



Contribution ID: 39

Type: Poster

diffcalc-core: Diffraction condition calculation package for a six-circle diffractometer

Tuesday, September 20, 2022 5:52 PM (2 minutes)

The Python 3 package `diffcalc-core` implements diffraction condition calculation for a six-circle x-ray diffractometer according to the methodology described in H. You. Angle calculations for a '4S+2D' six-circle diffractometer. *J. Appl. Cryst.* (1999). 32, 614-623. Diffractometer operation modes are selected based on three constraints that can include combination of detector, sample, reference vector, scattering plane, incident, exit beam or χ -plane orientations. All solutions fulfilling the diffractometer equation are returned for a requested reciprocal orientation. Configurations that correspond to a continuous solution space are flagged as insufficiently constrained. UB matrix can be set directly or calculated using reference reflections and/or known crystal orientations. Methods are provided to refine UB matrix based on a single reflection data or using a least-square fitting procedure with data from multiple reflections. The package source is available on GitHub (<https://github.com/DiamondLightSource/diffcalc-core>) under terms of Apache Software License ver. 2.0.

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Track Classification: NOBUGS 2022