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Examples of Crystal Structures with Whole Molecule Disorder. G.D. Enright, J.A. Ripmeester, Steacie Inst. for Molecular Sciences, National Research Council, Ottawa (ONT.), Canada.

Small molecule crystal structures that exhibit whole-molecule disorder present considerable challenges in collection, solving, and refinement. Diffraction patterns from such crystals contain significant diffracted intensity outside of the Bragg reflections in the form of diffuse scattering or as satellite reflections. Examples of both types will be presented.

In the first example we present the single-crystal structure of the high temperature polymorph of caffeine. Our study confirms some features of a recent PXRD structure determination except the space group is R-3c and the molecule is disordered over *six* symmetry related positions. The molecules are π -stacked along the c axis. The diffraction pattern contains intense diffuse bands that occur at *d*-spacings that correspond to the distance (and subharmonics) between molecules.

In a second example we will present the structure of a five-membered heterocyclic carbene. The diffraction patterns indexed as F-centered orthorhombic with a weak set of satellite peaks. The primary cell was solved in space group Fdd2 with the molecules fully disordered about a two-fold axis.

For both examples it was necessary to greatly expand the number of trial sets to find an initial solution and a large number restraints were applied to stabilize the refinement.