CRYSCALC

how to create a global CIF file from several individual CIF files?

A global CIF file, containing several structures coming from individual CIF files can be created with **CRYSCALC** following the sequence :

- create a new folder and copy CIF files to concatenate
- launch in this folder the following command

  `d:\cifs>cryscalc CREATE_CIF_BUFFER`

  A `CIF_files.buf` file is created: it contains the list of CIF files present in the current folder. If an editor has been previously defined in the `CRYSCALC.INI` setting file, this file is automatically edited for an optional reordering of the files list.
- Quit the text editor
- launch in this folder the following command

  `d:\cifs>cryscalc CREATE_GLOBAL_CIF`

  By default, the `CIF_files.buf` buffer file is used, but the buffer file name can be modified and then specified as optional argument.
  Example:
  `d:\cifs>cryscalc CREATE_GLOBAL_CIF buffer_1-4.buf`

  A `CIF_files_global.cif` file is created: it contains all the CIF files ! If an editor has been previously defined in the `CRYSCALC.INI` setting file, this file is automatically edited.

Remarks
- The two previous CRYSCALC instructions can be merged into a `bat` file (for example a `global_cif.bat`), that can be launched from the command line :

  `d:\cifs>global_cif`

- Dy default, the loop with `_publ_author_name` and `_publ_author_address` fields present in the first part of the global CIF file, called `AUTHORS INFORMATIONS`, contains only the name and address of the person defined in the [AUTHOR] / [USER] section of the `cryscalc.ini` setting file. This authors list can however be defined in an external file, named as `authors_list.txt` and has to be present in the current directory. The syntax of such a file is as follows:

  [AUTHOR]
   Name, first_name
   address

  Note that:
    - input items can contain characters with accents

* available lower case characters

à (Alt+ 0224)   á (Alt+ 0225)   â (Alt+ 0226)   ä (Alt+ 0228)   ã (Alt+ 0227)   å (Alt+ 0229)
ç (Alt+ 0231)
è (Alt+ 0232)   é (Alt+ 0233)   ê (Alt+ 0234)   ë (Alt+ 0235)
ì (Alt+ 0236)   í (Alt+ 0237)   î (Alt+ 0238)   ï (Alt+ 0239)
ñ (Alt+ 0241)
ò (Alt+ 0242)   ó (Alt+ 0243)   ô (Alt+ 0244)   ö (Alt+ 0246)   õ (Alt+ 0245)
ù (Alt+ 0249)   ú (Alt+ 0250)   û (Alt+ 0251)   ü (Alt+ 0252)

* available upper case characters

À (Alt+ 0192)   Á (Alt+ 0193)   Â (Alt+ 0194)   Ä (Alt+ 0196)   Ã (Alt+ 0196)   Å(Alt+ 0197)
È (Alt+ 0200)   É (Alt+ 0201)   Ê (Alt+ 0202)   Ë (Alt+ 0203)
Ì (Alt+ 0204)   Í (Alt+ 0205)   Î (Alt+ 0206)   Ï (Alt+ 0207)
Ñ (Alt+ 0209)
Ò (Alt+ 0210)   Ó (Alt+ 0211)   Ô (Alt+ 0212)   Ö (Alt+ 0214)   Õ (Alt+ 0213)
Ù (Alt+ 0217)   Ú (Alt+ 0218)   Û (Alt+ 0219)   Ü (Alt+ 0220)

− addresse has to be input in a single line
  * In order to get address on several lines in the final CIF file, the "\\" separator character can be used.
  * In the case of multiple addresses, they simply have to be written on different lines

Example:

```
[AUTHOR]
ROISNEL, Thierry
Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226 \\
F-35000 Rennes, France

[AUTHOR]
DORCET, Vincent
Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226 \\
F-35000 Rennes, France

[AUTHOR]
CORDIER, Marie
Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226 \\
F-35000 Rennes, France
```

CRYSCALC

how to extract individual CIF files from a multiple structures global CIF file?

Once this global CIF file has been created, it is possible to extract individual CIF files using the following command line:

```
d:\cifs>cryscalc EXTRACT_CIF CIF_files_global.cif
```