Structure Solution Advanced

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Version 1.0.0

Free Structure Solution Programs.

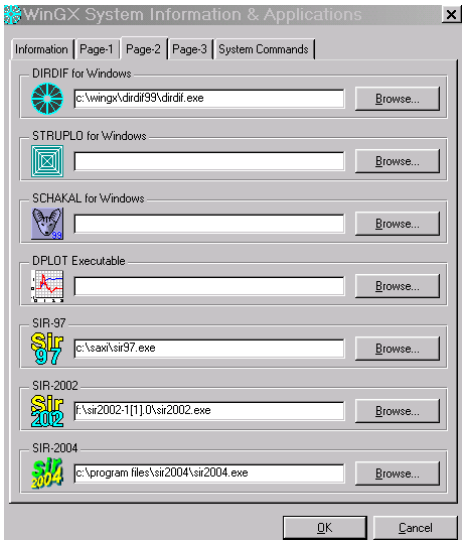
Download and install the program WINGX

http://www.chem.gla.ac.uk/~louis/software/index.html

Download and install Dirdif-99.2 for Windows (be sure to read the READ.ME instructions on how to install the software)

http://www.chem.gla.ac.uk/~louis/software/dirdif/index.html

The program SIR97 comes with the WINGX program. SIR2002 and SIR2004 must be obtained from the facilities manage.



Start WINGX and point to File/Systems/Applications. Goto tab Page-2.

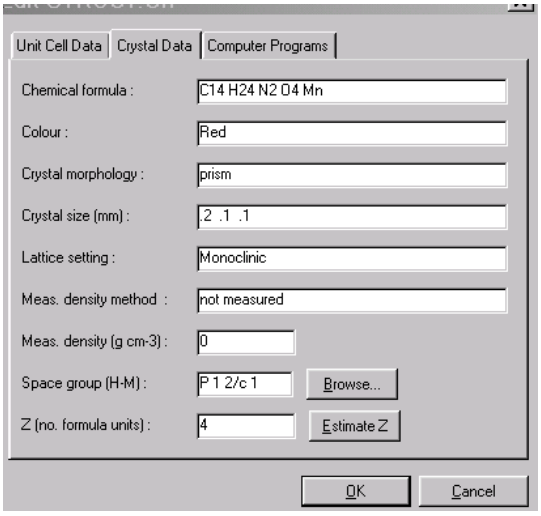
Find DIRDIF and SIR97. If you have downloaded SIR2002 and SIR2004 find them now.

Point to OK. Now your ready to begin

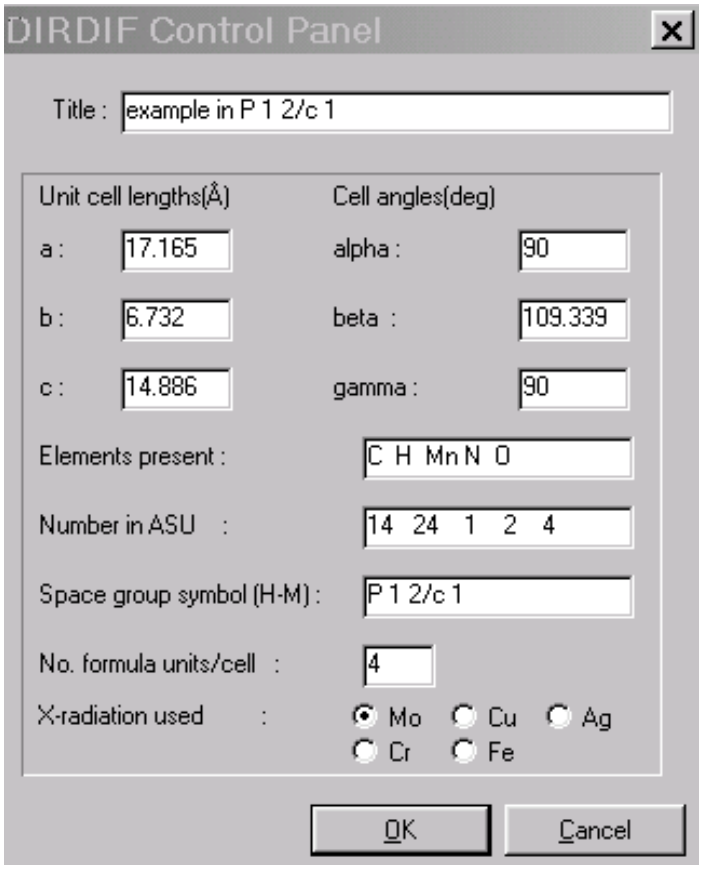
Point to File/Change Project/Select New Project

Find the *.ins file and double click it. Check the information that is displayed for errors and point to OK.

Point to Solve DIRDIF interactive. Input the Chemical Formula, Color, and Crystal Size. Point to OK. The computer will tell you it has written a structure file. Point to OK for the next screen

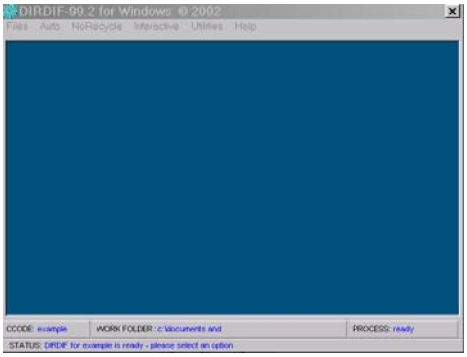


The DIRDIF control panel will pop up. Point to OK to continue. You can change the formula or space group.



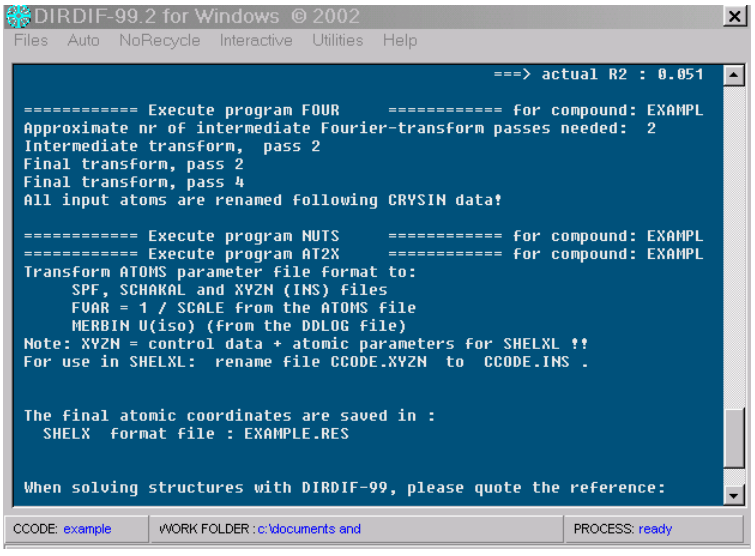
HINT The closer your formula is to the real formula the better your structure solution chances!

You will now see the DIRDIF screen.



Point to AUTO/PATTY. Dirdif will automatically run and create a SHELX.RES file

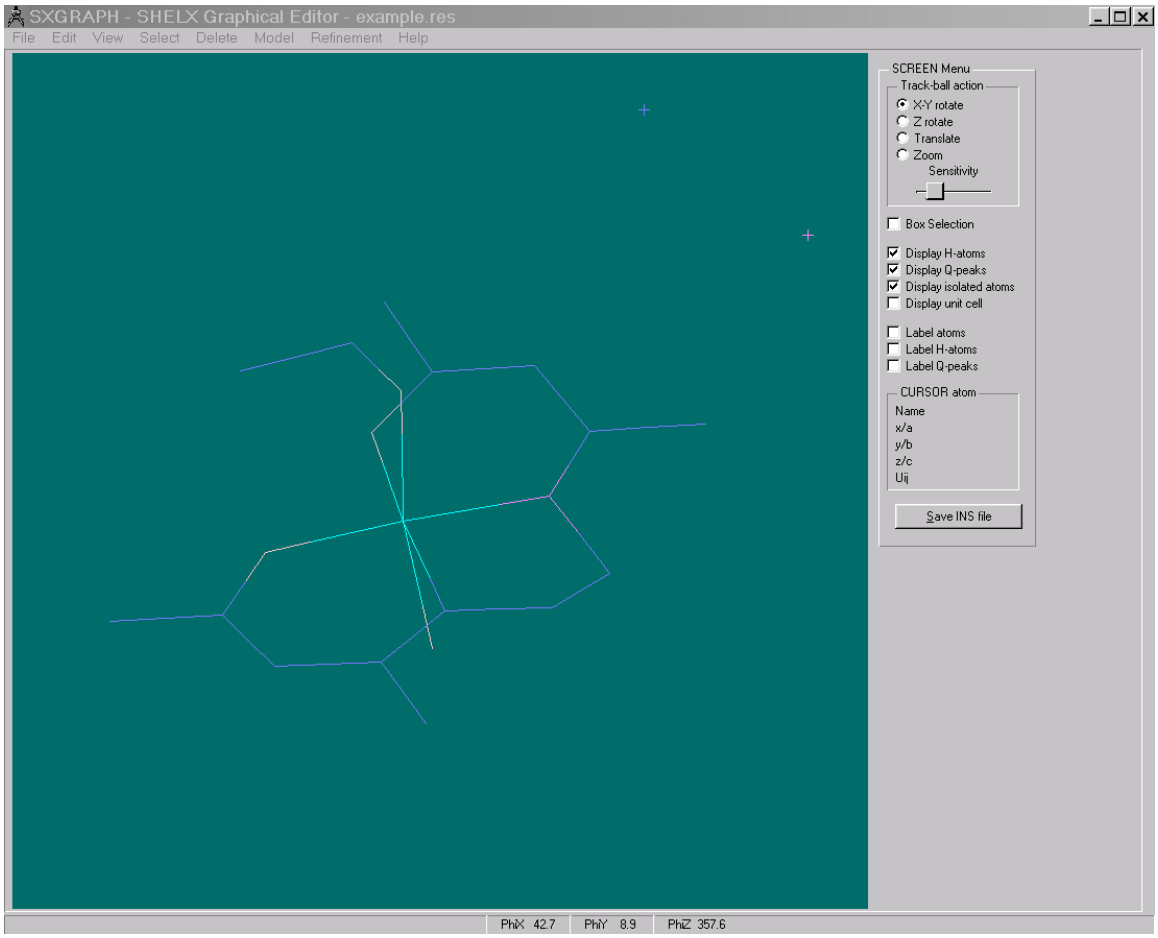
In this case the R2 is good 0.05 anything below 0.18 is solved. The RES file was written to the disk.

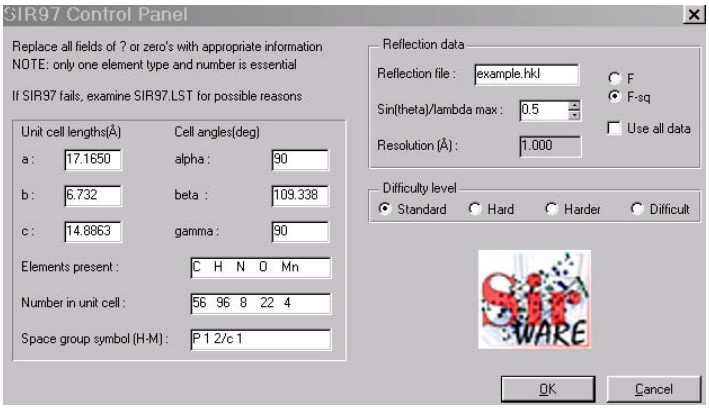


Now remove the = sign in the TITL and read it with XSHEL or XSEED.

TITL XYZN file = SHELXL INS file, from DIRDIF output for EXAMPL
CELL 0.71073 17.16500 6.73200 14.88600 90.0000 109.3390 90.0000
ZERR 4.000 0.00200 0.00090 0.00200 0.0000 0.0020 0.0000

If you want you can use WINGX to check the structure. Point to Model/SXGRAPH.

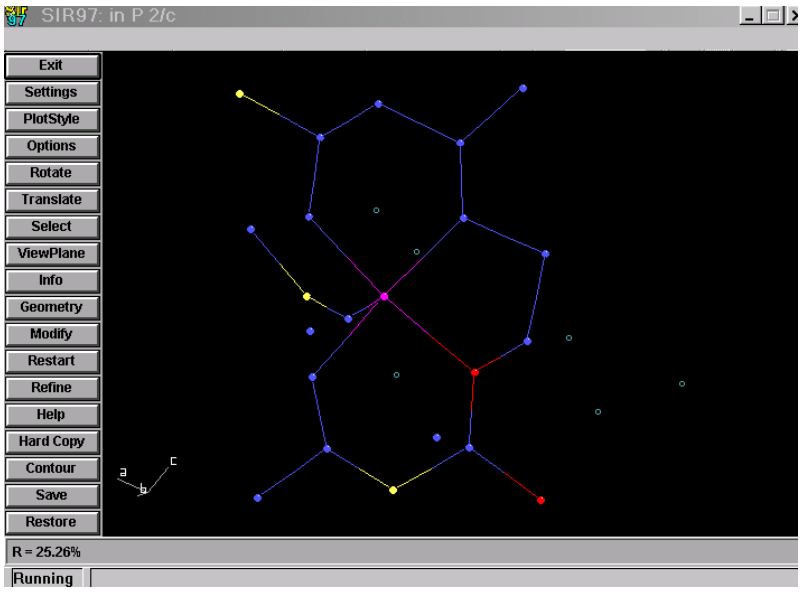




Now try SIR97. Point to Solve/Sir-97/GUI control. As with DIRDIF you can modify the cell contents and/or space group. The most useful control is the Difficulty Level.

Point to OK. Keep pointing to OKs until the solution begins.

SIR-97 found a solution but it mislabeled the atoms. When asked to go on point to no. Exit the program

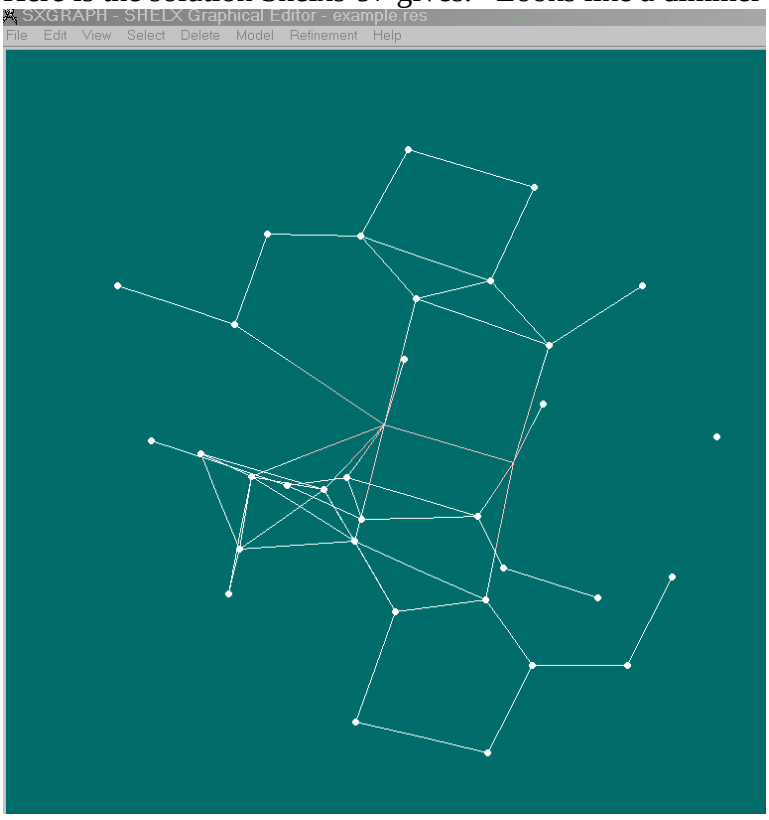


You will need to use X-seed or xshel to relabel the atoms. But this is the solution.

For fun run SHELXS.

Point to Solve/SHELXS-97

Here is the solution Shelxs-97 gives. Looks like a dimmer but its not its a FALSE minima structure.



This happens in structure solution programs sometimes. It is good to try as many programs as you can to see if each program gives a similar solution.