

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>cryscalcc 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>cryscalcc 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>cryscalcc 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 `cryscalcc.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)	ä (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)	Ä (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)		

- adresse 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>cryscalcc EXTRACT_CIF CIF_files_global.cif
```