

系列 Cu(II/I)配聚物的合成、结构及光电性能

金晶¹ 徐晓婷¹ 丛盛美¹ 李雷¹ 张广宁² 牛淑云^{1,*}
(¹辽宁师范大学化学化工学院, 辽宁 大连 116029; ²辽宁师范大学功能材料化学研究所, 辽宁 大连 116029)

Syntheses, Structures and Photoelectron Property of a Series of Cu(II/I) Coordination Polymers

JIN Jing¹ XU Xiao-Ting¹ CONG Sheng-Mei¹ LI Lei¹
ZHANG Guang-Ning² NIU Shu-Yun^{1,*}

(¹School of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, Liaoning Province, P. R. China; ²Institute of Chemistry for Functionalized Materials, Liaoning Normal University, Dalian 116029, Liaoning Province, P. R. China)

*Corresponding author. Email: syniu@sohu.com; Tel: +86-411-82159044.

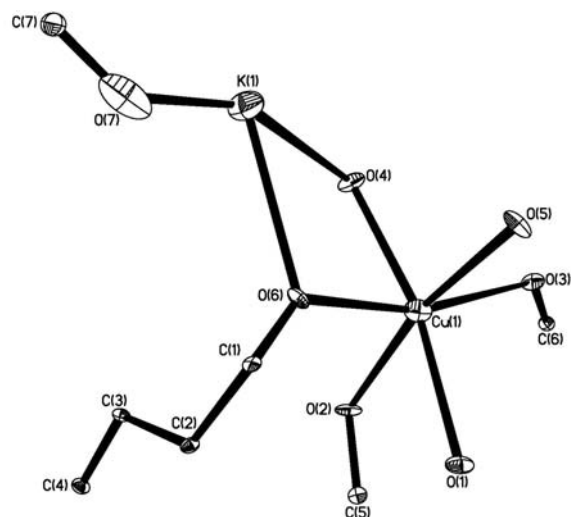


图 S1 配合物(1)的不对称单元

Fig.S1 Asymmetric unit of complex (1)

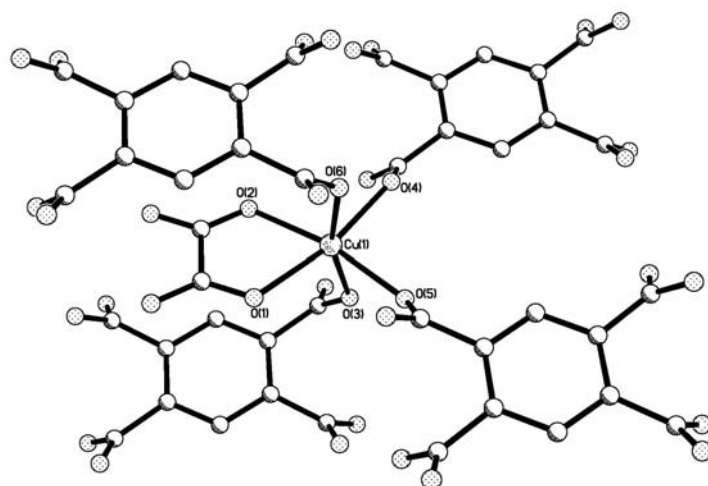


图 S2 配合物(1)中 Cu(II)离子的配位环境

Fig.S2 Coordination environment of Cu(II) ion in complex (1)

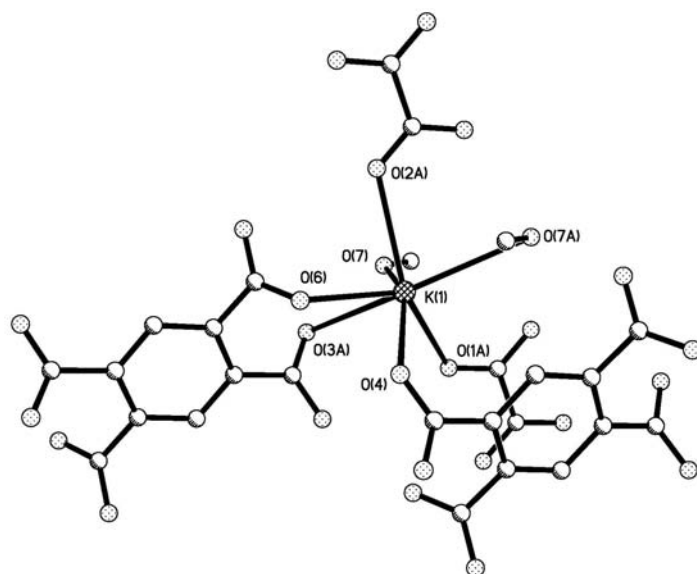


图 S3 配合物(1)中 K(I)离子的配位环境

Fig.S3 Coordination environment of K(I) ion in complex (1)

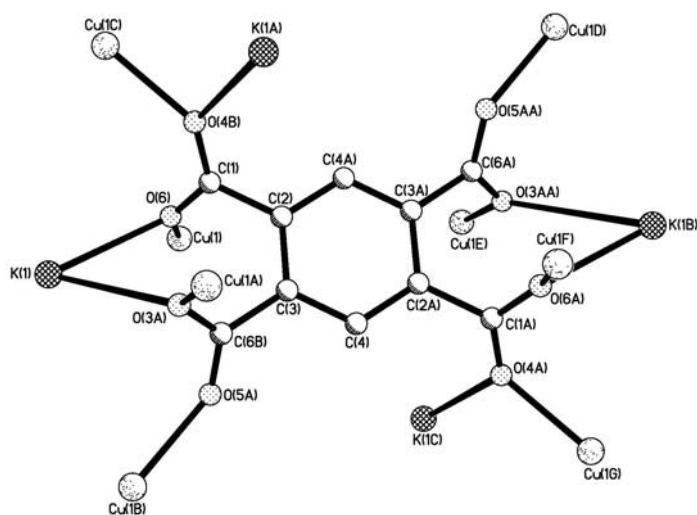


图 S4 配合物(1)中均苯四甲酸根离子的配位模式

Fig.S4 Coordination mode of btct anions in complex (1)

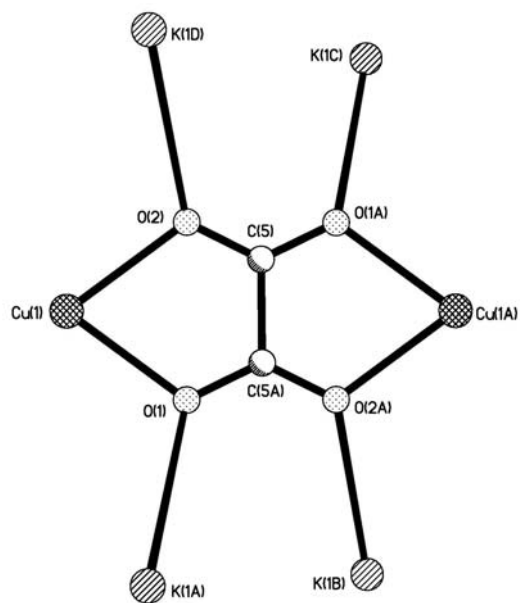


图 S5 配合物(1)中草酸根离子的配位模式

Fig.S5 Coordination mode of ox anions in complex (1)

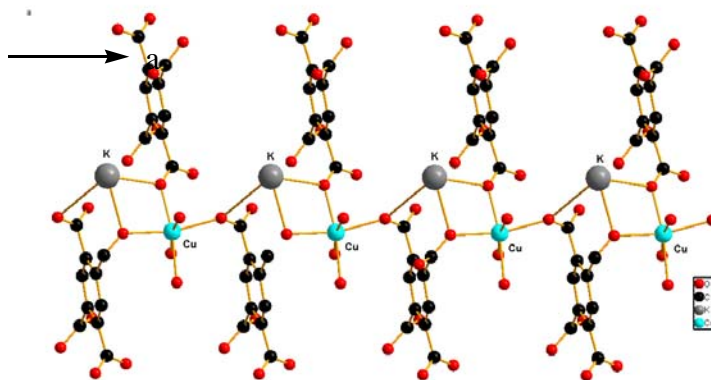
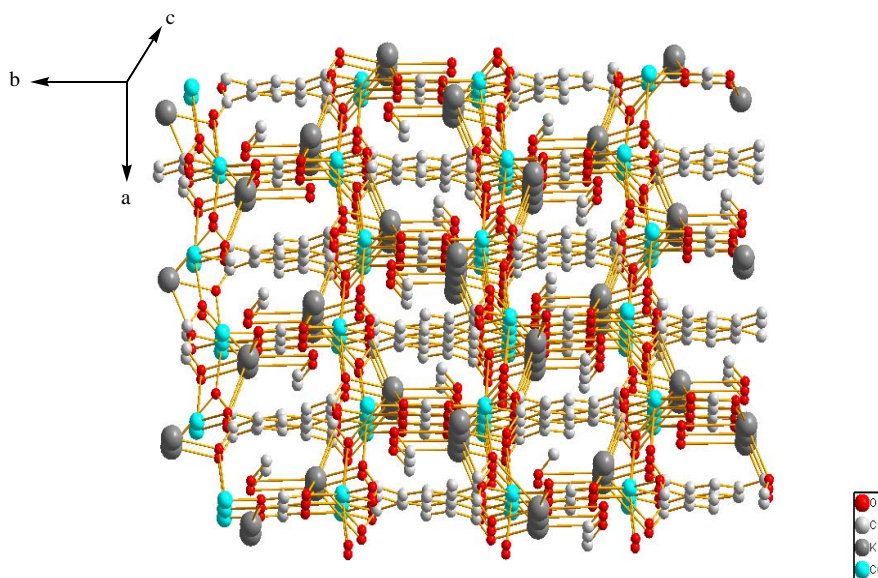


图 S6 配合物(1)沿 a 方向的 1D 无限链

Fig.S6 1D chain of complex (1) along a axis



图S7 配合物(1)的3D无限结构

Fig. S7 3D framework of complex (1)

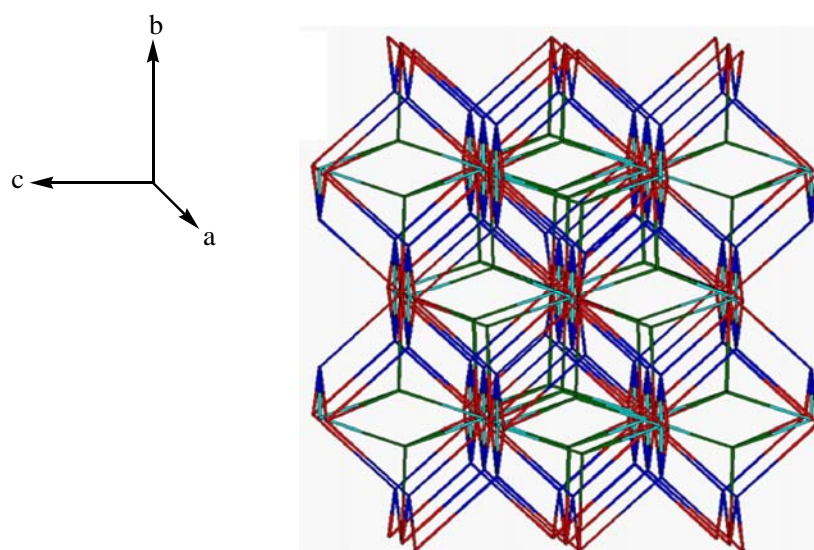


图 S8 配合物(1)的 4-节点(4, 5, 6, 12)-连接拓扑图

Fig. S8 4-nodal (4, 5, 6, 12)-connected topology of complex (1)
(red) btec node; (cyan) ox node; (blue) Cu node; (green) K node

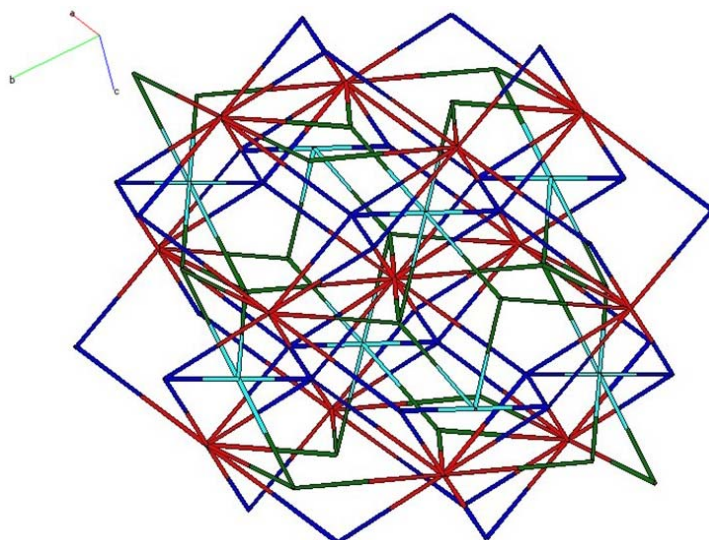


图 S9 配合物(1)的 4-节点(4, 5, 6, 12)-连接拓扑图

Fig. S9 4-nodal (4,5,6,12)-connected topology of complex (1)
(red) btec node; (cyan) ox node; (blue) Cu node; (green) K node

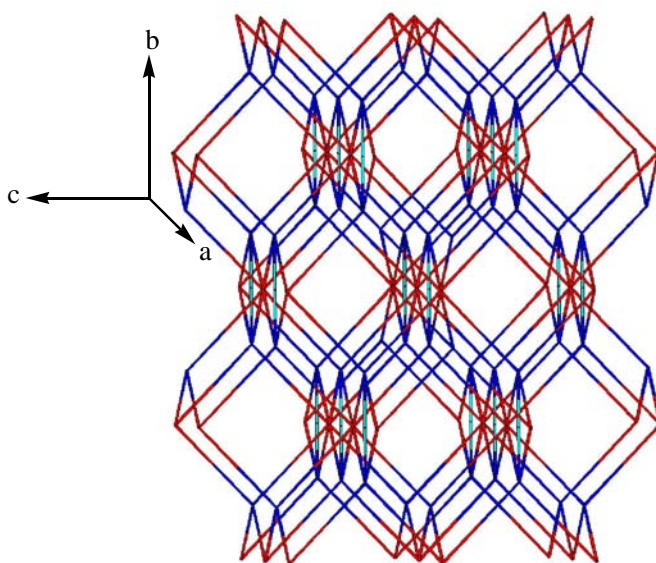


图 S10 配合物(1)的 3-节点(2, 5, 8)-连接拓扑图

Fig.S10 3-nodal (2, 5, 8)-connected topology of complex (1)
(red) btec node; (cyan) ox node; (blue) Cu node (K(I) node is omitted for clarity)

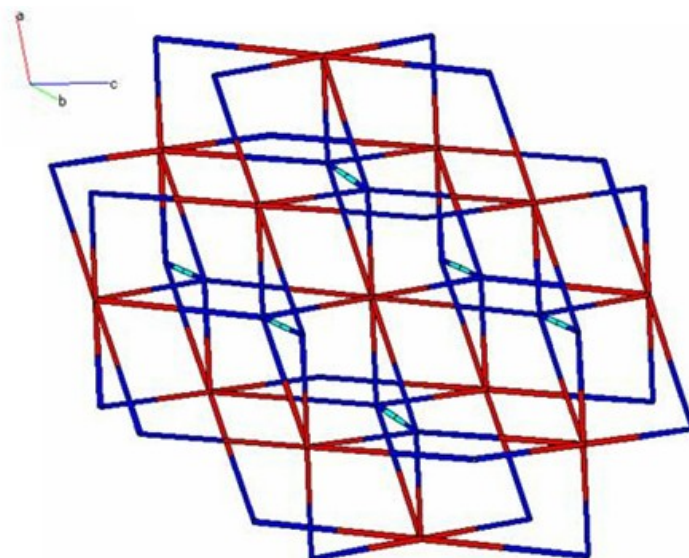


图 S11 配合物(1)的 3-节点(2, 5, 8)-连接拓扑图

Fig.S11 3-nodal (2, 5, 8)-connected topology of complex (1)

(red) btec node; (cyan) ox node; (blue) Cu node (K(I) nodes are omitted for clarity)

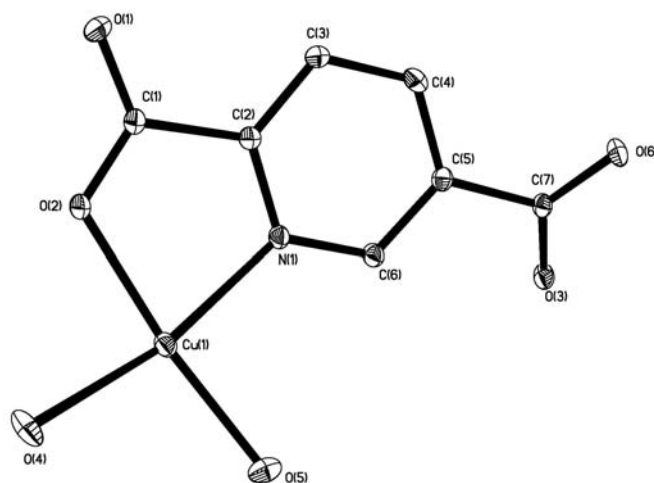


图 S12 配合物(2)的不对称单元(游离水分子被删掉)

Fig. S12 Asymmetric unit of complex (2) (dissociative water molecules are omitted)

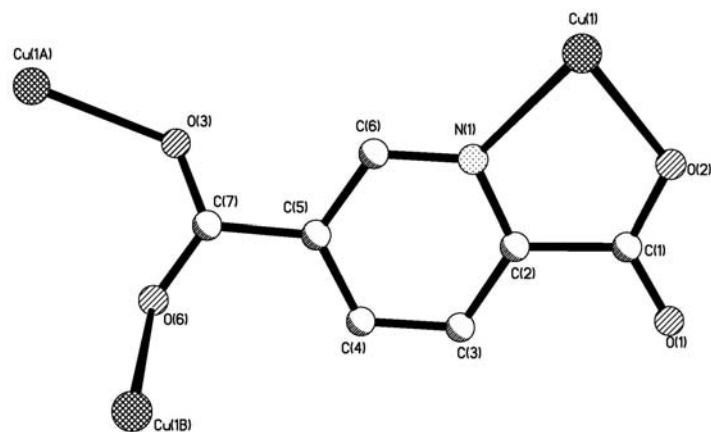


图 S13 配合物(2)中 2,5-pdc²⁻的配位模式

Fig. S13 Coordination mode of 2,5-pdc²⁻ in complex (2)

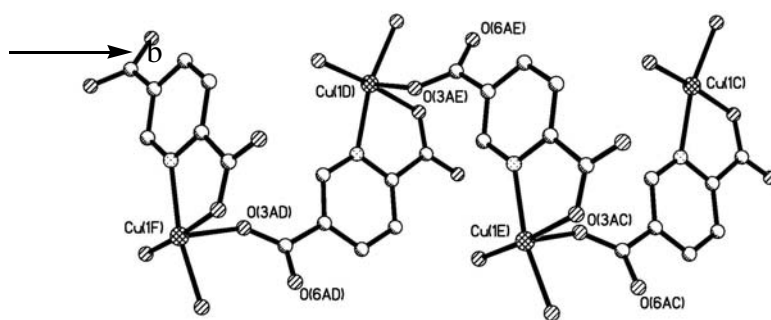


图 S14 配合物(2)沿 *b* 方向的 1D 无限链

Fig. S14 1D chain of complex (2) along *b* axis

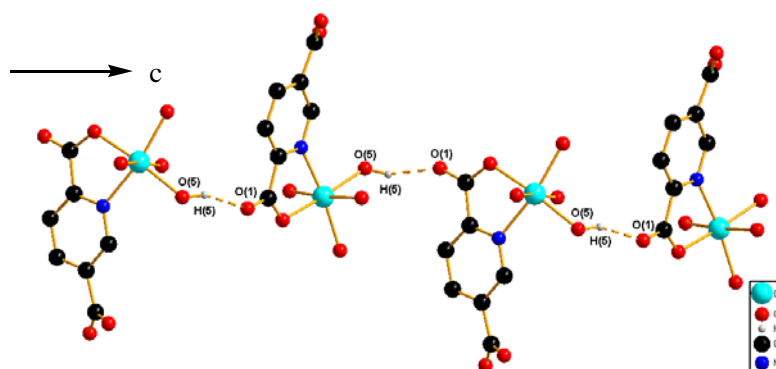


图 S15 配合物(2)沿 *c* 方向的 1D 氢键链

Fig.S15 1D hydrogen-bonded chain of complex (2) along *c* axis

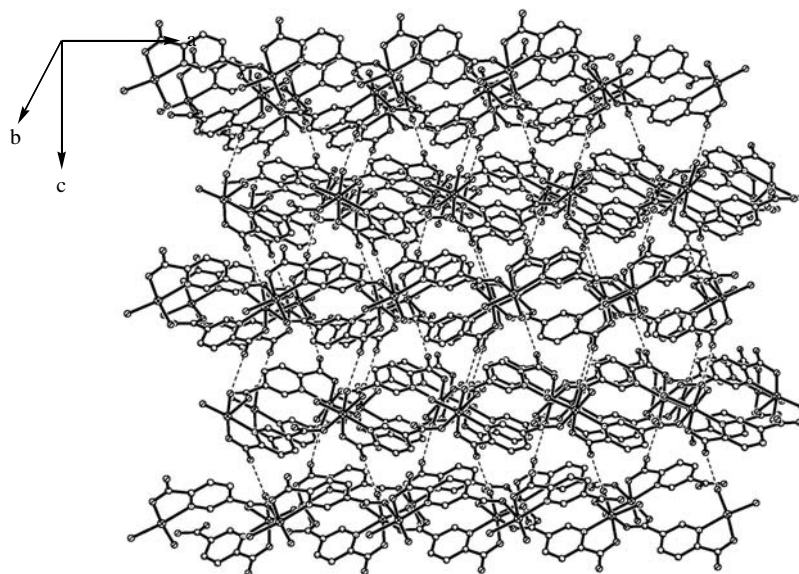


图 S16 配合物(2)的 3D 氢键网络结构

Fig.S16 3D hydrogen-bonded network structure of complex (2)

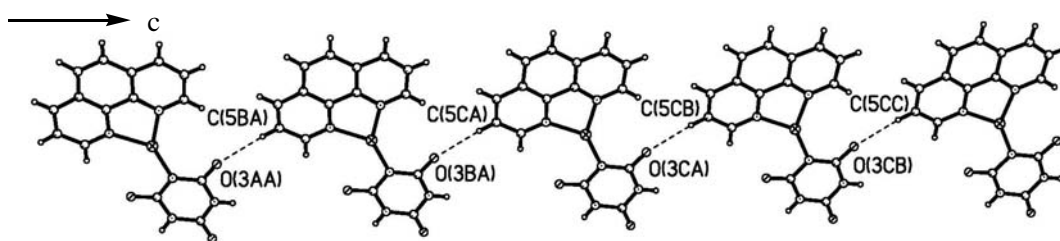


图 S17 配合物(3)沿 c 方向的氢键

Fig. S17 1D hydrogen-bonded chain of complex (3) along c axis

SPS 的测定

样品的准备. 将样品研碎后均匀的放在两块ITO导电玻璃间, 并使ITO导电面和样品相接触, 形成ITO/样品/ITO的三明治结构. 将装好样品的ITO玻璃放于样品池中, 并与自建外场的正负极相接, 放在上面的ITO玻璃接正极, 下面接负极.

样品池的安装. 将装好样品的样品池放到实验装置上, 并且同锁相放大器相连接. 让通过单色仪的光会聚在样品池上, 经过调制解调器斩波后垂直照射到样品的表面上, 保证光斑完全照射在样品上. 这时, 锁相放大器将能够检测到经过不同频率的光照射所产生的信号, 并将其放大.

数据转换及处理. 经光照射所产生的光电压信号, 通过锁相放大器收集, 并

将其转换为数据文件，最后经尾处理机程序处理得到SPS的光谱数据和谱图.

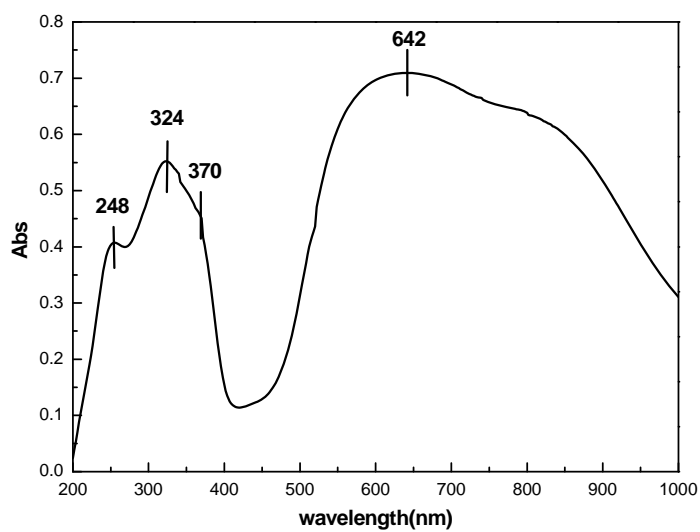
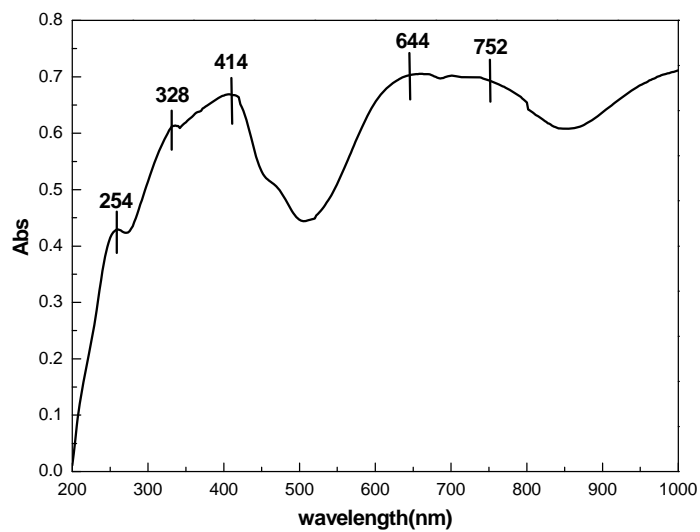


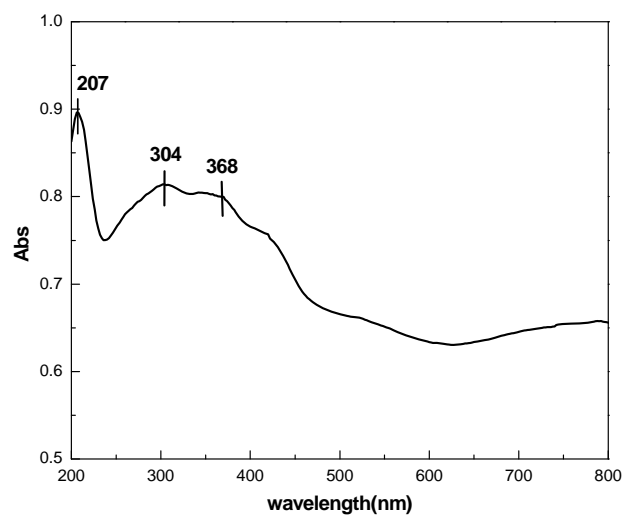
图 S18 配合物(1)的 UV-Vis 吸收光谱

Fig. S18 UV-Vis spectrum of complex (1)



图S19 配合物(2)的UV-Vis吸收光谱

Fig. S19 UV-Vis spectrum of complex (2)



图S20 配合物(3)的UV-Vis吸收光谱

Fig. S20 UV-Vis spectrum of complex (3)

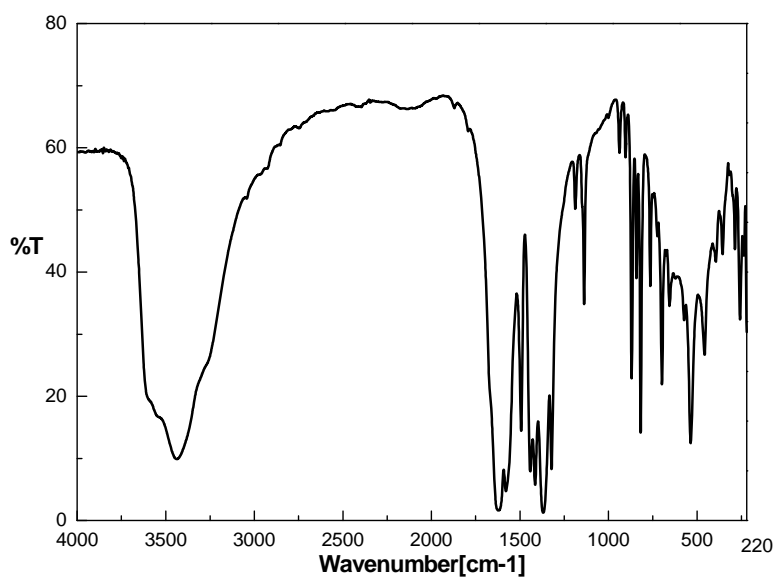


图 S21 配合物(1)的红外光谱

Fig. S21 IR spectrum of complex (1)

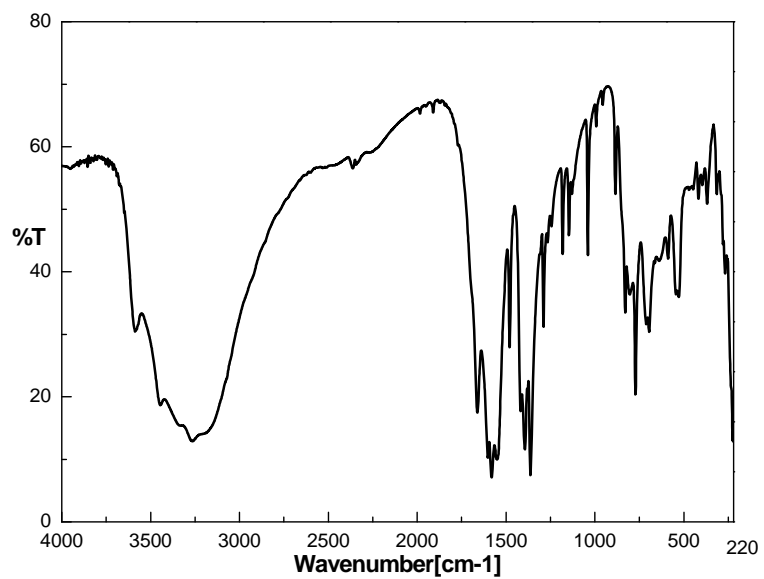


图 S22 配合物(2)的红外光谱

Fig. S22 IR spectrum of complex (2)

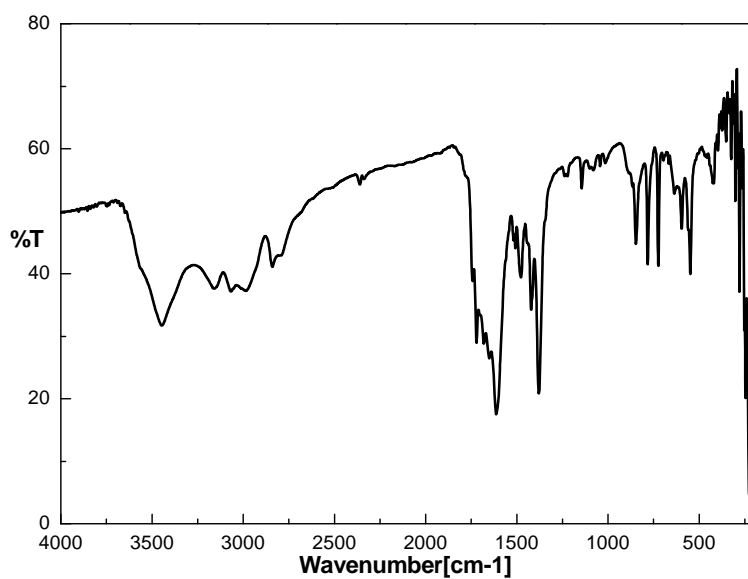


图 S23 配合物(3)的红外光谱

Fig. S23 IR spectrum of complex (3)