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MS41.P09

The Transferability of Atomic Multipoles in Amino Acids and Peptides

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Popular force fields usually employ point charges. Supplementing atomic charges with higher electrostatic multipole moments leads to more accurate charge distribution models. New generation force fields based on multipole models require high level of transferability of atomic multipoles. The aim of this work was to analyze the level of transferability achievable with the use of different methods of molecular density partitioning.

Molecular densities (MDs) were calculated for selected natural amino acids as well as di- and tripeptides in geometries as observed in X-ray diffraction experiment. The MDs were obtained through Fourier space fitting of pseudoatom model to the electron densities resulting from *ab initio* DFT calculations at B3LYP/6-31G** level. Such procedure was selected in order to be compatible with the idea of building a pseudoatom database [1-3] pursued in the charge density crystallography. Atomic multipole moments expressed in local coordinate system were calculated on the basis of three density partitions: directly from pseudoatoms, from atomic densities computed via stockholder partitioning and from atomic basins derived via topological analysis. Standard deviations from averaging over multipole moment components of atoms that are considered equal in their chemical environments (atoms representing the same atom type) were chosen as a measure of transferability.

The advantage of stockholder partition as yielding the best transferability within considered atom types was observed. The results were compared to the calculations of atomic multipoles directly from molecular wave functions (in atomic basins partition).

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MS41.P10

Bond Characterization of trans-4,4'-azo-1,2,4-triazole: A Combined Experimental and Theoretical Charge Density Study

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The experimental charge density distribution of a planar centrosymmetric molecule, trans-4,4'-azo-1,2,4-triazole, has been investigated in terms of a pseudo-atomic multipolar expansion

(Hansen-Coppens formalism) using high resolution single-crystal X-ray diffraction data at 100K. A parallel computation based on DFT calculation at the B3LYP level using 6-31G(d,p) basis set was performed on the molecule in gas phase. The electron density will be presented in terms of deformation density as well as the Laplacian distribution. Bond characterizations are expressed in terms of topological properties at the bond critical points; typical covalent character on N—N, N—C bonds are observed. The π bonding-delocalization of the molecule will be further illustrated by the Fermi-hole distribution. A π−π interaction with the inter-planar distance of 3.2 Å is allocated through the BCP and the associated bond paths. The agreement between experiment and theory is good on all intra-molecular interactions; the atomic charges, molecular electrostatic potentials, and natural bond orbital analyses will also be presented.
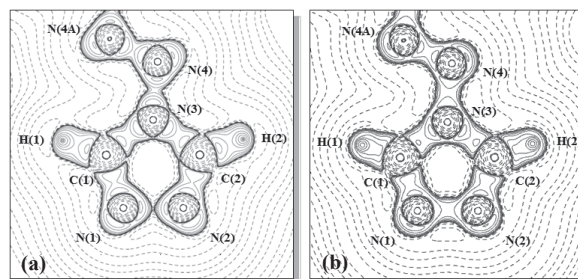

Figure. Laplacian map, $\nabla^2\rho(r)$ in the plane of N1-N2-N4 from (a) the experimental (b) the theoretical charge density.

Keywords: charge density, multipole model, π−π interaction

MS41.P11

New version of UBDB databank and LSDB program, verification and applications

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The theoretical databank of aspherical pseudoatoms (UBDB) has been designed as a set of parameters to be used in standard refinement of crystal structures, as a starting point in high-resolution studies, or also in reconstruction of molecular densities and the evaluation of a number of electrostatic properties of studied molecules. The UBDB consists of all atom types found in peptides, proteins and some other biologically relevant molecules [1]. It had been already shown that the databank corresponds very well to the electron density in a number of amino acids, when compared to conventional *ab initio* methods at the B3LYP/6-31G** level, and also, reproduces the electrostatic interaction energies quite well (~1kcal per mole).

The UBDB was recently extended by over 100 new atom types present in RNA, DNA and in other molecules of great importance in biology and pharmacy. The atom types' definitions were modified and new atom keys added to provide more precise description of the atomic charge distribution. H-X bond lengths were updated according to Allen et al. (2010) [2] and implemented in the LSDB program as well as used for modelling the appropriate atom types. The new version of LSDB and databank is available on the website [3].

UBDB databank was extensively tested. Electrostatic interaction energies calculated on the basis of databank of aspherical atom models (EP/MM method) [4] were compared to the corresponding results obtained directly from wave functions at the same level of theory (B3LYP/6-31G**) (SPDFG program) [5] and to some other theoretical methods [6]. Various small complexes were analysed to cover most of different interaction types and to test the newly added