

铜(II)与 α,β -不饱和酸根和乙酰胺配合物的合成、表征、晶体结构和磁性

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收稿日期 修回日期 网络版发布日期 接受日期

摘要 合成了铜(II)与丙烯酸根和乙酰胺及铜(II)与 α -甲基丙烯酸根和乙酰胺两种配合物,进行了元素分析、红外光谱、电子光谱、ESR谱和变温磁化等研究,确定配合物的组成为 $\text{Cu} \sim 2\text{A} \sim 4(\text{C} \sim 2\text{H} \sim 5\text{NO}) \sim 2$,其中 $\text{A} = \text{CH} \sim 2 = \text{CHCOO}^-$, $\text{CH} \sim 2 = \text{C}(\text{CH} \sim 3)\text{COO}^-$; $\text{C} \sim 2\text{H} \sim 5\text{NO} =$ 乙酰胺,测定了它们的晶体结构。 $\text{Cu} \sim 2(\text{CH} \sim 2 = \text{CHCOO}) \sim 4(\text{C} \sim 2\text{H} \sim 5\text{NO}) \sim 2(1)$ 晶体属单斜晶系, $\text{P}2_1/c$ 群;晶胞参数: $a = 1.5333(5)\text{nm}$, $b = 1.0044(3)\text{nm}$, $c = 1.6184(7)\text{nm}$, $\beta = 115.28(3)^\circ$; $Z = 4$; 最终偏离因子 $R = 0.0701$ 。 $\text{Cu} \sim 2[\text{CH} \sim 2 = \text{C}(\text{CH} \sim 3)\text{COO}] \sim 4(\text{C} \sim 2\text{H} \sim 5\text{NO}) \sim 2(2)$ 晶体属三斜晶系, $\text{P}1$ 群;晶胞参数: $a = 0.93327(11)\text{nm}$, $b = 1.12484(11)\text{nm}$, $c = 1.3740(6)\text{nm}$, $\alpha = 94.90(2)^\circ$, $\beta = 108.409(14)^\circ$, $\gamma = 110.556(5)^\circ$; $Z = 2$; 最终偏离因子 $R = 0.0351$ 。配合物中Cu(II)具有畸变的四角锥形配位环境,两个Cu(II)由四个 α,β -不饱和酸根桥联,在Cu(II)的端位各有一个乙酰胺分子以O原子配位。Cu(II)-Cu(II)间具有一对称中心。配合物1中Cu(II)-Cu(II)间距离为0.26302(13)nm,配合物2中Cu(II)-Cu(II)间距离为0.26383(4)nm。变温磁化率研究表明,两种配合物中Cu(II)-Cu(II)间具有强烈的反铁磁性偶合作用。

关键词 [铜络合物](#) [乙酰胺P](#) [晶体结构](#) [甲基丙烯酸P](#) [元素分析](#) [红外分光光度法](#) [电子自旋共振](#)

分类号 [0611.662](#)

Syntheses, characterization, crystal structure and magnetic properties of copper(II) α,β -unsaturated carboxylate complexes with acetamide

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Abstract Two copper(II) α,β -unsaturated carboxylate complexes with acetamide, $\text{Cu} \sim 2(\text{CH} \sim 2 = \text{CHCOO}) \sim 4(\text{C} \sim 2\text{H} \sim 5\text{NO}) \sim 2(1)$ and $\text{Cu} \sim 2[\text{CH} \sim 2 = \text{C}(\text{CH} \sim 3)\text{COO}] \sim 4(\text{C} \sim 2\text{H} \sim 5\text{NO}) \sim 2(2)$, have been synthesized and characterized by elemental analyses, IR, ESR, electronic spectra and magnetic studies. The single crystal X-ray diffraction study of two complexes shows that complex 1 crystallizes in the monoclinic space group with $\text{P}2_1/c$, $a = 1.5333(5)\text{nm}$, $b = 1.0044(3)\text{nm}$, $c = 1.6184(7)\text{nm}$, $\beta = 115.28(3)^\circ$, $Z = 4$, and $R = 0.0701$, while complex 2 is triclinic, with space group $\text{P}1$, $a = 0.93327(11)\text{nm}$, $b = 1.12484(11)\text{nm}$, $c = 1.3740(6)\text{nm}$, $\alpha = 94.90(2)^\circ$, $\beta = 108.409(14)^\circ$, $\gamma = 110.556(5)^\circ$, $Z = 2$ and $R = 0.0351$. Two copper(II) atoms are bridged by four α,β -unsaturated carboxylate groups, with each copper(II) atom coordinated with an acetamide molecule in the axial position, forming a distorted square pyramidal configuration. The symmetric center is between the two copper(II) atoms. The Cu-Cu bond distance is 0.26302(13) nm for the complex 1 and 0.26383(4) nm for the complex 2. The Cu-Cu distance and magnetic studies suggest that there exist antiferromagnetic interaction between two copper(II) atoms.

Key words [COPPER COMPLEX](#) [ACETAMIDE P](#) [CRYSTAL STRUCTURE](#) [METHYLPROPENOIC ACID P](#) [ELEMENTAL ANALYSIS](#) [INFRARED SPECTROPHOTOMETRY](#) [ELECTRON SPIN RESONANCE](#)

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