

**s8b.m1.o1** **Benefits of high quality data and how this can be achieved.** C. Nave, *CLRC Daresbury Laboratory, Warrington WA4 4AD, UK.*

Keywords: methods crystallography, data collection, acquisition.

Many protein crystallography experiments require the highest quality data. For example, measurement of small differences between signals, as in anomalous scattering applications, places particular demands on statistical accuracy. However, obtaining the highest quality measurement for each diffraction spot can conflict with a need to obtain a complete or high resolution data set from a single crystal. This is because radiation damage will lead to a loss of information, or even false information, after a certain exposure time. It is therefore of some importance to understand the data requirements in terms of completeness, redundancy, resolution and statistical accuracy for particular types of experiment. Examples of the benefits of obtaining high quality data for some particular cases will be given.

The quality of data, which can be obtained from a particular crystal, can be analysed in terms of the size of the crystal, its perfection, unit cell dimensions and lifetime in the beam. The data actually obtained can be degraded by the experimental protocol, the diffraction set up and deficiencies with the analysis software. The extent to which current experimental set ups approach the ideal will be examined to illustrate what steps can be taken to improve data quality, particularly for the most demanding applications.

**s8b.m1.o2** **Choices in Data collection and Processing** P.R. Evans, *MRC Laboratory of Molecular Biology, Hills Road, Cambridge, UK.*

Keywords: methods crystallography, data collection, acquisition.

The quality and correctness of a crystal structure ultimately depends on the quality of the diffraction data used to calculate it. Derivation of a good or optimum set of structure amplitudes from a crystal requires a series of choices of best protocol, and often compromises arising from conflicting requirements or from constraints beyond the experimenter's control. The talk will discuss the important practical decisions needed, under the headings of

- sources and beams
- crystals and crystal handling
- detectors and strategy
- indexing and integration
- data reduction and scaling
- quality assessment

The current state of the art of data collection from macromolecular crystals was summarized at a CCP4 study weekend in 1999, published as an issue of *Acta Cryst D* [1]

[1] *Acta Cryst section D* (1999), D55: 1631-1772.