

Quick and Dirty HOWTO for the Crysfire Indexing Suite

This document is written to provide a description of the fastest method to start a couple of indexing runs using Crysfire.

!!THIS IS NO SUBSTITUTION FOR THE CRYSFIRE MANUAL!!

Step 1. Install Crysfire by doing the following:

- a. Download the Crysfire package from <http://www.ccp14.ac.uk/>.
- b. Unzip the package to a directory of your choice.
- c. Add the above directory to your path variable.
- d. Check that you did it correctly by calling 'crysfire' from the command line.

Step 2. Save your diffractogram data to the Crysfire format (*.cdt)

- a. Easiest programme I know to do that with is Powder3D ;-). Check <http://www.fkf.mpg.de/xray> to download the current version. Install it and the IDL VMTM from <http://www.rsinc.com/idl> to get things up and running.
- b. Import your data, do a peak search (and refinement) and save your data to a Crysfire formatted file (check the manual for step by step advice). You can also call Crysfire automagically if you have installed it correctly (see Step 1.).

Step 3. Call Crysfire correctly

- a. ATTENTION, this sometimes goes wrong when doing it first, so take heed!
- b. Open a DOS window → quickest way 'windows button+r' type in 'cmd'.
- c. Change into the directory containing you data using 'cd'.
- d. Call Crysfire by typing 'crysfire'.
- e. Accept the displayed agreement with 'Y'.

Step 4. Load data and index

- a. Load your data by typing 'LO' and select the correct file.
- b. Index by typing 'IN' and then the required programme e.g. 'IT' for ITO.
- c. Keep hitting 'Enter' accepting defaults until the indexing routine starts.
- d. When the routine finishes the results are sorted and analysed.
- e. Several text windows open and can be dismissed, Crysfire waits for a response after each window.
- f. Iterate with different indexing algorithms until you have enough candidates.

Step 5. (Recommended)

- a. Analyse the candidates with Checkcell, download from <http://www.ccp14.ac.uk/>.

Written by B. Hinrichsen 25 May 2005-05-25