

## CRYSCALC

how to convert CIF or INS file?

**CRYSCALC** allows to perform file conversion from CIF or INS/RES files:

- to **CaRIne** format (.ACE)
- to **Powder Cell** format (.ACE)
- to **FPStudio** format (.FST), included in the **FullProf Suite**
- to **SHELXL** format (.INS)
- to **Pymol** format (.CIF)
- to cartesian coordinates format (.XYZ)
- to **FullProf** format (.PCR)
- to **CRYSCALC** format (.CFL)

by launching **CRYSCALC** in command line, with CIF or INS file given as first argument:

```
d:\cifs>cryscalcalc cif_file.cif
```

The kind of file conversion is directly managed by some keywords values (0 or 1) in the `cryscalcalc.ini` setting file:

```
[COMMAND LINE ARGUMENTS]
create_ACE = 0 ! .ACE file for CARINE
create_CEL = 0 ! .CEL file for PowderCELL
create_CIF = 0 ! .CIF file
create_FST = 1 ! .FST file for FPStudio
create_INS = 0 ! .INS file for SHELX
create_CIF_PYMOL = 0 ! .CIF file for PYMOL
create_XYZ = 1 ! .XYZ (Cart. coord.)
create_PCR = 0 ! .PCR file for FullProf
create_CFL = 0 ! .CFL file for CRYSCALC
```