03.2-11 CRYSTAL STRUCTURE OF GLYCINE ORTHOPHOSPHATE
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Studies on amino acid phosphate compounds are expected to be an important source of information for understanding the protein-nucleic acid interactions and with that end in view, the crystal structure of the title compound was studied. Glycinium orthophosphate (NH₂(CH₃COON)₂H₂PO₄) crystallizes in a tetra-molecular-unif cell, with dimensions a = 9.63, b = 7.89, c = 9.24 Å, β = 114° and the space group is P2₁/c.

Good single crystals were grown from a saturated aqueous solution containing glycine and orthophosphoric acid in stoichiometric proportions. Three-dimensional intensity data were collected by the multiple film equi-inclination Weissenberg technique using CuKα radiation. The crystal structure, solved by the Patterson and the Fourier methods, was refined to an R value of 0.08 for 1000 observed reflections. All hydrogen atoms except one were located. The amino acid exists as a positive ion (NH₂CH₃COON) in this structure and there is a strong C-O-H-C-O hydrogen bond between the carboxyl and the phosphate oxygens. The phosphate groups themselves are linked by hydrogen bonds and form extended chains along the b and c axes.

03.2-12 STUDIES ON CONFORMATION OF PROLYL RESIDUE IN PEPTIDES: THE CRYSTAL AND MOLECULAR STRUCTURE OF L-PROLYL-L-METHIONINE MONOHYDRATE.
By V. S. Yadava and H. M. Padmakumaran, Neutron Physics Division, Bhabha Atomic Research Centre, Trombay, Bombay 400 085, India.

The prolyl residue can have two conformations φ, ψ one with Cα and Cβ atoms on the same side of NCα Cα Cα plane and the other with Cβ on the opposite side of Cα (Ramachandran et al. 1970, Biochem. et Biophys. Acta, 221, 163-181).

L-Prolyl-L-methionine crystallizes in the monoclinic space group P2₁ with a = 19.385(4), b = 5.482(1), c = 6.414 Å, β = 93.21(8)° and Z = 2. From the Trombay computer-controlled diffractometer data (1072 observed reflections), the crystal structure was solved by direct methods and refined by the least-squares procedure to an R index of 0.084.

The crystal structure is a disordered one. The pyrroloidine ring exists in two conformations in the ratio of 3:2, with Cα atom of the ring statistically situated on both sides of NCα Cα Cα plane. The bond lengths and bond angles for the peptide have values close to those expected except those for the pyrroloidine ring. The molecule is in the extended conformation (φ = 166°, ψ = 70°) and in trans configuration (ω = 168°). The sulphur and the terminal methyl group have large thermal parameters. The hydrogen bonds through the water molecule stabilize the structure.

03.2-13 CRYSTAL STRUCTURE OF N-(p-AMINOBENZOYL)-L-GLUTAMIC ACID HYDROCHLORIDE.
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N-(p-Aminobenzoyle)-L-glutamic acid (C₉H₉N₂O₄), a major portion of folic acid, is a sulfanilamide antagonist. The title compound crystallizes in the monoclinic space group P₂₁ with a = 11.819(3), b = 4.929(1), c = 12.0855(1) Å, β = 102.4(1)°, Z = 2. The structure was solved by direct methods and refined by block-diagonal least-squares technique, with anisotropic temperature parameters for nonhydrogen atoms and isotropic ones for hydrogens, to an R value of 0.15 for 819 diffractionometer data. Para-aminobenzoic acid part of the molecule is linked to glutamic acid via a peptide-like linkage with C-N distance of 1.35 Å. The side chain in glutamic acid is buckled with Cβ gauche to C with respect to Cβ-Cβ (X = 77.2°).

The α-carboxylic C is trans to C with a torsion angle of C-C-C-C = -179.5°. The α-carboxylic group and the α-amino nitrogen are not coplanar, the angle of rotation (φ) of the C=N bond from the plane of the α-carboxylic group being 26°. All the available hydrogen atoms take part in hydrogen bonding and the structure is stabilized by a three-dimensional network of hydrogen bonds of types N-H...O, O-H...O and N-H...C. No intramolecular hydrogen bonds have been observed.

03.2-14 THE X RAY ANALYSIS OF HUMAN A.C.T.H. FRAGMENTS
by G. Préavigou, B. Bussetta, S. Georgette and M. Hospital, Laboratoire de Cristallographie, Université de Bordeaux I - 33405 - Talence-Cedex - France.

Among several crystallization trials with numerous fragments (or analogs) of human A.C.T.H., only two gave large enough crystals for X-ray study. The tetrapptide L-tyrosyl-L-prolyl-L-asparginyl-L-glycine, the 23-26 fragment, crystallizes by free diffusion between a concentrated peptide solution in methanol-water and chloroform. The crystal is orthorhombic, a = 8.866(2), b = 12.858(3), c = 18.146(4) Å, space group P 212121, with four molecules per unit cell. The final R value is 0.033. The molecule exists in the crystal as a right-handed helix. The peptide chain main chain is in extended conformation. The rather high density (1.44 Mg. m⁻³) is explained by a strong intermolecular hydrogen bond network. There is no intramolecular hydrogen bond.

The tetrapeptide L-methionyl-L-glutamyl-L-phenylalanine, the 4-7 fragment of A.C.T.H., crystallizes in the orthorhombic system with Z = 4, a = 20.5 Å, b = 27.7 Å, c = 4.8 Å.