

## W0108

**Structure Determination from Weak Anomalous Signals.** George M. Sheldrick, Lehrstuhl für Strukturchemie, Universität Göttingen, Germany.

Macromolecular structure determinations based on the anomalous scattering of native sulfur and phosphorus exploit intensity differences of the order of 1% between Friedel opposites, so careful data collection with the elimination of all possible systematic errors is an essential prerequisite. A high true redundancy, which except in cases of high symmetry requires a kappa or 3-circle goniometer, enables a sophisticated statistical analysis for the rejection of aberrant data and the estimation of optimal anomalous differences and their esds (Blessing, 1997; similar techniques have been implemented by the author in the programs SADABS and XPREP). Recent developments in the programs SHELXD (Usón & Sheldrick, 1999; Schneider & Sheldrick, 2002) for the location of the sites and SHELXE (Sheldrick, 2002) for phasing and improvement of the resulting density attempt to make more use of chemical knowledge such as typical interatomic distances, the presence of disulfide bridges and NCS. For examples of S-SAD phasing using these programs see Debreczeni *et al.* (2003).

Blessing (1997). *J. Appl. Cryst.*, 30, 421-426.

Debreczeni *et al.* (2003). *Acta Cryst.* D59, 393-395; 688-696; 2125-2132.

Schneider & Sheldrick (2002). *Acta Cryst.* D58, 1772-1779.

Sheldrick (2002). *Z. Kristallogr.* 217, 644-650.

Usón & Sheldrick (1999). *Curr. Opin. Struct. Biol.* 9, 643-648.