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Refining magnetic structures using representational theory and SARAh - learning from simplicity and serendipity

As we approach the centenary of Neel' s models of antiferromagnetism and ferrimagnetism, it is remarkable to note that magnetism and magnetic orderings remain frontiers of research rather than turn-the-handle studies. Quantum mechanics, the framework originally used to dismiss these initial models is now seen to allow possibilities that are still being discovered. For over 60 years, the need to describe and analyse magnetic structures has involved a range of group theoretical techniques, with formalisms based on the Shubnikov groups and representation theory becoming the most common. Underlying the modern application of these is a framework of phase transitions that was proposed by authors such as Landau, Dzyaloshinski, and Dimmock.

SARAh was originally developed in 1999 [1] as to perform the calculations of representation theory and as a meta-programme (a front end) to allow the analysis of magnetic diffraction data with GSAS and FullProf directly in terms of the mixing (weighting) coefficients of the magnetic basis functions. This talk will explain some of the theoretical background behind the new software [2], webSARAh and SARAh webRefine FP, which brings together representation theory, Shubnikov groups, order parameters groups and Landau theory, and integrates the analysis with FullProf. It will also introduce SERENDIPITY, a protocol to determine exchange interactions compatible with a given magnetic structure. The example application of SERENDIPITY to the analysis of powder inelastic neutron scattering data collected from the frustrated magnet claringbullite will be briefly explained [3].

[1] A.S. Wills, A new protocol for the determination of magnetic structures using Simulated Annealing and Representational Analysis- SARAh, Physica B: Condensed Matter 276, 680 (2000).
[2] A.S. Wills http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-web-representational-analysis/
[3] M. Georgopoulou, B. Fåk, D. Boldrin, J. R. Stewart, C. Ritter, E. Suard, J. Ollivier, and A. S. Wills
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