

Charge-density studies in small molecules and proteins: sources and detectors

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Charge density analysis [1] of accurate high-resolution single-crystal X-ray diffraction data is a matured branch of crystallography. At ultra-high resolution the deformation of the electronic cloud of atoms due to chemical bonding and interactions is highlighted via multipole modeling of electron densities. The derived electron densities and the electrostatic potentials can be utilized to calculate electrostatic interaction energies. Hydrogen bonds can be characterized by performing topological analysis of electron densities at the bond critical points. Although this technique is well-established for small molecules [2] this methodology has recently been adopted for macromolecules [3] as the number of biological macromolecular structures at ultra-high resolution (less than 1 Angstrom) are increasing gradually. However, the accuracy of charge density models and so the chemical bonding features are highly dependent on the quality of diffraction data, which is directly linked to the characteristic of the radiation sources and the performance of the detectors used, other than the sample history. This presentation will review some of the best recent reports of charge density studies in small molecules and proteins using various facilities and also highlight some new results from charge density analysis in organic chromophores using second generation home source and advanced detector. The various cases considered in this presentation may help users to evaluate the best combination of sources and detectors to be used for their respective samples to perform accurate charge density analysis.

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