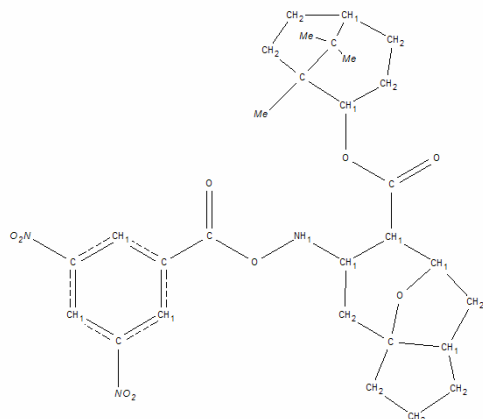


CRYSTALS workshops

Jo Peach's Crystal

Peach - Summary information

The data set for this crystal structure was collected for Dr Jo Peach in Oxford.



The cell is orthorhombic with $a=6.415$, $b=19.871$, $c=21.298$. The data collection used Copper radiation. Once again the space group is $P 2_1 2_1 2_1$

Using the GUIDE import the SHELX *peach.ins* file. Remember that the space group is $P 2_1 2_1 2_1$.

Using the GUIDE import the SHELX reflection file, *peach.hkl*.

Solve the structure in Sir 92 and read the results back into CRYSTALS.

Correct any wrongly typed hetero atoms by reference to the diagram above. (usually just the NO_2 groups)

Proceed with the refinement. (Switch to "Ellipse" view to check the results are reasonable).

Add Hydrogen atoms to the structure. Does the auto-refinement seem to have worked?

Continue the refinement - look at the thermal ellipses - they indicate the quality of the structure.

Continue the refinement. Check extinction.

Continue the refinement. Optimise the weights.

Finish the refinement. Validate your results and produce a CIF ready for publication.

To close CRYSTALS choose **Exit Crystals** from the **File** menu.

Alternatively, to get back to the workshop starting point, choose **Demo** from the **Help** menu.