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研究论文

具有纳米孔结构的配位聚合物$[Co_2(HO\text{-}BDC)_2(bpe)_2(H_2O)_2]_n\cdot n(py)\cdot nH_2O$的合成、晶体结构与热稳定性

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摘要 在水-吡啶混合体系中, 以5-羟基-1,3-苯二甲酸(简作HO-H_2BDC)、1,2-二(4-吡啶)乙烷(简作bpe)为配体与$Co(NO_3)_2\cdot 6H_2O$反应, 培养出$[Co_2(HO\text{-}BDC)_2(bpe)_2(H_2O)_2]_n\cdot n(py)\cdot nH_2O$(py=pyridine)的紫色单晶, 该晶体属三斜晶系, *P*1空间群, 晶胞参数*a*=1.0245(3) nm, *b*=1.1467(3) nm, *c*=1.2430(4) nm, *α*=68.915(5)°, *β*=67.163(4)°, *γ*=71.373(4)°, *V*=1.2279(6) nm^3, *Z*=1, M_r=979.70, D_c=1.325 Mg/m^3, *F*(000)=506, *μ*=0.740 mm^{-1}, R_1=0.0515, wR_2=0.1058. 该配位聚合物中在*ac*平面上具有规则平行四边形纳米尺寸的孔, 其孔径大小约为1.025 nm×1.354 nm, 而且通过氢键相互作用连成具有双层结构的2D网络结构. TGA曲线表明, 配位聚合物的失重发生在110~150 ℃之间, 总失重约为80.1%, 最终产物为Co_2O_3.

关键词 钴配位聚合物 5-羟基-1,3-苯二甲酸 1,2-二(4-吡啶)乙烷 晶体结构 氢键

分类号 0614

Synthesis, Crystal Structure and Thermal Stability of Coordination Polymer $[Co_2(HO\text{-}BDC)_2(bpe)_2(H_2O)_2]_n\cdot n(py)\cdot nH_2O$ with Nanoscale Channels

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Abstract A novel coordination ploymer $[Co_2(HO\text{-}BDC)_2(bpe)_2(H_2O)_2]_n\cdot n(py)\cdot nH_2O$[where HO-$H_2$BDC is 5-hydroxyisophthalic acid and bpe is 1,2-bis(4-pyridyl)ethane, py is pyridine] with nanoscale channels was synthesized and characterized via elemental analysis, IR spectra and single-crystal X-ray diffraction. The crystal belongs to triclinic crystal system, space group *P*1, with *a*=1.0245(3) nm, *b*=1.1467(3) nm, *c*=1.2430(4) nm, *α*=68.915(5)°, *β*=67.163(4)°, *γ*=71.373(4)°, *V*=1.2279(6) nm^3, *Z*=1, M_r=979.70, D_c=1.325 Mg/m^3, *F*(000)=506, *μ*=0.740 mm^{-1}, the final R_1=0.0515 and wR_2=0.1058 for 3625 observed reflections with $I>2\sigma(I)$. The coordination polymer has a 2D rectangular grid framework parallel to the ac plane with a dimension of 1.025 nm×0.1354 nm via strong hydrogen-bonding interactions. TGA curves of the coordination polymer show three main weight losses in the range of 110—150 ℃, 200—300 ℃ and 320—450 ℃ corresponding to the removal of non-coordinatated water molecules, non-coordinatated py molecules and the water and bpe molecules attached to metal, respectively, and the final resid

ue is identified to be Co_2O_3.

Key words Co coordination polymer 5-Hydroxyisophthalic acid 1 2-Di(Pyridine)ethane Crystal structure Hydrogen bond

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