Acta Cryst B
STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

ISSN 2052-5206

Introduction to the magnetic structures special issue

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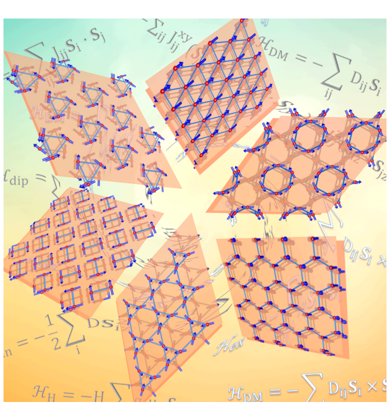
Keywords: magnetic structures; magnetic symmetry; representation analysis; magnetic neutron diffraction; magnetic CIF.



Magnetic crystallography deals with the structural characterization of magnetically ordered materials, where magnetic ordering implies the breaking of time-reversal symmetry. Similar to the role of space groups in conventional crystallography, magnetic space groups (also referred to as Shubnikov groups) are essential for classifying and describing commensurate magnetic structures. Although these groups were first systematically compiled by Zamorzaev (1957), their use in experimental and theoretical studies remained limited for many decades, largely due to the absence of standardized notation and accessible software. As a result, the magnetic structure community traditionally relied on the representation analysis method, established by E. F. Bertaut and later extended by Yu. A. Izyumov, both to determine and describe magnetic structures.

This situation changed significantly in the early 2000s, when new computational tools based on magnetic symmetry became widely available, driven by the growing interest in multiferroic and spin–orbit-coupled materials. These developments included standardized machine-readable listings of magnetic space groups, and the extension of available refinement programs to support magnetic symmetry for both commensurate and incommensurate cases. In addition, symmetry-based tools for the analysis of magnetic phase transitions were also developed, providing a more rigorous framework for understanding the coupling between magnetic, structural and electronic degrees of freedom.

These innovations have marked the beginning of a new era in magnetic structure analysis. Under the patronage of the IUCr, the magCIF standard was introduced as an extension of the conventional CIF format to accommodate magnetic symmetry. Similar to space groups in ordinary crystallography, magnetic symmetry groups in magCIF provide a unified and unambiguous format for the description and communication of magnetic structures. The magCIF format is now supported by most programs available for refinement and analysis, and has been the basis for the development of a comprehensive database of magnetic structures.

In this context, this special issue highlights how magnetic crystallography, now supported by a wide range of freely available computational tools, has become an efficient and accessible methodology for a wider research community. It aims not only to raise awareness of these resources but also to promote the adoption of standardized best practices for determining and reporting magnetic structures.

This virtual issue opens with a report from the IUCr commission on Magnetic Structures, which presents a set of guidelines for communicating and publishing commensurate magnetic structures (Perez-Mato *et al.*, 2024). These guidelines recommend the systematic application of magnetic space groups when describing or reporting commensurate magnetic structures. In this way, a standardized methodology similar to that of conventional crystallography can be applied. With the presently available software and databases, this can be done in a straightforward manner, regardless of the method used to determine the structure. These guidelines are followed by some examples of their application (Damay, 2024), a review of the UNI symbols as a recommended unified notation for magnetic space groups (Campbell *et al.*, 2024) and a brief account of how the long-standing divide between magnetic group symmetry and representation analysis has disappeared and how both approaches can be applied in a complementary manner (Rodriguez-Carvajal & Perez-Mato, 2024). The issue also includes reviews of some of the available software for analysis and modeling (Wills, 2025; Tasci *et al.*, 2025) and for magnetic structure refinement (Von Dreele & Elcoro, 2024; Henriques *et al.*, 2024; Rodriguez-Carvajal *et al.*, 2025). These are followed by a series of case studies in which magnetic structure analysis plays an essential role and the guidelines are applied. They include reviews of compound families (Garcia-Muñoz *et al.*, 2024; Garlea & Sarkis, 2025) as well as reports of specific materials analyzed using the new standards (Muñoz *et al.*, 2024; Pomjakushin, 2024; Nambu *et al.*, 2024; Calder *et al.*, 2024; Cadogan *et al.*, 2024; Attah-Baah *et al.*, 2024; Manuel *et al.*, 2025). The collections ends with a study of an incommensurate magnetic system (Colin *et al.*, 2025), showing how the superspace group formalism provides a similar degree of standardization for incommensurate cases.

This collection of articles showcases the latest advances in methods for determining commensurate magnetic structures and the standardization in their description. Each contribution follows the guidelines for magnetic structure communication and thus serves as a practical example of a clear, consistent, and standardized approach to reporting magnetic structures. We hope this collection will encourage a broader community to adopt these best practices when reporting new structures.

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