

CRYSCALC

how to extract .res and .hkl files from a CIF file?

Since SHELXL-ver.2014 structural refinement program (G. Sheldrick), CIF files created by **SHELXL** are embedding **res** and **hkl** files; as **SHREDCIF** program, distributed by G. Sheldrick, **CRYSCALC** can also extract these files from a **cif** file, even if it contains several structures.

This can be done by launching **CRYSCALC** in command line, with **EXTRACT** keyword as first argument and CIF file as second argument:

```
d:\cifs>cryscalc extract cif_file.cif
```

For CIF files created by **OLEX²** software that embeds **res** file and contains **hkl** data in the **_refln_index_xxx** loop, the extraction can be done with **EXTRACT_OLEX** keyword in the command line:

```
d:\cifs>cryscalc extract_olex cif_file.cif
```

Note that CIF files created by **OLEX²** software can also be detected if 'Olex2' is specified by the **_audit_creation_method** string.