

Summary

In the scope of this work three visualization programs and a data-base application for transferring multipole parameters were developed. These programs and methods were used in four charge-density studies.

Moliso enables the transparent visualization of color-mapped iso-surfaces together with the molecular structure, which could optionally include thermal ellipsoids. Beside the iso-surface, a cut-plane could also be displayed. For the correct transparent visualization a new approach was developed, which makes normally necessary sorting of polygons dispensable.

Molecool is a simple molecule-visualization program, which can directly read XD-files. It can display local coordinate systems and thermal parameters. The crystal environment can be calculated and a hydrogen bonding table will be plotted.

Rlat4XDS helps analyzing the reciprocal space if the program XDS has been used. It can exclude regions of the reciprocal space from the cell determination and correct the X-Ray data for phosphorus-absorption of the CCD-detector.

InvariomTool transfers theoretically calculated multipole parameters, called invarioms, from a data base into XD input files. It assigns invariom names to each atom of the structure. A database of invarioms can also be built up with this program. Additionally it can be used to generate XD input files for multipole refinement automatically, without using Invarioms. With the invariom approach it is possible to determine the charge density of low resolved X-Ray data sets. This enables the replacement of the independent atom model in future.

The charge-density study of the halogenated fullerene $C_{60}F_{18}$ shows C-C bonds of very different strength which could be found in good agreement with the theory. The electrostatic potential (ESP) shows a strong dipolarization of the molecule. Weak inter-molecular interactions could be analyzed with the use of

the electron density mapped on Hirshfeld surfaces.

The validity of the nearest neighbor approach could be shown for all carbon and oxygen atoms in thymidine by application of two different invariom models and a classical multipole refinement. A perfect agreement between the two invariom models could be found. Only small differences between the invariom models and the classical refinement were found while these differences could be assigned to the crystal environment. Relative bond strengths of thymidine could be found by the topological analysis of the electron density (ED) and the integration of the ED in the electron localization function (ELF), which was calculated from an "experimental" wavefunction, in agreement with the expectation from resonance structure formulae. The experimental ELF was used here for bond characterization for the first time. Effects of the crystal environment could be best studied with the analysis of the ESP and the Hirshfeld surfaces.

Adenosine was described with an invariom model and two classical multipole models with a different degree of freedom in the refinement. Also a good agreement between the models could be found here. The relative bond strengths do not vary that much as in thymidine, but the same trends could be found in the topological analysis of the ED and the integration of the ED in the ELF basins of adenosine.

The Watson- & Crick base pair 9-methyl-adenine-1-methyl-thymine lies almost completely on a crystallographic mirror plane in the crystal. The results of the topological analysis of the ED and the ELF-Integration agree well with the findings in Adenosine and Thymidine. The intermolecular contacts could be analyzed by the study of the gradient vector field of the ED and the ESP. The two hydrogen bonds which are also present in the DNA are equally strong but show different electrostatic behavior.

With the methods and approaches developed in this work it is possible to get experimental charge density faster and from lower resolved X-ray data. The results could be better understood and presented with the appealing visualization approaches.