Electrostatic and Related Properties from Accurate Charge Density Analyses

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Properties of atoms and molecules in crystals are now commonly extracted from a combination of X-ray diffraction experiments and theoretical results from a variety of approaches. Modern quantitative charge density studies typically involve use of CCDs and/or synchrotrons, *T* below 120 K and frequently nearer 10 K, careful data reduction and correction for systematic effects, and detailed modelling of atomic motion. Multipole refinement yields topological properties of the electron density in almost all studies, while valuable electrostatic properties are seldom reported. Yet there is a wealth of such properties accessible from the X-ray experiment: electrostatic potential, electric field and field gradient, atomic charges, electric moments of molecules in the crystal, and even intermolecular interaction energies.

If we accept that "theory is a good thing but a good experiment is forever" [1], we must ask: Are we maximizing the information that can be obtained from charge density data sets? If not, why not, and how might this be redressed? This presentation will seek answers to these questions from a discussion including results from a selection of recent studies. Limitations of some of the common approaches will be highlighted, and some solutions will be proposed, along with comments on related properties that might be explored.

[1] Kapitza P.L., *Experiment, Theory, Practice,* (D. Reidel, Boston),1980, 160.

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