

Jana2020 - Magnetic option

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The decision to create a new program for solving regular, modulated and magnetic structures stems from the fact that the graphical interface of the Jana2006 program [1] does not allow further improvement. The main aim was to create a program that would significantly facilitate solving and refining complicated crystal structures. A new original drawing procedure, JanaDraw, lies in the centre of this effort as it enables editing of structure parameters directly through the plot. JanaDraw displays regular as well as modulated structures and includes visualisation of the magnetic moments. The procedure makes full use of magnetic and superspace magnetic symmetry. Moreover, it naturally uses all specific options used in Jana, like rigid body groups, local symmetry, and special modulation functions. Editing of structural parameters can be done directly on atoms selected from the current structure plot, and this new feature greatly simplifies refining and completing the structure model. JanaDraw also supports so-called animations, where a modulated structure is continuously modified and redrawn according to its modulation functions.

At each refinement cycle, the processing can be monitored through the variation of statistical parameters such as R-factors. Users can directly see changes in the position of atoms, the shape of ADPs, or the magnitude of the magnetic moment in the JanaDraw plot. Similarly, profile changes during the refinement using powder data can be monitored with the Profile viewer. Both of these options can be extremely helpful in the refinement of difficult structures.

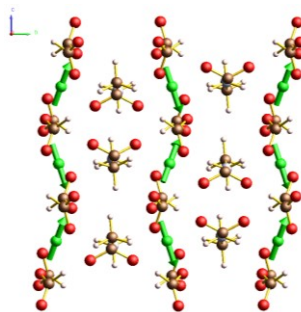


Figure 1. Magnetic and structural incommensurability in $[\text{CH}_3\text{NH}_3][\text{Ni}(\text{COOH})_3]$ [2]

For magnetic structures, the program allows representation analysis based on irreducible representations of the parent structure. In addition, more advanced methods can be used by direct connection to the ISODISTORT system [3] and the Bilbao Crystallographic server [4]. Jana2020 also contains significantly improved procedures for analysing possible twinning of the crystal during the transition from a higher magnetic group to a subgroup. This feature is extensively used for phase transitions studies. For magnetic structures with $k = 0$ and commensurately modulated magnetic structures, the possibility to refine the magnetic modes has been implemented as an alternative to the refinement of magnetic moments.

In the lecture, we will present applications of the latest version of the Jana2020 program.

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