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Full Papers

1,1-环丁烷二羧酸单、双核铜配合物的合成、晶体结构、热分析和磁性

李明星*, [a], 戴惠[1], 邵敏[1], 石磊[1], 林昆华[1], 程智萱[1], 翁林红[2]

[1]上海大学理学院化学系, 上海200444，中国

[2]复旦大学化学系，上海200433, 中国

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摘要 1,1-环丁烷二羧酸根（cbdc）与$Cu(ClO_4)_2$和邻啡罗啉（phen）在乙醇-水溶液中反应，合成二个铜配合物：[Cu(cbdc)(phen)(H_2O)]·2H_2O（**1**）和[Cu_2(cbdc)(phen)$_2$ (H_2O)$_2$] (ClO_4)$_2$·H_2O（**2**）。晶体**1**属单斜晶系，*P*2(1)/*c*空间群，晶胞参数*a*=0.9428(4), *b*=1.2183(5), *c*=1.6265(7)nm, *β*= 102.418(5) °, *V*=1.8246(13) nm^3, *Z*=4, *R*=0.0445, wR_2=0.0947。铜离子被cbdc、phen和H_2O五配位，形成四方锥结构。分子间通过π…π重叠和氢键作用，堆积成三维超分子结构。采用TG-DSC热分析详细研究了该配合物的热分解过程。晶体**2**属单斜晶系，*P*2(1)/*c*空间群，晶胞参数*a*=0.8897(3), *b*=1.9130(8), *c*=1.9936(8)nm,*β*=99.04(2) °, *V*=3.351(2)nm^3, *Z*=4, *R*=0.0540, wR_2=0.1102。该化合物为羧基桥联的双核铜配合物，Cu(1)被cbdc和phen平面四配位，Cu(2)被cbdc、phen和二分子水五配位，形成变形的三角双锥结构。变温磁化率研究（2-300 K）表明，该配合物的磁性遵从居里定律，对该配合物的磁性和结构关系做了讨论。

关键词 铜配合物、1,1-环丁烷二羧酸、晶体结构、热稳定性、磁性。

分类号

Synthesis, Crystal Structures, Thermal Analysis and Magnetic Property of Mono- and Bi-nuclear 1,1-Cyclobutanedicarboxy- late Copper Complexes

LI Ming-Xing*,[1], DAI Hui[1], SHAO Min[1], SHI Lei[1], LIN Kun-Hua[1], CHENG Zhi-Xuan[1], WENG Lin-Hong[2]

[1] *Department of Chemistry, College of Science, Shanghai University, Shanghai 200444, China*

[2] *Department of Chemistry, Fudan University, Shanghai 200433, China*

Abstract Two new copper complexes, [Cu(cbdc)(phen)(H_2O)]•2H_2O (**1**) and [Cu_2(cbdc)(phen)$_2$(H_2O)$_2$](ClO_4)$_2$•H_2O (**2**) (cbdc＝1,1-cyclobutanedicarboxylate and phen＝1,10-phenanthroline), were synthesized by reaction of cbdc with Cu(ClO_4)$_2$ and phen in ethanol aqueous solution. Complex **1** crystallizes in monoclinic system with space group *P*2(1)/*c* and *a*＝0.9428(4) nm, *b*＝1.2183(5) nm, *c*＝1.6265(7) nm, *β*＝102.418(5)°, *V*＝1.8246(13) nm^3, *Z*＝4, *R*＝0.0445, wR_2＝0.0947. The structure of **1** is discretely mononuclear, which is packed by π…π interaction forming a 3D supramolecular structure where Cu(II) ion is five-coordinated and has square-pyramidal coordination geometry. Its thermal decomposition procedure detail was studied by thermal analysis TG-DSC. Complex **2** belongs to monoclinic system with space group *P*2(1)/*c* and *a*＝0.8897(3) nm, *b*＝1.9130(8) nm, *c*＝1.9936(8) nm, *β*＝99.04(2)°, *V*＝3.351(2) nm^3, *Z*＝4, *R*＝0.0540, wR_2＝0.1102. The structure of **2** is a discrete binucleus, where Cu(1) is four-coordinated by phen and cbdc in a square-planar geometry while Cu(2) is five-coordinated by phen, one O of cbdc and two H_2O, which can be best described as distorted trigonal-bipyramidal geometry. Cu(1) and Cu(2) are linked by carboxylic group of cbdc in a bidentate bridging fashion. Variable-temperature magnetic susceptibilities of **2** in 2—300 K showed that its magnetic behavior obeyed Curie law.

Key words copper complex 1 1-cyclobutanedicarboxylate crystal structure thermal analysis magnetic property

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通讯作者 李明星 mx_li@mail.shu.edu.cn