# XD Toolkit Manual

***Before you start a new refinement:***

*1)* In the folder that the SHELX structure solution was carried out, there should be a res and an hkl file.

*2)* Copy the res file to your project folder, and rename it “shelx.ins”.

*3)* Copy the hkl file to your project folder, and rename it “shelx.hkl”.

*4)* Alternatively, 2 and 3 can be done in XD Toolkit by clicking “File – Load Starting Files from Struture Solution Folder”. This will prompt you to first select your structure solution folder, and thenyour new project folder.

## Wizard

The Wizard tab takes some user input, and then goes through an entire standard refinement strategy from start to finish.

**Guide**

***1)*** Type a name for your compound (max. 8 characters) in the “*Compound ID*” box, and click initialize compound.

*NOTE:* If you have a large structure this may take a short while, but shouldn’t take longer than a minute.

***2)*** Enter your desired sin(θ/λ) cutoffs.

***3)*** If you have H atoms in your structure, go to the “*RESET BOND*” tab. Click “*Automatically add reset bond instructions*”.

If the program says it cannot add reset bond instructions for any H atoms, go to the “*Manually add reset bond instructions*” section, and input an appropriate bond length for these atoms.

*NOTE:* Clicking the “*Get other bond lengths*” button in the “*Manually add reset bond instructions*” section will take you to a paper with tables of standard bond lengths from neutron diffraction.

***4)*** Go to the “*CHEMCON*” tab. Check the box that says “*Make atoms inputted below chemically equvialent*”. Now type atoms that are chemically equivalent into the input box below and click “*Add CHEMCON*”. Do this for all groups of atoms that are chemically equivalent.

*NOTE:* You can use any of the other CHEMCON options but they are only appropriate in certain situations so always look at your structure before using them.

***5)*** Choose if you want to introduce higher-order multipoles one by one, and if you want to try lowering local symmetry at the end of the refinement, with the relevant check boxes in the wizard tab.

Both of these options are recommended, but doing them both makes the refinement strategy twice as long, so you may not wish to use one/both of them for larger structures.

***6)*** Click "*Test*". If everything is fine then you will get the message "*Ready to run XD Wizard*" folllowed by an estimated running time. Otherwise you will get instructions telling you what else you need to do.

***7)*** Click "R*un XD Wizard*".

## Manual Refinement

## RESET BOND

## CHEMCON

## Results

## Tools

## Backup

## XD Programs