Input data

Required data

The below list should contain all the information which is necessary to reconstruct reciprocacal space volume data for typical use cases. The aim is to collect enough information to capture a reasonably general use case. Not all of the individual use cases may require all of the information below. For example, a fixed detector setup will simply have an empty sequence of detector rotations, and an amorphous sample does not make use of the orientation matrix as there are no defined hkl-directions.

Some of the information is static, meaning it never changes for a given experimental setup (e.g.: sequence of instrument rotations, pixel size for a given detector), while other data is changing only occasionally (center pixel coordinate should be static unless the detector is remounted). Many parameters may vary from scan to scan or from sample to sample (UB matrix), while most data will potentially change with every scan point (instrument rotation angles, wavelength,

Source

- Radiation wavelength: lambda
- Polarization factor

Instrument

- Sequence and directions of sample circle rotations (static for given instrument)
- Sequence and directions of detector circle rotations (static for given instrument)
- Rotation angles for sample rotations
- Rotation angles for detector rotations

Sample

- Orientation Matrix UB

Detector

- Detector orientation at instrument zero angles.
- Center pixel coordinates: Pixel which is hit by the direct beam at all instrument angles zero (Is this a well-defined quantity? What happens if detector is mounted parallel to the x-ray beam?)
- Distance of the center pixel to the intrument rotation center
- Pixel size
- Image dimensions in pixels
- Flatfield calibration file: Correct for inhomogeneities of the detector response and mask out bad pixels.
- Region(s) of interest
- Bin sizes for pixel binning.
- If beam defining slit is used: orientation and position of slit

Helpful data

- sample lattice constants: a, b, c, alpha, beta, gamma

Notes