Single-crystal X-ray diffraction applied to electron density analysis

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Abstract

Single-crystal X-ray diffraction (SCXRD) permits to determine molecular structures in crystalline systems. To this end, crystallographers fit the Independent Atoms Model (IAM) against the collected X-ray structure factors. However, after structure determination, electron density residuals indicate that some information has not been taken by the model. These residuals, which are ~3% of the total SCXRD, contain the contribution of all intra- and inter-molecular interactions to the electron density distribution in a crystal (EDC). To absorb this significant information, the multipolar model (MM), which works on the modelling of valence electrons, was developed in late 70's. Actually, most of EDC studies use MM to analyze how atoms and molecules interact through the space. In this lecture, we will see the experimental factors having an influence on the quality of the EDC model (either IAM or MM), and how MM is defined. In the last part, we will see some MM applications that permit to understand the intensity and nature of interatomic interactions, and how molecules organize in space through them.