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Solution of magnetic structures in JANA2020

Abstract

JANA2020 is a program developed for the solution and refinement of regular, twinned, modulated, and composite crystal structures. In addition, JANA2020 includes a magnetic option for solving magnetic structures from powder and single-crystal neutron diffraction data. This tool uses magnetic space and superspace symmetry to describe modulated magnetic structures. The basics of the underlying formulation of magnetic structure factors and the use of magnetic symmetry for handling modulated and non-modulated magnetic structures will be presented, together with the general features of the magnetic tool. Examples of structures solved in the magnetic option of JANA2020 are given to illustrate the operation and capabilities of the program.

BACKGROUND

Junior scientist, head of the group of Magnetic Structures at the department of Structure Analysis of the Institute of Physics – Czech Academy of Sciences. Main topics of research are frustrated and highly correlated systems. She has extensive experience in the synthesis of new materials containing f-elements and characterization of their structure and electronic properties under multi-extreme conditions using x-rays and neutron scattering techniques. Margarida works in magnetic structure determination and magnetic crystallography in aperiodic systems. She is part of the development team of Jana2020 and an active lecturer on its magnetic option for scientists and students of worldwide renown facilities and universities. She is also a member of the Commission for Magnetic Structures of IUCR.

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