

CRYSCALC

how to create an import.CIF file on a Bruker diffractometer?

After a data collection on a APEXII or D8Venture Bruker AXS diffractometer, integrating diffraction frames with SAINT and data reducing with SADABS/TWINABS software respectively, generate the following files in the \work folder:

- P4P file, containing cell parameters, symmetry and Bravais Lattice, chemical formula, crystal features ...
- HKL file, containing integrated intensities list (h, k, l, F^2, sig_F^2)
- ABS file, containing absorption corrections outputs

Creation of import.cif can be performed using the following instruction:

```
d:\guest\job_ID\work>cryscalcc P4P=job_ID_0m.p4p HKL=job_ID_0m.hkl ABS=job_ID.p4p
```

or only:

```
d:\guest\job_ID\work>cryscalcc P4P=job_ID_0m.p4p
```

In this case, P4P and ABS file names will deduced from the P4P file name.

Remarks

- on a D8Venture diffractometer, files name is preceeding by the "Mo_" or "Cu_" characters string, depending on the X-ray source that has been used.
- data collection features (X-ray voltage and current, experiment and detector temperatures, ...) and scan features (crystal-detector distance, scan time, frame width, motors positions ...) are extracted from the header of the first frame of each measured scan.
- import.CIF is containing all the previous features and can be opened directly with **WinGX** interface or **CRYSCALC**.