

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>crystalcalc create_archive job.cif
```

By default, `res` and `hkl` files are embedded into the final archive.cif file (named in this case `crystalcalc_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 `crystalcalc_archive.cif`) and without screen outputs respectively.

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