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The Extended PLATON/SQUEEZE Tool in the Context of Twinning and SHELXL2014

A. Spek[1]

[1]*Utrecht University, Crystal and Structural Chemistry, Utrecht, The Netherlands*

The completion of a single crystal structure determination is often hampered by the presence of disordered solvent molecules of crystallization. The often not interesting details of that solvent disorder and its contribution to the calculated structure factors has to be modelled in some way in order to obtain publishable results. Current refinement programs include suitable constraints and restraints for a stable refinement of a discrete disorder model. This is often the preferred procedure, in particular when charge balances and valence states are relevant. Unfortunately, a discrete disorder model is not always feasible. Examples include solvent molecules in infinite channels or structures including unknown solvents or solvent mixtures. In such cases the iterative back-Fourier transformation of the content of the disordered solvent volume in a difference density map can be attempted as the contribution to the calculated structure factors. Back-Fourier transformation of disordered solvent regions was prototyped by us nearly 25 years ago (van der Sluis & Spek, 1990) around the, at that time widely used, SHELX76 refinement program. The original reason for its development was the structure determination of a pharmaceutical that contained infinite channels filled with ridges of electron density in the difference density map rather than discrete density peaks (van der Sluis & Spek, 1990). The preliminary implementation of a successful prototype procedure (called BYPASS) was complex and found not to be easily distributable due to its dependence on many (local) ad-hoc programs. A new distributable version, compatible with the next generation refinement program SHELXL97, was implemented as the SQUEEZE tool in the program package PLATON Spek, 2009). The new SHELXL2014 refinement program allows for an even more elegant implementation of the SQUEEZE tool including the possibility to apply it also for twinned structures. Examples and restrictions will be discussed.

[1] *van der Sluis, P & Spek, A.L. (1990a) Acta Cryst. A46, 194-201.,* ***[2]*** *Spek, A.L. (2009) Acta Cryst. D65, 148-155.,* ***[3]*** *van der Sluis, P & Spek, A.L (1990b) Acta Cryst. C46, 883-886.*

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