3. 2-10 THE CRYSTAL AND MOLECULAR STRUCTURE OF BIS-(2'-DEOXYCYTIDINE-5'-MONOMETHYLPHOSPHATO)Zn(II) PENTAHYDRATE. Rolf-Dietrich Stigler, Petra Kollat and John J. Stezowski, Institut fuir Organische Chemie, Biochemie und Isotopenforschung der Universitat Stuttgart, Pfaifenwaldring 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 $\mathbb{N}(3)$ of cytosine to give a complex that displays crystallographic 2-fold symmetry.

The crystals display space-group symmetry P3.2l with $a=11.087(2)$ and $c=26.553(6)$ for $a$ crystal at 2120 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 $c=12.949(9)(T \sim 120 \mathrm{~K})$. We are attempting to grow larger crystals of this form for a structure determination as well.
 SINE SYN-ANHYDRONUCLEOSIDES. By G. Gurskaja, G.Javadova, S. Zavgorodny, T. TsiTevich, 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 $\mathbb{N}$-glycosidic bond and posessing all the functional groups of natural nucleosides have been synthesized and X-ray studied. 8, $1^{1}$-Anhydro-8-hydroxy-9-(2- $\beta-D-p$ sicofurenosyl)adenine (AOPA) - space group P1, cell dimensions: $a=6.941(2), b=9.764(1), c=14.341(4) \AA$, $\alpha=110.084(13), \beta=97.925(26), \gamma=87.024(17)^{\circ}$, $Z=2(A O P A) \cdot 12 \mathrm{H}_{2} \mathrm{O}$. Symmetrically independent molecules are conformationally different. 6,1'-Anhydro-6-hydroxy-1-(2- $\beta-\mathrm{D}-\mathrm{p}$ sicofuranosyl)cytosine (AOPC) - space group $\mathrm{P}_{1}$, cell dimensions: $a=6.148(1), b=9.630(1), c=9.664(1)$ A, $\beta=90.351(5)^{\circ}, Z=2$ (AOPC). (Dokl. Akad. Nauk USSR (1983) 273, 340). In the structures under study we have observed three sugar conformations ( ${ }^{3}$ in AOPC and ${ }^{2} T_{3}$ and $3^{2}$ 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 AOFA molecules about the exocyclic bonds 64'-05' and the N-glycosidic bond are very close. The appropriate torsional angles are equal to $177 \pm 3^{\circ}\left(05^{\prime} 65^{\prime} \mathrm{C4} 4^{\circ} \mathrm{C} 3^{\prime}\right)$ and $66^{\circ} \pm 10$ (04'G1'N9(N1)C4(C2)).
03. 2-13 THE CRYSTAL STRUCTURE OF DIPEPTIDE CYCLO-L- METEIONYL- D- PROLIL. By V.M. Padmanabhan and V.S. Jakkal", Neutron Physica Division, Bhabha Atomic Research Centre, Trombay, Bombay 400085, India.

The title compound ( $\mathrm{C}_{10} \mathrm{~N}_{2} \mathrm{O}_{2} \mathrm{SH}_{16}$ ) crystallises in the orthorhombic space group $P 2_{1} 2_{1} 2_{1}$ with $Z=4$ and $a=9.782(4), b=11.068(3), c=10.069(5) \mathrm{A}^{\circ}$. The structure was solved by Patterson method and DIRDIP programme and refined to an R-index of 0.073 (non hydrogen atoms only ) for 1391 reflections taken by the diffractometer fabricated indigenously in Trombsy. 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 cbain conformation favours the theoretical predictions and is gauche-trans-gauche.

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