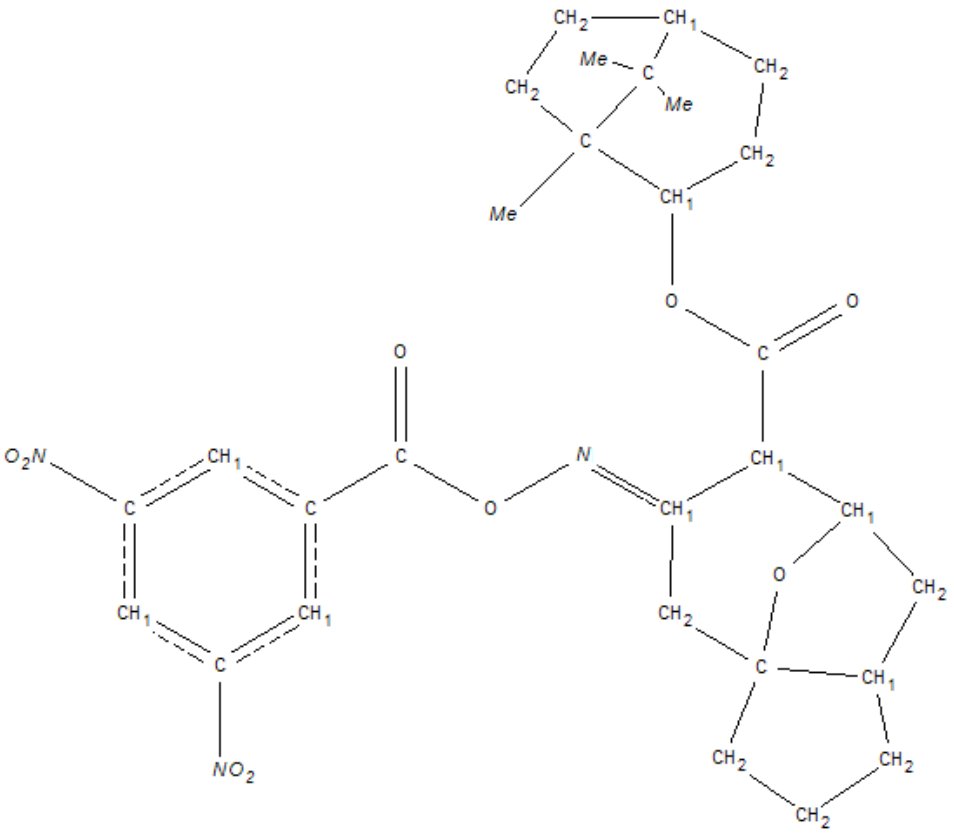
CRYSTALS workshops

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 21 21 21.

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.