MS23-05 | New Tools in Jana2006/Jana2020 to Study and Characterization of Pi-Pi Stacking of Incommensurate Modulated Structures: α & ß-Mn(dmp)Cl_2

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Understanding packing and interactions inside solids is important knowledge for crystal engineering aiming to build new desired compounds with specific physical and chemical properties [1], as well as for understanding properties such as luminescence [2]. Two important interactions in organic, organometallic or protein structures are highlighted: hydrogen bonding [3] and π interactions (π-anion, π-cation and π-π-stacking) [4]. Both types of interaction are characterised by specific distances and angles, which can be easily determined and visualized using graphic software such as Diamond[5] or Mercury[6] for 3D structures. However, in case of modulated structure (3+1)D, this visualisation and interpretation is not so straightforward. In this contribution, we describe new tools developed for Jana2006/Jana2020 software in order to find and visualize π-π-stacking in (3+1)D modulated structures. The improvement of the π-π stacking vizualisation allowed us to understand the difference between two new polymorphs, α and β-Mn(dmp)Cl_2, which we use as a case study.

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