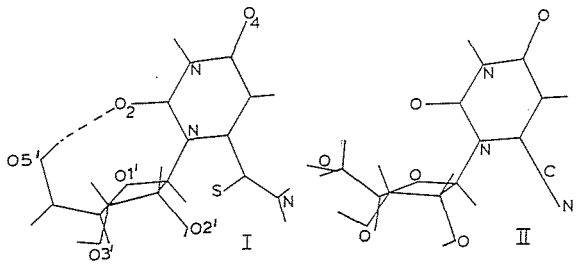
bulk that influences the conformation, rather than the nature of the group. The plane of the thiocarboxamido group is nearly perpendicular to the pyrimidine plane with C–S = 1.655A, and C–N = 1.318A, typical for such functional groups. The conformation of the glycoside 5'–hydroxy is gauche–gauche with respect to the furanose ring and has the 5'–hyroxyl hydrogen pointed toward, and 2.84A from, O2 to form an intramolecular hydrogen bond. This intramolecular hydrogen bonding is observed in many of the uridine structures studied, in particular those with a 6–substituent. This feature is considered a stabilizing effect for a syn conformation. The closest intramolecular contacts that the thiocarboxamido makes is S...O1' = 3.66A and N...O2' = 3.98A. However, in the cyano compound, the 5'–hydroxyl is in a gauche–trans conformation and its hydrogen forms an intermolecular hydrogen bond. The cyano group is nearly coplanar (24°) with the pyrimidine ring. In both structures, the furanose hydroxyls form a newtwork of intermolecular hydrogen bonds with adjacent molecules in the lattice.



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03.2–17 THE STRUCTURE OF N–ACETYL–α,α–DIETHYLGLYCINE–N'–METHYLAMIDE MONOHYDRATE, $C_9H_{18}N_2O_2 \cdot H_2O$. By Z. Gałdecki* and B. Luciak, Institute of General Chemistry* and Institute of Physics, Technical University of Łódź, Żwirki 36, 90–924 Łódź, Poland.

In recent years an interest in α,α–dialkylamino acids and their peptides has increased because of the presence of α–methylalanine and α–ethylalanine in ionophore antibiotics and in peptide hormone analogues. It was stated that diethylglycine (Deg) incorporation into peptide chain is more difficult than methylalanine. It is accounted for steric hindrances (Redliński A., private communication). In order to explain this problem and to determine the conformation of Deg residues in linear peptide, crystal structure investigations of the title compound (Ac–Deg–NHMe) have been undertaken. The compound crystallizes in two forms. We examined a structure of the more stable form, with melting point at 684K, which crystallizes in the monoclinic space group $P2_1/c$ with unit cell parameters: $a = 7.139(1)$, $b = 11.823(2)$, $c = 15.778(3)$ Å, $\beta = 122.23(1)^\circ$, $Z = 4$, $D_m = 1.20$, $D_x = 1.204 Mgm^{-3}$. The intensities of 1523 independent reflections were collected using CuKα radiation. The structure was solved by direct methods (MULTAN) and refined by full–matrix least–squares to a final $R = 0.046$. The positions of all H atoms were found from ΔF syntheses and were refined isotropically. The parameters of the remaining atoms were refined assuming anisotropic temperature factors. The view of the molecule along [010] is shown in the picture. The X–ray study revealed one molecule of crystallizing water, which forms two hydrogen bonds O···O with the peptide molecules. Their lengths are 2.763 and 2.801 Å. The hydrogen bonds connect the peptide molecules into chains parallel to [201]. The torsion angles in Ac–Deg–NHMe are: $\omega_0 = 171.2(6)$, $\varphi_1 = 68.9(8)$, $\psi_1 = 19.5(9)$, $\omega_1 = 178.5(7)^\circ$. Comparison of the torsion angles values with those for α–helical and 3_{10}–helical conformations indicates that in the crystal of Ac–Deg–NHMe the Deg residues exist in a conformation more close to 3_{10}– than to α–Helix. On the basis of the atomic parameters from X–ray study the INDO and IEHT calculations were carried out using the programs QCPE141 and FORTICON. The results of the calculations will be discussed.

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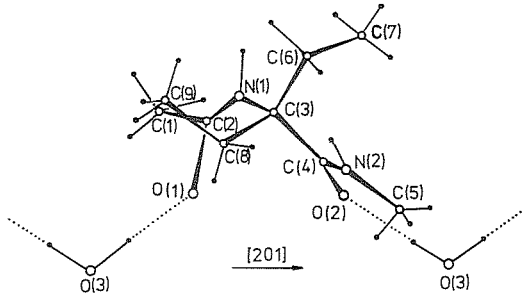

03.2–18 STRUCTURAL STUDY OF $[CoPO_8C_{10}N_4H_{11} \cdot (H_2O)_4] \cdot 3H_2O$. By E. Molins, A. Caubet, C. Miravitlles, X. Tejada and V. Moreno. Facultat de Física and Facultat de Química, Universidad de Barcelona. Fac. de Química, Tarragona. Instituto "Jaime Almera", C.S.I.C., Apartado 30102, Barcelona. Spain.

In our departments we are working on metal complexes of purine and pyrimidine nucleotides (V. Moreno et al. Inorg. Chem. to be published). In order to make a decisive confirmation of Co–5'IMP etablished by means of spectral and chemical techniques, it was undertaken its study by X–ray diffraction methods. The crystals are pale violet with a = 6.877(3), b = 10.909(6), c = 26.102 (9) A, $P2_12_12_1$ and Z = 4. The Co and P atoms were located by direct methods (MULTAN 11/82) and the remaining atoms by succesive Fourier synthesis. At this stage the structural model doesn't correspond with the expected one. Full matrix least–squares refinement was carried out with the SHELX–76 program. The final R–value is 0.080. The final structural model shows that, during the synthesis, the ribose ring is broken and the fragment C3P–O3P is caught by the Co–atom and used for connect it to the phosphate group. Similar processes can occur in biological reactions.