EUHEDRAL tutorial

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www.crystal.chem.uu.nl/distr/euhedral

www.cryst.chem.uu.nl/platon

EUHEDRAL

Optimization of the crystal shape for an analytical absorption correction.

Principle: Minimization of R2

$$R2 = w_1 * R_{int} + w_2 * R_{psi}$$

$$R_{int} = \frac{\sum |I - I_{mean}|}{\sum I}$$

$$R_{psi} = \frac{1}{n} * \sum \frac{I_{max}}{I_{min}} - 1$$

Defaults: $w_1 = 10$, $w_2 = 0.1$

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There are four possibilities to optimize the crystal shape:

- volume: refining the distances of all faces simulatiously.

- distance: refining the distances of all faces separately.

- tilt: tilt the faces with respect to each other.

- crystrot: change the orientation of the crystal on the diffractometer.

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EUHEDRAL is not a stand-alone program. It uses the absorption correction routines ABST or ABSG of the program PLATON.

References:

- PLATON: A.L. Spek, *J. Appl. Cryst.* **36** (2003) 7-13.

- ABST: N.W. Alcock, *Cryst. Computing* (1970) 271-278.

- ABSG: P. Coppens, *Cryst. Computing* (1970) 255-270.

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There are different algorithms for the optimization:

- volume: parabolic refinement
- distance: parabolic refinement or simplex method
- tilt: trial-and-error
- crystrot: trial-and-error or simplex method

Step 1

Read the ins and hkl file with commands *readins* and *readhkl*.

Set the correct point group with the command *pg*.

Note: Cell parameters and direction cosines must be consistent (otherwise PLATON will stop).

Note: Only the standard settings of the point groups are known to EUHEDRAL. If necessary you can transform the dataset with PLATON (before you use EUHEDRAL).

Step 2

Reduce the number of reflections, using the command *filter*. With the graphical output the user can check, whether the complete crystal is covered by incoming and outgoing beam (different projections are offered by the program).

Filterparameters:

- angdistmax: angular distribution of reflections in psi
- intmin: minimal intensity
- nhklmin: minimal redundancy per reflection
- thetamin: minimal theta

Step 3

Perform a volume refinement. This is a check, whether the crystal description is appropriate.

If the volume factor approaches 0, there is some severe error in the model.

Possible solutions:

- crystrot: assuming the crystal dimensions are correct, but the indexing of faces failed.

- bestsphere: assuming that nothing is known about the crystal shape.

Step 4

At this stage we should have a roughly correct crystal description.

We can now fine-tune the description with the commands *volume*, *distance*, and *tilt*. These commands can be repeated until a minimum R2 value is reached.

Step 5

If we have chosen a small subset of reflections in the beginning (to speed up the refinement), we can now increase the subset by running *filter* again.

If we have chosen a centric pointgroup in the beginning (to speed up the refinement), we can now set the correct pointgroup with the command *pg*.

Step 6

When the result of the refinement is satisfactory, we leave the program EUHEDRAL. We then apply the absorption correction to the complete dataset using PLATON and *name.ins*.

Note on non-merohedral twins:

- The EUHEDRAL refinement should be done on a HKLF4 dataset of non-overlapping reflections of one twin domain.

- For the PLATON absorption correction on the HKLF5 file, the checking of direction cosines must be switched off. (All direction cosines should be based on the same orientation matrix).