

## W0179

**Optimizing Refined Molecular Fragments in a Cell.** Douglas R. Powell, Univ. of Kansas, Lawrence, KS 66045, dpowell@ku.edu.

The program CLEAN implements a method of moving covalently-bonded groups to simplify descriptions of intermolecular hydrogen and ionic bonding and to optimize the arrangements of these groups in the cell. The optimization includes using translations permitted by the affine normalizer of the respective space group. Molecular groups sitting on crystallographic centers, mirrors, rotation axes, etc., are first expanded by the point group symmetry and then reduced to the symmetry-unique set of atoms through an optimized choice of atoms. Separate molecular groups that are hydrogen-bonded to other group(s) are moved to be nearest to a group that has already been positioned.

The program TIDY<sup>1</sup> performs a similar optimization for inorganic compounds that lack covalently-bonded groups. TIDY is also particularly useful at identifying the appropriate structure type of a compound, greatly simplifying structural comparisons.

<sup>1</sup> L. M. Gelato & E. Parthe, *J. Appl. Cryst.*, 1987, 20, 139-143.