s2.m9.o3 Intermolecular Interactions in Molecular Materials from the Topological Analysis of the Electron Density Point of View.

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We present the characterization of different classes of materials (exhibiting molecular magnetism, charge transfer properties and resonance assisted H-bonds) containing hydrogen bonds, using experimental charge density analysis.

In the molecular magnetic materials, weak intermolecular interactions play an important role in the magnetic behavior at the macroscopic scale since they are involved in charge transfer, frontier orbital overlap and polarization mechanisms. A precise description of the electron density and its topology may help in understanding and developing new molecular magnetic materials.

The topology of the electron density is also precious for analyzing the interactions governing charge transfer between donor and acceptor in charge-transfer complexes, in peculiar in determining the pathway of the weak intermolecular interactions.

In the case of materials containing strong intramolecular hydrogen bonds, such interactions are very difficult to characterize because of the frequent dynamic and/or static (tautomerism, …) disorder affecting H atoms.

The presentation will be devoted to inter- and intra-molecular interactions in materials cited above, with an emphasis on tautomeric O-H—O/O—H-O resonance assisted hydrogen bonds. The correlation between the topological properties of the electron density at the bond critical points and the geometrical parameters characterizing hydrogen bonds will be discussed.

s2.m9.o4 Experimental and theoretical electron density and electrostatic properties as a tool for understanding activity of HIV-1 integrase inhibitor precursors.

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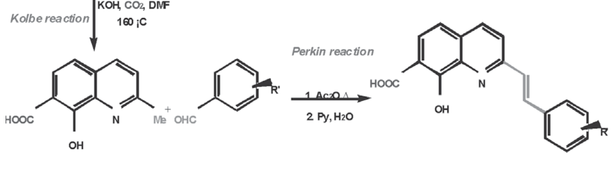
Keywords: Electron Density; Pharmacology; Structure / Reactivity

Styrylquinoline derivatives are potent inhibitors of the HIV-1 virus integrase activity. The biologically tested molecules contain one aromatic part connected to the quinoline group through different chemical spacers (carbon chain, urea, peptidic bond…). The most promising molecule in the inhibition of the HIV-1 integrase is the (*E*)-8-hydroxy-2[2-(4,5-dihydroxy-3-methoxyphenyl)-ethenyl]-7-quinolinecarboxylic acid (**1**) where the spacer is a C=C double bond (scheme). The crystallization of this molecule is particularly difficult giving rise to very small needle-shape crystals which are instable in time. The low temperature crystal structure was of very poor quality but has revealed a planar *trans* molecular conformation. In order to recover the molecular property, we have synthesized and crystallized the two precursors of this molecule: the 3',4',5'-methoxy-dihydroxy benzaldehyde aromatic part (**2**) and the 8-hydroxy-7-quinolinic acid (**3**). In the present study, high resolution X-ray diffraction data were collected at 100 K on a Smart CCD diffractometer. The diffraction intensities are fitted to the Hansen-Coppens multipole model. The electron density topological properties and the electrostatic potential are used to characterize the chemical bonds and the electrophilic/nucleophilic characters of the two precursors. The experimental results are compared to *ab initio* quantum mechanic calculations for (**2**) and (**3**) isolated molecules. These theoretical calculations were also carried out for (**1**). In the case of the two precursors (**2**) and (**3**) electron densities are used as reference in order to reveal the role of the chemical spacer in the charge transfer and electron delocalization between the two parts of the styrylquinoline derivative inhibitors.



(3) (2) (1)