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研究论文

一个新颖的三核镍配合物[Ni$_3$(C$_{13}$H$_9$N$_2$O)$_5$(CH$_3$OH)(CH$_3$CH$_2$OH)]Cl的合成、晶体结构及性质研究

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摘要 在甲醇-乙醇混合溶剂中, 含有N, O给体的二齿配体2-(2-羟苯基)苯并咪唑与NiCl$_2$•6H$_2$O在常温下反应合成得到标题化合物, 采用元素分析、红外光谱、紫外光谱、热分析以及X射线单晶衍射法对其进行了组成和结构表征. 结果表明该化合物为三斜晶系, 空间群*P*-1, 晶胞参数: *a*＝1.2046(2) nm, *b*＝1.4891(3) nm, *c*＝2.1342(4) nm, *α*＝96.787(3)°, *β*＝104.862(3)°, *γ*＝99.993(3)°, *V*＝3.5904(12) nm^3, *Z*＝2, *D*$_c$＝1.349 g/cm^3, *F*(000)＝1516, GOF＝1.008, *R*$_1$＝0.0583, *wR*$_2$＝0.1455 [*I*＞2*σ*(*I*)]. 在标题化合物的晶体结构中, 晶体学不对称的三个配位中心Ni(II)原子配位环境各不相同, 五个配体提供的五个氧配位基中有四个起着桥联的作用, 形成了一个新颖的V型金属簇状化合物. 变温磁化率研究表明标题化合物在整体上表现为弱的反铁磁性耦合作用.

关键词 2-(2-羟苯基)苯并咪唑 三核镍配合物 晶体结构 热分解 磁性质

分类号

Synthesis, Crystal Structure and Thermal Decomposition of a Novel Trinuclear Nickel Complex [Ni$_3$(C$_{13}$H$_9$N$_2$O)$_5$(CH$_3$OH)(CH$_3$CH$_2$OH)]Cl

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Abstract The trinuclear complex [Ni$_3$(C$_{13}$H$_9$N$_2$O)$_5$(CH$_3$OH)(CH$_3$CH$_2$OH)]Cl was obtained by the reaction of the bidentate N,O-donor ligand 2-(2-hydroxyphenyl)benzimidazole with NiCl$_2$•6H$_2$O in methanol-etha- nol at room temperature. The structure and chemical composition of title complex were determined by elemental analysis, IR spectrum, UV-Vis spectrum, thermal analysis and X-ray diffraction analysis. The crystal structure belongs to triclinic system, space group *P*-1 with *a*＝1.2046(2) nm, *b*＝1.4891(3) nm, *c*＝2.1342(4) nm, *α*＝96.787(3)°, *β*＝104.862(3)°, *γ*＝99.993(3)°, *V*＝3.5904(12) nm^3, *Z*＝2, *D*$_c$＝1.349 g/cm^3, *F*(000)＝1516, GOF＝1.008, *R*$_1$＝0.0583, *wR*$_2$＝0.1455 [*I*＞2*σ*(*I*)]. The X-ray crystal structure of the trinuclear complex reveals that the three unsymmetric Ni(II) atoms, which have different coordinated environment, were bridged by four of five oxygen atoms from five ligands and a novel V-model metal cluster complex was formed. The low-temperature (300～1.8 K) magnetic measurement of the title complex reveals that it was weakly antiferromagnetically coupled.

Key words 2-(2-hydroxyphenyl)benzimidazole trinuclear nickel complex crystal structure thermal decomposition magnetic property

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