Abstract :

Nowadays, X-ray diffraction equipment allows us to detect weak X-ray intensities. This ability increases the quantity of structural information obtained from experimental data. Furthermore, the development of in situ and operando measurements heightens the need for perfect modeling and interpretation of the electronic density of crystalline structures [1]. Although, the software CrysAlisPro [2] connected with Olex2 [3] seems to be able to solve single crystal structures for us. However, the interpretation of residual density and the determination of more complex structures such as aperiodic, twined or disordered structures still need advanced knowledges in crystallography field, which can not be compensated by a software. The equipment automation and the performance of the software allow the re/investigation of structures that we would have rejected or where a part of the solution would have been ignored, such as a compound with a large solvent disorder. In case of pharmaceutical compounds, it is essential to know the composition and the exact structure of the active molecule but some other elements may be present and may disrupt the active process (excipient or solvent). For example, in case of Trospium Chloride, a drug used to treat incontinence and overactive bladder, the determination of the presence of two disordered polymorphs in the same crystal were vital for the production of the proper compound [4].
After a brief introduction about disordered structures, I will present how we can model the arrangement of different disordered solvents using the software Jana2006 [5] (anharmonic ADP, rigid body and splitting the atomic position) to understand phase transitions of [Zn-(C7H4NO4)2]·3H2O [6]. Then, I will discuss an unexplainable methanol-solvent disorder in polyphosphate of cadmium, which could finally be modeled using the group/subgroup theory. Finally, I will speak about the polyoxometalate structures, polyvalent functional compounds [7] for which the automatic procedure of CrysAlisPro and Olex2 are not working well.

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