C - 70

03. CRYSTALLOGRAPHY IN BIOCHEMISTRY AND PHARMACOLOGY

03.2-10 THE CRYSTAL AND MOLECULAR STRUCTURE OF 8(2'-DEUTEROCYTIDINE-5'-MONOMETHYLPHOSPHATE) - ZINC PENTAHYDRATE. By Petra Kollat and John J. Staszewski, Institut für Organische Chemie, Biochemie und Isotopen-Forschung der Universität Stuttgart, Pfaffenwaldring 55, 7000 Stuttgart 80, FRG and Sandra Miller and Luigi G. Marzilli, Department of Chemistry, Emory University, Atlanta, GA 30322, USA.

We report a crystal structure determination for a metal-nucleotide complex in which zinc is complexed with an unusual chemical modification of mononucleotide. An oxygen atom of the phosphate moiety has been methylated to give rise to a mononucleotide model that more closely resembles the chemical properties of an "monomer" in an oligomer or a polymer.

The zinc ion displays a tetrahedral coordination geometry resulting from interactions with four nucleotide molecules. The metal ion binds with an oxygen of the phosphate and nitrogen N(3) of cytosine to give a complex that displays crystallographic 2-fold symmetry. The crystals display space-group symmetry P212121 with a = 11.087(1), b = 9.630(1), c = 9.664(1) Å and a = 177±0.5, b = 90±0.5, c = 90±0.5 (Dokl. Akad. Nauk USSR 1983) 272, 340. In the structures under study we have observed three sugar conformations (C3 in AOP and C3 in AOPA) and two conformations of the five-membered anhydrocycle. In AOP molecules the anhydrocycle and the base are coplanar whereas in the strongly hydrated AOP molecules the anhydrocycle has a non-plane conformation resembling that in solution. The conformations of AOP and AOPA molecules about the exocyclic bonds are very close. The appropriate torsional angles are equal to 177±0.5 0 (O6'O5'O4'O3') and 66±1° (O4'O1'N9'(N1)O4'(O2'))

03.2-11 CRYSTAL STRUCTURE OF L-TYROSYL-L-VALINE MONOHYDRATE. By B.Barazitiyan, T.P.Seshadri and M.A. Vinayakumar, Department of Physics and ICMR Centre on Genetics and Cell Biology, Indian Institute of Science, Bangalore 560 012, India.

We report here the crystal structure of L-tyrosyl-L-valine monohydrate as a part of our investigation on peptides which are possibly involved in specific interaction with nucleic acids.

The dipeptide crystallizes in orthorhombic space group P2_12_12 with four molecules per unit cell of dimensions a = 5.629(1), b = 8.702(2), c = 31.600(8) Å. Intensity data (z = 60°) were collected with 2θ/ω scans on CAD-4 diffractometer. The structure obtained from direct methods has been refined block diagonally to R = 7.1 %. The molecule exists as zwitterion. The peptide bond is planar. The tyrosine side chain conformational angles are θ_21 = 8.5° and θ_22 = -100.°. The valine side chain conformation has χ_11 = 174.° and χ_12 = -59.7°. The OH group forms two hydrogen bonds with amino and carboxyl ends of the peptides. The tyrosine residues do not show any ring stacking.

03.2-12 X-RAY STRUCTURE OF ADENINE AND CYTOSINE SYN-ANHYDRONUCLEOSIDES. By G.Surakaya, G.Basedova, G.Bevgorodny, P.Tamlevich, V.Florentiev and B.Gottlieb, Institute of Molecular Biology, the USSR Academy of Sciences, Moscow, the USSR.

A new type of adenine and cytosine anhydronucleosides characterized by a syn-conformation about the N-glycosidic bond and possessing all the functional groups of natural nucleosides have been synthesized and X-ray studied. 6,1'-Anhydro-6-hydroxy-9-(2-β-D-psicofuranosyl)adenine (AOPA) - space group P2_1, cell dimenssions: a = 6.941(1), b = 9.764(1), c = 14.341(4) Å, α = 110.054(13), β = 97.925(52), γ = 97.024(17)°, 2Z(AOPA) = 12 H2O. Symmetrically independent molecules are conformationally different. 6,1'-Anhydro-6-hydroxy-1-(2-β-D-psicofuranosyl)cytosine (AOPC) - space group P2_1, cell dimensions: a = 6.148(1), b = 6.630(1), c = 9.564(1) Å, β = 90.351(5)°, 2Z(AOPC) = 2Z(AOPA) = 12 H2O. In the structures under study we have observed three sugar conformations (3B in AOP and 3B and 3C in AOPA).