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## 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>cryscalc ; 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 cryscalc.ini setting file, conversion to CIF file can be realized by the following command line :
   ```
   d:\cifs>cryscalc si.pcr
   ```