

9.1. PRINCIPLES OF MONOCHROMATIC DATA COLLECTION

Even after the source and overall time have been allocated or planned, the strategy is still the result of a compromise between several competing requirements. Some are general, others depend on the characteristics of a particular crystal or detector. As seen in the previous section, it is not possible to define protocols relevant for all applications. Rather, it is important to consider the relative importance of the parameters that can be varied to the problem in question and make the appropriate decisions.

Synchrotron beamlines become brighter, detectors faster and data-processing software ever more sophisticated. Existing software has advanced to the stage where many decisions regarding the geometric restraints on data completeness and minimalist data

collection are automatically proposed to the user. Decisions regarding the qualitative completeness, with respect to the optimum resolution limit, exposure time and redundancy, are more nebulous concepts and are not yet addressed in an automated manner. This must be the area of major advance in the next years.

Thus data collection may have become easier from a technical point of view, but several crucial scientific decisions still have to be made by the experimenter. It is always beneficial to sacrifice some beam time and interpret the initial diffraction images, so as to avoid mistakes which may have an adverse effect on data quality and the whole of the subsequent structural analysis.

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