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P.14.07.4
Interactions in Selected Dicarboxylic Acids Derived from Electron Charge Density
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High-resolution X-ray diffraction data were collected for tartaric acid, malic acid and its adduct with urea at 80 K to obtain accurate crystal data and experimental electron density. The measurements were performed on Nonius KappaCCD difractometer equipped with Oxford Cryosystems 700 Series Cryostream Cooler. The quality of tartaric acid data was compared with that of the data obtained using a point detector at 105 K.

Data was interpreted using the multipole formalism [1] to derive the electron density and related properties such as the electrostatic potential and atomic moments. The electron density and its Laplacian extracted from the data were analyzed in terms of the topological properties of covalent bonds and non-bonded interactions [2].

Charge density and topological properties for the studied crystal structures were carried out to explore the character and role of both inter- and intra-molecular hydrogen bonds.

The interesting features related to the differences of electron density distribution were found for the same functional groups (hydroxyl and/or carboxyl). The differences caused by molecular interactions have influence on the molecular symmetry. The results are compared to those obtained for analogous molecules.

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P.14.07.5
Experimental Electron Density Distribution of Bis(thiosemi-carbazide)-Zinc(II) Dinitrate
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Over three hundred transition metal complexes with thiosemicarbazide-based (TSC) ligand have been characterized by classical X-ray diffraction and seem to play a role in supramolecular chemistry [1]. In addition, a great number of TSC derivates present a very wide of potent pharmacological application [2, 3], while two of them (3-AP) and (5-HP) are used in clinical phase I or II against ribonucleotide reductase [4]. Understanding the interactions between the organic part and the divalent cation is essential in that case, since the mechanism involves a chelate compound with a divalent cation. Here, we present the electronic and electrostatic properties of the most simple TSC ligand coordinated with zinc(II). Cation behavior will be discussed in comparison with a zinc aspirinate compound [5].

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P.14.07.6
Electron Density, the Driving Tool towards Dynamics and Reactivity of Systems ?
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The fast development of photo-induced and time resolved diffraction leads to fundamental questioning about the proper modelisation of systems out of equilibrium.

Based on the role of Hellmann-Feynman force and its impact onto molecular dynamics, we have modelled the evolution of the charge density of simple molecules along a reaction path. Moreover, we have addressed the change of charge density in a molecular chain undergoing strong distortions, such as those initiating na soft mode transition.

The planned developments are strongly connected with the Cluster Partitioning Model recently developed in our group [1,2] which allows for a description of one particle density matrix of complex systems through a superposition of local contributions taking into account realistic environmental effects.

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P.14.07.7
Estimating ADP's of Hydrogen Nuclei for Charge Density Analysis
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Charge density analysis of X-ray diffraction data requires accurate treatment of the motion of all nuclei in order to deconvolute nuclear motion from the electron distribution. Presently, nearly 80% of charge density studies on molecular crystals assume isotropic motion of hydrogen nuclei, in large part due to the difficulty of performing accurate neutron diffraction studies on all systems of interest. However, failure to model the motion correctly not only alters the topology of the electron density close to the nuclei where the thermal motion has been simplified, but also in the vicinity of neighbouring nuclei [1].

Methods for approximating hydrogen atom ADP's based on a combination of rigid-body analysis and allowances for internal modes have been shown to be quite successful [1,2]. We have recently developed a new method for estimating hydrogen atom ADP's from first principles, using two layer "ONIOM" calculations [3] which mimic the effects of the crystal field and yield internal (high frequency) and external (low frequency) contributions to the nuclear motion. Results obtained for small molecules are consistent with neutron experiments at a variety of temperatures.

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P.14.07.8
Bonding in 5-Membered Cyclic Alkynes: Charge Density in 1-Zirconacyclopent-3-yne
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Small cyclic alkynes are, in general, unstable because of ring strain. Recently, 1-zirconacyclopent-3-yne complexes, *viz* 5-membered cyclic alkynes, were synthesized.[1] The bonding nature