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铜〔Ⅱ)与咪唑及2-羰基丙酸水杨酰腙混配体配合物的合成、晶体结构及热分解研究

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摘要 以2-碳基丙酸水杨酰腙、咪唑与五水硫酸铜在水中反应，首次制得混配体配合 物Cu(C10H8N2O4)（C3H4N2）（H2O）[C10H8N2O4^2-为2-羰基丙酸水杨酰腙负离子 ； C3H4N2为咪唑]，并在甲醇溶剂中培养出单晶．该单晶为深绿色，属单斜晶系， 空间群为P2（1）/c，晶胞参数a=1.50583(5) nm,b=1.08411(3)nm,c=0.94366(2)nm, α=90°，β=101.5583(11)°,γ=90°,V=1.50927(7)nm^3,Z=4,μ=1.479mm^-1, Dc=1.628Mg/m^3,F(000)=756.00,R=0.0340,ωR=0.0777,GOF=1.025。晶体测试结果 表明，配合物中Cu(Ⅱ)的配位数为5，处于四方锥配位环境，其中配体2—羰基丙酸 水杨酰腙的羧基以单齿配位．腙基上C≡N的N配位以及碳基(C≡0)的0配位，咪唑的 3位N参与了配位，这四个配位原子处于四方锥的锥底，另一个配位原子来自H20中 的0，它处于四方锥的锥顶．在晶胞中，除分子内存在氢键外，分子间也存在氢键 ．根据TG-DTG曲线研究了配合物的热分解过程，利用Kissinger公式计算了配合物 主要分解阶段的表观活化能．

关键词 铜络合物 咪唑 丙酸 P 腙 P 晶体结构 热分解 活化能 硫酸铜

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Synthesis, Crystal Structure and Thermal Decomposition of Copper(II) Complex with Imidazole and 2-Oxo-propionic Acid Salicyloyl Hydrazone

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Abstract In water, a copper(II) complex with 2-oxo-propionic acid salicyloyl hydrazone and imidazole Cu(C10-H8 N2O4)(C3H4N2)(H2O) [C10- H8 N2O42- is the dinegative ion of 2-oxo-propionic acid salicyloyl hydrazone, C3H4N2 is imidazole] has been synthesized. The dark-green crystals of the complex were obtained in methanol, and the crystal structure was determined by single crystal X-ray diffraction analysis. The results show that the complex is monoclinic of space group P2(l)/c, the cell parameters are as follows: a = 1.50583(5) nm, h = 1.08411(3) mn, c = 0.94366(2) nm, α=90°, β= 101.5583(11)°, γ= 90°, F= 1. 50927(7) nm3, Z = 4, μ= 1.479 mm-1, Dc = 1.628 Mg/m3, F((XK)) =756.00, R = 0.0340, ωR=0.0777, GOF = 1.025. In the complex, Cu atom is square- pyramidally coordinated by carboxyl monodentate ligand, one N atom of hydrazone C =N and one O atom of carbonyl of 2-oxo-propionic acid salicyloyl hydrazone, one N atom of imidazole, these four atoms are located at the bottom of the square-pyramid, the other coordinating atom is O atom of H2O locating at the apical position. In the crystal, there are hydrogen bonds either in or between the molecules. The thermal decomposition for the complex was studied and the apparent activation energy was obtained by the Kissinger formulae.

Key words COPPER COMPLEX GLYOXALINE METHYLACETIC ACID P HYDRAZONE P CRYSTAL STRUCTURE THERMAL DECOMPOSITION ACTIVATION ENERGY COPPER SULFATE

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