研究简报

有机二磺酸锰配合物

宋玉梅* 庞 洁
(南京大学配位化学研究所,配位化学国家重点实验室,南京 210093)

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; 锰
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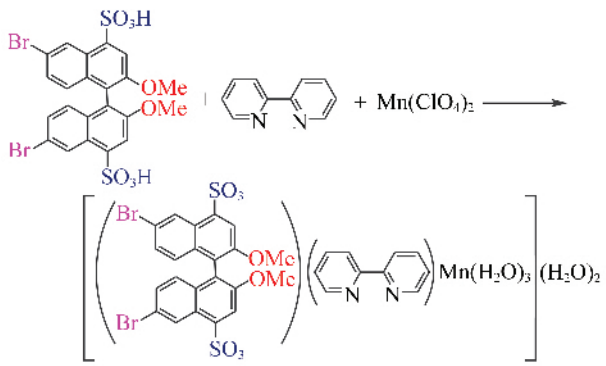
Organic-Disulfonate Ligand Manganese(Ⅱ) Coordination Compound

SONG Yu-Mei* PANG Jie
(*Coordination Chemistry Institute,State Laboratory of Coordination Chemistry, Nanjing University, Nanjing* 210093)

Abstract: The crystal structure of $[Mn(BDA)(bpy)_2(H_2O)](H_2O)_2$ (**1**)(BDA=6,6′-dibromo-2,2′-dimethoxy-1,1′-binaphthylene-4,4′-disulfonate, bpy=2,2′-bipyridine) composes of a manganese center which is surrounded by two nitrogen atoms from 2,2′-bipyridine and four oxygen atoms from three water and sulfonate group of BDA that also participate in H-bonding interactions to form 3D network as well as some uncoordinated water. CCDC: 277922.

Key words: crystal structure; 6,6′-dibromo-2,2′-dmethoxy-1,1′-binaphthylene -4,4 ′-disulfonic acid; manganese(Ⅱ)

Hydrothermal treat of racemic 6,6′-dibromo-2,2′-dmethoxy-1,1′ -binaphthylene-4,4-disulfonic acid (H_2BDA) and $Mn(ClO_4)_2\cdot 6H_2O$ in the presence of 2,2′-bipyridine (2,2′-bpy) affords a novel compound **1** (Scheme 1) in which Mn center displays a slightly distorted octahedron composed of two N atoms of 2,2′-bpy, one of three oxygen atoms of sulfonate group and two O atoms of water, as shown in Fig.1[1~5]. Furthermore, the dihedral angle between naphthalene rings has about 89.4°, almost perpendicular to each other while one of two sulfonate failed to take part in the coordination to Mn atom to result in the formation of discrete monomeric compound **1**. As expected, there are many strong H-bonds between water and sulfonate group to result in the formation of three-dimensional network as shown in Fig.2, and the bond lengths of C-C, C-O, C-S, S-O, C-Br C-N and Mn-N as well as Mn-O are unexceptional (see Fig.1 footnote).



Scheme 1

Experiment

Hydrothermal treatment of $Mn(ClO_4)_2\cdot 6H_2O$ (0.3 mmol), 6,6′-dibromo-2,2′-dmethoxy-1,1′-binaphthylene-4,4′-disulfonic acid (0.6 mmol), 2,2-bipyridine

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*通讯联系人。E-mail:songyumei@163.com
第一作者:宋玉梅,女,25 岁,博士生;研究方向:手性相转移催化剂合成及不对称催化。

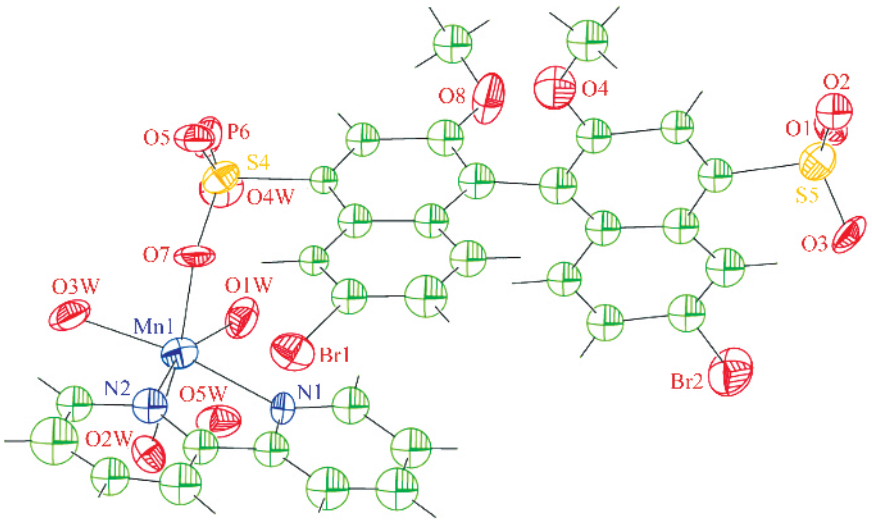

Fig.1 Perspective view of coordination compound **1** with a Mn center having a slightly distorted octehedron

Key bond distances (nm) and angles (°):

Mn(1)-O(7) 0.207 2(17), Mn(1)-O(2W) 0.214 7(15), Mn(1)-O(1W) 0.216 9(19), Mn(1)-O(3W) 0.218 8(17), Mn(1)-N(2) 0.222(2), Mn(1)-N(1) 0.226(2)

O(7)-Mn(1)-O(2W) 171.8(7), O(7)-Mn(1)-O(1W) 97.1(7), O(2W)-Mn(1)-O(1W) 89.6(6), O(7)-Mn(1)-O(3W) 91.3(6), O(2W)-Mn(1)-O(3W) 83.2(6), O(1W)-Mn(1)-O(3W) 96.6(7), O(7)-Mn(1)-N(2) 85.4(7), O(2W)-Mn(1)-N(2) 89.7(7), O(1W)-Mn(1)-N(2) 162.2(7), O(3W)-Mn(1)-N(2) 101.0(8), O(7)-Mn(1)-N(1) 93.3(7), O(2W)-Mn(1)-N(1) 91.3(7), O(1W)-Mn(1)-N(1) 91.1(8), O(3W)-Mn(1)-N(1) 170.6(8), N(2)-Mn(1)-N(1) 71.2(8)

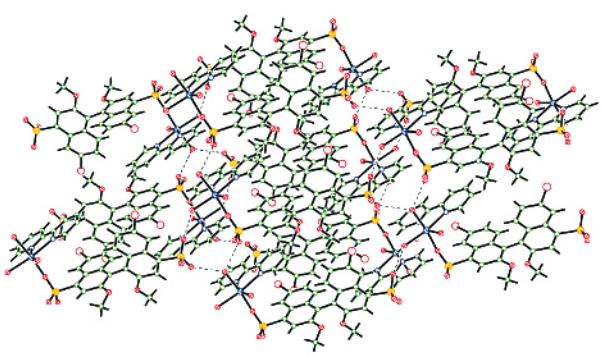

Fig.2 Presentation of 3D network through H-bonds of compound **1**

(1.2 mol), water (1.0 mL) and alchonol (1.0 mL) over two days at 120 ℃ yielded colorless block crystals[6~9]. The yield was about 65% based on acid 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. $C_{32}H_{32}Br_2MnN_2O_{13}S_2$, M=931.48, triclinic, $P\bar{1}$, a=0.815 5(19) nm, b=1.223 3(3) nm, c=1.560 0(4) nm, α=85.088 1(6)°, β=84.147(6)°, γ=77.932(6)°, V=1.880 9(7) nm^3, Z=2, 12 540 unique data (θ_{max}=33.5°), R=0.230 (1 948 [$I \geqslant 2\sigma(I)$] reflections), wR=0.539 (all data), ρ_{max}=865 e·nm^{-3}; water-H were not located. Programs used: SAINT, SADABS, SHELX-97, ORTEP.

CCDC: 277922.

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