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 reducting 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>cryscalc P4P=job_ID_0m.p4p HKL=job_ID_0m.hkl ABS=job_ID.p4p
```

or only:

```
d:\guest\job_ID\work>cryscalc 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**.