

03.2-10 THE CRYSTAL AND MOLECULAR STRUCTURE OF BIS-(2'-DEOXYCYTIDINE-5'-MONOMETHYLPHOSPHATE)-Zn(II) PENTAHYDRATE. Rolf-Dietrich Stigler, Petra Kollat and John J. Stezowski, Institut für Organische Chemie, Biochemie und Isotopenforschung 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 approximately 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 $P3_121$ with $a = 11.087(2)$ and $c = 26.553(6)$ for a crystal at $\sim 120\text{K}$. Small crystals of a second modification have also been grown. They display the same Laue symmetry and systematic extinctions but the following lattice parameters: $a = 17.984(9)$ and $c = 12.949(9)$ ($T \sim 120\text{K}$). We are attempting to grow larger crystals of this form for a structure determination as well.

03.2-11 CRYSTAL STRUCTURE OF L-TYROSYL-L-VALINE MONOHYDRATE By B.Ramakrishnan, T.P.Seshadri and M.A. Viswamitra, 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 $P2_12_12_1$ with four molecules per unit cell of dimensions $a = 5.629(1)$, $b = 8.702(2)$, $c = 31.600(8)$ Å. Intensity data upto $\theta = 60^\circ$ were collected using $\text{CuK}\alpha$ radiation on CAD-4 diffractometer. The structure obtained from direct methods has been refined block diagonally to $R = 7.1\%$. The molecule exists as zwitter-ion. The peptide bond is planar. The tyrosine side chain conformational angles are $\chi^{21} = 81.5^\circ$ and $\chi^{22} = -100.9^\circ$. The valine side chain conformation has $\chi^{11} = 174.2^\circ$ and $\chi^{12} = -59.7^\circ$. The CH 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.Gurskaya, G.Javadova, S.Zavgorodny, T.Tsilovich, V.Florentiev and B.Gottikh, 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. 8,1'-Anhydro-8-hydroxy-9-(2- β -D-psicofuranosyl)adenine (AOPA) - space group $P1$, cell dimensions: $a=6.941(2)$, $b=9.764(1)$, $c=14.341(4)$ Å, $d=110.084(13)$, $\beta=97.925(26)$, $\gamma=87.024(17)^\circ$, $Z=2(\text{AOPA}) \cdot 12 \text{H}_2\text{O}$. Symmetrically independent

molecules are conformationally different. 6,1'-Anhydro-6-hydroxy-1-(2- β -D-psicofuranosyl)cytosine (AOPC) - space group $P2_1$, cell dimensions: $a=6.148(1)$, $b=9.630(1)$, $c=9.664(1)$ Å, $\beta=90.351(5)^\circ$, $Z=2(\text{AOPC})$. (Dokl. Akad. Nauk USSR (1983) 273, 340). In the structures under study we have observed three sugar conformations (3E in AOPC and 2T_3 and 2T in AOPA)

and two conformations of the five-membered anhydrocycle. In AOPC molecules the anhydrocycle and the base are coplanar whereas in the strongly hydrated AOPA molecules the anhydrocycle has a non-plane conformation resembling that in solution. The conformations of AOPC and AOPA molecules about the exocyclic bonds C4'-C5' and the N-glycosidic bond are very close. The appropriate torsional angles are equal to $177 \pm 3^\circ$ ($05'C5'C4'C3'$) and $66 \pm 1^\circ$ ($04'C1'N9(N1)C4(C2)$).

03.2-13 THE CRYSTAL STRUCTURE OF DIPEPTIDE CYCLO-L-METHIONYL-D-PROLYL. By V.M. Padmanabhan and V.S.

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The title compound ($\text{C}_{10}\text{H}_{20}\text{O}_2\text{S}_2$) crystallises in the orthorhombic space group $P2_12_12_1$ with $Z = 4$ and $a = 9.782(4)$, $b = 11.068(3)$, $c = 10.069(5)$ Å. The structure was solved by Patterson method and DIRDIF programme and refined to an R-index of 0.073 (non hydrogen atoms only) for 1391 reflections taken by the diffractometer fabricated indigenously in Trombay. The pyrrolidine ring is close to half chair form with a (pseudo) two-fold axis passing through the nitrogen atom. The endocyclic torsion angles indicate that it belongs to class B conformation and proline is collagen type. The piperazine ring has a boat-like form. The methionine side chain conformation favours the theoretical predictions and is gauche-trans-gauche.

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