化学学报 2005 63 (6): 550-554 ISSN: 0567-7351 CN: 31-1320/06

研究简报

新型一维梯状双链配位聚合物{[Cu(malate)(2,2'-bipy)]•3H$_2$O}$_\infty$的合成、晶体结构与表征

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收稿日期 2004-6-15 修回日期 2004-11-23 网络版发布日期 接受日期

摘要 合成了铜(II)与羟基丁二酸和2,2'-联吡啶形成的配位聚合物{[Cu(malate)(2,2'-bipy)]•3H$_2$O}$_\infty$ (其中malate＝羟基丁二酸根, 2,2'-bipy＝2,2'-联吡啶), 通过X射线衍射测定了单晶结构, 并进行了元素分析、红外光谱、紫外光谱、热分析等研究. 配合物属单斜晶系, 空间群*P*2(1)/*c*; 晶胞参数: *a*＝0.70132(10) nm, *b*＝1.9730(3) nm, *c*＝1.18998(16) nm, *β*＝94.551(3)°; *Z*＝2; 最终偏离因子*R*＝0.0483. 配合物中每个铜(II)原子与来自2,2'-联吡啶的两个氮原子和两个羟基丁二酸根的三个氧原子配位, 形成畸变的三角双锥结构单元. 每个羟基丁二酸根以*R*构型方式桥联两个三角双锥结构单元, 沿*a*轴方向无限延伸形成一维链. 两条平行链以面对面的方式重叠, 彼此吡啶环之间存在强的(-(相互作用, 加之C$_{吡啶环}$—H…O$_{羧基}$弱相互作用形成新颖的梯状双链结构, 比邻的梯状双链又通过分子间O$_{羟基}$-H…O$_{羧基}$氢键沿*a*轴方向共同构筑了具有隧道的三维结构.

关键词 羟基丁二酸铜(II) 配位聚合物 晶体结构

分类号

Syntheses, Characterization and Crystal Structure of a Novel Polymeric Complex {[Cu(malate)(2,2'-bipy)]·3H$_2$O}$_\infty$ (malate＝malate dianion) with Ladder-Shaped Double Chains Structure

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Abstract Copper(II) malate polymeric complex with 2,2'-bipy, {[Cu(malate)(2,2′-bipy)]•3H$_2$O}$_\infty$, has been synthesized and characterized by means of elemental analysis, thermal analysis, IR and UV-vis spectroscopy. The single crystal X-ray diffraction study shows that the complex is monoclinic, with space group *P*2(1)/*c*, *a*＝0.70132(10) nm, *b*＝1.9730(3) nm, *c*＝1.18998(16) nm, *β*＝94.551(3)°, *Z*＝2 and *R*＝0.0483. Each Cu(II) atom is coordinated by two nitrogen atoms from 2,2'-bipy and three oxygen atoms from two different malate dianions with a distorted trigonal bipyramidal geometry. The malate dianion adopts an *R* conformation bridging two copper centers, giving rise to a 1-D polymeric chain along the crystallographic axis *a*, and two parallel 1-D chains are constituted to form a novel ladder-shaped double chain structure through (-(interactions between the pyridine rings and C$_{pyridine}$—H…O$_{hydroxyl}$ weak interactions. On the other hand, the neighboring double chains are extended into a 3-D structure with channels via intramolecular O$_{hydroxyl}$-H…O$_{carboxyl}$ hydrogen bonds in the direction of axis *a*.

Key words copper(II) malate polymeric complex crystal structure

DOI:

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