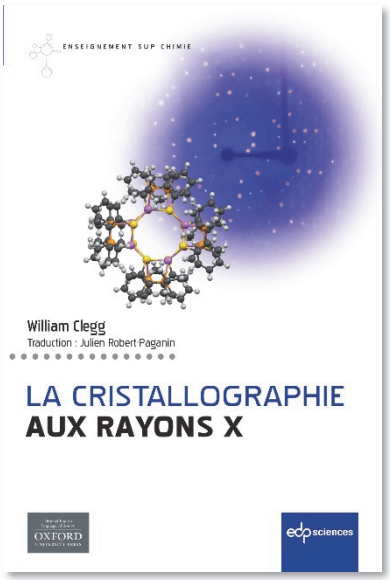

Clegg_files.zip

The following files are provided here for use by readers and instructors.

1D-Fourier.xls: a Microsoft Excel spreadsheet providing 1D Fourier synthesis calculations as described in Chapter 2, section 2.7, page 51. In order to use the buttons for selection of various Fourier coefficients and sets of phases (signs), it is necessary to enable macros.

A folder of files for each of 9 example structures described in the book:

VACYII - density/symmetry calculation example 1
YUXXIY - density/symmetry calculation example 2
ICSD4067 - density/symmetry calculation example 3
TEQSOX - example used to illustrate structure completion
VOXTOR - case study 1
FAJJOP - case study 2
XAYCAB - case study 3
XIBVUB - case study 4
HOQQOV - case study 5

The folder names are the CSD REFCODES for the structure (except ICSD4067, which is not in the CSD, but is entry number 4067 of the ICSD).

For each structure, the following files are provided, and can be used to illustrate structure solution, refinement, and manipulation:

name.cif - a complete CIF with embedded diffraction data (hkl) and refined structure model (res)
name.docx - a Microsoft Word document containing formatted tables of the structural results from the final refinement
name.hkl - the measured diffraction data (corrected for absorption etc.) consisting of indices, intensity and sigma(I) for each reflection
name.lst - detailed commentary output from the final refinement using SHELXL-2014
name.res - the final refined structural model in SHELXL format
name.xyz - orthogonal coordinates for the atoms in the structure, for use with various graphics and modelling programs
name_x.cif - the CIF with hkl and res components removed
Some of these files (cif, res, xyz) can be read by popular graphics and geometry programs, both commercial and free

Note: for ICSD4067 the original data are no longer available; the hkl file here contains calculated intensities (from the model);

it can be used for illustration purposes, but not for sensible refinement, as it matches the refined structure exactly; the CIF is taken from the ICSD.