Determination of Crystal System and Space Group

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The determination of a crystal system from single-crystal diffraction data is a deceptively simple process of identifying the maximum point symmetry in the diffraction pattern, also known as the Laue symmetry. For most crystals of biological macromolecules, this is straightforward, but it can be complicated when the crystals possess pseudo-symmetry, are twinned, and/or yield only poor-quality data. For crystals of chiral biological macromolecules, assignment of a space group within the Laue group is then based on identification of all translational symmetry operators, *i.e*. screw axes and centering (excepting trigonal group 32). Identification of screw axes in the diffraction data depends on the quality of the data and the success of data processing, and should generally be regarded as a hypothesis until the structure is solved. Fortunately, many downstream programs for phasing take into account space group alternatives based on screw symmetry assignment. Issues that arise in the assignment of crystal system and space group will be illustrated by a variety of examples.