Advances in the application of magnetic and non-magnetic superspace-group symmetry

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Superspace-group symmetry is essential to the unambiguous description of modulated structures, and a correct understanding of their physical properties. An exhaustive enumeration of superspace groups in up to 3+3 dimensions were announced previously [1-2]. We now announce an exhaustive enumeration of magnetic superspace groups in up to 3+3 dimensions (over 250,000 groups). With these tables in hand, we have developed an algorithm and tool that detects the unique superspace-group (magnetic or non-magnetic) of an arbitrary modulated structure, given the amplitudes and phases of its modulations, and identifies it in the exhaustive symmetry-group table. This capability has been integrated into both the FINSYM and ISOCIF packages of the ISOTROPY software suite [3], and to JANA2000. The ISODISTORT package [4], which uses group-representations to generate incommensurate structure models based on a given parent structure [5], now automatically identifies the unique magnetic superspace-group of each magnetically modulated child structure. Anyone can access these data sources and tools online to generate, symmetrize, transform, or otherwise explore magnetic or non-magnetic modulated structure models.

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