

The unified (UNI) system of magnetic space-group symbols

Branton Campbell¹, Harold T. Stokes², J. Manuel Perez-Mato³, Juan Rodriguez-Carvajal⁴
¹Brigham Young University ²Brigham Young University, ³University of the Basque Country,
⁴Institut Max Von Laue - Paul Langevin
branton.campbell@gmail.com

The 1651 three-dimensional magnetic space groups (MSGs) are essential to the crystallographic description of many magnetic materials [1]. The two commonly used systems of MSG symbols, with accompanying numbers and settings, are those of Belov-Neronova-Smirnova (BNS) and Opechowski-Guccione (OG). Both have advantages and disadvantages. Both present challenges of interpretation to novice and expert users alike, which can inhibit understanding and lead to errors in published magnetic structures. To address each of these challenges going forward, we have introduced a new unified (UNI) MSG symbol [2], which combines a modified BNS symbol with essential information from the OG symbol. The UNI symbol is easier to interpret correctly than previous MSG symbols, at the expense of some compactness. Among other advantages, the UNI MSG symbol (1) is true to the spirit of the Hermann-Mauguin symbols and settings used in the International Tables for Crystallography, (2) clearly conveys the magnetic point group (MPG) of the MSG, (3) explicitly communicates the translational part of the time-reversal generator of each type-4 MSG, (4) separates the time-reversal from other generators for clarity, (5) distinguishes each type-1 MSG from the corresponding non-magnetic space group, (6) and reveals the conventional lattice centering of both the MSG itself and the underlying non-magnetic space group.

[1] S. V. Gallego, et al., *J. Appl. Cryst.* 49, 1750-1776 (2016).

[2] B. J. Campbell et al., *Acta Cryst.* A78, 99-106 (2022).