**o.m12.p3** **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*
Keywords: dehydro amino acids, α,β-dehydrophenylalanine, solid state structure.

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-dehydrophenyloalanineglycine-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(3)°. 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(5)° 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.

**o.m12.p4** **Nicotinamide Adducts of Cobalt(II) Arylcarboxy-lates** . H. Necefoglu[a], T. Hökelek[b], (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-diethylnicotinamide is an important respiratory stimulant.

The structure determination of three compounds $[Co(3\text{-}X\text{-}C_6H_4COO)_2(C_6H_6N_2O)_2(H_2O)_2]$, where X is H (complex I), OH (complex II) and $NH_2$ (complex III), was undertaken to determine the ligand properties of NA and benzoate ligands. The monomeric $[Co(3\text{-}X\text{-}C_6H_4COO)_2(C_6H_6N_2O)_2(H_2O)_2]$ 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 ($Co\text{-}O_{COO}$ 2.085(1), 2.099(3) and 2.082(4) Å, respectively) and water O atoms ($Co\text{-}O_{aq}$ 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 $[Co(4\text{-}O_2N\text{-}C_6H_4COO)_2\ (H_2O)_4]$ (2.59 Å)[1] and $[Co(4\text{-}H_2N\text{-}C_6H_4COO)_2\ (H_2O)_4]$ (2.592(3) Å)[2].

There are intra- and intermolecular hydrogen bonds between the nicotinamide $N_{amide}$ and $O_{CO}$ atoms and between water O atom and nicotinamide $O_{CO}$ atoms (coplexes I and II), and between the non-coordinated $O_{COO}$ and $O_{OH}$ atoms (complex II), and between the non-coordinated $O_{COO}$ and $O_{aq}$ atoms (complex III).

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