

**s2.m1.p21** Topological properties of the electron density distribution in amino-acid phosphates. W. Maniukiewicz<sup>(1)</sup>, E. Molins<sup>(2)</sup> and R.H. Blessing<sup>(3) (1)</sup>  
*Institute of General and Ecological Chemistry, Technical University of Łódź, 90-924 Łódź, ul. Zwirki 36. Poland, (2)*  
*Institut de Ciència de Materials de Barcelona, CSIC, Campus de la UAB, 08193 Bellaterra (Barcelona), Spain. (3)*  
*Hauptman-Woodward Institute, 73 High Street, Buffalo, New York 14203, USA.*  
 Keywords: AIM theory, charge density, protein phosphorylation.

The protein phosphorylation involves condensation of phosphate with the side-chain hydroxyl group of serine, threonine or tyrosine residues. This produces important changes in various physicochemical properties of the protein molecule. The Hansen-Coppens [1] multipole model of charge density has been fitted to low temperature high-resolution X-ray diffraction data for the racemic and the nonracemic crystals of serine and threonine phosphates. A comparative analysis of resulting model parameters is performed in terms of Bader's topological theory (AIM) [2]. The critical points of the electron density have been located in order to characterize the covalent bonds and intermolecular interactions. The results show that chemically similar bonds in different molecules are topologically equivalent.

This work was supported by the Polish Scientific Research Council (KBN) under grant 3T09A 064 14

**s2.m1.p22** Electron density analysis of L-histidinium dihydrogen orthophosphate orthophosphoric acid from X-ray and neutron diffraction data I. Mata<sup>a</sup>, E. Espinosa<sup>b</sup>, W. Maniuckiewicz<sup>a</sup>, E. Molins<sup>a</sup>, S. Veintemillas<sup>a</sup>, A. Cousson<sup>c</sup>, W. Paulus<sup>c</sup>, C. Lecomte<sup>d</sup>,  
<sup>a</sup>*Institut de Ciència de Materials de Barcelona, Campus UAB 08193 Bellaterra, Spain, (b)*  
*Laboratoire d'Ingénierie Moléculaire pour la Séparation et les Applications des Gaz, Faculté des Sciences Gabriel Université de Bourgogne, 6 boulevard Gabriel, 21100 Dijon, France, (c)*  
*Laboratoire Léon Brillouin CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France, (d)*  
*Laboratoire de Cristallographie et Modélisation des Matériaux Minéraux et Biologiques, Faculté des Sciences, Université Henri Poincaré, Nancy I, BP 239, 54506 Vandoeuvre-les-Nancy Cedex, France.*  
 Keywords: charge spin densities, L-histidinium.

Crystal structure, thermal vibrations and electron density of L-histidinium dihydrogen orthophosphate orthophosphoric acid (LHP) (formally  $C_6H_{10}N_3O_2 + H_2PO_4 \cdot H_3PO_4$ , monoclinic system, space group  $P2_1$ ), have been analysed from single crystal X-ray ( $T=140K$ ,  $a=9.084(3)$ ,  $b=8.913(1)$ ,  $c=8.786(2)$ ,  $\beta=111.03(2)$ ) and neutron diffraction data ( $T=130K$ ,  $a=9.037(6)$ ,  $b=8.906(5)$ ,  $c=8.749(5)$ ,  $\beta=110.93(9)$ ). LHP is a material which presents non linear optical properties.

The X-ray diffraction data (27597 measured reflections from which 7762 are unique,  $R_{int}=0.0242$ ) were collected with  $MoK\alpha$  radiation and scintillation counter up to a maximal resolution of  $\sin(\theta)/\lambda=1.35\text{\AA}^{-1}$ . The neutron diffraction data consist on 4475 collected reflections, from which 3423 are unique ( $R_{int}=0.045$ ), up to  $\sin(\theta)/\lambda=0.88\text{\AA}^{-1}$  using  $\lambda=0.8302\text{\AA}$ .

Crystal structure was refined against neutron and high order X-ray data ( $\sin(\theta)/\lambda > 1.0\text{\AA}^{-1}$ ), and the resulting structural parameters were combined in a new model, which was used as the starting point in a multipolar X-(X+N) refinement. In this refinement, a pseudoatoms model of the electron density distribution was fitted to the X-ray structure factors, previously corrected from anomalous scattering. This correction was performed in a previous multipolar refinement against the X-ray structure factors with not merged Friedel pairs.

At the end of the X-(X+N) refinement ( $R=0.017$  for 6521 reflections with  $I > 3\sigma(I)$ ), the highest discrepancies in the residual density maps (of about 3 times the variance of the maps) were observed close to the phosphorus atoms positions. The rigid bond test shows a very good deconvolution between the thermal vibration and the electron density parameters.

The electrostatic potential and the topological properties of the electron density distribution in the unit cell of the LHP will be presented, in order to characterize the intermolecular interactions. The electron density parameters of the L-histidinium moiety have been included in the multipolar data bank of peptides, created on the LCM<sup>3</sup>B with the aim of transfer to crystallographic studies involving proteins.

[1] N.Hansen & P.Coppens. *Acta Cryst.* **A34** (1978), 909-921.

[2] R.F.W. Bader. *Atoms in Molecules: a Quantum Theory* (Clarendon Press, Oxford, 1990)