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Most of nucleoside 5'-monophosphates have been extensively investigated as regards their structure for long, but potassium salts of them have never been studied by the use of X-ray crystallography. The results of structural investigations on five mono- and dipotassium salts of two purine [K₂(AMP)6H₂O, K(IMP)3H₂O] and two pyrimidine [K₂(CMP)6.25H₂O, K(UMP), K₂(UMP)5H₂O] ribonucleotides will be presented. The K⁺ salts crystallize with Z' = 1-4 for the respective crystal. In all the mono-/dianions, the orientation of the base with respect to the sugar ring is *anti*, which is typical for nucleotides. The ribose rings in AMP and UMP salts exist in ideal envelope conformations: ²E in two dianions in K₂(AMP)6H₂O and two dianions in K₂(UMP)5H₂O, and ³E in the monoanion in K(UMP). The sugar rings in the remaining crystals are slightly deformed from the ideal pucker, with the nearest descriptors being: ³T₂ for the IMP monoanion, ²T₁ for two CMP dianions and ³T₄, ²E for two remaining CMP dianions. The orientation of the phosphate relative to the ribose ring is the same in all the anions: *gauche-gauche*, which is characteristic of the 5'-nucleotides. The arrangement of the terminal phosphate atoms relative to the ester C5' is *antiperiplanar* (*ap*) for one of O atoms and *+/-synclinal* (*+/-sc*) for the others in most of the presented nucleotides. However the phosphate group in the IMP monoanion is disordered and exists in two orientations: typical *ap/sc* and quite uncommon *sp/ac*.

Keywords: nucleotides, ribonucleotides, biological compounds

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Sesquiterpene lactones isolated from a medicinal plant of the Venezuelan Andes

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Sesquiterpene lactones are perhaps the most studied members of the terpenes because a large number of them exhibit pharmaceutical activity. The structures of two sesquiterpene lactones, Tenuline and Gaillardiline, isolated from a medicinal plant of the Venezuelan Andes (*Ambrosia cumanensis*) will be presented in this contribution. Tenuline, C₁₇H₂₂O₅·2(H₂O), crystallizes in the orthorhombic system, space group P2₁2₁2₁, with unit cell parameters a=6.9501(2), b=9.5145(3), and c=25.7739(8) Å, V=1704.34(9)Å³, Z=4, d_c=1.334 g cm⁻³. Due to the presence of the water molecules in the structure, there is an extensive hydrogen bonding network which helps stabilize the structure. There are eight inter- and one intra-molecular hydrogen bond. Gaillardiline, C₁₇H₂₂O₆, crystallizes in P2₁2₁2₁ with unit cell parameters a=9.0749(3), b=11.1830(3), c=15.8804(4) Å, V=1611.62(8) Å³, Z=4, d_c=1.329 g cm⁻³. Three inter- and four intramolecular hydrogen bonds help to stabilize the structure. Both hydrogen bond networks can be described using graph set theory. They will be discussed in detail. We thank R. Benson (Rigaku-USA), for support with data collection using Cu radiation. This work was funded by FONACIT-Venezuela, through grant LAB-97000821.

Keywords: natural products, sesquiterpene lactones, crystal structure

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Organic two-photon absorbing materials for technological applications and photodynamic therapy

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Two-photon absorbing (TPA) chromophores are used in the technology for three-dimensional microfabrication by lithographic process and in biomedical applications as fluorescent markers for TPA microscopy and as photosensitizers in PTA photodynamic therapy. Advantage of TPA chromophores in comparison with conventional one-photon absorbing chromophores is an opportunity to achieve a very high spatial resolution in three dimensions and so treat tumors without damage to neighboring healthy organs. We studied structures of a large series of substituted benzylidenepiperidones, organic chromophores with general formula Donor-π-bridge-Acceptor-π-bridge-Donor. Structure – properties relations between geometric and spectroscopic characteristics of materials, important for their PDT applications, have been established. Dark toxicity and toxicity under irradiation have been characterized and discussed in connection with spectroscopic properties of materials.

Keywords: two-photon absorbing materials, photodynamic therapy, spectroscopy

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The structure of water nanopipe, a hollow-type water nanowire, in crystal host

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One-dimensional (1D) water nanostructures are important for better understanding the structure and behavior of water molecules at the atomic level. Previously we reported the first water nanowire in the crystal structure of L-tryptophan pyridoxal-5-phosphate Schiff base, obtained from its aqueous solution [1,2]. Here, we report the second water nanowire, called water nanopipe, in the crystal obtained from another batch of aqueous solution of the Schiff base. This nanopipe is a hollow-wire type nanowire, where the diameter and unit length (equals to the length of c-axis) are 1.649 nm and 0.473 nm. The structure is constructed in such a way that five water molecules form a small cluster unit, and three of the small units are linked around a three-fold axis to form a large cluster unit consisting of 15 water molecules. These large units are then piled up by nine hydrogen bonds parallel to c-direction and form an infinite water nanopipe. In this structure, seven kinds of hydrogen bonds are formed by five independent water molecules: the O--O distances are 0.246, 0.247, 0.272, 0.281, 0.290, 0.293 and 0.295 nm and the hydrogen-bonded O-O-O angles range from 82 to 135°. This nanopipe structure is assumed to be much more stable than the nanowire structure, because the more hydrogen bonds are formed along to the piling-direction in the nanopipe than the nanowire, and the very long needle crystals up to 2.6 cm are obtained for the nanopipe structure. Therefore, it would be considered that the present nanopipe structure provides a structural scaffold between the nanoworld (nm) and the real world (cm) in the