X-Ray Crystal Structure of Glycyl-L-tryptophanatocopper(II) Trihydrate

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Summary A new copper–peptide complex has been prepared and its structure elucidated by *X*-ray analysis using photographic methods: it is the first reported metal–peptide structure where one of the peptide residues is tryptophan.

A DEEP-BLUE solution containing glycyl-L-tryptophanatocopper(II) trihydrate may be prepared by the reaction of equimolar amounts of (a) freshly-precipitated $Cu(OH)_2$ and glycyl-L-tryptophan or (b) $CuCO_3$ and glycyl-L-tryptophan. Both reactions are carried out in aqueous solution and the reaction may be accelerated by warming. The complex separates as deep blue plate-like crystals.

Crystal data: The crystals are orthorhombic, space group $P2_12_12_1$, (D_2^4); $a = 7{\cdot}74$, $b = 13{\cdot}78$, $c = 14{\cdot}81$ Å, D_m (flotation) = 1·57, $D_c = 1{\cdot}58$ g cm^{-3}, $Z = 4$.

The structure was solved using three-dimensional Patterson and Fourier methods. The intensities of the 1120 independent reflections were visually estimated from Cu-K_α Weissenberg photographs. After two cycles of full-matrix least-squares refinement the residual, R, has a value of 0·134.

The Figure shows a view of the structure seen down the $-b$-axis. For clarity the square plane of the Cu atom has been translated parallel to the c-axis so that atoms C(3) and C(5) are not eclipsed. The co-ordination about the Cu atom is square planar, the positions being occupied by an oxygen and two nitrogen atoms of the glycyl-L-tryptophan ligand and a water molecule. There is no evidence of any further interactions involving the copper atom.

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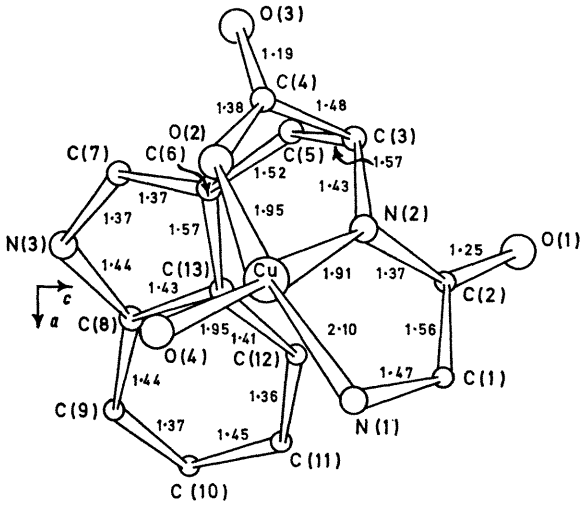

FIGURE. *View of the molecule down the* —b-*axis.*

[1] Hans C. Freeman, *Adv. Protein Chemistry*, 1967, **22**, 337.
[2] R. A. Pasternak, *Acta Cryst.*, 1956, **9**, 341.

Chains of molecules lie parallel to the *ac* plane at $y = 0$ and $y = \frac{1}{2}$. Hydrogen bonds involving water molecules link adjacent molecules in the chain through the co-ordinated water molecule and the peptide oxygen atom. Further hydrogen bonding with water molecules occurs between the chains through peptide oxygen atoms.

The bond lengths shown in the Figure are provisional, and further refinement of the structure is continuing. No significance is attached to discrepancies between these and published values in similar structures,[1,2] at the present stage.

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