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Refinement of Disorder with SHELXL. Peter Müller, MIT, Dept. of Chemistry, 77 Massachusetts Ave, 2-325, Cambridge, MA 02139, pmueller@mit.edu.

The structure determined from a diffraction pattern is the spatial average over the whole crystal. In the ideal crystal all unit cells are identical, with all molecules in exactly the same conformation, orientation and position as in the cells to its left, right, top, bottom, front and back. Sometimes, however, parts of molecules (and in some extreme cases even whole molecules) are found in more than one crystallographically independent orientation. One can distinguish three cases:

1. More than one molecule in the asymmetric unit
2. Twinning
3. Disorder

With disorder the orientations of some atoms differ randomly in the different unit cells of the crystal. In most cases it suffices to describe a disorder by formulating two different positions per disordered atom and, in addition, the ratio between the two alternative positions.

In this presentation, the parameterization of disorder will be illustrated, and, based on several examples, the refinement of disorder with the program SHELXL will be demonstrated. This will include a detailed description of how to use restraints and constraints in refinements of disorder.