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Magnetic, electric and toroidal polarisation modes describing the physical properties of crystals - the NdFeO3 case

Tuesday, 21 March 2023 16:00 (2 hours)

We present a general classification [1, 2] to answer the question: which groups allow to describe a given magnetic, electric and toroidal polarisation mode? These three classifications are based on magnetic point groups used in two contexts: (i) the magnetic point group of the magnetic crystal class and (ii) the magnetic site symmetry point group of the Wyckoff position of interest. The following statements are true for magnetic, electric and toroidal modes: (i) there are 64 unique modes: 3 pure ferro-, 13 mixed ferro- with antiferro- and 48 pure antiferro-, (ii) a continuous reorientation of any moment is possible only in triclinic or monoclinic symmetry [3], (iii) canted antiferro- ordering is possible only in monoclinic or orthorhombic symmetry.

To visualise the similarities of magnetic, electric and toroidal modes, we propose a new Rotation-Inversion (RI) notation [1] of magnetic point groups which does not prioritise or distinguish any of three generalised inversions: space inversion -1, time inversion 1'and the space-and-time inversion -1'. In RI notation each operation is presented as a product of one proper rotation and one generalised inversion. The general classifications of modes are presented for the case of NdFeO3.

References

[1] P. Fabrykiewicz, R. Przeniosło and I. Sosnowska, Acta Cryst. A (in press)
[2] P. Fabrykiewicz, R. Przeniosło and I. Sosnowska, Acta Cryst. A77 (2021) 327
[3] R. Przeniosło, P. Fabrykiewicz and I. Sosnowska, Acta Cryst. A74 (2018) 705

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