CRYSCALC

how to create reports and tables of structural data from a CIF file?

Different formats of experiment reports, containing experimental and refinement details as well as tables of structural data (atomic positions, anisotropic atomic displacement parameters, bond length, angles, torsion angles, hydrogen boundings) can be created by launching **CRYSCALC** in command line, given the kind of report as first argument and `cif` file as second one.

- text format (`.txt` extension)

```
d:\cifs>cryscalc report_text cif_file.cif
```

`cif_file_structural_report.txt` file is created.

- HTML format (`.html` extension)

```
d:\cifs>cryscalc report_html cif_file.cif
```

`cif_file_structural_report.html` file is created. If a browser has been defined in the `cryscalc.ini` setting file, the HTML report file is directly opened by the browser.

```
[EXTERNAL APPLICATIONS]
browser = "c:\Program Files (x86)\Mozilla Firefox\firefox.exe"
```

- Latex format (`.ltx` extension)

```
d:\cifs>cryscalc report_latex cif_file.cif
```

`cif_file_structural_report.ltx` file is created. If a Latex to pdf converter has been defined in the `cryscalc.ini` setting file, the `pdf` file is created and directly opened (pdfviewer has to be previously associated to `pdf` files on your computer).

```
[EXTERNAL APPLICATIONS]
pdflatex = "C:\Program Files\MiKTeX 2.9\miktex\bin\x64\pdflatex.exe"
```

Remarks

- if a picture file of the measured crystal is present in the current folder, it is embedded into the `html` and `pdf` reports. The name of this picture has to be `sample_ID.jpg` or `sample_ID.png`.
- if a picture file of the structural model is present in the current folder, it is embedded into the `html` and `pdf` reports. The name of this picture has to be `sample_ID.gif`.
- `sample_ID` is extracted by **CRYSCALC** from the `data_sample_ID` CIF line in the CIF file.