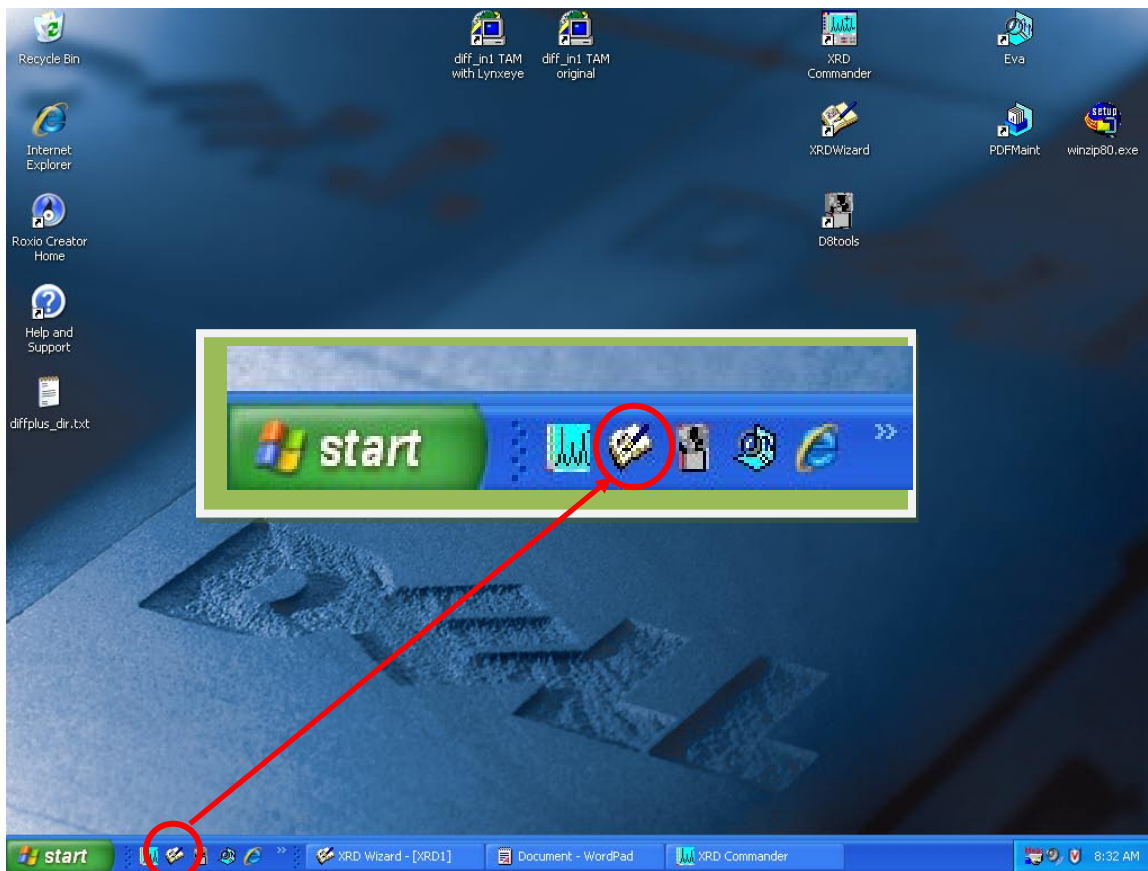


Step by Step tutorial
for
Powder XRD Short-Arm
Data Collection

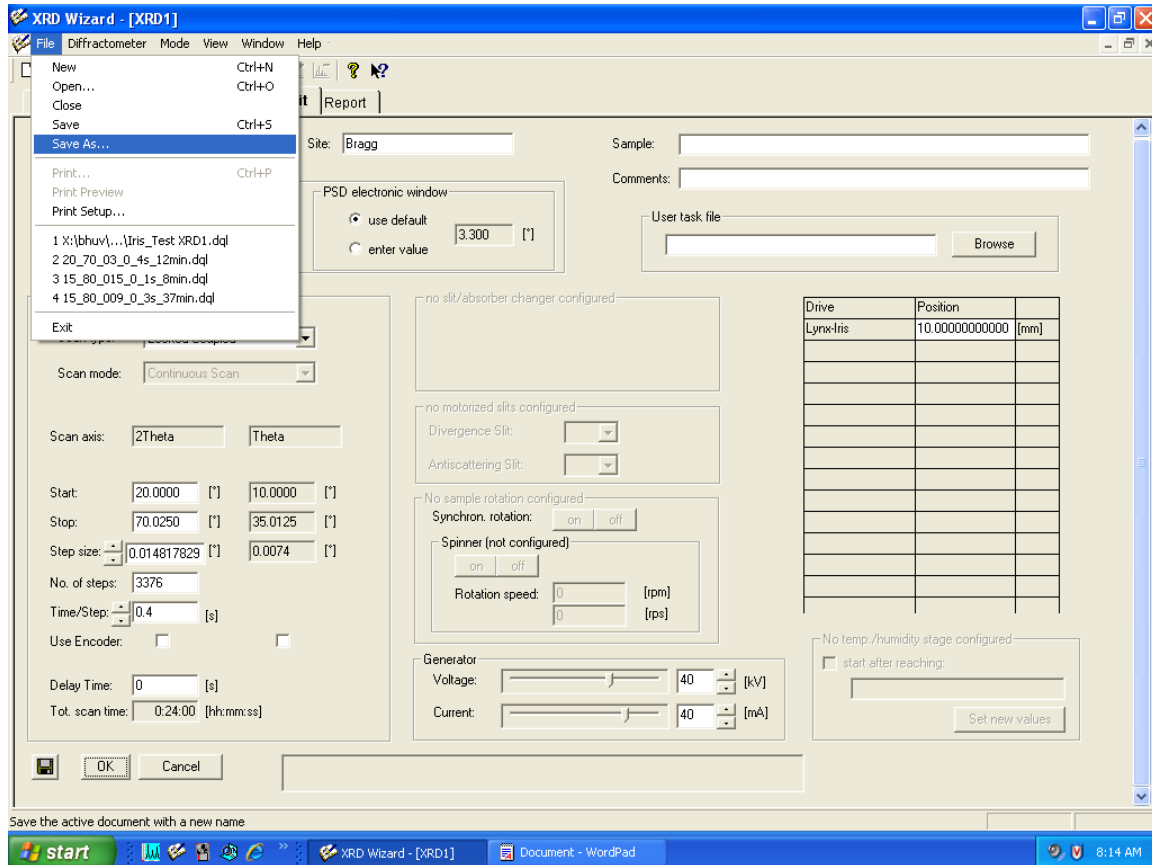
Creating the Parameter File

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

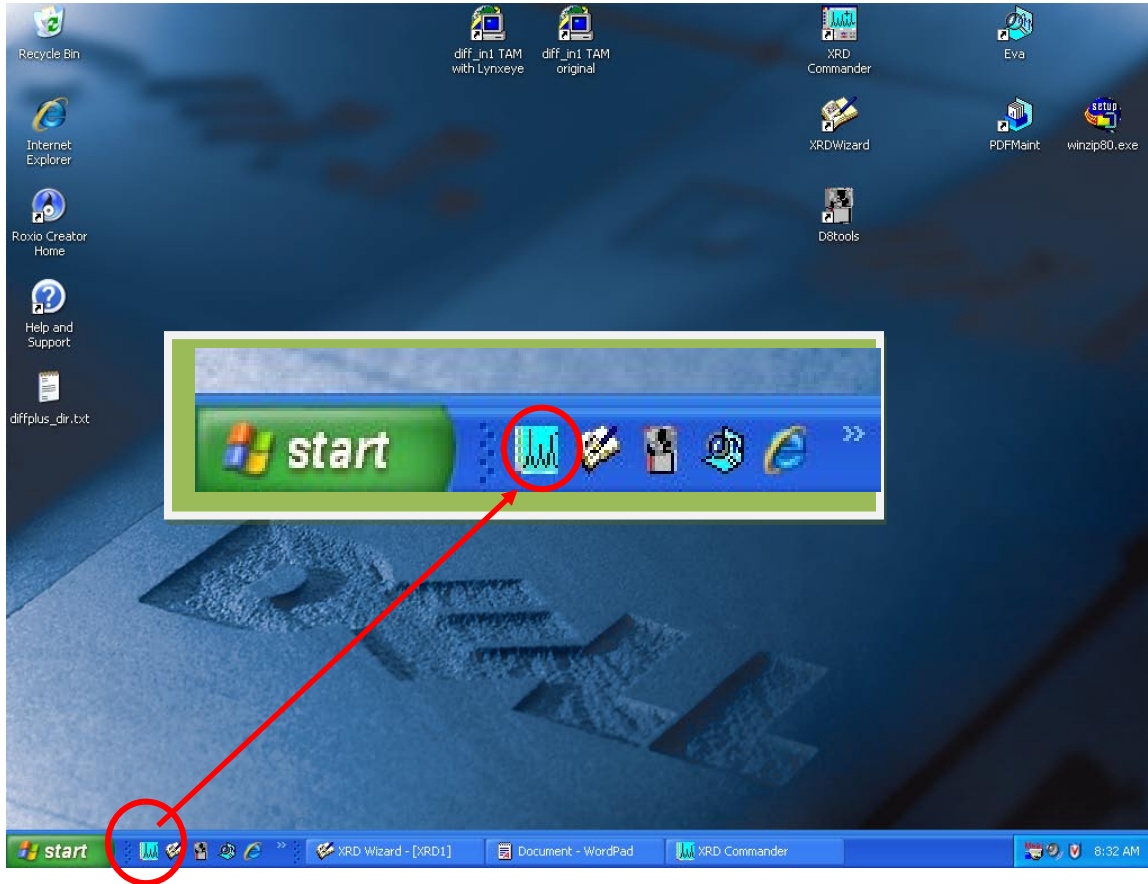


Step 4. Go to File → save as, and put the “dqj” file in the desired directory



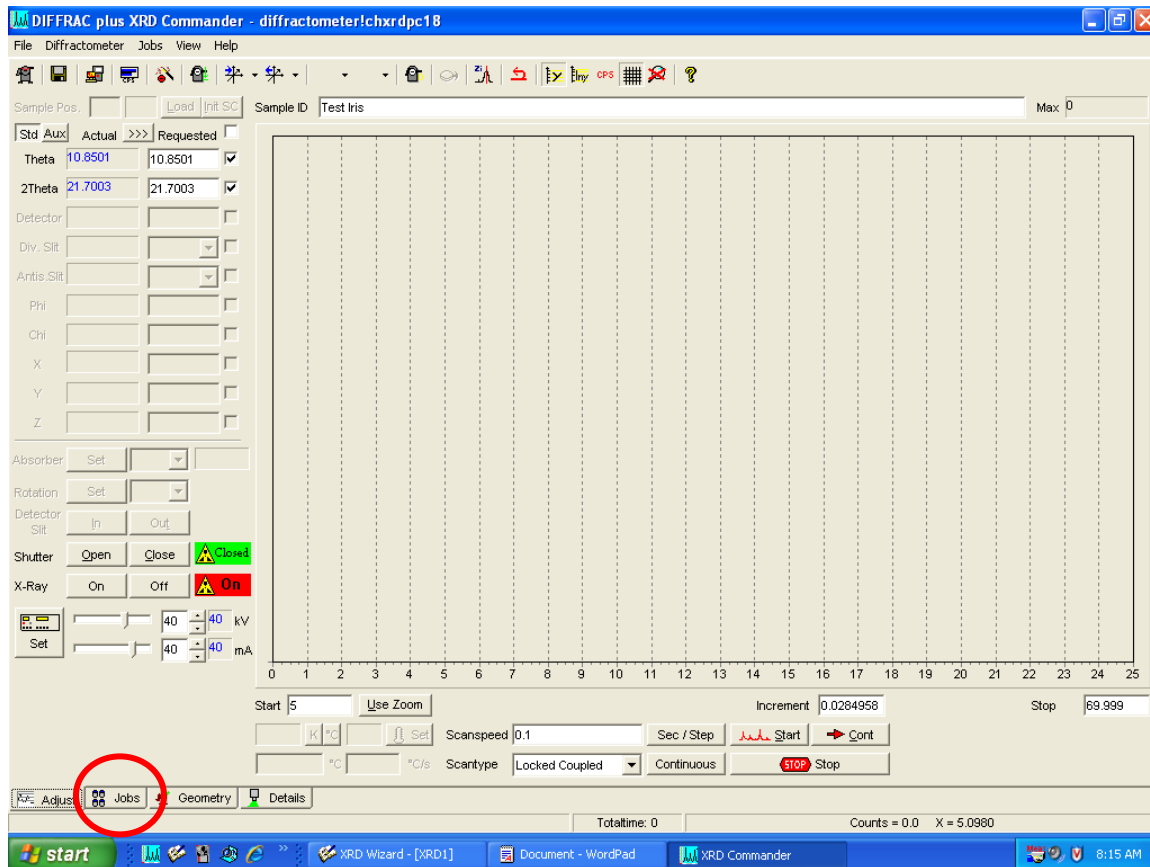
Data Collection Using COMMANDER

Step 5. Now start the Commander:



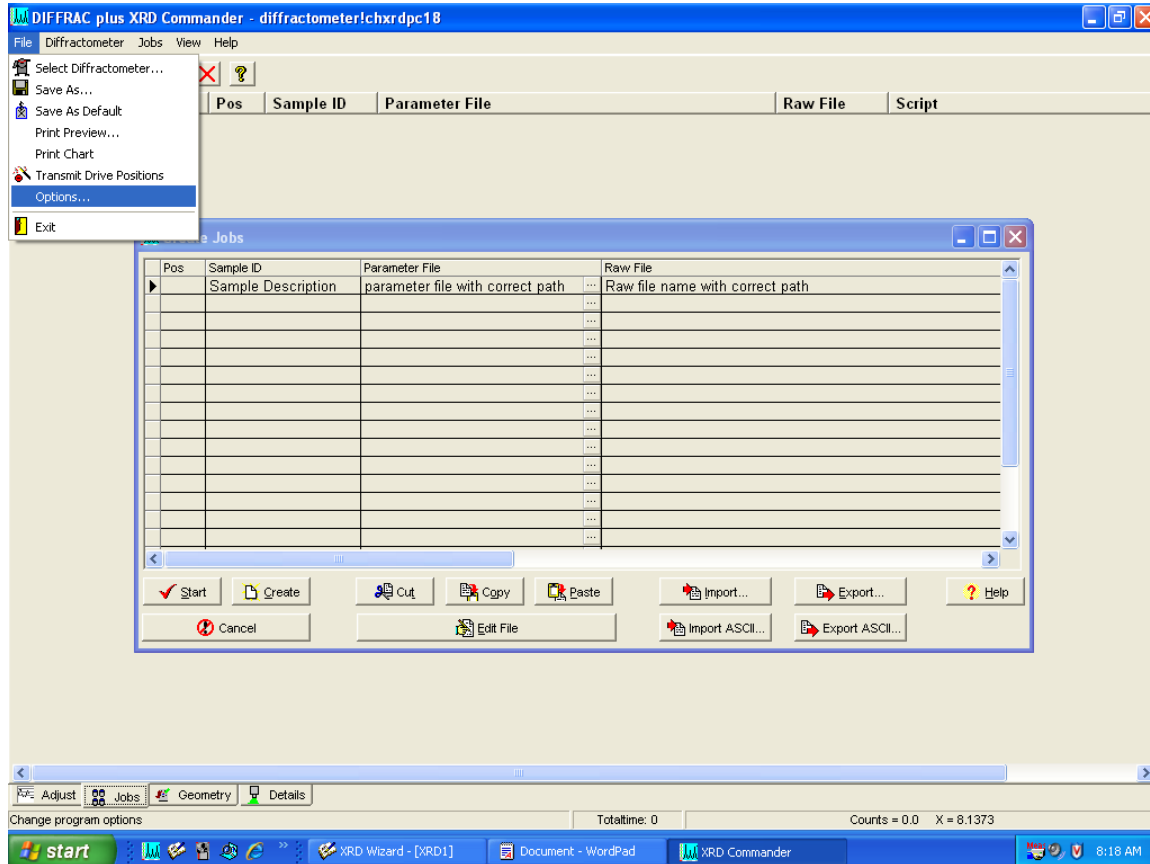
Step 6. You will be getting the following window.

1. Now select the Jobs Tab:



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

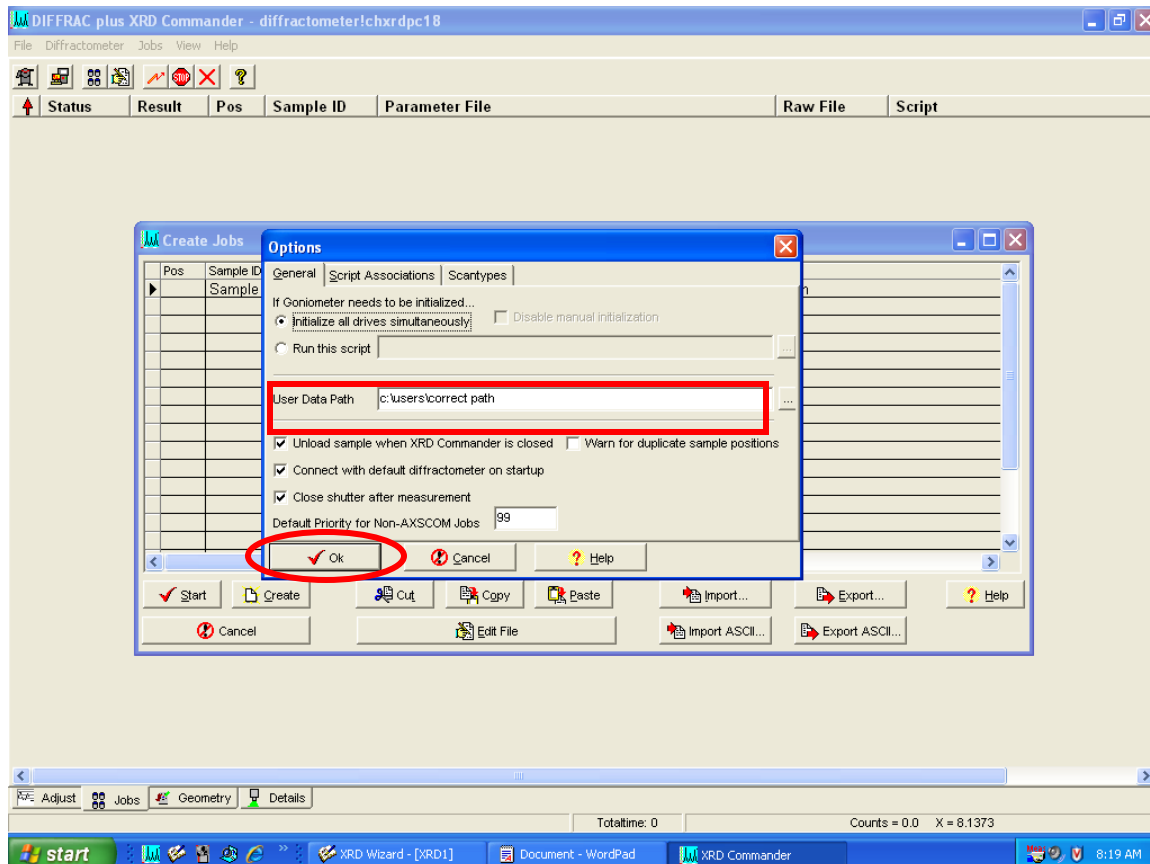
1. Go to File → Options



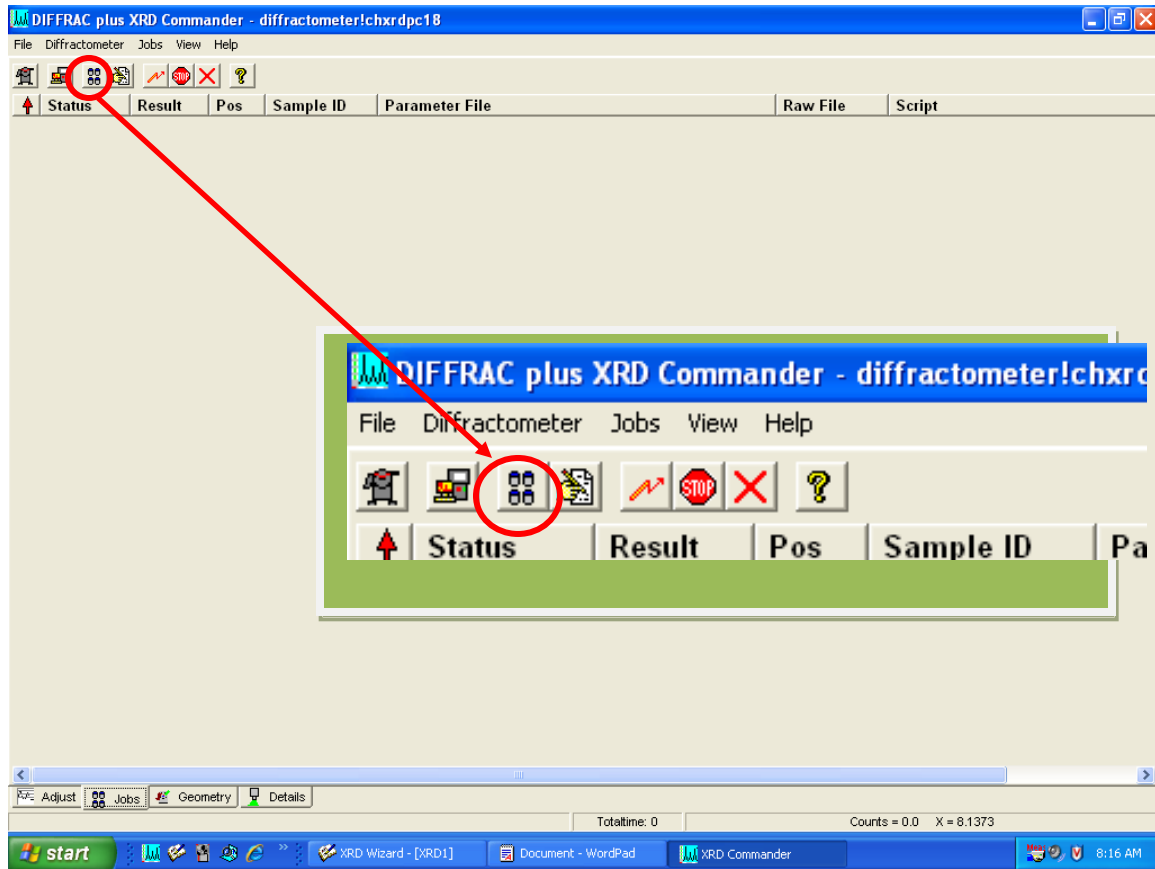
Step 8. Now in field titled “User Data Path” type the correct path (or browse for it).

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.



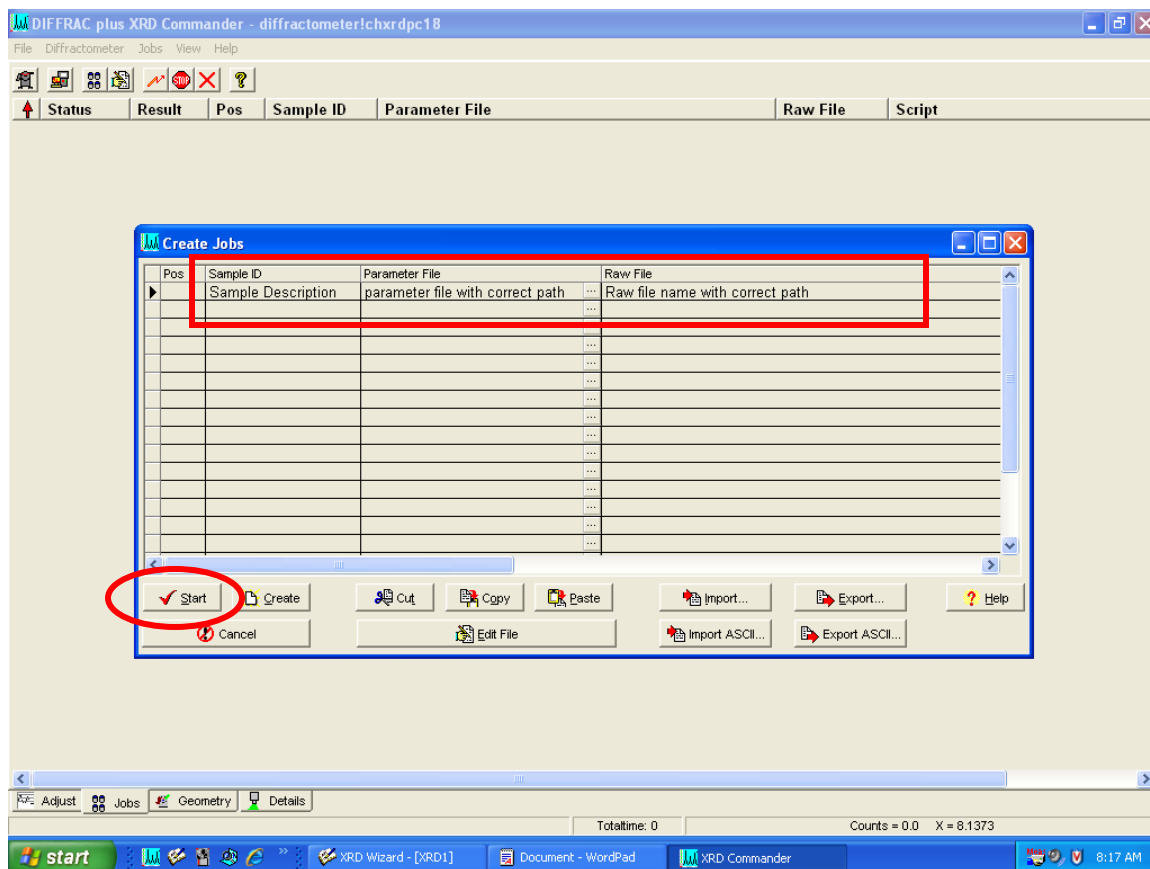
Step 9. Click on the icon for create jobs (or you can also go to Jobs --> Create Jobs)



Step 10. In the following window:

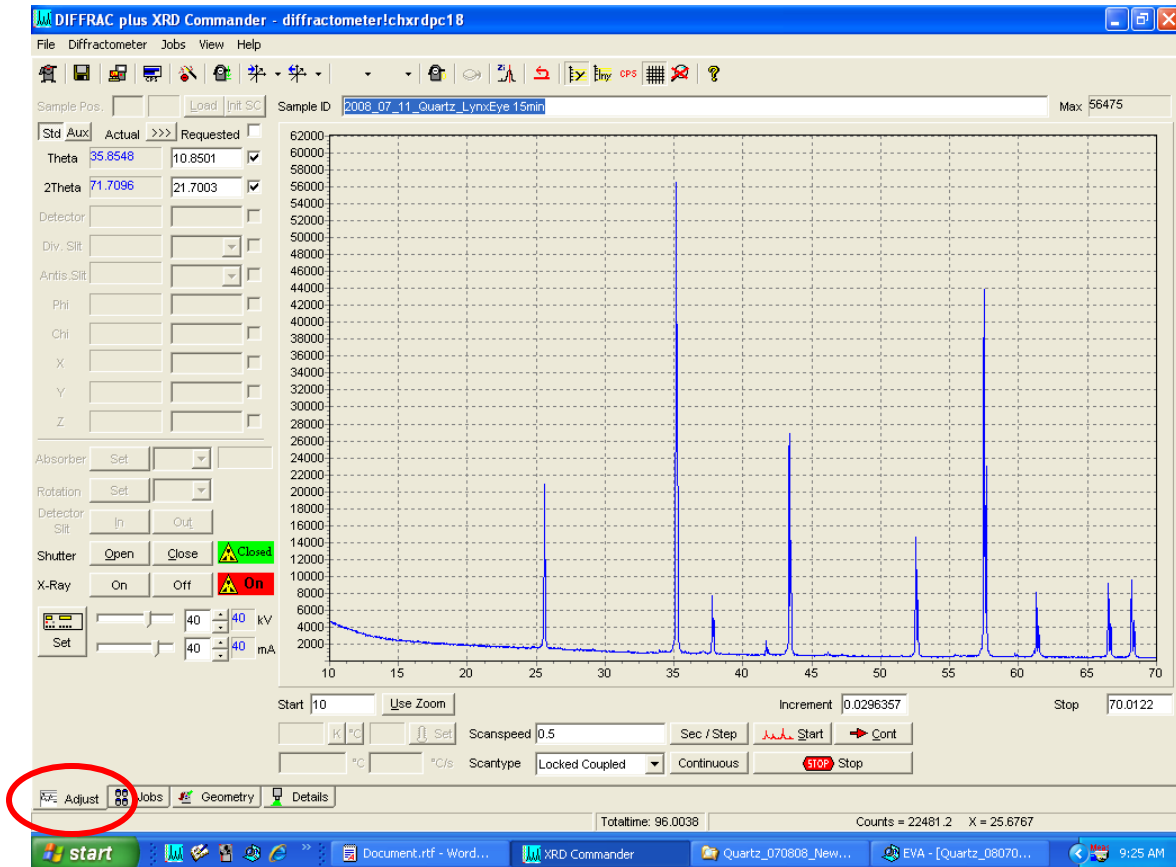
1. Enter the Sample ID. This is a description of your sample
2. Browse for the appropriate DQL file under Parameter File
3. Enter the Raw File name under Raw File column. If you have not put the correct User Data Path in the File --> Options menu, you can also browse for the location of the directory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

Then go for **Start**.



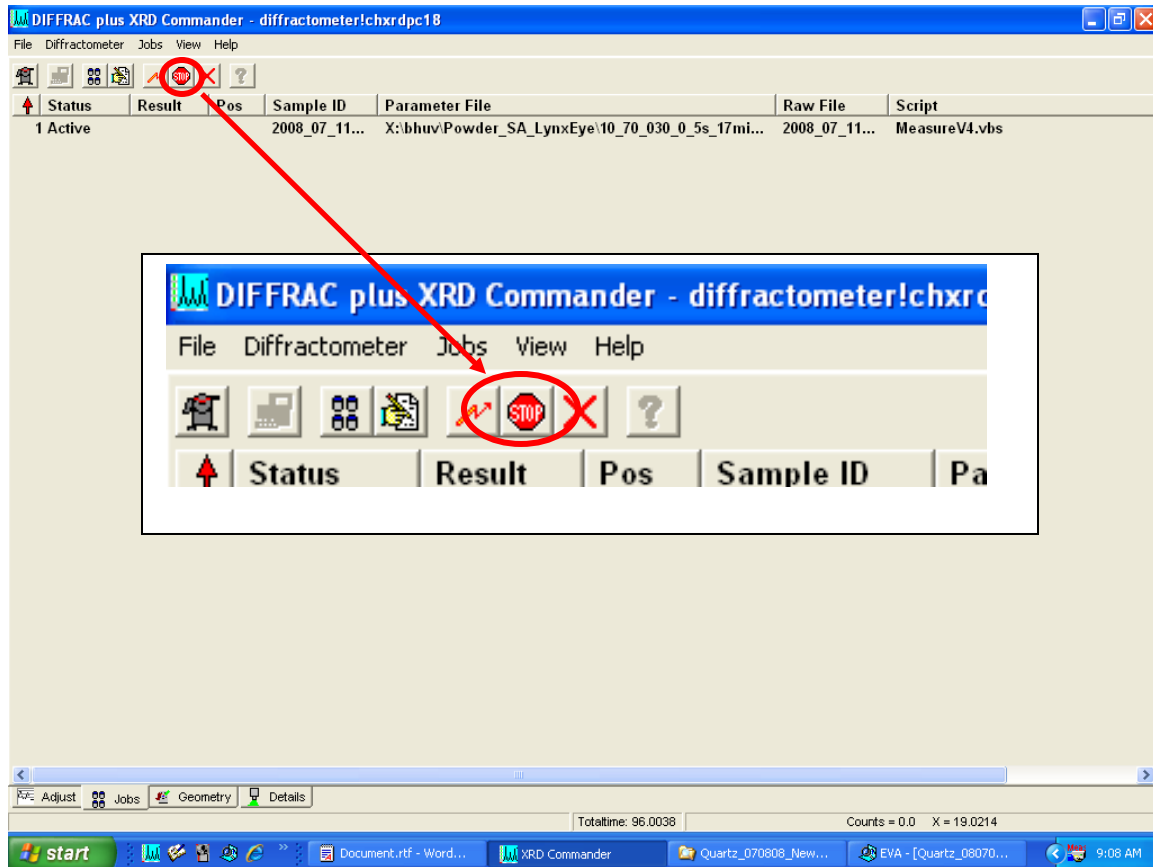
Step 11. To view the data being collected, click on the Adjust Tab.

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.



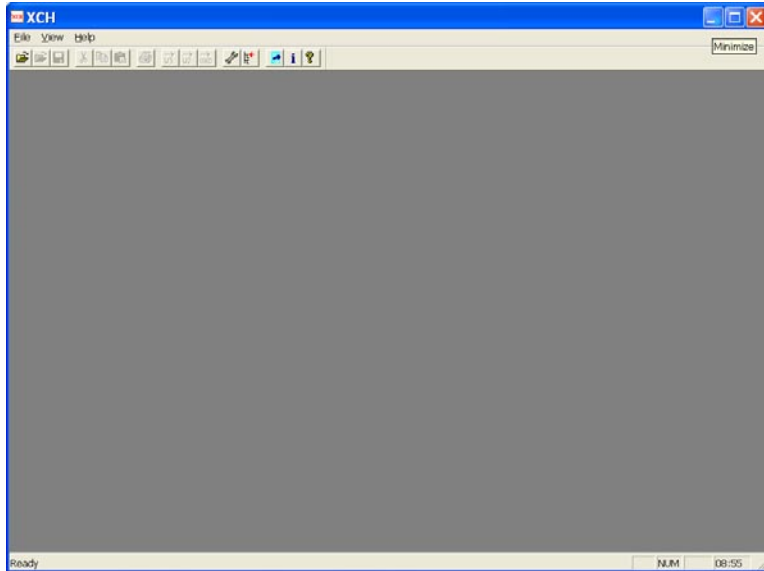
Appendix1.

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

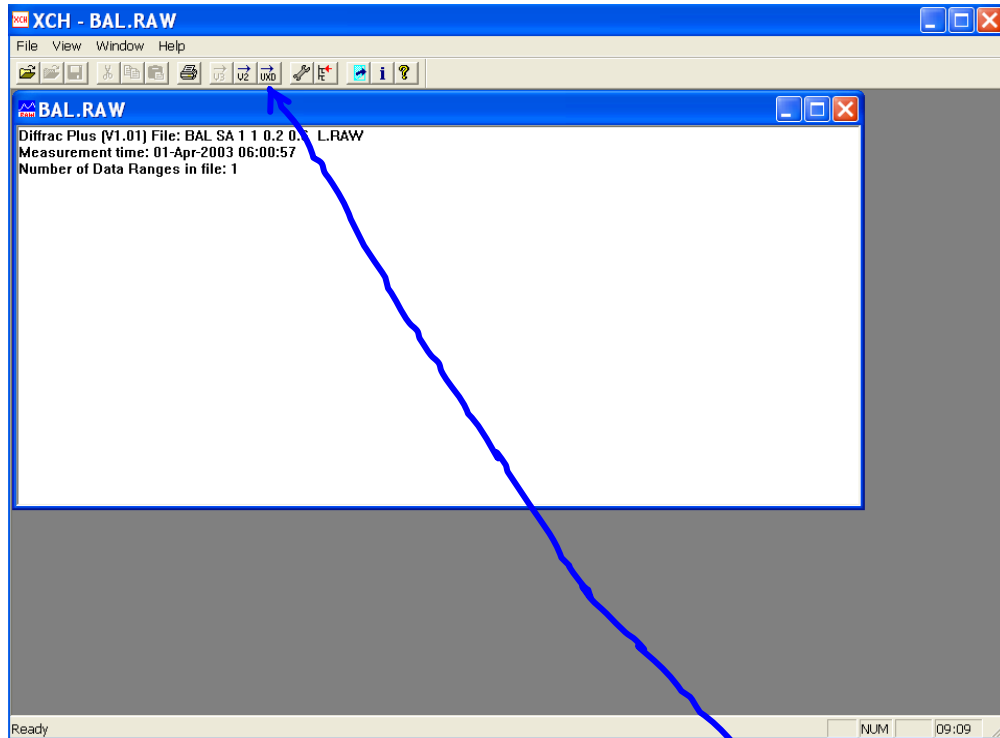


Appendix 2. To convert .RAW file to an ASCII (.UXD) file.

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



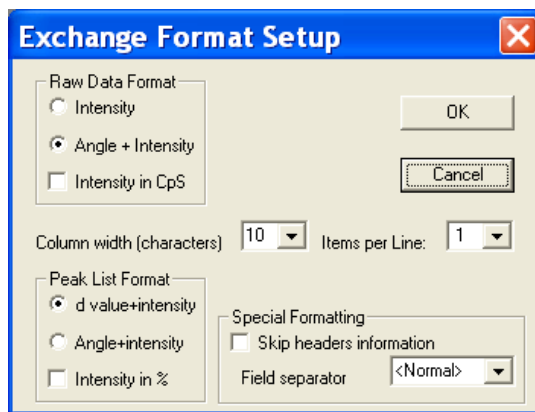
- Open your .RAW (say BAL.RAW) file



- 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

- **Nattamai Bhuvanesh**
X-ray Diffraction Lab.
Department of Chemistry
Texas A&M University
College Station, TX 77845