

CRYSCALC

how to install?

CRYSCALC is a crystallographic calculations program, free of charge. First install of **CRYSCALC** can be performed using the `cryscalc_setup.exe` setup program. All the different files (executable, setting file, ...) will be copied in a folder defined by the user and **CRYSCALC** and **PATH** environment variables will be defined and modified.

For a manual install of **CRYSCALC**, the executable `cryscalc.exe` file can be download from the **CRYSCALC** web site at the following URL address:

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

This `cryscalc.exe` file has to be copied in a folder that will be accessible via the **PATH** environment variable.

CRYSCALC is using a setting file, called `cryscalc.ini`, where the user has to adapt the contain to its own computer environment (definition of editor, browser ...) and also to its working environment (definition of a diffractometer setup, softwares, calculations options ...). An example of this setting file can be downloaded at:

<http://www.cdifx.univ-rennes1.fr/progs/cryscalc/cryscalc.ini>

and has to be copied in the same folder than the `cryscalc.exe` file.

Remark

- To get all facilities of **CRYSCALC**, it is recommanded to define the **CRYSCALC** environment variable, that has to point to the folder where **CRYSCALC** has been installed (ex: `d:\progs`). Furthermore, some special options of **CRYSCALC** can not be fully executed if **WinPLOT** has not been installed previously, i.e. visualization of a simulated powder diffraction pattern, plot of X-ray/neutrons scattering and absorption cross-sections, plot a $F_c = f(F_o)$ curve.
- Updating **CRYSCALC** can be performed directly inside the program, using the "Update CRYSCALC" option in the main menu or the **UPDATE** keyword in interactive mode. If a browser is correctly defined in the setting file, the latest version of **CRYSCALC** will be downloaded from the web site. User has then just to save this `cryscalc.exe` in the folder where it has been installed.