s5.m3.p1 **Refining Crystal Structures from Electron Diffraction Data.** A. Stewart & C.J. Gilmore *Dept. of Chemistry, University of Glasgow, Glasgow G12 8QQ, Scotland,UK.*

Electron crystallography poses as many problems in validating and refining crystal structures as it does in solving them. Very few published crystal structures derived in this way have been subjected to least squares refinement[1]. Here we show the results of refining a series of compounds from numerous sources[2,3] including:

1. Urea
2. Polybut-1-ene
3. Polyethylene
4. The Si(111) 7x7 surface
5. $CuCl.3(H_2O)$
6. 2,6-bis(4-dimethylamino-benzylidene)-cyclohexanone.

Refinement is not a trivial exercise; restraints on bond lengths are required, weighting schemes are difficult because of a lack of standard deviations for the intensities; the final R factors usually exceed 40%, and thermal parameters can be hard to control. We have extended the traditional methods of matrix inversion in least squares to include singular value decomposition techniques which are far more robust than the usual Choleski method employed by least squares programs.

Refinement methods are useful in obtaining the best possible model from the data and validating the proposed model.

[1] Dorset, D..L. & Gilmore, C.J. (2000) *Acta Cryst.* **A56**, 62-67.
[2] Dorset, D.L. (1995), *Structural Electron Crystallography.* New York:Plenum.
[3] Voigt-Martin, I.G., Kothe, H., Yakimansky, A.V., Tenkovtsev, A.V., Zandbergen, H., Jansen, J. & Gilmore, C.J. (2000). *Ultramicroscopy* **83**, 33-59.