# MS05 - Structural information in drug design

Chairs: Dr. Rob van Montford, Prof. Andreas Heine

## MS05-P01

### Crystal structure and vibrational study of diphenylhydrazine dihydrogenophosphate monocrystal DPHDP $(C_6H_9N_2)_2H_2P_{2\&1}$

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Chemical preparation, crystal structure and vibrational study are reported for a new diphenylhydrazine dihydrogenophosphate monocrystal DPHDP $(C_6H_9N_2)_2H_2P_2O_7$ .This organic cationic diphosphate $(C_6H_9N_2)_2H_2P_2O_7$ was synthesized by the method of ion exchange resin**.** $(C_6H_9N_2)_2H_2P_2O_7$ crystallizes in the monoclinic system, with a merit factor of 0.0285, space group $P2_1/c$, a = 7,1991 (2) Å, b = 8,0209 (4) Å, c =31,2070(2) Å, β = 93,577(1)°, Z = 4, V = 1798.5 (1) $Å^3$. The crystal structure was refined down to R = 0.027, R = 0.069 for 1830 reflections satisfying criterion $I \geq 2\sigma(I)$. The structural resolution shows the existence of $H_2P_2O_7^{2-}$ ion chains linked together by hydrogen bonds. The organic cations $C_6H_9N_2^+$ and the phosphate chains are linked together by hydrogen bonds. Diphosphate group adopt an eclipsed configuration. A network of O-H... O hydrogen bonds reinforce the cohesion of the structure. The vibrational study by IR absorption spectroscopy of the title compound reveals the presence of three bands and confirms the existence of non-equivalent positions of water molecules in the structure.

$(C_6H_9N_2)_2H_2P_2O_7$ is a non linear optical NLO product as it is not centrosymetric.

References:

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**Keywords: Crystal structure, vibrational study, X-ray diffraction.**

## MS05-P02

### Chemical preparations, crystal data and vibration Spectroscopic Study of single crystal L-arginine phosphate monohydrate

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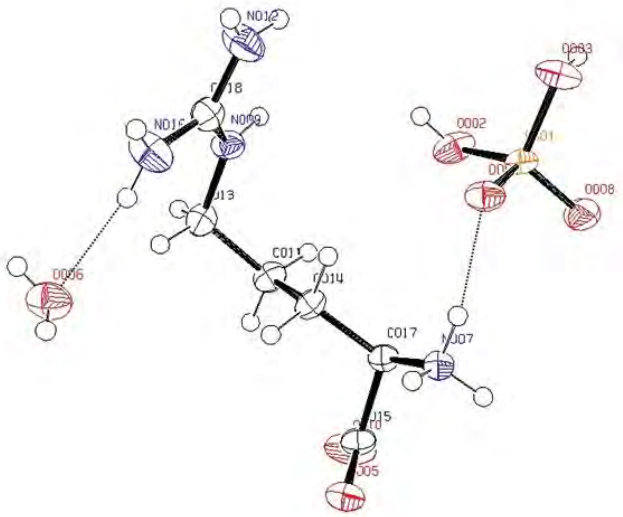
A single-crystal was selected from the reaction product of a stoichiometric mixture of phosphoric acid ($H_3PO_4$) to which was added the Arginine ($C_6H_{14}N_4O_2$) and its crystal structure determined from three-dimensional X-ray diffraction data. The structure is monoclinic, space group $P2_1$, $a$=7.3450(14) Å, $b$=7.9176(15) Å, $c$=10.8796(22) Å, $\beta$=97.98(2)°, $V$=626.57(186) $Å^3$ and $Z$=2, least squares refinement was converged to R1=0.0456, wR2=0.1433 for 3278 unique reflections. The structure consists of chains formed by edge sharing of PO4 tetrahedra, water and arginine. The stacking along b axis consists of these chains bridged by layers formed by PO4 water and arginine by hydrogen bonds. The Raman and infrared spectra of single crystal LAP were recorded to determine the symmetries of the vibrations of the various molecular groups such as $NH_3^+$, $NH_2$, $CH_2$, CH, $COO^-$, $H_2O$ and $H_2PO_4$ present in the crystal.

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