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Macromolecular Crystal Diffraction Data Collection: Opinions About Best Practices. J.W. Pflugrath, Rigaku Americas, Corp., 9009 New Trails Dr., The Woodlands, TX 77381 USA.

While the minimum requirements for a diffraction data set are completeness in the unique Miller indexes to a given resolution, many other factors play a role in achieving good statistics and good redundancy required for optimal phasing and crystal structure refinement. Many aspects of optimizing the diffraction data collection experiment with 2D detectors are dealt with, including choice of crystal, exposure time, rotation width per image, axes to scan, scan setting angles, multiple scans, rotation ranges, potential collisions, multiple detector positions, spot overlap, and tolerance for completeness. In this talk we will delve more into the computational aspects of modern best practices used by the algorithms in the d*TREK suite. d*TREK is 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 IP and CCD detectors. In the end, we learn that careful experimental technique pays off more than clever computational algorithms.