Using Electron Diffraction Data. C.J. Gilmore and A.
Stewart Department of Chemistry. University of Glasgow,
Glasgow G12 8QQ, Scotland, UK.
Keywords: electron diffraction, refinement, maximum entropy.

Electron crystallography is still the Cinderella of the crystallography world: specimen preparation can be difficult; data are hard to collect and have problems with sample thickness, dynamical scattering and sampling; structure solution is problematic, and refinement and structure validation are also non-trivial. Yet there is an ever-increasing body of knowledge in structural science derived from this method, and many samples can only be studied in this way.

In this talk we discuss two complementary problems:
1. Structure solution especially using maximum entropy methods which are well suited for this purpose.
2. Structure refinement using least squares.

Unconstrained and unrestrained refinement is not usually successful1 and we will report on the use of:
• Constraints such as rigid bodies.
• Restraints such that bond lengths are constrained to be equal and constrained also to a chemically sensible value and yet still allowed some freedom of refinement.
• Matrix manipulations using singular value decomposition and eigenvalue filtering. These methods enable the user to determine which parameters are sensitive to the experimental data. Quite often this is not obvious.

The structures come from the literature and are available on a database in cif format.

We acknowledge support from Eastman Kodak, Rochester, USA.