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

*Tuesday, 20 September 2022 17:52 (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.

## Email address of presenting author

irakli.sikharulidze@diamond.ac.uk

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**Primary author:** SIKHARULIDZE, Irakli (Diamond Light Source)

**Presenter:** SIKHARULIDZE, Irakli (Diamond Light Source)

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