CRYSTALS workshops

Twinning

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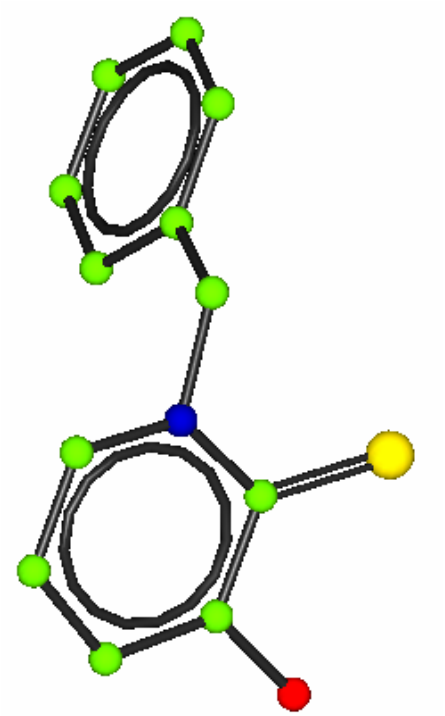
AS19A2: Non-merohedral Twin

Summary information

This crystal was synthesised by Andrew Smith and the data was collected by Simon Parsons in Edinburgh.



The cell is monoclinic **P 21/n**

Instructions

From the workshop dialog, choose AS19A2 Twin.

Using the GUIDE import the SHELX *as19a2.ins* file.
Remember that the space group is P 21/n.

Using the GUIDE import the SHELX reflection file, *as19a2.hkl.*

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

Sir92 will place the N incorrectly. Use the dialog to correct the atom types.

The structure won't refine very well (it will stick at R>14%)

Use ROTAX to find the twin law (hint: it's the one with the lowest figure-of-merit). And then complete the refinement.

The R factor will fall to about 11%. Use the toolbar item Analyse to see the Fo-Fc plot. There is a very strong reflection not lying on the plot. You might decide to omit it (by right-clicking on it)