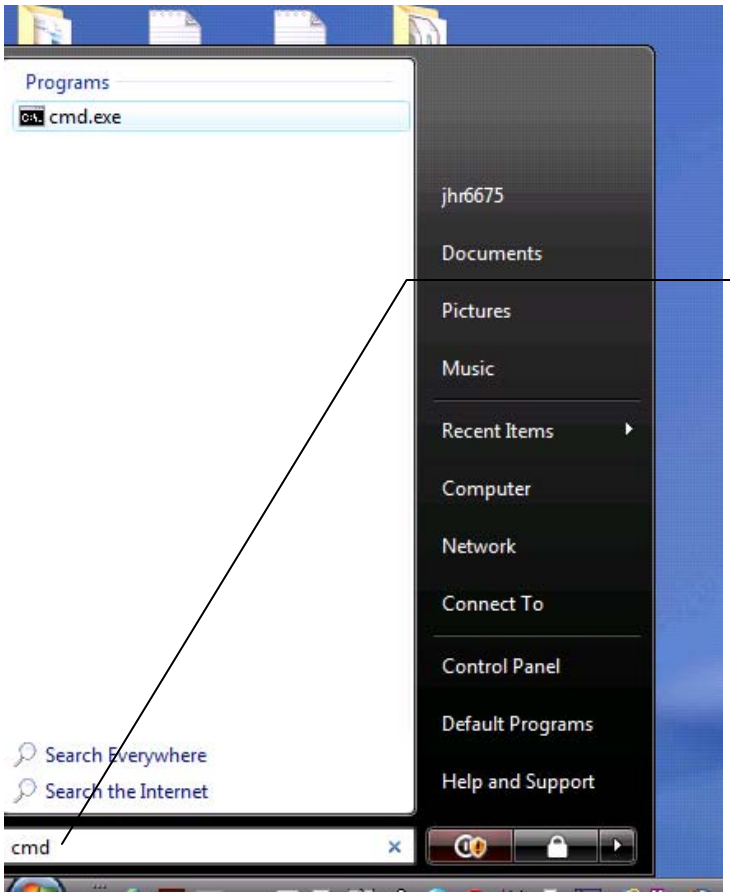
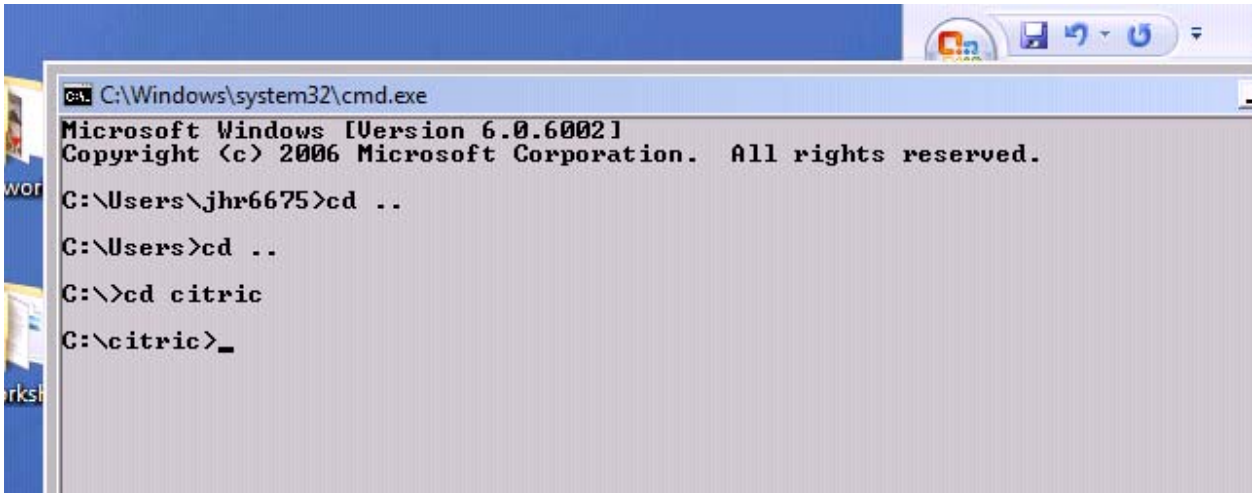
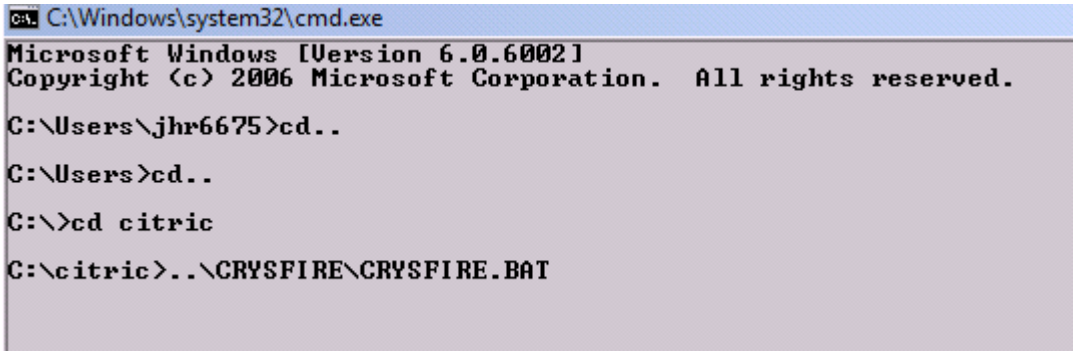
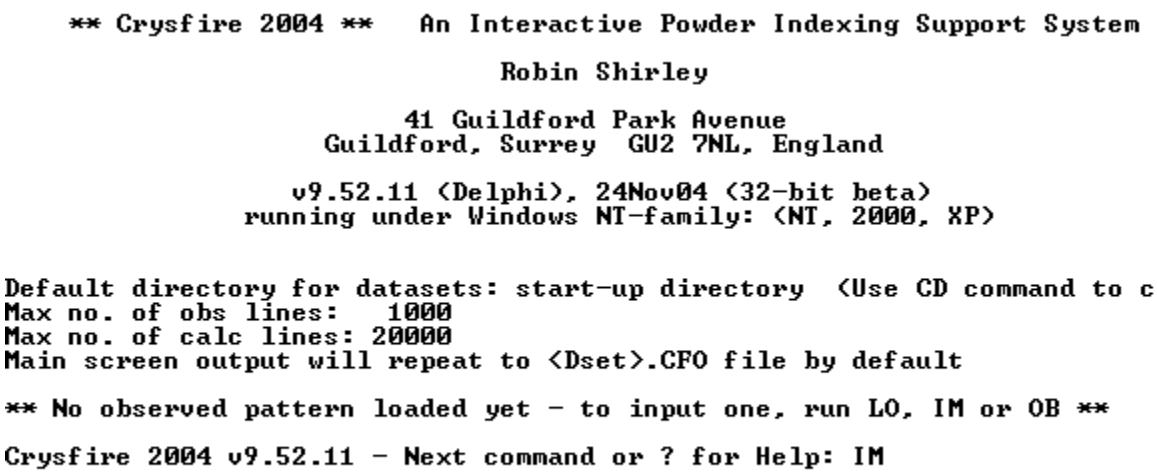
- Down load CRYSFIRE, PowderCell and Citric zip files.
- Unzip all folders.
- Move Citric, CRYSFIRE and PowderCell folders to the C: drive
- Call up a command window
- 

- Navigate (with the cd command) to the citric folder
- 

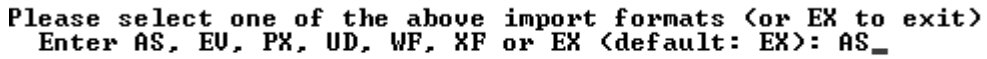
- Type "..\CRYSFIRE\CRYSFIRE.BAT" at the command prompt



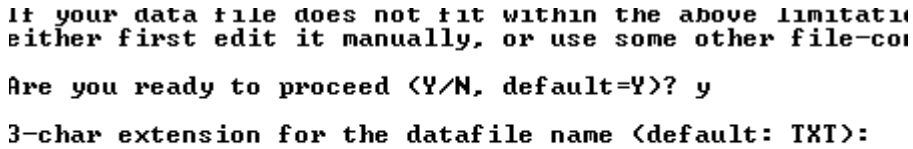
-
- Follow the prompts
- Type IM at the prompt
-



- The AS at the next prompt



-
- When asked to proceed type Y and at the next prompt hit a RETURN (no name)



-
- At the next screen enter "citric"

```
Drive / directory information followed by listing of textfiles
in the currently selected directory, sorted into name order:  *.TXT

 Directory/File specification is:  .\*.TXT

 CITRIC.TXT

Name of ASCII datafile to be loaded (omitting .TXT, default = exit): citric_
```

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o Use the defaults for the next 7 queries. After the How many fields query you will see

```
Reading data file...

Reading peaks list...

 No.   2Theta       d           Q

  1    11.479    7.702519    168.5522
  2    14.905    5.938965    283.5166
  3    15.185    5.830017    294.2120
  4    16.973    5.219682    367.0387
  5    17.928    4.943613    409.1769
  6    18.180    4.875866    420.6264
  7    19.016    4.663240    459.8587
  8    19.720    4.498271    494.2068
  9    19.877    4.463233    501.9968
 10    20.538    4.320992    535.5908
 11    22.267    3.989129    628.4110
 12    22.320    3.979939    631.3167
 13    23.075    3.851261    674.2083
 14    23.721    3.747836    711.9325
 15    24.295    3.660571    746.2810
 16    24.424    3.641615    754.0705
 17    24.995    3.559703    789.1735
 18    27.117    3.285702    926.2829
 19    28.316    3.149241   1008.2964
```

o

o For the working name enter citric

```
 13    23.075    3.851261    674.2083
 14    23.721    3.747836    711.9325
 15    24.295    3.660571    746.2810
 16    24.424    3.641615    754.0705
 17    24.995    3.559703    789.1735
 18    27.117    3.285702    926.2829
 19    28.316    3.149241   1008.2964

Type ENTER to continue or F (and ENTER) to Finish without further pauses:

 20    28.785    3.099011   1041.2471
 21    29.283    3.047393   1076.8198

What is the working name for this new dataset (1 to 8 chars): citric
```

o

o Save the dataset to citric and continue

```
Save the current dataset in Crysfire (CDT) format

Dataset name (max 8 letters/digits, default: citric) or *Q to quit: citric_
```

o

o Give it a title and hit return (twice)

- You should see the Crysfire 2004 v9.52.11 line and the command prompt
- Type index and return
- Now select the indexing programs. We will run several as an internal check for the unit cell.
- Type TP first.
- Accept all default values
- Start the program. When it is complete a text file will appear. Close it for now.
- Hit a return and a 2nd text file will appear. This is a summary of what TP found. The figure of merit is off the scale (that is good).
- Close this text file. (you may need to do this twice).
- Repeat the process for the next indexing program.
- At the Crysfire 2004 v9.52.11 line type Index
- Chose DV this time
- Here is the summary file

Running summary of all solutions logged so far for this dataset name,
sorted in descending order of I20 then Merit (as defined by each program)

I20	Merit	Volume	V/V1	BL	IndexProg	Date	Time	Pedig	a	b	c
20********		904.933	1.00	P	TAUPv3.3a	23Feb10	15:59:40	Ort__1	6.2985	9.3265	15.4050
20	5500.6	904.933	1.00	P	DICVOL91/log	23Feb10	16:04:50	Ort__1	15.4050	9.3265	6.2985
20	4950.1	904.930	1.00	P	DICVOL91/log	23Feb10	16:04:50	Mon__7	19.8997	9.3265	6.2985
20	4623.2	904.935	1.00	P	DICVOL91/log	23Feb10	16:04:50	Mon__4	16.6429	9.3265	6.2985
20	4367.2	904.935	1.00	P	DICVOL91/log	23Feb10	16:04:50	Mon__2	15.4050	6.2985	9.3265
20	4155.1	904.935	1.00	P	DICVOL91/log	23Feb10	16:04:50	Mon__1	9.3265	15.4050	6.2985
20	3998.5	904.937	1.00	P	DICVOL91/log	23Feb10	16:04:50	Mon__6	18.0082	6.2985	9.3265
20	3693.3	904.930	1.00	P	DICVOL91/log	23Feb10	16:04:50	Mon__5	11.2541	15.4050	6.2985
20	3265.0	904.935	1.00	P	DICVOL91/log	23Feb10	16:04:50	Mon__3	15.4050	9.3265	6.2985

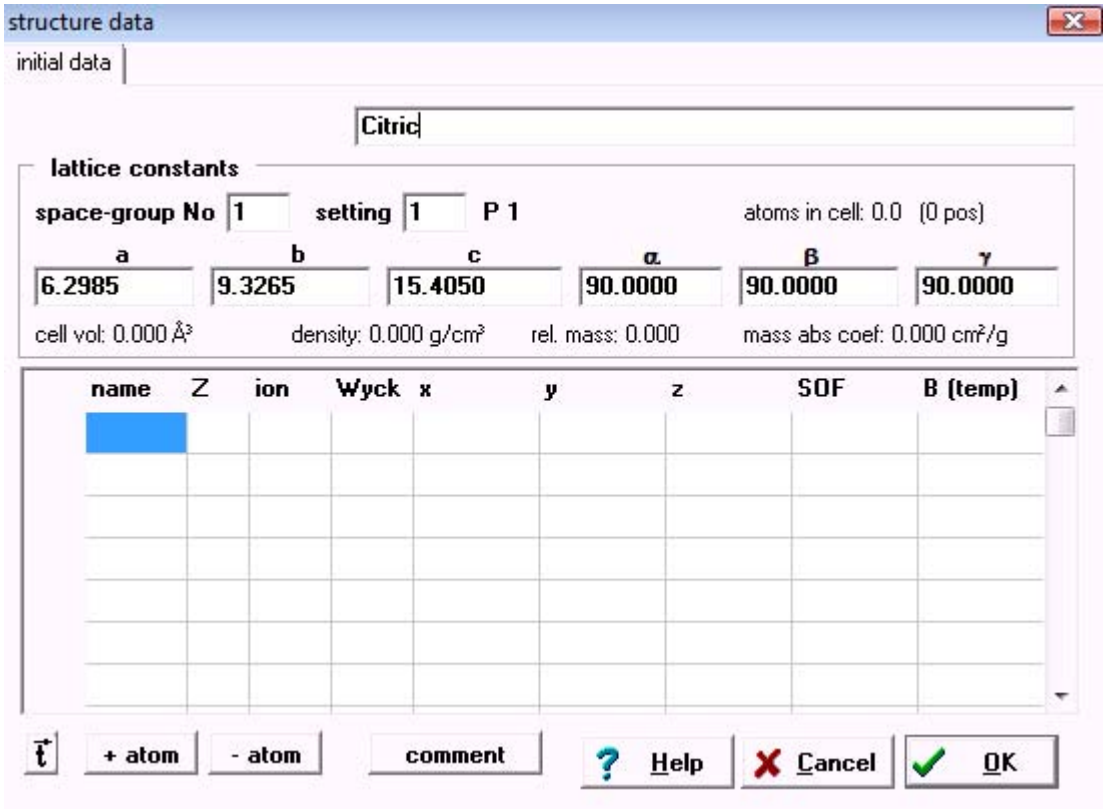
-

- Notice that there are several DP outputs the one with the highest Merit is of interest.
- Try out other indexing programs.
- If you do you may see something like this

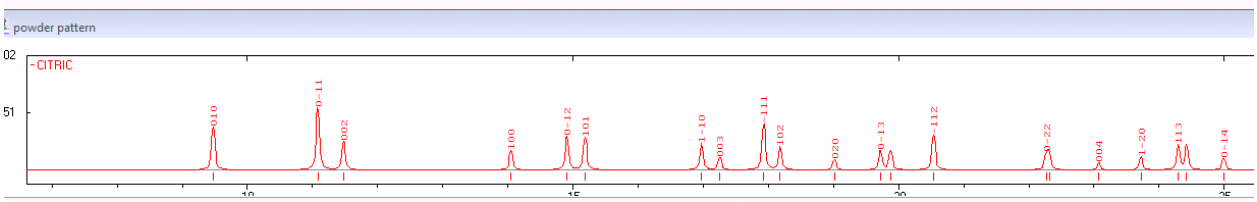
2017691.8		904.94	1.00	P	ITO12/log	23Feb10	16:06:29	461	9.3265	15.4051	6.2985
2014646.88		904.934	1.00	P	FJZNv6.22a	23Feb10	16:07:05	241	9.3265	15.4050	6.2985
20********		904.933	1.00	P	TAUPv3.3a	23Feb10	15:59:40	Ort__1	6.2985	9.3265	15.4050
20	5500.6	904.933	1.00	P	DICVOL91/log	23Feb10	16:04:50	Ort__1	15.4050	9.3265	6.2985

- ITO, FJZM, TAUP and DICVOL will find solutions. The highest are for the orthorhombic cell 6.2985 9.3265 and 15.4050 (a,b and c are interchangeable!)
- CRYSFIRE has found a solution.
- It is time to go to PowderCell.

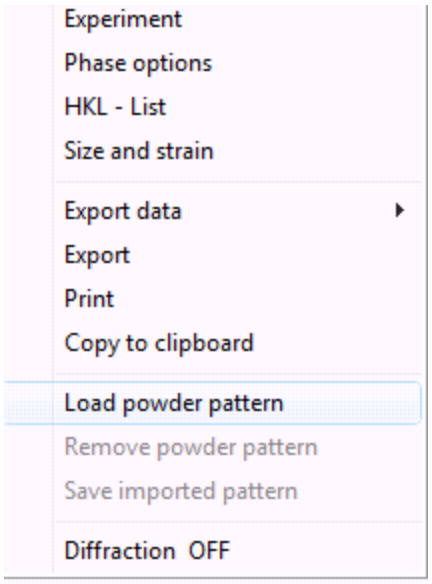
- Powder Cell .. Navigate your way to the powder cell folder (in explorer) and double click the PCW icon
- Goto file/new and input the cell in the Structure Data box. For now allow the space group to be P1.



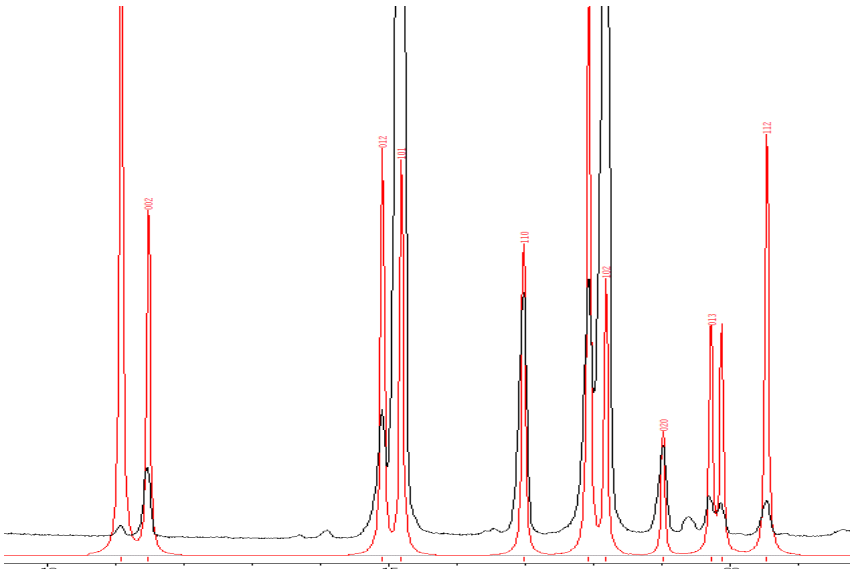
- Point to Ok. The program will say no valid atom coordinates. Ignore this.
- An idealized pattern will appear at the bottom of the screen



- That's good. Load the powder data.



- It will ask if you want to take the range from the measurement. Answer YES (Ja).
- Maximize the pattern window.
- You will now see a lot of peaks in red that do not belong there. That is because you are still in the P1 space group. Point to Structure and then point to Edit initial data.
- For space-group number change that to 19 (P212121).
- Point to OK.
- You should now see good overlap between the observed pattern (black) and the predicted pattern (red)



- If you wish to clean up the patterns run a few Refinements.

- Notice that there are a few peaks in the observed Citric acid pattern that are missing from the calculated. This is an impurity, most likely the anhydrous form of citric acid.
- This concludes this tutorial.
- You may wish to continue by inputting the coordinates of citric acid in PowderCell and refining the pattern.