

Vibrational Spectra of the Cu(II) Complexes of Aspartic and Glutamic Acids

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SUMMARY. The infrared and Raman spectra of $\text{Cu(asp).2H}_2\text{O}$ and $\text{Cu(glu).2H}_2\text{O}$ (asp = L-aspartate; glu = L-glutamate) were recorded and discussed in relation to their crystal structures. Some comparisons with Cu(II) complexes of other amino acids are also made.

RESUMEN. "Espectros Vibracionales de los Complejos de Cu(II) con los Ácidos Aspártico y Glutámico". Se registraron los espectros infrarrojos y Raman de los complejos $\text{Cu(asp).2H}_2\text{O}$ y $\text{Cu(glu).2H}_2\text{O}$ (asp = L-aspartato; glu = L-glutamato) y se los discute en base a sus estructuras cristalinas. Se realizan algunas comparaciones con otros complejos de Cu(II) con amino ácidos.

INTRODUCTION

As a part of a research project devoted to the synthesis and characterization of copper complexes with pharmacological activity, we are investigating some general physicochemical properties of Cu(II) complexes of α -amino acids. As it is well known, many of these complexes possess an effective anti-rheumatic and/or anti-inflammatory activity ¹⁻⁵. In previous papers we have investigated the vibrational spectra of the complexes derived from amino acids containing hydrophobic ⁶ and hydroxylic ⁷ residues.

We have now extended these studies to the two acidic α -amino acids present in almost all proteins, i.e., L-aspartic and L-glutamic acid. Both complexes present the same stoichiometry, i.e., $\text{Cu(aa).2H}_2\text{O}$.

$\text{Cu(glu).2H}_2\text{O}$ is orthorhombic, space group $\text{P2}_1\text{2}_1\text{2}_1$ and $Z = 4$. The coordination about the copper ions is approximately square planar, involving the N atom and one α -carboxylate oxygen atom of one glutamate moiety, a β -carboxylate oxygen of another amino acid group and the oxygen atom of one of the water molecules. The Cu-O and Cu-N distances range from 1.97 to 2.00 Å. Two additional glutamate oxygen atoms at 2.30 and 2.59 Å complete a severely distorted octahedron ⁸.

$\text{Cu(asp).2H}_2\text{O}$ crystallizes in the monoclinic space group C2 with $Z = 4$. The coordination of the Cu(II) cation is a distorted tetragonal pyramid. The shortest equatorial bonds occur at the base of the pyramid with a water oxygen, the nitrogen atom and an α -carboxylate oxygen of one aspartate ion and a β -carboxylate oxygen of another aspartate ion. The oxygen atom of the second water molecule occupies the apical position ⁹.

EXPERIMENTAL

(L-aspartato)diaquacopper(II), $\text{Cu(Asp).2H}_2\text{O}$, was obtained by mixing hot aqueous solutions of copper(II) acetate and L-aspartic acid and digesting the generated precipitate at 50 °C during one hour ¹⁰. The similar complex of L-glutamic acid, $\text{Cu(Glu).2H}_2\text{O}$, was prepared in a similar way using copper(II) nitrate ⁸. The composition of both complexes was confirmed by elemental chemical analysis.

The IR spectra were recorded with a Perkin Elmer 580 B spectrophotometer, using the KBr pellet technique. Raman spectra were obtained with a Bruker IFS 66 FTIR instrument provided with a FRA 106 Raman accessory. The samples were excited with the 1064 nm line of a Nd:YAG laser.

KEY WORDS: Cu(II) complexes, Aspartic Acid, Glutamic Acid, IR and Raman Spectra.

PALABRAS CLAVE: Complejos de Cu(II), Acido Aspártico, Acido Glutámico, Espectros IR y Raman.

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