The magnetic option in Jana2006

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The new magnetic option implemented in Jana2006 is capable of handling different sets of diffraction data to consistently solve and describe commensurate and incommensurate magnetic structures based on symmetry considerations [1]. The representation analysis uses the magnetic symmetry of the paramagnetic phase and its irreducible representations.

Jana2006 uses directly the symmetry operations from Shubnikov space and superspace groups to describe the relevant symmetry modes for the spin configuration and its constraints consistent with the parent paramagnetic space group and the magnetic propagation vector(s). This procedure renders a better performance dealing with non-modulated and modulated magnetic structures and simplifies the algoritms for handling the diffraction data of modulated magnetic phases [2]. Furthermore, the assignment of a symmetry group for a magnetic phase conveys unambiguously other important features such as magneto-structural couplings. To further explore the aspects of the magnetic ordering, the magnetic option of Jana2006 is connected to Bilbao Crystallographic Server [3] and ISODISTORT [4].

Here we will review the fundamental concepts of magnetic symmetry and the superspace formalism, and present the working flow and the capabilities of the magnetic option of Jana2006. Several examples of magnetic ordering models will be presented for both commensurate and incommensurate types of magnetic structures.

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2. V. Petríček, J. Fuksa, M. Dušek, *Acta Crystallogr. A* 66 (2010) 649.

3. J.M. Perez-Mato, *et al*., Aroyo, *Annu. Rev. Mater. Res.* 45 (2015) 13.1.

4. ISOTROPY Software Suite, iso.byu.edu (06/2019).