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水合双邻羟基苄氨乙酸铜配位结构的**EXAFS**研究

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摘要 用参数化经验公式, 从已知晶体结构的无水双邻羟基苄胺铜(II)[Cu(o-OC6H4CH2NH2)2, 1]的EXAFS数据中分离出振幅和相移, 拟合另一已知晶体结构的水合双邻羟基苄胺铜(II){[Cu(o-OC6H4CH2NH2)2.H2O].1/2.H2O, 2}的结构参数并进行检验后, 代入未知结构的水合双邻羟基苄氨乙酸铜(II)[Cu(o-HOC6H4CH2NHCH2CO2)2.H2O, 3]中进行曲线拟合, 得到配位原子、键长和配位数等结构信息. 结合红外光谱, 推断标题化合物中, Cu(II)与两个苄基氮和两个羧基氧形成一个平面四边形的配位结构.铜与羧基氧键长2.00A, Cu-N键长1.99A, 另有一个较远的配位水分子, 铜与水的氧距离2.95A. 配体上的酚基氧没有与Cu(II)配合. 因此, 邻羟基苄氨乙酸(HBG)与Cu(II)配位时表现为二啮形式.

关键词 苯酚 P 晶体结构测定 苯乙胺 P X射线衍射分析 曲线拟合 铜络合物 水合物 付里叶变换 配位场理论 甘氨酸 P

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Coordination structure of bis(N-o-hydroxybenzylglycine) copper (II) hydrate determined by EXAFS spectroscopy

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Abstract EXAFS measurements were performed on the K-edge for CuL2 (I; HL = o-hydroxybenzylamine), [CuL2(H2O)].0.5H2O (II) and CuL12.H2O (III; HL1 = N-o-hydroxybenzylglycine, n = 1) on a x-ray spectrometer in transmission mode. The crystal structures of I and II are known and used as the model and ref. compound, resp. Parameterized amplitude and phase shift were curve fitted from the Fourier filtering data of I and transferred to deduce the structural parameters of I for certification. By curve fitting the EXAFS of III with the certified amplitude and phase shift function, the coordination structural information of bond lengths, coordination nos. and the type of coordination atoms were obtained. Combined with IR spectroscopy and ionic conductivity studies, the conclusion can be inferred that Cu(II) in III is linked with 2 benzyl N atoms, 2 carboxylate O atoms and has square coordination, planar wherein the Cu-O (carboxylate O) bond length is 2.00 ? and Cu-N 1.99 ? There is another O atom located 2.95 ?away from the central Cu. The phenol O atom in III is not coordinated with Cu(II), therefore, here N-o-hydroxylbenzylglycine behaves as a bidentate ligand.

Key words PHENOL P CRYSTAL STRUCTURE DETERMINATION PHENYLETHYLAMINE P X-RAY DIFFRACTION ANALYSIS CURVE FITTING COPPER COMPLEX HYDRATE FOURIER TRANSFORM LIGAND FIELD THEORY GLYCINE P

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