6-furfurylamino-purine (Kinetin) is a highly potent growth factor (cytokinin) which is implicated in many aspects of plant growth. It promotes cell division and differentiation. A 1:1 crystal complex of kinetin and picric acid was crystallized and we present its crystal and molecular structure as an appropriate model compound for studying the structural properties of cytokinins in an ionic environment.

The complex, C_{11}H_{15}N_{6}O_{5}, crystallizes in the monoclinic system, space group P2_1/n, with cell dimensions (at 18 °C): a = 4.995(1) Å, b = 13.931(3) Å, c = 26.065 Å, β = 90.99(2)°, V = 1.63 g/cm³ and Z = 4. The structure was solved from diffractometer data by direct methods and refined by a cascade matrix least-squares technique to R = 0.05 using 2040 observed reflections.

The present structure provides the first description of the adenosine moiety with the N(3)H and N(7)H tautomers. The molecular geometry of the adenine ring found in this structure differs considerably from the assumed in theoretical calculations on the N(3)H tautomer of purine. The kinetin cation assumes a similar conformation from the N(7)H and N(3)-H···N(9) hydrogen bonds. The two layers of unlike molecules while Form I has 1 H_2O and 3 C_H_4H_4Cl solvated molecules. The crystals are not isomorphous, although the peptide molecules are isostuctured. Both crystals have space group P2_1/c with a = 13.307(2) Å, b = 24.820(4) Å and c = 11.231(2) Å for Form I and a = 16.716(2) Å, b = 24.067(3) Å, and c = 10.918(1) Å for Form II. The unusual intramolecular hydrogen bond in the β-bend encompassing the sequence L-Phe-LAla occurs in both crystal forms. The β-bend has torsional angles characteristic of a Type II' bond (for a D,L sequence) rather than the expected Type I (for an L,L sequence). The φ,ψ values for L-Phe and L-Ala are +60°, -122° and +97°, respectively (in Form II). The aberrant residues, L-Phe, lies in the D-region of the φ,ψ map that is forbidden to L-residues. In the present structure, φ,ψ in the atypical β-bend is at a distance of only 2.84 Å from H_2O. To achieve a separation even as large as 2.84 Å required an increase of 2° per value for the C_6H_5Cl and C_6H_4Cl angles from the average values that have been observed in other peptides. One water molecule is buried in an excessively hydrophobic region to provide hydrogen bonds to two amide and two carbonyl moieties. The stability of the conformation of cyclic peptides in different solvent environments is demonstrated.

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bulk that influences the conformation, rather than the nature of the group. The plane of the thiacarboxamide group is nearly perpendicular to the pyridazine plane with $\beta = 86.8^\circ$, and $\beta = 81.8^\circ$, typical for such functional groups. The conformation of the glycoside 5'-hydroxy is gauche-trans with respect to the uridine ring and has the 5'-hydroxyl hydrogen pointed toward, and 2.844 Å 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 substituent. This feature is considered a stabilizing effect for a conformation. The closest intramolecular contacts that the thiacarboxamide 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 intramolecular hydrogen bond. In both structures, the furanose hydroxyls form a network of intermolecular hydrogen bonds with adjacent molecules in the lattice.

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03.2.17 THE STRUCTURE OF N-ACETYLC-dC-dC-dD-dI-ETHYLGLYCINE-N'-METHYLAMIDE MONOHYDRATE, C9H15N3O4.H2O. By Z. Galdecki and B. Lucia. Institute of General Chemistry and Institute of Physics, Technical University of Łódź, 031 Łódź, Poland.

In recent years an interest in $\alpha$, $\alpha$-disalkylamino acids and their peptides has increased because of the presence of $\alpha$-methylalanine and $\alpha$-ethylalanine in ionophore antibiotics and in peptide hormones analogues. It was stated that diethylglycine (Deg) incorporation into peptide chain is more difficult than methylalanine. It is accounted for steric hindrances (Redlinski, private communication). In order to explain this problem and to determine the conformation of Deg residues in a 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 68ºC, which crystallizes in the monoclinic space group P21/c with unit cell parameters:

- $a = 7.139(1)$, $b = 11.823(2)$, $c = 15.778(3)$ Å
- $\beta = 122.23(1)^\circ$, $Z = 4$, $D_0 = 1.20$, $D_2 = 1.24(4) g cm^{-3}$

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 $R = 0.086$. The positions of all H atoms were found from difference syntheses and were refined isotropically. The parameters of the remaining atoms were refined assuming anisotropic temperature factors. The view of the molecules 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 2.762 and 2.801 Å. The hydrogen bonds connect the peptide molecules into chains parallel to [010]. The torsion angles in Ac-Deg-NHMe are:

- $\chi_1 = 171.2(6)$, $\chi_2 = 68.9(8)$, $\chi_3 = 19.5(9)$, $\chi_4 = 178.5(7)^\circ$

Comparison of the torsion angles values with those for $\alpha$-helical and $\beta$-helical conformations indicates that in the crystal of Ac-Deg-NHMe the Deg residues exist in a conformation more close to $\beta$- than to $\alpha$-Helix. On the basis of the atomic parameters from X-ray study the INDO and IICHT calculations were carried out using the programs QCPET141 and FORTICON. The results of the calculations will be discussed.

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03.2.18 STRUCTURAL STUDY OF [CoPO4Cl0.79(1.4H2O)]. 3H2O. By E. Molins, A. Caubet, C. Miravitlles, X. Tejada and V. Moreno. Facultad de Fisica and Facultad de Quimica, Universidad de Barcelona. Fac. de Quimica, Terragona. Instituto "Jaime Almera", C.S.I.C., Apartado 30102, Barcelona, Spain.

In our department 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-O-IPM established by means of spectral and chemical techniques, it was undertaken its study by X-ray diffraction methods. The crystals are pale violet with $a = 6.877(3)$, $b = 10.906(3)$, $c = 26.102(9)$ Å, $P_2_12_1$, and $Z = 4$. The Co and P atoms were located by direct methods (MULTAN 11/82) and the remaining atoms by successive 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 $3P-03P$ is caught by the Os atom and used for connect it to the phosphate group. Similar processes can occur in biological reactions.