cif2hkl

A program that computes structure factors |F^2| for neutrons, x-rays, and electrons

cif2hkl - CrysFML based utility for generating .lau/.laz files for e.g. McStas and McXtrace.

Purpose: Reads a CIF/CFL/SHX/PCR crystallographic description and generates a HKL F^2 reflection list.

Installation

```
make
make test
sudo make install
```

On a recent Debian/Ubuntu/Mint system, use:

```
sudo apt install cif2hkl
```

Optionally you can build a Debian package with any of: - `make deb`

Syntax

```
cif2hkl --xtal file.cif cif2hkl --powder file.cif
```

Use

The cif2hkl program is a command line tool, that uses arguments. The syntax and help are obtained with:

```
cif2hkl --help
```

It reads a file with crystal structure information, and computes the |F^2| structure factors. The supported input file formats are:

Extension	Format	Link
CIF	Crystallographic Information File	https://en.wikipedia.org/wiki/Crystallographic_I
PCR	FullProf control input file	https://www.ill.eu/sites/fullprof/
CFL	CrysFML input file	https://code.ill.fr/scientific-software/crysfml
SHX	ShelX input file	https://shelx.uni-goettingen.de/
INS	ShelX instruction file	https://shelx.uni-goettingen.de/

Extension	Format	Link
RES	ShelX result	https://shelx.uni-goettingen.de/

The general syntax is:

```
cif2hkl [options][-o outfile] file1 file2 ...
```

and can treat files in series. The result is a file with a readable header and reflection list with columns

```
[ H K L Multiplicity Sin(Theta/Lambda) d_spacing |F|^2 ]
```

which is used by e.g. McStas neutron and McXtrace X-rays ray-tracing software. However electronic scattering structure factors can also be computed.

The available options on the command line are:

```
--help     or -h    Show this help
--version  or -v    Display program version
--out FILE          Specify the name of the next output file.
   -o FILE            Default is to add .hkl to the initial file name.
--lambda LAMBDA     Set the incoming probe wavelength [Angs].
   -l    LAMBDA       Default is 0.5
--powder   or -p    Generate a list of unique HKL reflections (for powders). Default.
--xtal     or -x    Generate a list of all HKL reflections (for single crystals).
--mode MODE         Computes F2 for M any of NUC,XRA,ELE (neutrons, Xrays, electrons).
   -m  MODE
--verbose           Display processing details.
--no-output-files   Just read the CIF/CFL/ShellX file (for checking).
```

Example: cif2hkl -o CaF2.laz CaF2.cfl

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