Invarioms for Automated Low Order Data Charge Density Analysis – Optimizing Conditions

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Considerable effort is necessary for an experimental charge density study with respect to the X-ray diffraction experiment and the modeling of the high resolution data. By introduction of invarioms [1], that define an intramolecular transferable atom using the nearest neighbor approximation [2], invariomic multipole parameters can be predicted. For this purpose we use theoretical calculations [3] on model compounds that mimic the same chemical environment as an atom in a given structure. For the molecular electron density theoretical structure factors [4] are calculated and a multipole refinement then yields the parameters needed. This way approximated aspherical structure factors and an improved geometry can be derived for a crystal structure of interest. Properties derived from the density, i.e. Hirshfeld surfaces [5], the electrostatic potential, dipole- and multipole moments as well as topological properties are then accessible. It is emphasized that by using this procedure, standard low resolution data sets can be evaluated. The fact that a defined limited number of invarioms exists allows additionally the automation of the modeling process, for which a program is currently developed. The usage of theoretically derived multipoles has several advantages compared to the experimentally obtained [6] ones. In this work we want to investigate, how temperature and resolution of an experiment influences the fit when using invarioms compared to a spherical atom approximation (promolecule). To answer this question several data sets were measured on the same D,L-serine crystal at different temperatures of 293, 100 and ~20K. Different resolution cutoffs were also tried, using the same evaluation procedure. Similarly on the theoretical side, several DFT basis sets were compared to show that optimal density is used in our database.

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