

MS45 What is inside the black box?

MS45-01

Space groups, the final frontier: a tutorial guide to some entries in International Tables Volume A

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Abstract

Crystallographers of previous generations were well acquainted with the contents of International Tables Volume A (and its predecessor Volume I in the earlier series); most of this weighty tome is taken up with extensive graphical, mathematical and other information about each of the 230 space groups relevant to three-dimensional crystal structures. With the increasing use of automatic procedures in the collection and processing of diffraction data and the solution and refinement of crystal structures from the data, the need to refer to these tables has largely disappeared as far as many users are concerned, and younger practitioners may well never have opened the Big Book any more than they have opened Black Boxes. Automation, however, is not infallible and there is much to be said for knowing what useful information is available when it is needed. I will begin with a few basic concepts and principles regarding space group symmetry and then go on to examine a few specific space groups in some detail. Those who are familiar with Volume A can take time off and visit a parallel session!