CRYSCALC

What is it?

CRYSCALC has been created to perform basic crystallographic calculations or get crystallographic informations. It has been written in Fortran 95, and uses the crystallographic calculations facilities of the Crystallographic Fortran Modules Librairies written by J. Rodriguez-Carvajal (ILL-Grenoble, France) and J. Gonzalez (Univ. La Laguna, Spain).

Facilities implemented in **CRYSCALC**:

- unit cell volume calculation
- space group informations: space group features, Wyckoff positions, symmetry operators, extinctions ...
- calculation of d_hkl, Q_hkl, 2theta_hkl (including propagation wave vector)
- hkl generation for a given space group
- structure factor calculation (Xrays, neutrons, electrons)
- simulation of powder diffraction pattern (X, neutrons)
- geometric calculations: interatomic distances, angles, connectivity, bond valence sums (BVS), centroid coordinates, angles between 2 vectors in direct and reciprocal space, ...
- atomic features: weight, density, electronic configuration, ionic and Shannon radii, neutron data, X-rays data ...
- molecular informations: molecular weight, density ...
- absorption coefficient calculation (X-rays, neutrons) and transmission calculation
- transformation of unit cell, atomic coodinates and hkl files
- statistics on hkl file and sort of hkl data
- search for systematic extinctions and space group
- ADP parameters conversion
- create HTML report from a CIF file
- ...

CRYSCALC can be run through an input file containing a list of keywords, defining the type of crystallographic calculations that will be performed, or in an interactive mode, by entering keywords at the CRYSCALC prompt.

Crystallographic features can be read from different types of input files :

- `CFL`
- `INS/.RES` file (SHELXL)
- `CIF` file
- `PCR` file (FullProf)
- `CEL` file (PowderCELL)

Alternatively, particular jobs can be performed by **CRYSCALC** when special arguments are passed to CRYSCALC through the command line (see List of command line arguments section of the user's guide).

CRYSCALC is a free of charge and available for the scientific communauty at the following URL address:

http://www.cdifx.univ-rennes1.fr/progs/cryscalc/cryscalc.exe

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