group. On the other hand, atropisomers are stereoisomers resulting from hindered rotation about single bonds, and the dihedral angle between two naphthalene rings has 103.0° , closely perpendicular to each other to result in the formation of atropisomeric chirality. The presence of water leads in the formation of 3D network through strong H-bonds between water and sulfonate group. As expected, the

bond distance distances of C-C, C-Br, C-O, C-N, C-S, C-Br, S-O, Cd-N and Cd-O are normal as seen in the footnote of Fig.1.



Scheme 1

Experiment

Hydrothermal treatment of $\text{Cd}(\text{ClO}_4)_2$ (0.3 mmol),

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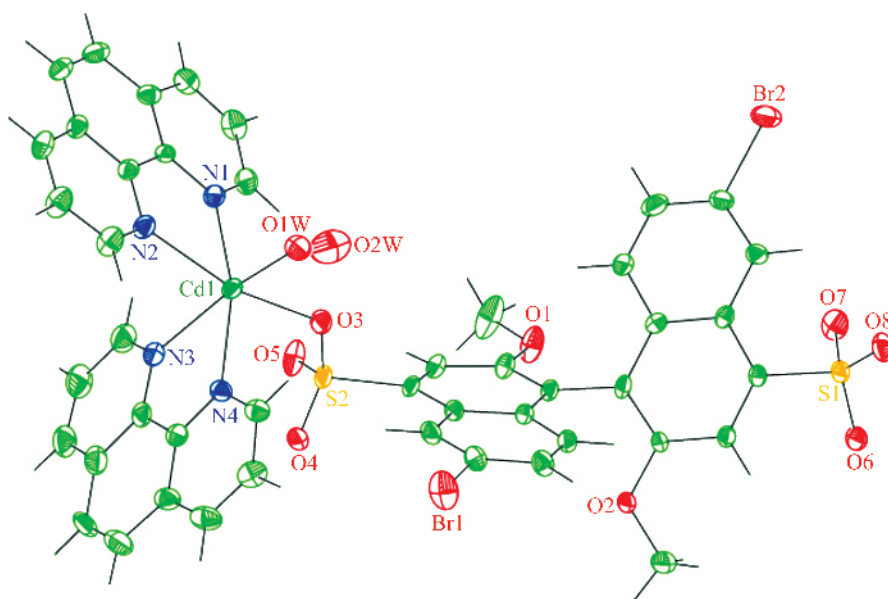


Fig.1 ORTEP view of compound **1** showing Cd center has a slightly distorted octahedron

Key bond lengths (nm) and angles (°):

Cd(1)-O(3) 0.226 1(4), Cd(1)-N(4) 0.230 2(4), Cd(1)-N(1) 0.231 6(4), Cd(1)-O(1W) 0.233 2(4),

Cd(1)-N(2) 0.034 2(4), Cd(1)-N(3) 0.238 9(5)

O(3)-Cd(1)-N(4) 93.67(15), O(3)-Cd(1)-N(1) 92.17(15), N(4)-Cd(1)-N(1) 162.80(16), O(3)-Cd(1)-O(1W) 94.16(14),

N(4)-Cd(1)-O(1W) 91.42(15), N(1)-Cd(1)-O(1W) 104.28(15), O(3)-Cd(1)-N(2) 164.21(15), N(4)-Cd(1)-N(2) 102.09(15),

N(1)-Cd(1)-N(2) 72.44(15), O(1W)-Cd(1)-N(2) 86.49(16), O(3)-Cd(1)-N(3) 93.99(15), N(4)-Cd(1)-N(3) 71.68(16),

N(1)-Cd(1)-N(3) 91.79(16), O(1W)-Cd(1)-N(3) 161.66(15), N(2)-Cd(1)-N(3) 90.09(17)

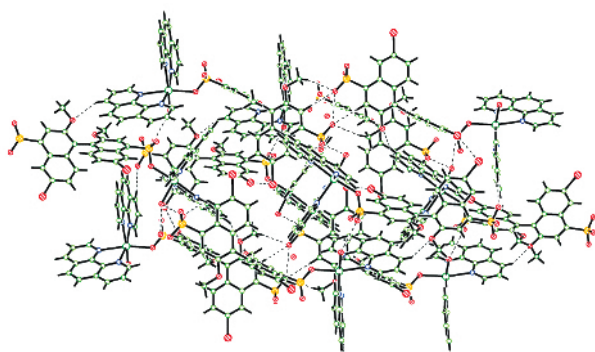


Fig.2 3D network representation of compound **1** through H-bonds

6,6'-dibromo-2,2'-dimethoxy-1,1'-binaphthylene-4,4'-disulfonic acid (0.6 mmol), 1,10-phenanthroline(phen) (1.2 mol), water (1.0 mL) and alchonol (1.0 mL) over two days at 130 °C yielded colorless block crystals^[6-9]. The yield was about 45% based on acid. Intensity data were collected at 296(2) K on a Bruker AXS SMART CCD for a colorless block 0.10 mm×0.10 mm×0.20 mm. $C_{46}H_{34}Br_2CdN_4O_{10}S_2$, $M=1139.11$, monoclinic, $P2_1/n$, $a=1.2402(9)$ nm, $b=1.3845(10)$ nm, $c=2.6262(18)$ nm, $\beta=101.207(10)^\circ$, $V=4.4230(5)$ nm³, $Z=4$, 16 064 unique data ($\theta_{max}=33.4^\circ$), $R=0.0742$ ($7492[I \geq 2\sigma(I)]$

reflections), $wR=0.2118$ (all data), $\rho_{max}=1120$ e·nm⁻³; water-H were not located. Programs used: SAINT, SADABS, SHELX-97, ORTEP.

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