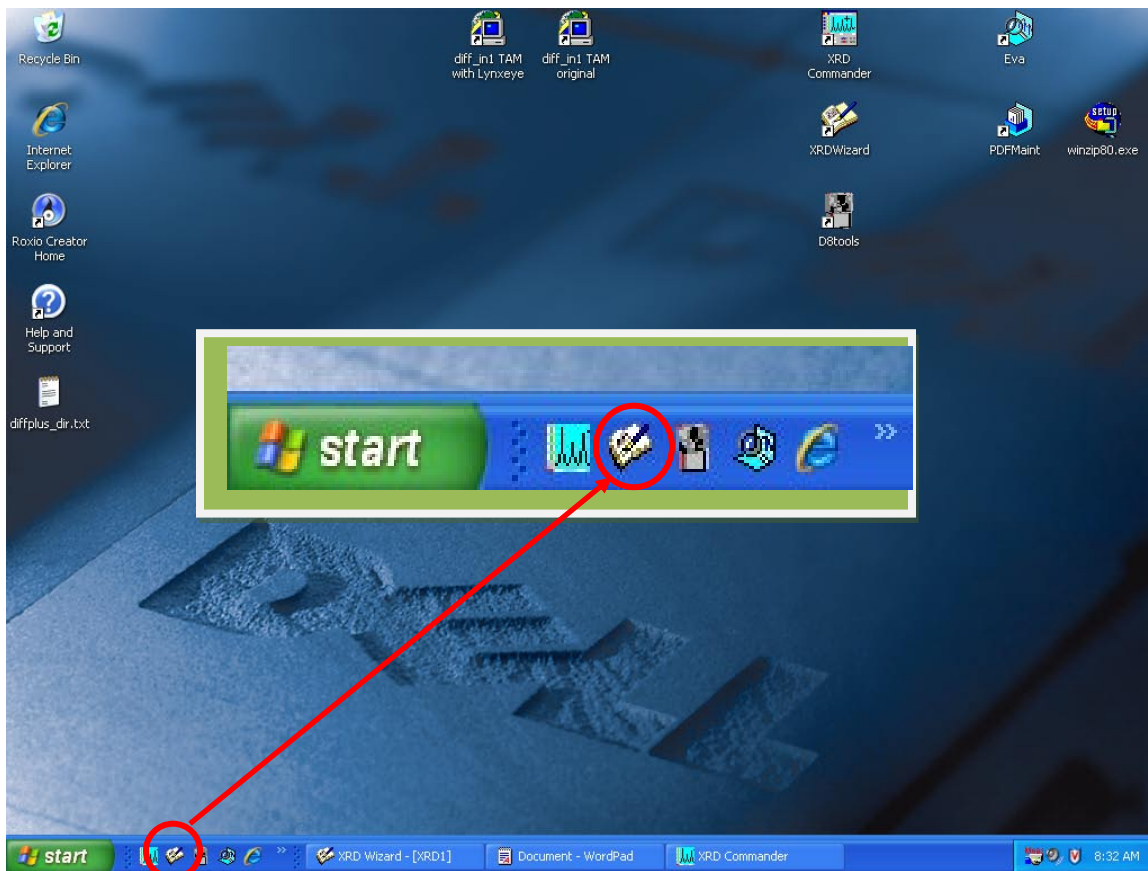


**Step by Step tutorial
for
Powder XRD Short-Arm
Data Collection**

Creating the Parameter File

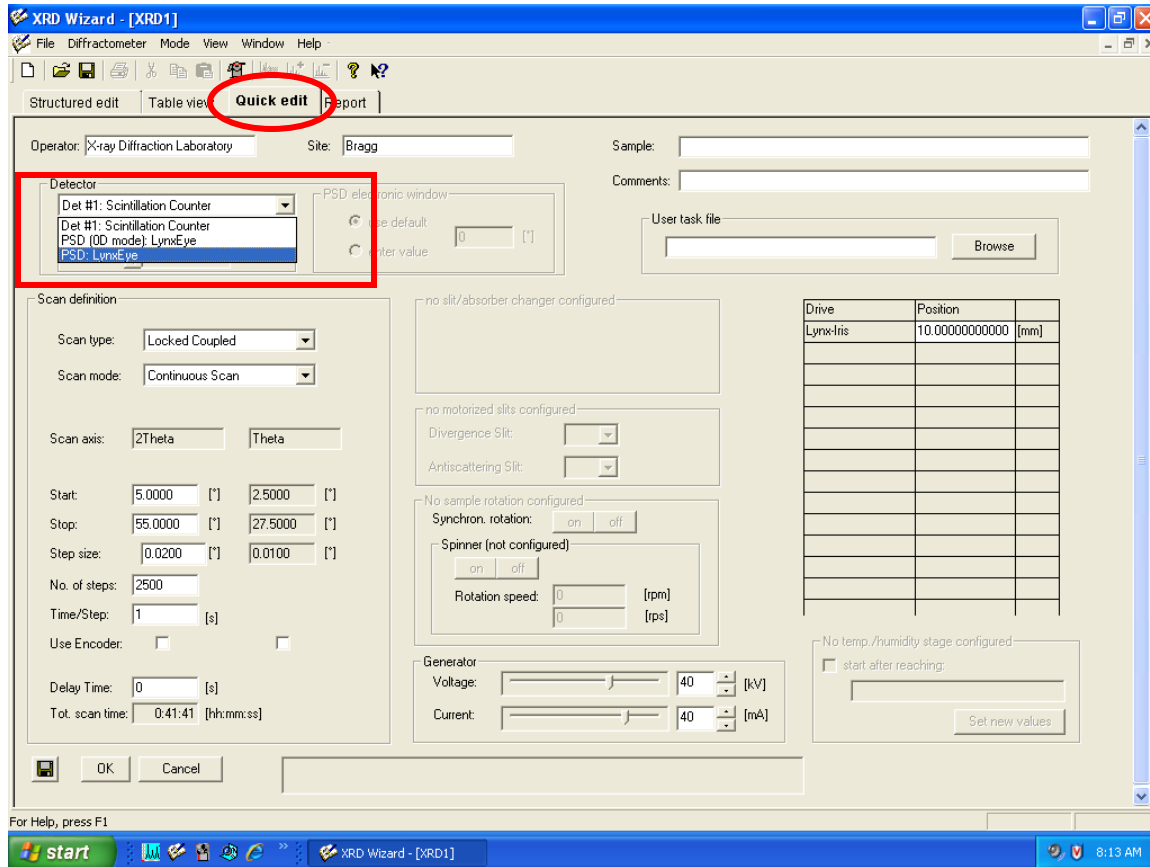
Step 1. First create a parameter (whateverfilenameyouwant.dql) file if you have not created one before for the required range and conditions (for the lynxEYE detector). If you already have a dql file, you can go to **Step 5** directly.

1. Click on the XRD wizard icon



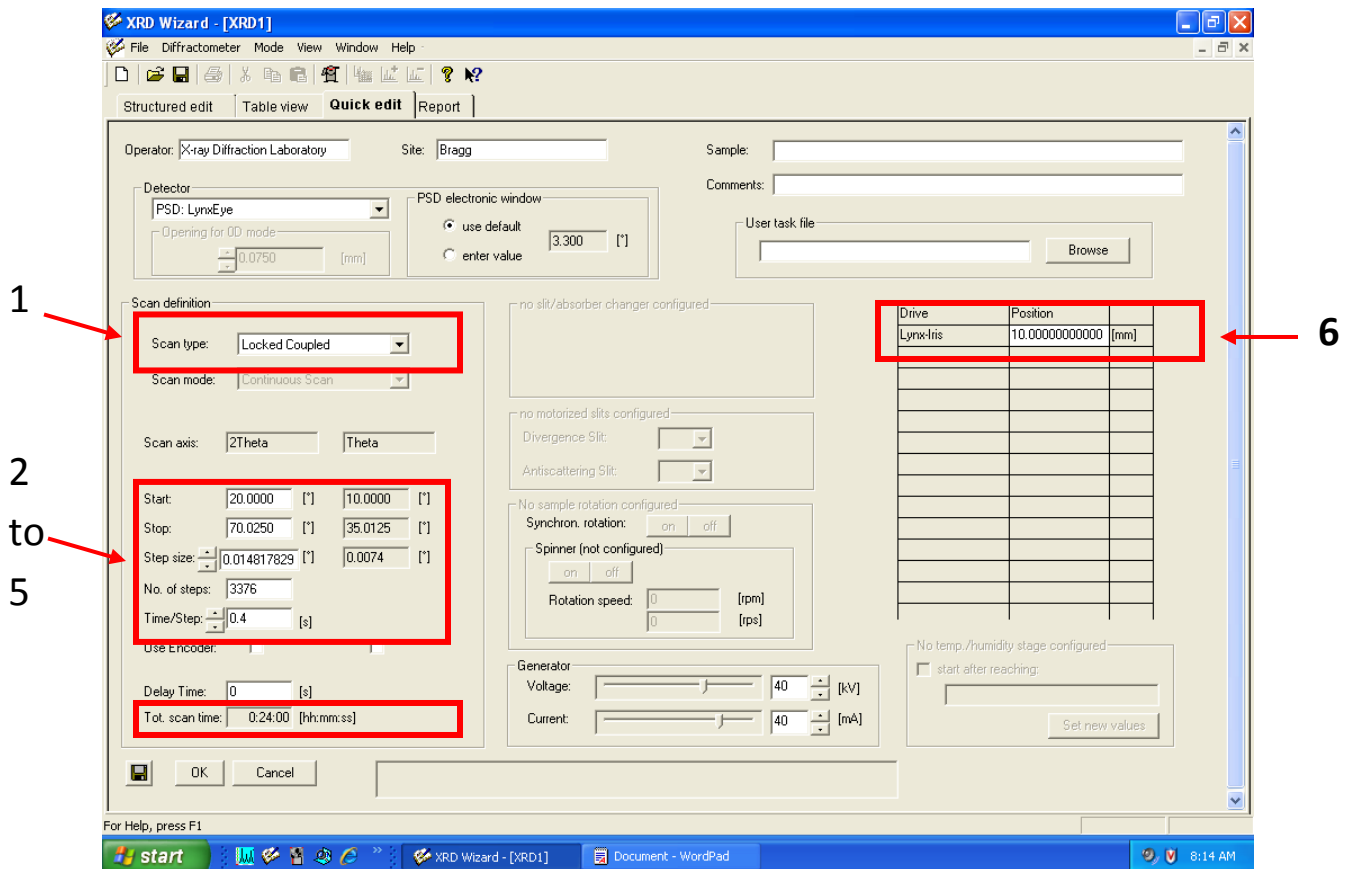
Step 2. You will get the XRD Wizard program window: Go to the Quick edit tab.

1. Select the Correct Detector: (usually) PSD: LynxEye

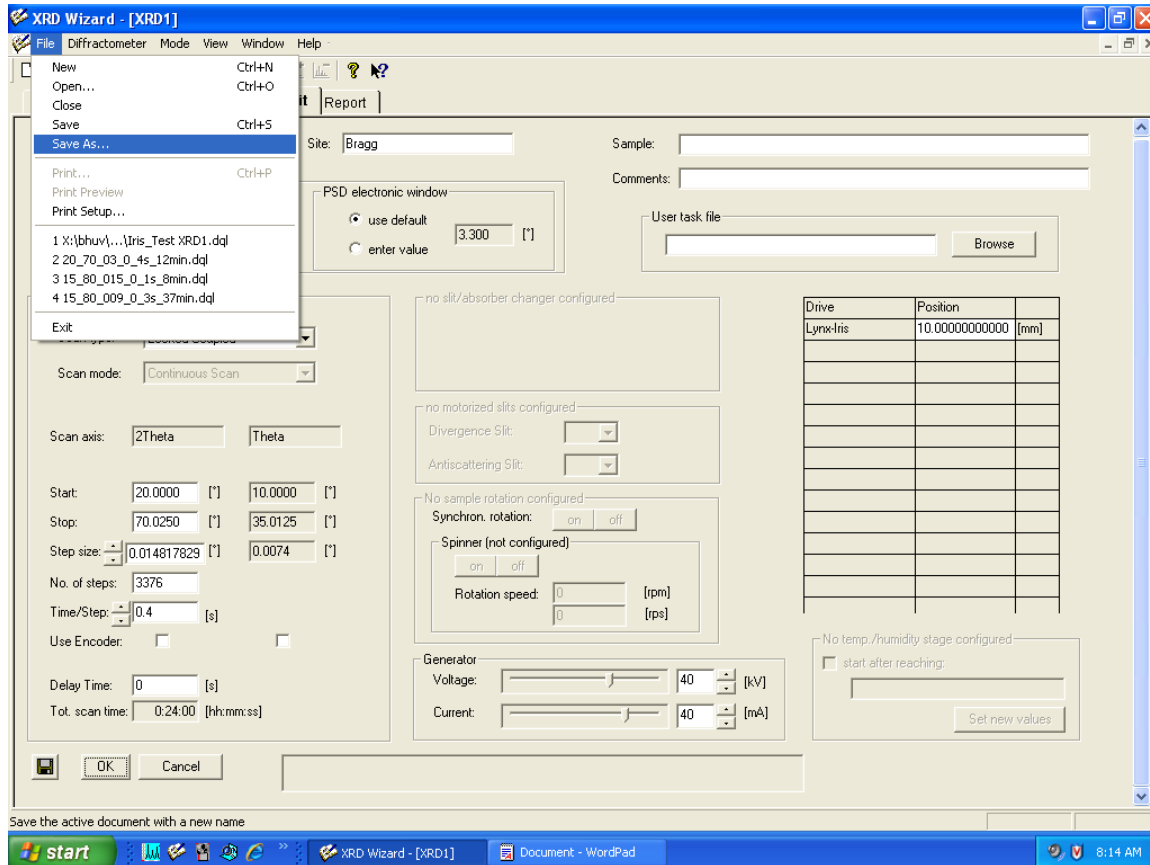


Step 3. Then under scan definition:

1. Make sure you are in “Locked-Coupled” mode in the “Scan Type”.
2. Enter the required “Start” 2-Theta value. If you are not sure, you can Start at 5 [°]. Lowest 2-Theta start allowed is 2 [°].
3. Enter the required “Stop” 2-Theta value. If you are not sure, you can Stop at 70 [°]. Highest reasonable 2-Theta stop is 120 [°]
4. Select or enter the required Step size. “0.015” [°] is a good value. If you think your peaks are broad, and you are wanting to get better intensities, you can enter a higher value, say 0.03.
5. Next enter a Time/Step. “0.4” s is a good value. If you want faster data, you can go as low as 0.1s at the cost of lower quality powder pattern. Longer Time/Step will give you better pattern at the cost of longer time [Variable Counting Time is possible – Talk to an expert for details].
6. In addition, you can select to open-up or close-down the IRIS (anti-scattering slit) width. If you are collecting your data starting from 20 degrees 2-theta or above, set a value of 13. If you are starting from 5 or 2 degrees, set a value of 6 or 2 respectively for Lynx-Iris Position. [Multi Range option, with different IRIS settings for different ranges in the same powder pattern is possible – talk to an expert for such data collection]
7. Check the Tot. scan time. You can optimize your parameters vs. available time according to this.



Step 4. Go to File → save as, and put the “dqj” file in the desired directory



The screenshot shows the XRD Wizard software interface. The File menu is open, and 'Save As...' is selected. The software is configured for a Bragg site. The scan mode is set to 'Continuous Scan'. The scan axis is '2Theta'. The start angle is 20.0000 °, and the stop angle is 70.0250 °. The step size is 0.014817829 °. The number of steps is 3376. The time per step is 0.4 s. The delay time is 0 s, and the total scan time is 0:24:00. The generator voltage is 40 kV and the current is 40 mA. The PSD electronic window is set to 3.300 °. The divergences are set to 10.0000 ° and 35.0125 °. The rotation speed is 0 rpm and 0 rps. The table shows the drive and position for the Lynx-Iris detector.

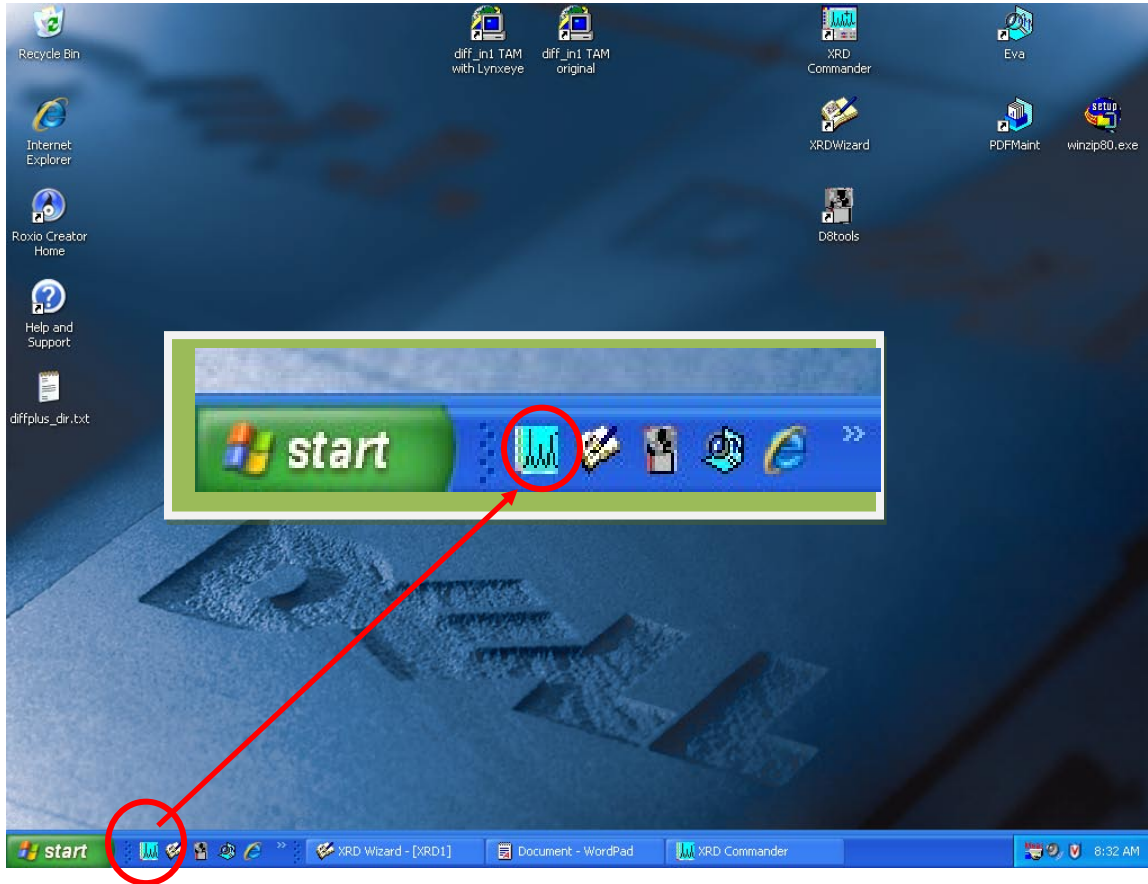
Drive	Position
Lynx-Iris	10.0000000000 [mm]

Save the active document with a new name

start | XRD Wizard - [XRD1] | Document - WordPad | 8:14 AM

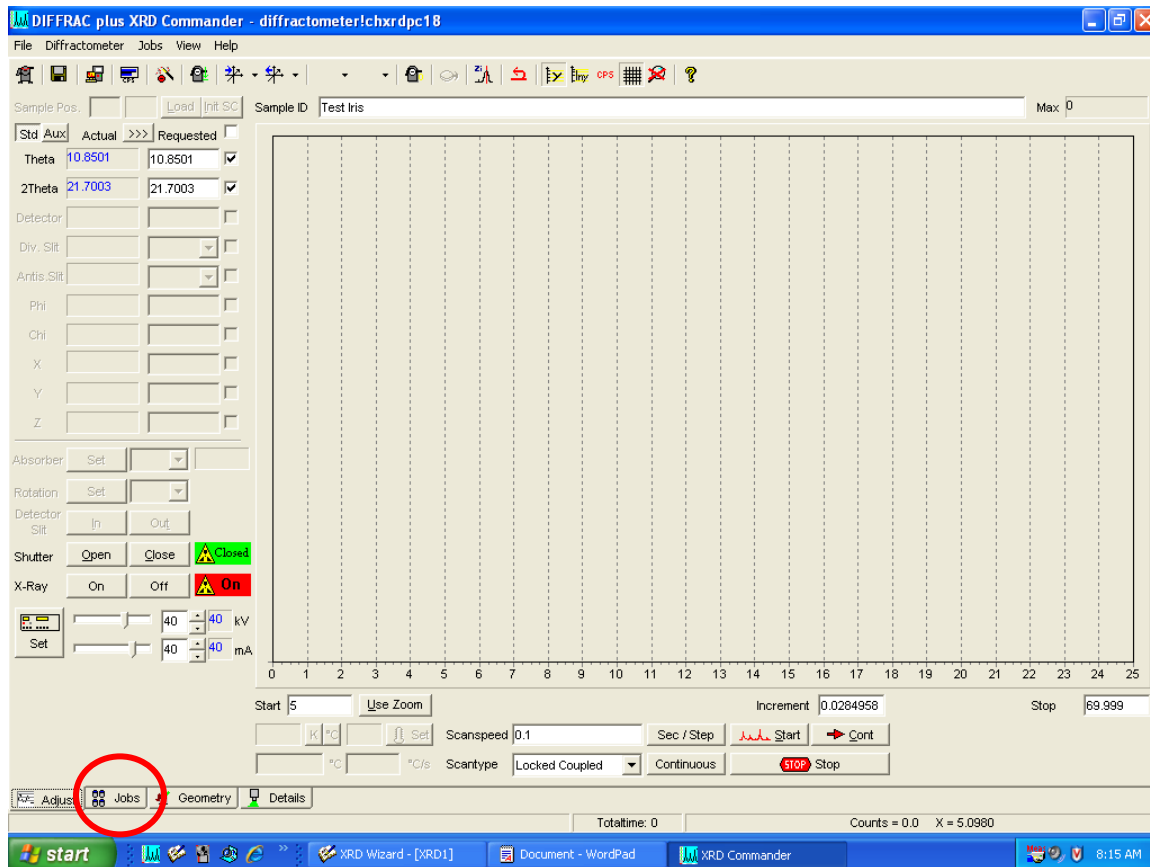
Data Collection Using COMMANDER

Step 5. Now start the Commander:



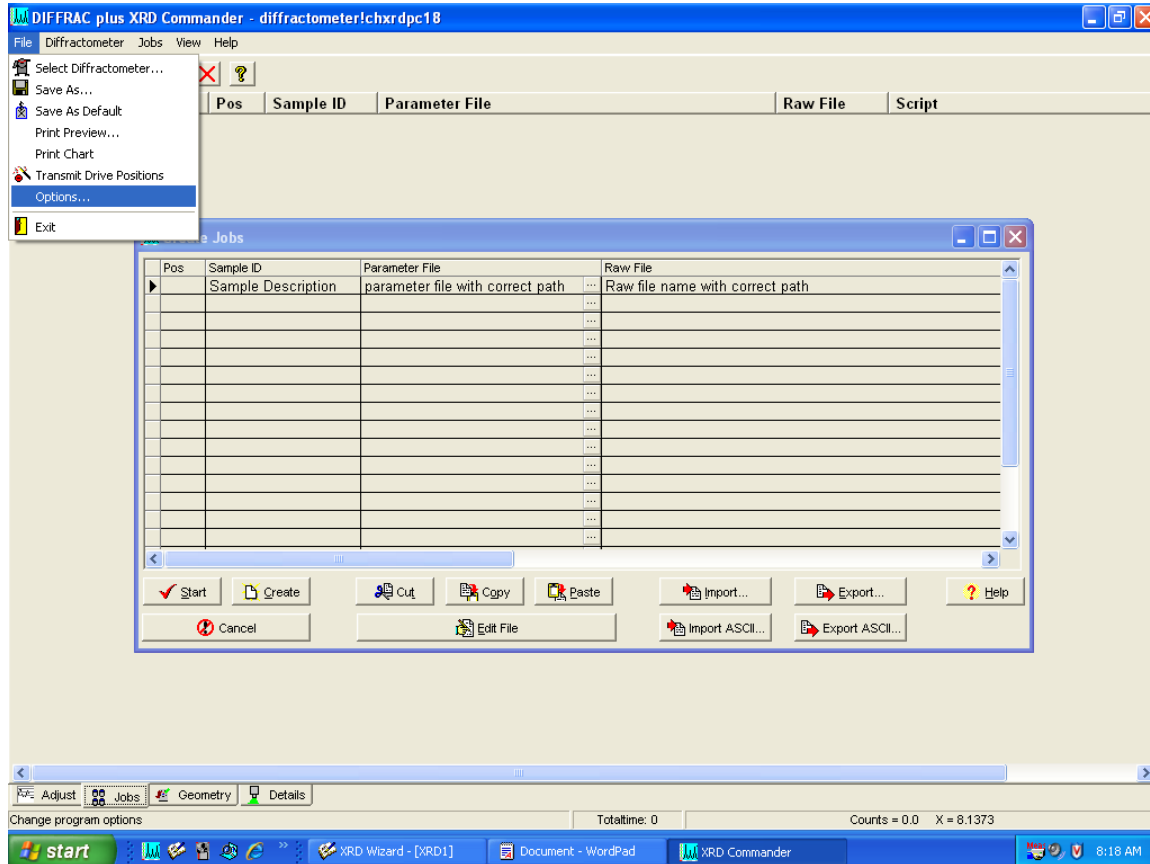
Step 6. You will be getting the following window.

1. Now select the Jobs Tab:



Step 7. To select the default directory where you want your data to be written:

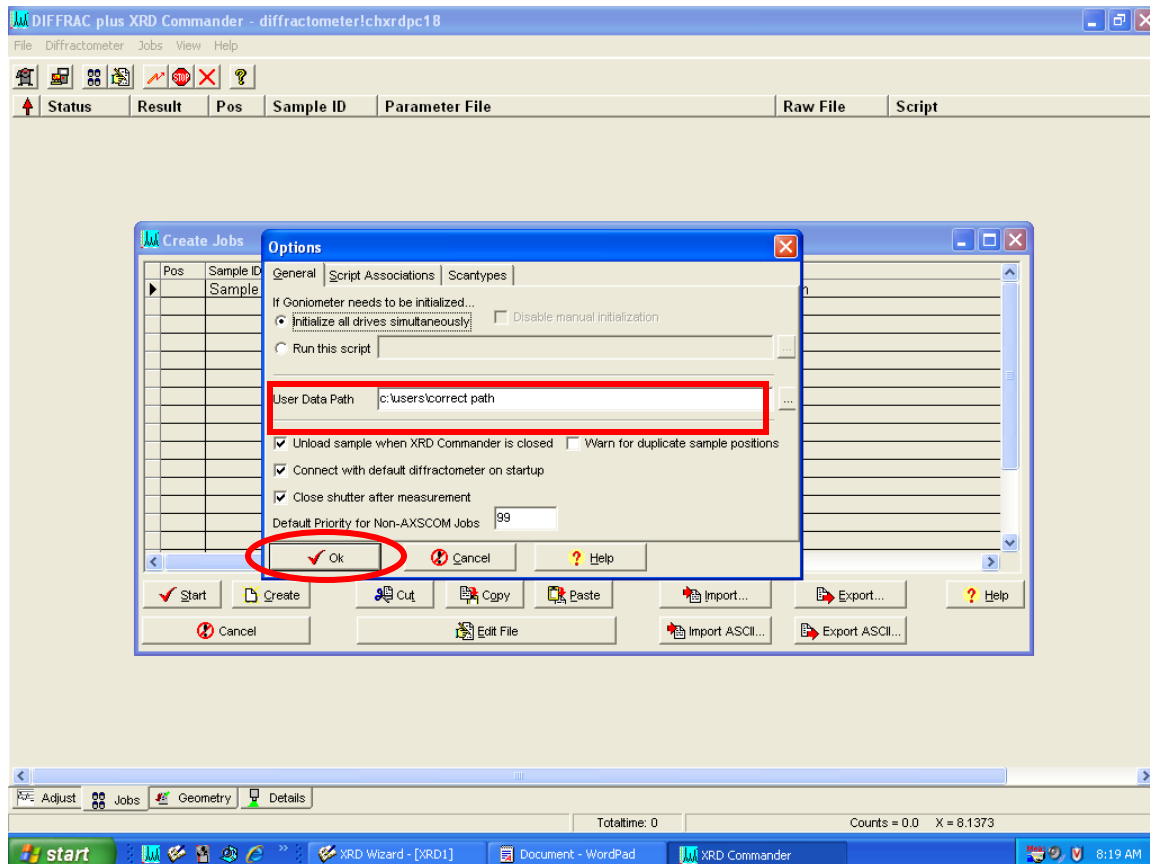
1. Go to File → Options



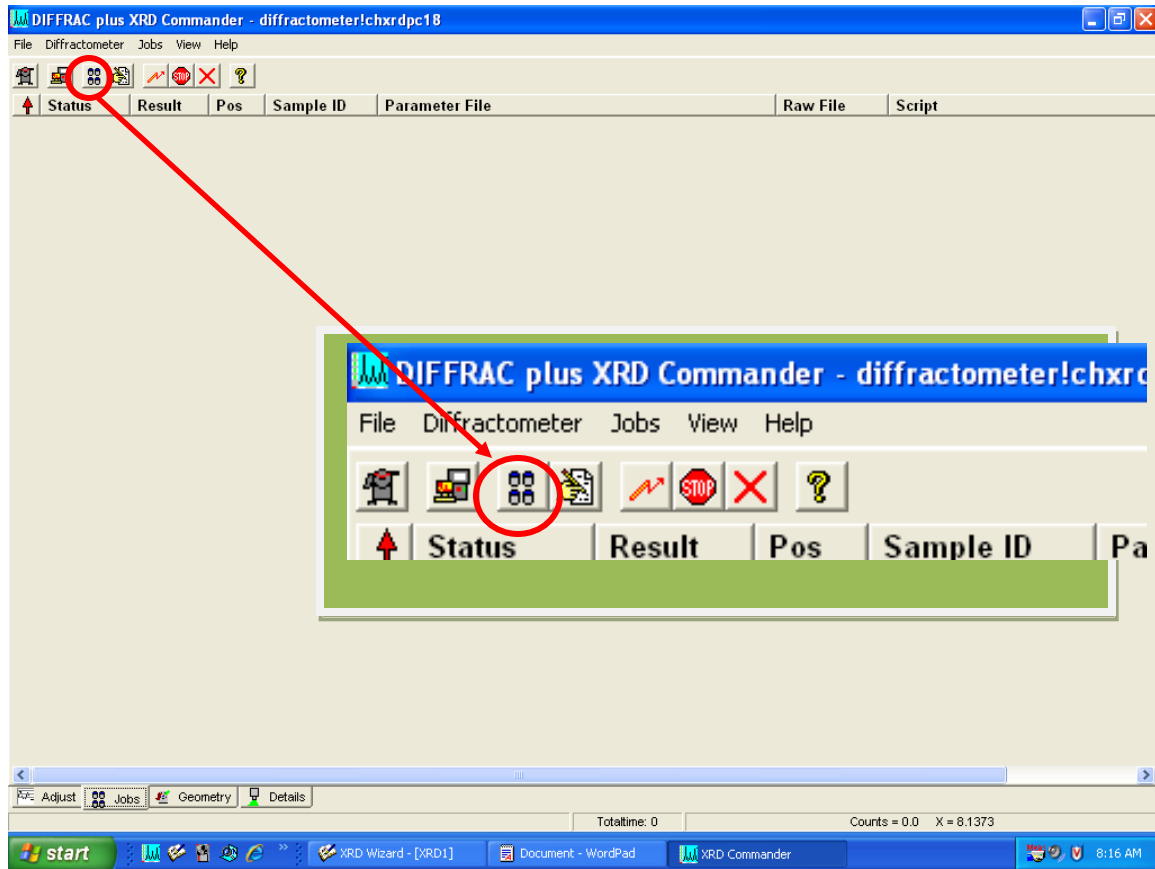
Step 8. Now in field titled “User Data Path” type the correct path (or browse for it).

1. Usually C:\users\facultyname\username
2. Click on OK in the Options window.

CAUTION: Please do not change anything in the Script Associations or Scan Types tabs.



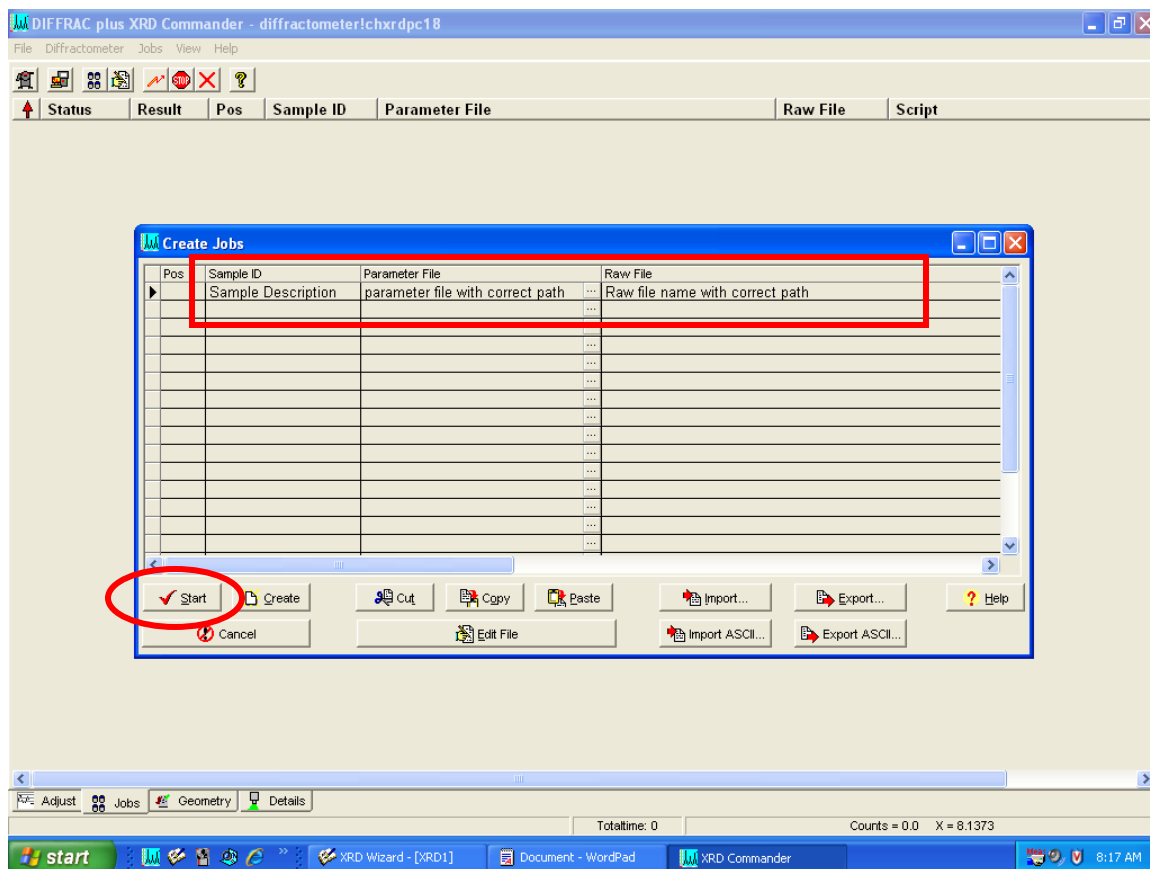
Step 9. Click on the icon for create jobs (or you can also go to Jobs --> Create Jobs)



Step 10. In the following window:

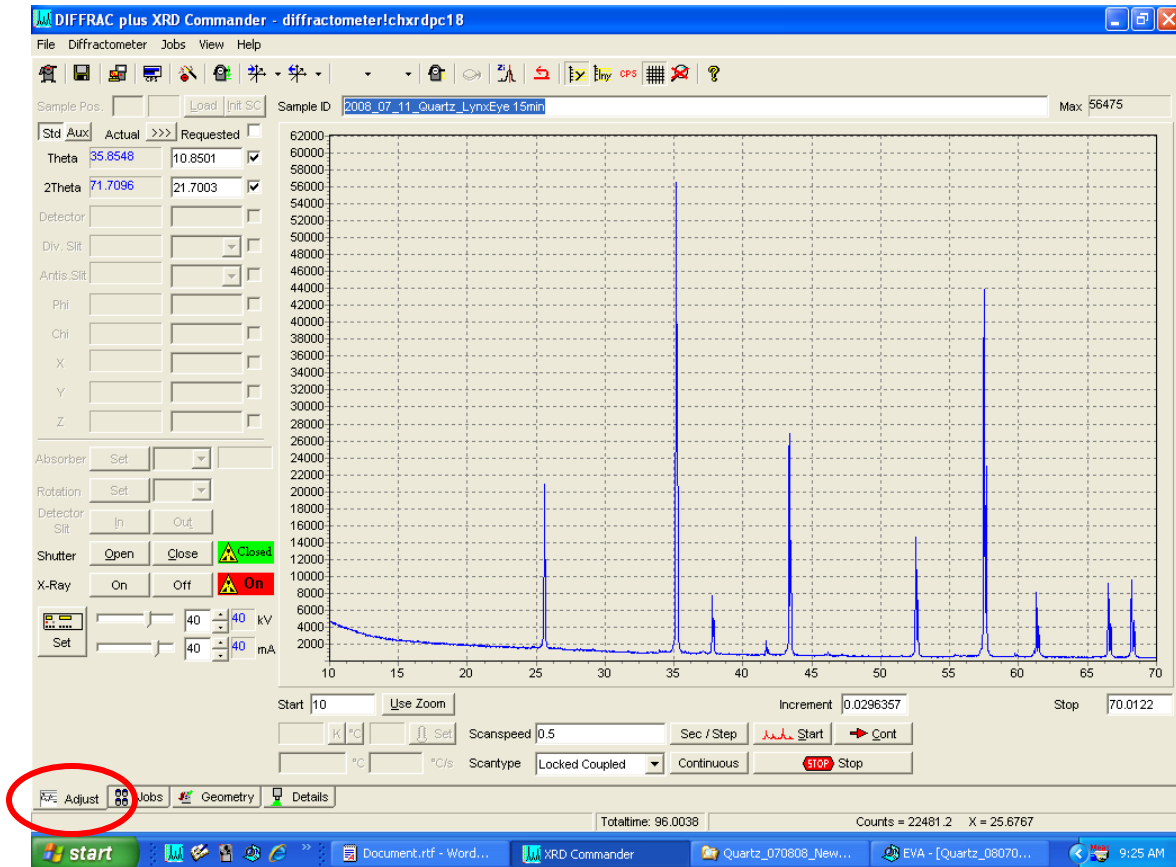
1. Enter the Sample ID. This is a description of your sample
2. Browse for the appropriate DQL file under Parameter File
3. Enter the Raw File name under Raw File column. If you have not put the correct User Data Path in the File --> Options menu, you can also browse for the location of the directory and give a Raw File name.

Then go for **Start**.



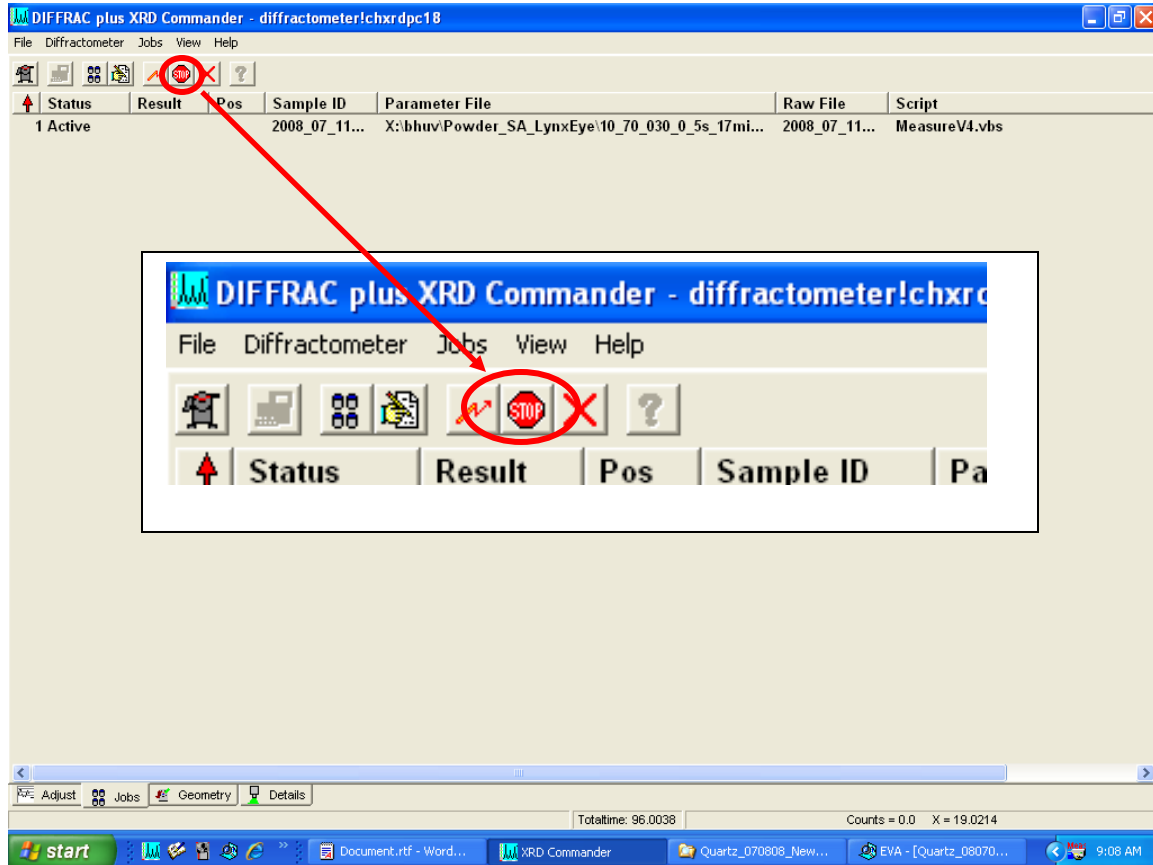
Step 11. To view the data being collected, click on the Adjust Tab.

1. In this window, you can zoom, unzoom, look for peak positions. .
2. Your raw file will be saved in the directory of your choice or (previously defined) default directory. Double click the data file or import it in EVA and have fun analyzing.



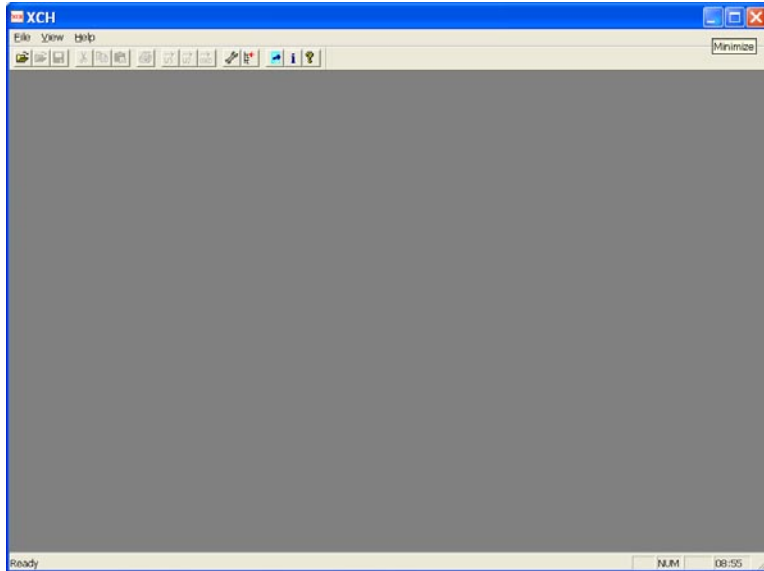
Appendix1.

1. If you want to stop the run for some valid reason, you can abort it using Halt all Jobs icon.

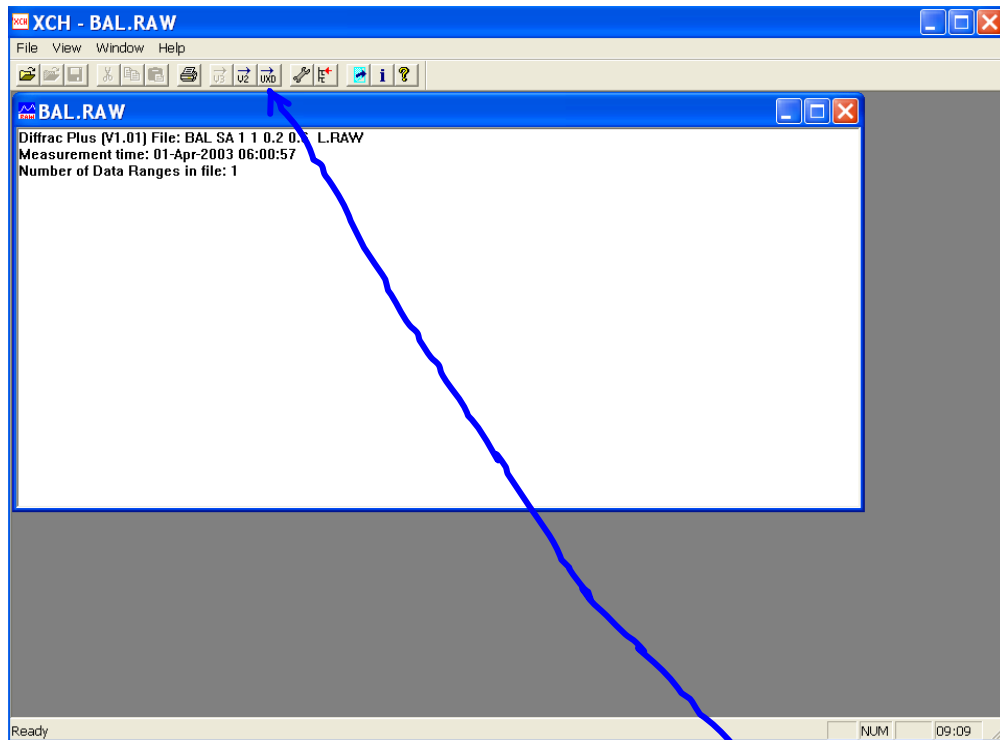


Appendix 2. To convert .RAW file to an ASCII (.UXD) file.

Open the [Diffrac Files Exchange](#) program.



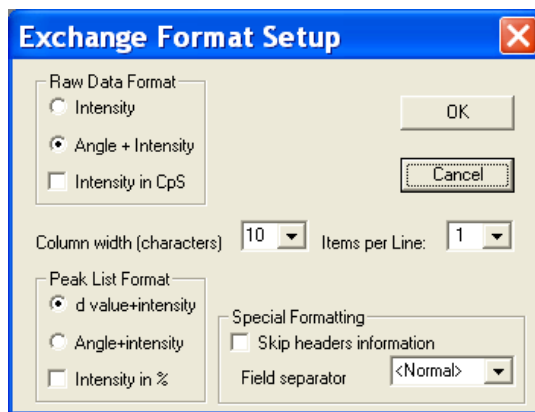
- Open your .RAW (say BAL.RAW) file



- Check the format of the output file:

File → UXD format

Check if all the values are as given in the following screen.



If the screen you get is not matching to the above, change it accordingly.

- Click OK.

- Now click the icon



- Select the folder you want to save the ascii file (say, BAL.UXD), and save it.

The UXD file will contain several header lines which you may(!!!) or may not want followed by a two column data. The first column will correspond to Two-theta and the second the corresponding intensities.

Happy Powder X-ray Diffraction

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