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Keywords: databases, charge density, electrostatic calculations

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Topological properties of hydrogen bonds: Charge density studies by the maximum entropy method

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The Maximum Entropy Method (MEM) is applied to low-temperature single crystal x-ray diffraction data of amino acids and peptides. The resulting electron density maps are analyzed according to Bader's Atoms in Molecules theory (Bader, 1994) towards the determination of the electron density and its Laplacian at bond critical points (BCPs). Energy densities at BCPs are calculated according to Abramov (1997), employing the local virial theorem. Geometrical, topological and energetic properties of 52 hydrogen bonds are studied. The electron densities, their principal curvatures and the energy densities at BCPs are found to depend systematically on the distance between hydrogen and acceptor atom. These relations appear different from the corresponding relations as described by Espinosa et al. (1999) for multipole densities. MEM electron densities at the BCPs of hydrogen bonds are higher than the multipole densities. The difference between MEM and multipole densities is more pronounced for stronger hydrogen bonds. The contribution of the prior density (overlapping spherical atomic electron densities) to the MEM density is studied. The prior density seems to contribute a large part to topological and energetic properties at BCPs of hydrogen bonds. However, the properties at BCPs of covalent bonds of MEM densities differ significantly from the prior. Thus, for research into chemical bonds an experimental electron density should not be substituted by a promolecule.
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Topology of the electrostatic potential in the analysis of molecular reactivities and hydrogen bonds

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The topology of the electrostatic potential (EP) has been studied for single molecules using geometries and electron distributions determined from high-resolution single-crystal X-ray diffraction experiments. Local maxima, corresponding to the nuclei, and local minima are associated to electrophilic and nucleophilic sites, respectively. Space can be partitioned in primary bundles, which are volumes formed by field lines with the same start and end. Influence zones of electrophilic and nucleophilic sites can be built by joining primary bundles with a common start (nucleophilic) or end (electrophilic). Zero flux surfaces and saddle points can be used for delimiting influence zones, as they appear on the surface of the primary bundles. In the bonding regions, the topologies of EP and the electron density (ED) are similar, appearing a saddle point of EP analogous to the bond critical point of ED. As seen from a theoretical study on hydrogen bonded complexes, the region between the saddle points of EP and ED is populated by electrons of the acceptor atom which are electrostatically attracted toward the hydrogen atom. As the topological properties at both saddle points show a similar behavior, the analysis of EP is useful for the characterization of hydrogen bonds. In another theoretical study, the effect of the chemical and crystallographic environment on the hydrogen bond has been simulated by external electric fields. The perturbations induced on both the topologies of ED and the interaction energy are related.

Keywords: electrostatic potential, topology, hydrogen bonds

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Avoiding multiple diffraction for accurate charge density measurement using synchrotron radiation

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Although contamination by multiple diffraction (MD) to the diffracted intensity is neglected in many cases of structure determination, its influence is not negligible for accurate measurement of charge density in crystal, especially with heavy elements, and must be avoided. Since in the researches with Synchrotron Radiation (SR) incident beams are highly collimated, it is generally believed that the MD has little effect on structure factor measurements. The aim of the present study is to see whether MD can be neglected or not. The authors measured integrated intensity from Yttrium Iron Garnet (YIG) crystal by a four-circle diffractometer with avalanche photo diode detector at Photon Factory BL14A. Two types of data collection were carried out, one at ordinary bisecting position and the other at the position avoiding MD by psi-rotation of the crystal (MD-free). In MD-free measurement, the perturbation due to MD in each structure factor was simulated from the orientation matrix, and optimal four angles were calculated to avoid MD. Then integrated intensities were measured at those positions by modifying the program controlling the diffractometer. 9910 reflections up to sin(theta)/lambda < 1.24 (wave length = 0.75Å, 2theta < 137 degrees) were measured in both cases. In the MD-free measurement only 91 reflections were measured at the bisecting position. The XAO analysis of the two data sets exhibited a significant improvement of the MD-free experiment compared to the intensity data measured at the ordinary bisecting setting.

Keywords: charge density, multiple diffraction, synchrotron radiation