

Quick Start Users Guide for Bruker SMART APEX II Diffractometer

APENDIX III

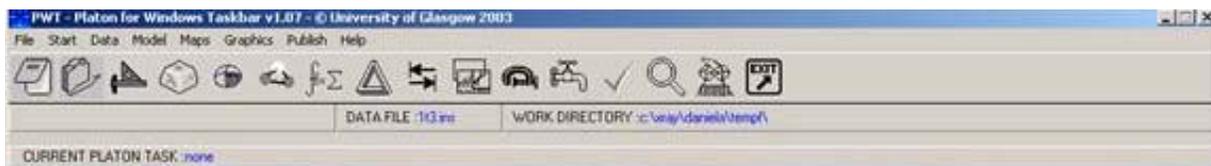
INTRODUCTION FOR FINDING ADDITIONAL SYMMETRY WITH PLATON

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Platon is a versatile SHELX97 compatible multipurpose crystallographic tool and is FREE for academic users. More information can be found from Platon homepage.

Suppose your files are **f10.***

- (1) In DOS mode, type **copy f10.res f20.res**, and then type **copy f10.hkl f20.hkl**. In this introduction, f20.* will be used while f10.* will be kept for backup.
- (2) Find the Platon program on the computer, double click **pwt.exe** to open Platon Taskbar and the following window will show up.

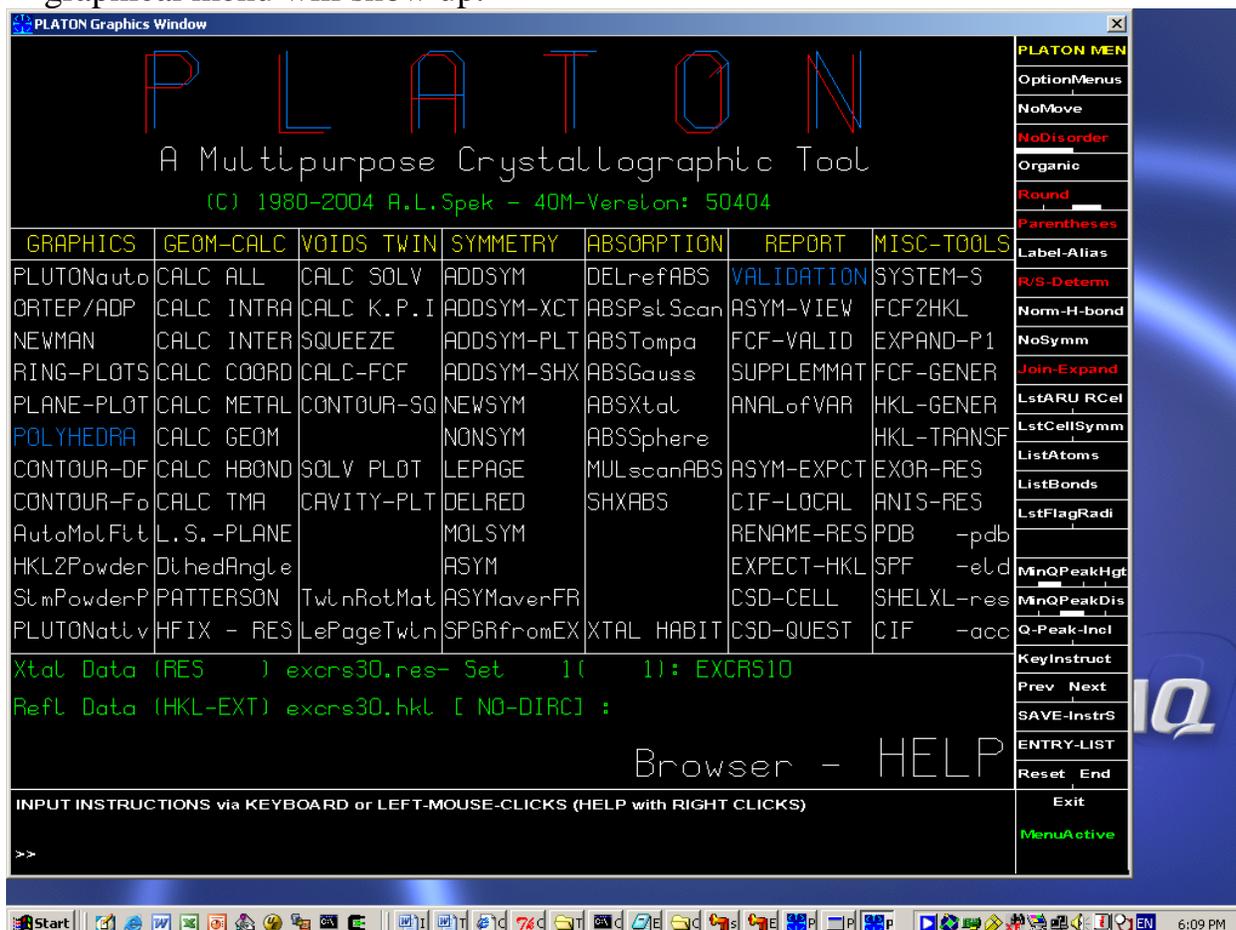


- (3) In Platon, click **File** and select **select Data File**. Either .ins or .res file can be used. However, **.res file is recommended**. Click **Files of type** and select **SHELX file (*.res)**, then find the target file **f20.res** by browsing the computer through the **Look in** window, then click **open** to select **f20.res** file.
- (4) Find the icon $\int f_x \Sigma$ on the toolbars and click it. A lot of numbers will come out on the screen at this time and it usually takes a few seconds but up to a couple of minutes. It's done when you see the bottom of the screen have something like following:

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR

You may see the summary of results from Platon on the screen.

- (5) Close Platon program and any other windows that were opened by Platon.
- (6) Use Windows Explorer to go to the directory of your files and double click **f20.lps** to open it. Go to the **end** of this file and find lines of **(Summary and Remarks : N = NOTE, W = WARNING, E = ERROR)**. Pay attention to those warning messages. **If additional symmetry was found**, you will see a message like this: **N: ADDSYM finds additional \(\pseudo\)symmetry in the structure \(\please check!\)**. Check that there are no solvent accessible voids; if there are, there may be disordered solvent that can be modeled or treated with SQUEEZE. PLATON also tells your about possible hydrogen bonds; if there are, insert HTAB in the .ins and run XL again. Close f20.lps.
- (7) If no additional symmetry was found, finish the structure as usual using files **f10.***. Otherwise, the structure needs to be converted to the proper space group. In Platon Taskbar, select the data file again click **Start** and select **Graphical Menu**. A graphical menu will show up.



- (8) Under the column of **SYMMETRY**, click **ADDSYM-SHX** and wait for a few seconds until it's done. Platon will make changes to **f20.res** file. Then click **Exit** on the right bottom corner to exit graphical menu. Close Platon program and any other windows that were opened by Platon.
- (9) Open **f20.res** with Notepad. The title has been changed to this:

TITL XXXXXX in P-1 P21/c

The first P-1 is the previous space group and P21/c is the new space group. Change the title properly by deleting previous space group P-1.

Sometimes, Platon uses non-standard settings. For example in this case, **P2(1)/c** should be used instead of **P2(1)/n**. Make sure that the new space group is correct by referring to the new symmetry operations.

- (10) SFAC and UNIT lines have been changed to:

```
SFAC C 2.31000 20.84392 1.02000 10.20751 1.58860 0.56870 0.86500 =
          51.65125 0.21560 0.00330 0.00160 11.500 0.68000 12.01000
SFAC H 0.49300 10.51091 0.32291 26.12573 0.14019 3.14236 0.04081 =
          57.79977 0.00304 0.00000 0.00000 0.624 0.35000 1.00800
UNIT 92 60
```

Manually create SFAC lines to be **SFAC C H**, and make sure the order of atom is the same as in atom list. Put this line just before **UNIT** instruction as usual. Delete current SFAC lines with a lot of numbers. New SFAC and UNIT lines should look like this:

```
SFAC C H
UNIT 92 60
```

IMPORTANT !

Several things have been changed from the initial .res file to that output by Platon. Make sure all commands present in the saved f10.res are copied appropriately into the new f20.res.

Platon may also change the atom codes in the atom list, make sure to fix these!

Save f20.res after change and then quit.

- (11) In DOS mode, type **copy f20.res f20.ins** to create f20.ins file.
- (12) In DOS mode, type **copy f10.pcf f20.pcf** to create f20.pcf file. **.pcf** file contains crystal information needed as a reference when **XCIF** runs. Open **f20.pcf** with Notepad, check **_symmetry_cell_setting** and **_symmetry_space_group_name_H-M** at the beginning of the file. In this case, change **_symmetry_cell_setting** from **Triclinic** to **Monoclinic**; Change **_symmetry_space_group_name_H-M** from **P-1** to **P2(1)/c**. Save f20.pcf and quit.
- (13) In DOS mode, run **XL f20**. Now the structure is in the new symmetry. Finish as usual. During XCIF, make sure the correct space group name is printed.