研究简报

有机二磺酸镉配合物

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Organic-Disulfonate Ligand Cadmium(Ⅱ) Coordination Compound

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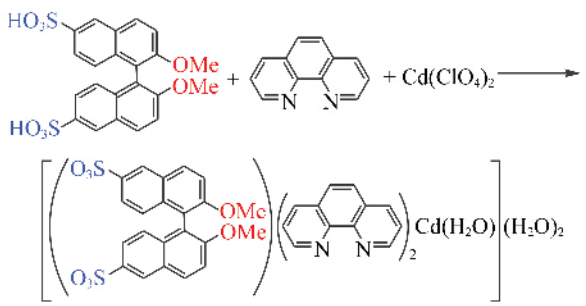
Abstract: The crystal structure of $[Cd(DBDA)(phen)_2(H_2O)](H_2O)_2$ (**1**) (DBDA=2,2′-dimethoxy-1,1′-binaphthylene-6,6′-disulfonate, phen=1,10-phenanthroline) composes of a cadmium center which is surrounded by four nitrogen atoms from 1,10-phenathroline as well as two oxygen atoms from water and sulfonate group of DBDA that also participates in H-bonding interactions to form 3D network. CCDC: 277920.

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

Under hydrothermal condition a novel cadmium coordination compound **1** was obtained through treatment of 2,2′-dimethoxy-1,1′-binaphthylene-6,6′-disulfonic acid (H_2DBDA), 1.10- phenanthroline (phen) and Cd $(ClO_4)_2$ in the presence of water and alcohol[1~5]. From the Fig.1 it can be found that the coordinational environment of Cd composes of four nitrogen atoms from two different phen rings, one oxygen atom of water and another oxygen atom from one of the sulfonate group of ligand DBDA to result in the formation of a slightly distorted octahedron. At the same time, both of two sulfonate groups lose their protons to reach the balance of electron charge of coordination compound **1**. Finally, two uncoordinated water and one coordinated water molecules interact with sulfonate group to form the strong hydrogen bonds to lead to the formation of 3D network. The key bond distances and angles have been listed in the footnote of Fig.1 and all of the bond lengths and angles are normal. In addition, the dihedron angle between two naphthalene rings of DBDA ligand is about 97.3°, closely perpen-



Scheme 1

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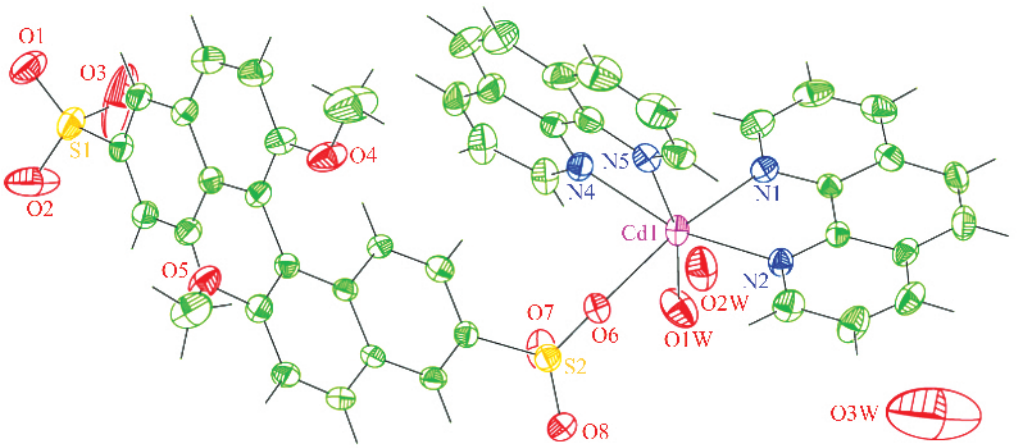

Fig.1 ORTEP view of compound **1** showing Cd center has a slightly distorted octahedron

Key bond lengths (nm) and angles (°):

Cd(1)-O(1W) 0.226 9(4), Cd(1)-N(2) 0.230 4(4), Cd(1)-N(1) 0.232 9(4), Cd(1)-N(4) 0.233 5(4), Cd(1)-N(5) 0.234 6(5), Cd(1)-O(6) 0.235 5(4)

O(1W)-Cd(1)-N(2) 97.22(17), O(1W)-Cd(1)-N(1) 88.57(15), N(2)-Cd(1)-N(1) 72.85(15), O(1W)-Cd(1)-N(4) 99.03(19), N(2)-Cd(1)-N(4) 162.29(16), N(1)-Cd(1)-N(4) 100.51(14), O(1W)-Cd(1)-N(5) 165.99(16), N(2)-Cd(1)-N(5) 93.17(16), N(1)-Cd(1)-N(5) 103.51(15), N(4)-Cd(1)-N(5) 72.09(17) O(1W)-Cd(1)-O(6) 83.72(14), N(2)-Cd(1)-O(6) 103.11(14), N(1)-Cd(1)-O(6) 170.81(13), N(4)-Cd(1)-O(6) 85.69(14), N(5)-Cd(1)-O(6) 84.80(14)

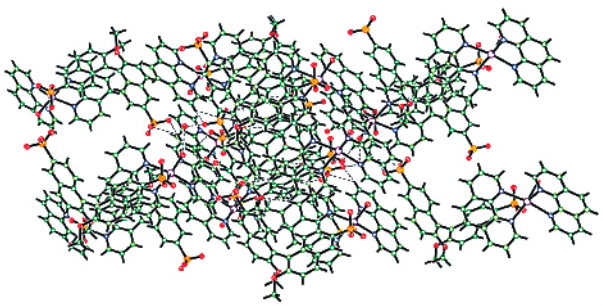

Fig.2 Packing view of compound **1**

dicular to each other.

Experiment

Hydrothermal treatment of $Cd(ClO_4)_2 \cdot 6H_2O$ (0.3 mmol), 2,2′-dimethoxy-1,1′-binaphthylene-6,6′-disulfonic acid (0.6 mmol), 1,10-phenanthroline (phen) (1.2mol), water (1.0 mL) and alcohol (1.0 mL) over two days at 130 ℃ yielded colorless block crystals[6~9]. The yield was about 40% 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. $C_{46}H_{38}CdN_4O_{11}S_2$, M=999.32, monoclinic, $C2_1/c$, a=1.533 4(8) nm, b=2.255 0(12) nm, c=1.285 5(7) nm, β=102.502(10)°, V=4.214 9(4) nm^3, Z=4, 15 351 unique data (θ_{max}=30.4°), R=0.093 2 (6 795 [$I \geqslant 2\sigma(I)$] reflections), wR=0.240 (all data), ρ_{max}=1 360 e·nm^{-3}; water-H were not located. Programs used: SAINT, SADABS, SHELX-97, ORTEP.

CCDC: 277920.

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