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Data Collection Strategy – Beyond Completeness and Redundancy. J.W. Pflugrath, Rigaku/MSC, Inc., 9009 New Trails Drive, The Woodlands, TX 77381.

The minimum requirements for a diffraction data set are completeness in the unique Miller indexes to a given resolution. Beyond that, good counting statistics and good redundancy are the next important. This talk will focus on all aspects of optimizing the diffraction data collection experiment with 2D detectors including choice of crystal, exposure time, rotation width per image, axes to scan, total degrees to scan, integration, and treatment of systematic, random, and erratic errors. Radiation damage, absorption, oblique incidence, anomalous scattering and other systematic effects will be addressed. The basis of the discussion will be the d*TREK suite, a flexible, customizable, device-independent software and toolkit which collects and processes single crystal X-ray diffraction images from two-dimensional position sensitive detectors such as imaging plate (IP) area detectors and charged-coupled device (CCD) detectors. The ultimate result of the processing is a list of Bragg reflections which appear on those images with their Miller indices (hkl), estimated intensities, and uncertainties. Almost all image formats are supported including Rigaku R-AXIS II, R-AXIS IV, R-AXIS IV++, HTC, RAPID, Mercury, Jupiter and Saturn detectors, as well as some non-commercial (i.e. NOIR-1) and most other commercial detectors. d*TREK is available for the major Unix platforms (Linux, Mac/OSX, OSF1, Solaris) and for Windows platforms through the CrystalClear™ graphical user interface.