

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

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**SUMMARY.** The infrared and Raman spectra of Cu(asp).2H<sub>2</sub>O and Cu(glu).2H<sub>2</sub>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 Cu(asp).2H<sub>2</sub>O y Cu(glu).2H<sub>2</sub>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  $\alpha$ -amino acids. As it is well known, many of these complexes possess an effective anti-rheumatic and/or anti-inflammatory activity <sup>1-5</sup>. In previous papers we have investigated the vibrational spectra of the complexes derived from amino acids containing hydrophobic <sup>6</sup> and hydroxylic <sup>7</sup> residues.

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

Cu(glu).2H<sub>2</sub>O is orthorhombic, space group P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> and Z = 4. The coordination about the copper ions is approximately square planar, involving the N atom and one  $\alpha$ -carboxylate oxygen atom of one glutamate moiety, a  $\beta$ -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 <sup>8</sup>.

Cu(asp).2H<sub>2</sub>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  $\alpha$ -carboxylate oxygen of one aspartate ion and a  $\beta$ -carboxylate oxygen of another aspartate ion. The oxygen atom of the second water molecule occupies the apical position <sup>9</sup>.

### EXPERIMENTAL

(L-aspartato)diaquacopper(II), Cu(Asp).2H<sub>2</sub>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 <sup>10</sup>. The similar complex of L-glutamic acid, Cu(Glu).2H<sub>2</sub>O, was prepared in a similar way using copper(II) nitrate <sup>8</sup>. 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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