X-Pert High Score Plus (ICC Database)

We will use the X-Pert Philips Diffractometer in ERC 333 today. This instrument is equipped with a program that searchers the International Tables for Crystallography database. The program is called "X-Pert High Score Plus". A procedure to search for a crystal structure using this program is given below. ***You should use this program to identify one unknown sample such as a piece of mounting clay or any crystalline material that you want.***

1) Run X-Pert High Score Plus.

2) File Open => Get .xrdml file from the diffractometer.

3) Treatment
   Determine Background
   Recalculate
   (Subtract if you think you need to i.e. especially if you used a glass coverslip under the sample.)

4) Treatment
   Search Peaks
   Adjust to the peaks you think are correct.

5) Peak list
   Delete peaks that you don't think are correct by hand

6) a) Reference Patterns
   Retrieve patterns by restrictions
   Chemistry Periodic Table if you know the elements in the material

or

b) Analysis
   Search and M.
   Execute (This finds any peaks that seem to match from the ITC database.

7) Click to pick pattens
   Right click to accept

8) Select the pattern tab at the bottom of the plot and select the best match

9) Double click for the pdf for the best pattern and save as to save the pdf.

You make the plot the top level and save as ASC to read the files in excel. Bring a flash drive to transfer the data to your pc.