Direct location of individual sulfur atoms from weak, medium resolution SAD data, Judit É. Debreczeni and George M. Sheldrick*, *Lehrstuhl für Strukturchemie, Georg-August Universität, Tammannstr. 4, 37077 Göttingen, Germany*. E-mail: gsheldr@shelx.uni-ac.gwdg.de

Keywords:SAD phasing; SHELX; substructure solution

Location of sulfur atoms in disulfide bridges represents a special case in heavy atom substructure solution, as the number of sites depends on the resolution of the anomalous data. At low resolution (lower than 2.8 Å) the two sulfur atoms of the disulfide unit coalesce to a super-sulfur atom, therefore half the real number of sulfurs should be searched. On the contrary, high resolution (better than 2.0 Å) anomalous data usually allow the direct resolution of disulfide units to single atoms [1].

The average diffraction limit of crystals from biological samples is only rarely higher than 1.5 Å and anomalous data are only reliable to 0.5 Å lower resolution. In such cases, i.e. when the anomalous signal extends to medium resolution, sulfur atoms of disulfide units cannot be resolved directly. However, modelling of the heavy atom substructure with super-sulfur atoms is not optimal and phases calculated are not sufficient to define the molecular envelope that reduces the efficiency of subsequent phase improvement steps.

This problem can be overcome by the direct location of two-atom disulfide units using the new algorithm implemented in each dual-space refinement cycle of *SHELXD*. Tests on known and previously unknown structures indicated that this innovation — apart from the marked improvement in phasing — improves the discrimination between correct solutions and noise peaks of the heavy atom substructure and allows the location of "hidden" single sulfur peaks. This approach played an essential role in successful phasing of a previously unknown structure solved recently [2].

[1] Debreczeni, J. É. *et al.* (2003). *Acta Cryst.* **D59**, 688-696.
[2] Debreczeni, J. É. *et al.* (2003). *Acta Cryst.* **D59**, 2125-2132.