CRYSCALC

how to create a final archive CIF?

CRYSCALC allows to create a final archive `.CIF` file, extracting useful structural and refinement parameters from the `CIF` file created by refinement program (ex: SHELXL), and diffractometer and crystal features, software names ... from `import.cif` file. This can be done by launching **CRYSCALC** in command line, with `create_archive` keyword as first argument and `CIF` as second argument:

```
d:\cifs>cryscalc create_archive job.cif
```

By default, `res` and `hkl` files are embedded into the final `archive.cif` file (named in this case `cryscalc_archive_hkl.cif` file) and extracted parameters are listed on the screen. Optional `no_hkl` and `no_out` arguments can be used to exclude hkl list from the final archive (named in this case `cryscalc_archive.cif`) and without screen outputs respectively.

```
d:\cifs>cryscalc create_archive cif_file.cif no_hkl no_out
```

Note that integration of `res`, `hkl` and `fcf` files can also be specified in the `[ARCHIVE_AND_REPORT]` section of the `cryscalc.ini` setting file through the following keyords:

```
include_RES_file             = 1      ! include .RES file in the archive_cryscalc.cif file
include_HKL_file             = 1      ! include .HKL file in the archive_cryscalc.cif file
include_FCF_file             = 1      ! include .FCF file in the archive_cryscalc.cif file
```