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研究论文

二维配位聚合物[Cu(ox)(4,4'-bpy)]$_n$的水热合成与结构表征

任红[1], 徐家宁[2], 于连香[2], 叶俊伟[3], 毕明辉[1], 张萍[2], 宋天佑[1]

1. 吉林大学无机合成与制备化学国家重点实验室,
2. 化学学院,
3. 超分子化学与材料教育部重点实验室, 长春 130012

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摘要 采用水热方法合成出一种新型配位聚合物[Cu(ox)(4,4'-bpy)]$_n$(ox=草酸根离子, 4,4'-bpy=4,4'-联吡啶), 并通过X射线单晶结构分析、元素分析以及红外光谱测定对该化合物进行了表征. 结果表明, 标题化合物属于单斜晶系, *Cm*空间群, 晶胞参数*a*=1.1921(7) nm, *b*=1.153(7) nm, *c*=0.5155(4) nm, *β*=113.38(3)°, *V*=0.6291(7) nm^3, *Z*=2. 该化合物是一个由{Cu(ox)}$_n$链通过桥联配体4,4'-bpy垂直相连并具有矩形格子结构的二维层状配位聚合物, 层与层之间交错排列, 通过$C_{4,4'\text{-bpy}}$—H…O_{ox}层间氢键作用, 进一步扩展成三维超分子网络结构.

关键词 水热合成 Cu(Ⅱ)配位聚合物 混合配体 层状结构 超分子网络

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Hydrothermal Synthesis and Structure Characterization of a 2D Coordination Polymer [Cu(ox)(4,4'-bpy)]$_n$

REN Hong[1], XU Jia-Ning[2], YU Lian-Xiang[2], YE Jun-Wei[3], BI Ming-Hui[1], ZHANG Ping[2]*, SONG Tian-You[1]*

1. Key Laboratory of Inorganic Synthesis and Preparative Chemistry,
2. College of Chemistry,
3. Key Laboratory for Supramolecular Structure and Materials of Ministry of Education, Jilin University, Changchun 130012, China

Abstract A new polymer [Cu(ox)(4,4'-bpy)]$_n$(1)(ox=$C_2O_4^{2-}$, 4,4'-bpy=4,4'-bipyridine) was hydrothermally synthesized and characterized *via* elemental analyses, IR spectrum and single crystal X-ray diffraction. The polymer crystallizes in a monoclinic system, space group *Cm*, *a*=1.1921(7) nm, *b*=1.153(7) nm, *c*=0.5155(4) nm, *β*=113.38(3)°, *V*=0.6291(7) nm^3, *Z*=2. Cu atom in the title compound is in an octahedral geometry with four O atoms from two bis-chelating oxalate ligands in equatorial plane and two N atoms from the 4,4'-bpy ligands in the axial position. The crystal structure possesses infinite {Cu(ox)}$_n$ chains connected with each other by the bridging 4,4'-bpy ligands in a perpendicular manner, leading to a 2D layered network with rectangular grids. The layers stacking in a staggered fashion are further assembled by $C_{4,4'\text{-bpy}}$—H…O_{ox} hydrogen bonds and lead to a 3D supramolecular architecture.

Key words Hydrothermal synthesis Copper(Ⅱ) coordination polymer Mixed-ligand Layered structure Supramolecular architecture

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通讯作者 张萍 zhangping@jlu.edu.cn