## Electron Density and Electrostatic Potential Study of an Organic Phosphate

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The electron density of the phosphate of L-histidinium phosphoric acid (LHP), experimentally obtained by X-ray and neutron diffraction data, is used for a detailed study involving *ab initio* calculations and topological analysis of both the electron density and the electrostatic potential [1][2].

As the L-histidinium presents a large dipolar moment and LHP crystals are non-centrosymmetric, this material has potential non-linear optical properties. These properties strongly depend on the crystal packing which, in this case, involve very short hydrogen bonds.

The results of this analysis on the LHP electron density allow a good characterization of the intermolecular interactions and a better understanding of the crystal packing. Moreover, the topological analysis of the electrostatic potential proves to be a useful tool to study the interaction of the molecules with its environment.

[1] Bouhmaida N., Dutheil M., Ghermani N.E., Becker P., *J. Chem. Phys.*, 2002, **116**, 6196. [2] Leboeuf M., Köster A.M., Jug K., Salahub D.R., *J. Chem. Phys.*, 1999, **111**, 4893.

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