Direct and Simple Experimental Crystallographic Method to Calculate Partial Charges with Atomistic Correspondence to *ab-initio* Methods

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Derivation of partial charges in small and large scale molecular systems is important for modeling of various experimental and theoretical properties like dipole moments, auto-correlation functions, charge disparity, understanding of dispersion, benchmark of classical MD simulations and electrostatic potential energy surface mapping. A correspondence between theoretical calculations (based on single/small number of molecules) is usually established with macroscopic IR/Raman spectra or dipole moment measurements. Such comparisons are indirect and lack a fine mapping of electrostatic potential from theory to experiment. In a new approach developed as the experimental part of this work, partial charges are calculated from crystallographic model refinement. The experimental method exhibits a satisfactory correspondence with partial charges obtained using quantum chemistry calculations. Particularly, gas phase partial charges from CHELPG method and condensed phase Lowdin charges correlate well and validate this experimental method.

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