

CRYSCALC

how to convert a PCR or INS/RES file to a CIF file ?

CRYSCALC allows to perform file conversion from PCR (**FullProf**) or INS/RES (**SHELXL**) input files containing structural features. This can be realized with the help of the **CREATE_CIF** keyword after reading structural features with the **READ_pcr** or **READ_INS** keyword. These operations can be realized by **CRYSCALC** through different ways:

1. in interactive mode

```
> Enter keyword:  
read_pcr si.pcr  
> Enter keyword:  
create_cif
```

2. in command line (*flash* mode)

CRYSCALC instructions can be given as arguments by condensing these keywords in a single line :

```
d:\cifs>cryscalcc ; read_pcr si.pcr ; create_cif ;
```

*Note that in this case, the different keywords to be executed by **CRYSCALC** are separated by ";" character.*

3. in command line

If `create_cif = 1` is specified in the [COMMAND LINE ARGUMENTS] section of the `cryscalcc.ini` setting file, conversion to CIF file can be realized by the following command line :

```
d:\cifs>cryscalcc si.pcr
```