

PLATON/SQUEEZE - An Effective Tool for Taking the Contribution of Disordered Solvent into Account in Crystal Structure Refinement. A.L. Spek, Bijvoet Center for Biomolecular Research, Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands

A significant number of compounds crystallize together with molecules of the solvent of crystallization. Solvent molecules often reside on a site with higher symmetry than their molecular symmetry, resulting in disorder. In other cases, solvent molecules fill up infinite channels around 3, 4 or 6 fold screw axes. The stacking in those channels is often incommensurate with the translation period of the ordered part of the structure, resulting in ridges of constant density without maxima in three dimensions.

Several approaches are available to take the contribution of disordered solvents to the structure factors into account. The conventional one is to fit a (constrained) disorder model in the disordered solvent area. Such an approach works well for toluene molecules disordered over an inversion centre. However, fitting a THF molecules in this way in a site with -3 symmetry will never be satisfactory. Another approach involves the refinement of population and/or displacement parameters for peaks picked up from a difference density map without any further interpretation.

The SQUEEZE technique is based on the concept that the total density shown in a correctly phased Fourier map can be split-up into a part that can be described and refined with discrete model parameters (i.e. positional and displacement parameters) and a (smaller) part corresponding to the disordered solvent. The contribution to the calculated structure factors of the disordered solvent is taken into account by back-Fourier transformation of all density found in the disordered solvent area. The procedure (see P. v.d. Sluis & A.L. Spek, *Acta Cryst.* A46, (1990), 194) is highly automated and compatible with the widely used SHELXL refinement package. A number of successful applications of the technique will be discussed in some detail along with its limitations. The program is available by anonymous ftp (xraysoft.chem.ruu.nl).