研究简报

消旋的有机二磺酸三邻菲咯啉锌配合物

黄雪峰*,[1] 钱 坤[2]
([1]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)
([2]南昌大学稀土中心,南昌 330013)

关键词: 无机手性; 6,6′-二溴-2,2′-二甲氧基-1,1′-二萘-4,4′-二磺酸; 锌
中图分类号: O614.24+1 **文献标识码**: A **文章编号**: 1001-4861(2005)09-1437-02

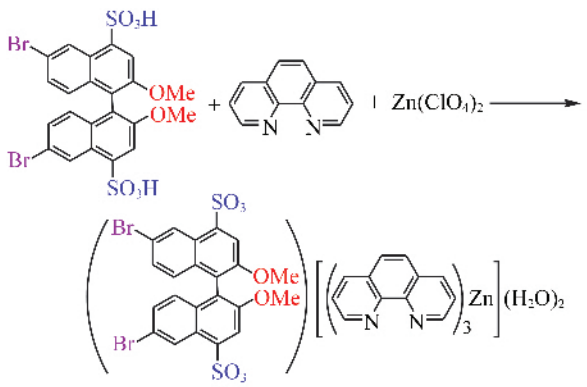
(*Δ*,*Λ*)-[Tris(1,10-phenanthroline)Zn(Ⅱ)] [(*R*,*S*)-6,6′-dibromo-2,2′-dimethoxy-1,1′-binaphthylene-4,4′-disulfonate]

HUANG Xue-Feng*,[1] QIAN Kun[2]
([1]*Coordination Chemistry Institute,State Laboratory of Coordination Chemistry, Nanjing University, Nanjing* 210093)
([2]*Center of Rare Earth, Nanchang University, Nanchang* 330013)

Abstract: Compound [Zn(phen)$_3$][BDA] (**1**) (BDA=6,6′-dibromo-2,2′-dimethoxy-1,1′-binaphthylene-4,4′-disulfonate, phen= 1,10-phenanthroline) composes of the anion part (racemic-(*R*,*S*)-6,6′-dibromo-2,2′-dimethoxy-1,1′-binaphthylene-4,4′-disulfonate) and the cation part which consists of a racemic octahedrally coordinated zinc center defined six nitrogen atoms from three phen rings to form an inorganic chirality that can be resolution by chiral organic ligand, the 3D framework was formed through the strong H-bonding interaction between sulfonate and water. CCDC: 277924.

Key words: inorganic chirality; 6,6′-dibromo-2,2′-dimethoxy-1,1′-binaphthylene -4,4′-disulfonic; Zinc(Ⅱ)

Compound **1** was prepared under hydrothermal conditions by the reaction of racemic 6,6′-dibromo-2,2′-dimethoxy-1,1′-binaphthylene-4,4′-disulfonic acid (H_2BDA), 1,10-phenanthroline (phen) and $Zn(ClO_4)_2\cdot 6H_2O$[1~5]. The local coordination geometry around each Zn center in **1** (Fig.1) is a slightly distorted octahedron defined six nitrogen atoms from three different phen ligands while the organic ligand H_2BDA loses its two protons and change to BDA which fail to coordinate to zinc atom. That is, the compound composes of anion(BDA) part and cation part [Zn(phen)$_3$] which can be defined as *Δ* or *Λ* in crystallography. It is worth noting that racemic [Zn(phen)$_3$] can be optical resolution if a chiral H_2BDA induced. In addition, there are two uncoordinated water existing in the crystal struc-



Scheme 1

收稿日期:2005-02-15。收修改稿日期:2005-06-01。
973 项目(No.G2000077500)资助。
*通讯联系人。E-mail:hxf-china@163.com
第一作者:黄雪峰,男,28 岁,博士生;研究方向:不对称合成及催化。

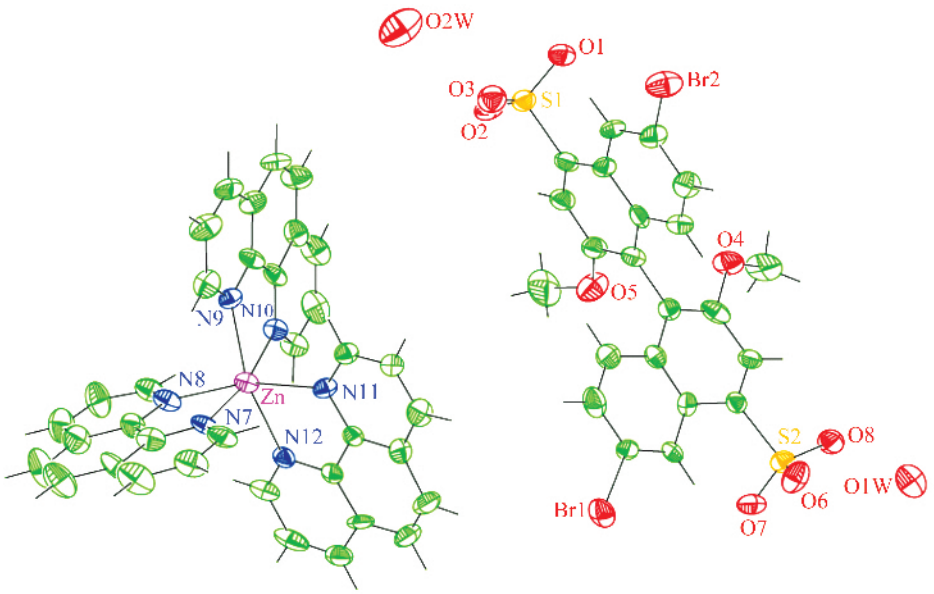


Fig.1 ORTEP of the molecule **1** at 30% probability

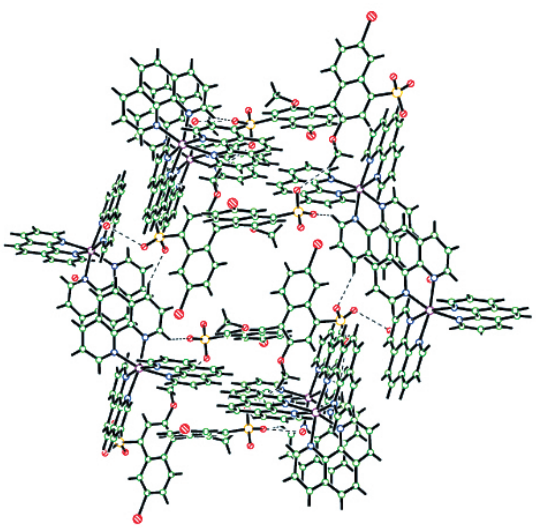


Fig.2 A crystal packing perspective view of **1**

ture to result in the strong hydrogen bonds between sulfonate group and water to form 3D network. As expected, the bond distance of C-C, C-O, C-S, S-O, C-Br and Zn-N are unexceptional, while the dihedron angle of BDA in compound **1** is almost perpendicular to each other.

Experiment

Hydrothermal treatment of $Zn(ClO_4)_2 \cdot 6H_2O$ (0.3 mmol), 6,6′-dibromo-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 alchonol (1.0 mL) over two days at 130 ℃ yielded colorless block crystals[6~9]. The yield was about 42% based on acid. Intensity data were collected at 293(2) K on a Bruker AXS SMART CCD $C_{58}H_{42}Br_2ZnN_6O_{10}S_2$, M=1 272.29, triclinic, $P\bar{1}$, a=1.210 8(3) nm, b=1.578 7(4) nm, c=1.851 5(5) nm, α=69.500(5)°, β=88.251(6)°, γ=67.923(6)°, V=3.051 0(14) nm^3, Z=2, 7 691 unique data (θ_{max}=26.0°), R=0.092 7 (3 087 [$I \geqslant 2\sigma(I)$] reflections), wR=0.325 (all data), ρ_{max}=1 480 e·nm^{-3}; water-H were not located. Programs used: SAINT, SADABS, SHELX-97, ORTEP.

CCDC: 277924.

References:

[1] Zeng X R, Xiong R G, Xu Y, et al. *Cryst. Struc. Commun. Acta Cryst. Sec C*, **2000**,**56**:943~944

[2] Xie Y R, Xiong R G, Xue X, et al. *Inorg. Chem.*, **2002**,**41**: 3323~3326

[3] Xiong R G, Zhang J, Chen Z F, et al. *J. Chem. Soc., Dalton Trans.*, **2001**:780~782

[4] Ye Q, Wang X S, Zhao H, et al. *Chem. Soc. Rev.*, **2005**,**34**: 208~225

[5] Xiong R G, You X Z, Abrahams B F, et al. *Angew. Chem. Int. Ed.*, **2001**,**40**:4422~4424

[6] SONG Yu-Mei(宋玉梅), PANG Jie(庞 洁). *Wuji Huaxue Xuebao(Chin. J. Inorg. Chem.)*, **2005**,**21**:1433~1434

[7] TANG Yun-Zhi(唐云志), ZHOU Ting(周 挺). *Wuji Huaxue Xuebao(Chin. J. Inorg. Chem.)*, **2005**,**21**:1435~1436

[8] XIE Yong-Rong(谢永荣), YE Qiong(叶 琼). *Wuji Huaxue Xuebao(Chin. J. Inorg. Chem.)*, **2005**,**21**:1439~1440

[9] XIE Yong-Rong(谢永荣), YE Qiong(叶 琼). *Wuji Huaxue Xuebao(Chin. J. Inorg. Chem.)*, **2005**,**21**:1441~1442