**E0046**

**Some Useful Concepts in Teaching Structure Determination and Structural Chemistry.** George M. Sheldrick, Lehrstuhl für Strukturchemie, Univ. Göttingen, Germany.

The automation of methods of determining crystal structures of both small and macromolecules (for which the author must take some of the blame) is leading to the potentially dangerous situation in which it is no longer considered necessary for students to understand details such as how the phase problem is 'solved' (or even that there are phases).

The Patterson method, especially Patterson superposition, provides a relatively non-mathematical way of gaining insight into crystallographic ways of thinking. Another concept that is widely ingored but in the author's opinion is useful in understanding both inorganic structures and the coordination of metal ions in proteins (e.g. Müller *et al*., 2003) is the *bond-valence method* (Brown, 2002). Structure determination projects, especially if presented as 'puzzle solving' exercises, e.g. where the chemical composition turns out to be unexpected or where there are minor problems in sorting out the space group or interpreting disorder, can also be useful in enhancing motivation and understanding: a tutorial by Fabio Dall'Antonia and Eftichia Alexopoulos used for such projects is available via http://shelx.uni-ac.gwdg.de/.

Brown, I.D. (2002). *IUCr Monograph on Crystallography* 12, OUP.
Müller, P. *et al*. (2003). *Acta Cryst*. D59, 32-37.