Crystal Structure of Boc-Gly-ΔPhe-Gly-Phe-4-pNA. K. Ejsmont, M. Makowski, J. Zaleski, *Institute of Chemistry, University of Opole, Oleska 48, 45-052 Opole, Poland, e-mail: zaleski@uni.opole.pl*

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One of the aims of contemporary protein research is the rational design of synthetic peptide mimics for structural motifs in proteins. Incorporation of non standard amino acids with well-defined stereochemical and functional properties turns out to be an attractive approach to impose localised restrictions on the polypeptide chain. In the last few years, a large body of studies has been devoted to determine the likely conformational consequences of the presence of dehydro residues, especially α,β-dehydrophenylalanine (ΔPhe). Incorporation of ΔPhe unit into a peptide decreases conformational flexibility and has a stabilising influence on the β-turn or α-helix in short sequences and 3_{10}-helical conformation in long sequences. The crystal and molecular structure of the tetrapeptide (Z–isomer) tertbuthyloxycarboxyloglycine-α,β-dehydrophenylalanineglycine-phenylalanine – 4 –anilide (Boc-Gly-ΔPhe-Gly-Phe-4-pNA) has been determined by the X-ray diffraction method. Space group P1, a = 10.392(2), b = 11.727(2), c = 15.501(3)Å, α = 65.83(3), β = 84.43(3), γ = 75.65(3º). There are two independent molecules (I and II) in the unit cell. They differ in conformation. The torsional angles ϕ and ψ for dehydrophenylalanine (ΔPhe) are ϕ = -51.0(5), ψ = -29.5(5) for I and ϕ = 59.4(5), ψ = 20.5(5º) for II. Two resultant conformations are stabilised by two intramolecular and three intermolecular N-H...O hydrogen bonds. These and other structural parameters of the title compound in comparison with peptides containing α,β-dehydrophenylalanine residues, will be presented and discussed.

Nicotinamide Adducts of Cobalt(II) Arylcarboxylates. H. Necifoglu¹, T. Hökelek², (a) Kafkas University, Department of Chemistry, Kars, Turkey (b) Hacettepe University, Department of Physics, Ankara, Turkey.

Keywords: nicotinamide complex, ligand properties, hydrogen bonds.

Nicotinamide (NA) is a form of niacin. A deficiency of this vitamin leads to loss of copper from the body, known as pellagra disease. The nicotinic acid derivative N,N-diethynicotinamide is an important respiratory stimulant.

The structure determination of three compounds [Co(3-X-C₆H₄COO)₂(C₆H₆N₂O₂)(H₂O)₂], where X is H (complex I), OH (complex II) and NH₂ (complex III), was undertaken to determine the ligand properties of NA and benzoate ligands. The monomeric [Co(3-X-C₆H₄COO)₂(C₆H₆N₂O₂)(H₂O)₂] molecules have the typical structure of NA complexes in which the metal atom has a trans-octahedral coordination. The complexes have a centre of symmetry with the monodentate benzoate ions and NA ligand acting as monodentate ligands. The four nearest symmetry related carboxylate (Co-O_COO 2.085(1), 2.099(3) and 2.082(4) Å, respectively) and water O atoms (Co-O_aq 2.141(1), 2.132(3) and 2.154(4) Å, respectively) forms a slightly distorted square planes around the Co atom, while the slightly distorted octahedral arrangement is completed by the pyridine N atoms of NA ligands at distances of 2.150(1), 2.139(4) and 2.153(3) Å, respectively.

There are hydrogen bonds between the water and carboxylate non-coordinated O atoms(O...O 2.580(2), 2.586(5) and 2.583(6) Å, respectively. Similar hydrogen bonds are observed in [Co(4-O₂N-C₆H₄COO)₂(H₂O)₂] (2.59 Å) and [Co(4-H₂N-C₆H₄COO)₂(H₂O)₂] (2.592(3) Å)2.

There are intra- and intermolecular hydrogen bonds between the nicotinamide Namide and OCO atoms and between water O atom and nicotinamide OCO atoms (complexes I and II), and between the non-coordinated OCO and OOH atoms (complex II), and between the non-coordinated OCO and Oaq atoms (complex III).