Magnetic, electric and toroidal polarization modes describing the physical properties of crystals. NdFeO$_3$ case

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We present [1] the answer to the question: which groups allow to describe a given magnetic, electric and toroidal (anapole) polarization 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. Magnetic, electric and toroidal modes are considered in restricted sense, i.e. as set-of-directions, disregarding the atomic positions. For magnetic, electric and toroidal orderings there are 64 modes: 3 pure ferro(magnetic/electric/toroidal) modes, 13 mixed ferro(magnetic/electric/toroidal) with antiferro(magnetic/electric/toroidal) modes, and 48 pure antiferro(magnetic/electric/toroidal) modes. The proposed classification of modes leads to useful observations: the electric and toroidal modes have many symmetry limitations similar to those already known for the magnetic modes [2, 3], e.g. continuous reorientations of the magnetic or electric or toroidal moments are possible only in triclinic or monoclinic symmetry. Similarly, antiferro(magnetic/electric/toroidal) ordering with a weak perpendicular ferro(magnetic/electric/toroidal) component 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 both space-and-time inversion, -1’. Each operation O from a magnetic point group is a product O = RI of one proper rotation R = 1, 2, 3, 4 or 6 and one generalized inversion I = -1, 1’ or -1’. Proper rotations transform magnetic, electric and toroidal polarizations in the same way while inversions in different ways. Starting from the magnetic point group which describes a certain mode of the magnetic moment, we can obtain another magnetic point group which describes the same mode for electric polarization by a specific permutation of generalized inversions which changes -1 to 1’ in RI decomposition of each operator of the magnetic point group as shown graphically in Fig. 1.

The general classifications of magnetic, electric and toroidal modes are presented for the case of NdFeO$_3$. The predicted monoclinic NdFeO$_3$ symmetry [1, 2] leads to a nontrivial Dirac multipoles motif which could be confirmed using neutron diffraction or resonant x-ray diffraction [4].

![Figure 1](https://example.com/figure1.png)

Figure 1. Schematic presentation of the action of permutations of generalised inversions -1, 1’ and -1’ on the magnetic moment, M, the electric polarization, P, and the toroidal polarization, T. Symbol R (with hat) represents the proper rotation.