Use of selected computing tools for study of molecular and supramolecular structures of (not only) coordination compounds

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Full characterization of the molecular and supramolecular structure of the studied compound is one of the main goals of single crystal X-ray structure analysis. This characterization includes calculations of various geometric parameters as well as graphical drawing of the formed structures. Standard computing tool for calculation of (not only) geometric parameters is the program *PLATON* [1] while for drawing of illustrations program *DIAMOND* [2] is used in our laboratory. Recently, program *CrystalExplorer* [3] became very popular as it, as an advanced tool for study of the (supra)molecular structure, allows among others to calculate Hirshfeld surfaces; this allows to visualize the packing modes and intermolecular interactions in a new way. In addition, program *Mercury* [4] can be also used for advanced study of (supra)molecular structure as it offers visualization of closely related molecules (e.g. solvatomorphs) by structures overlay or to explore the crystal packing forces using statistical data of CSD using the Full Interaction Maps. The use and usefulness of these advanced computing tools will be illustrated on two polymorphs of the Co(III) complex with Salen-type Schiff base and two solvatomorphs of Ni(II) complex based on 2,2'-bipyridine and oxalato ligands.

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