Poster

Crystal Structure Analysis in School

E. Irmer

University of Göttingen, XLAB – Göttingen Experimental Laboratory for Young People,

Justus von Liebig-Weg 8, D 37077 Göttingen/Germany

erhard.irmer@chemie.uni-goettingen.de

The measurement of diffraction data on single crystals requires professional expertise and highly specialised equipment that may not be available at school. But solving and refining of structures is now also possible for students [1, 2] thanks to simplified graphical user interfaces of the structure determination programs [3, 4]. In courses at the student laboratory and in teacher training courses, we try to provide the lowest possible barrier to X-ray structure analysis, where after training teachers can work alone with their students, and we place particular emphasis on students working as independently as possible.

Ideally, the structure determination is integrated into a practical lab course, for example on the synthesis of aspirin or the isolation of citric acid or caffeine. After a didactically reduced introduction to the theory, the students visit the university's X-ray structure analysis department, where they are shown how to prepare samples and measure them on the diffractometer. The students then receive a step-by-step tutorial on how to determine a simple organic structure. We focus on structure solution and refinement, starting from an ins-file with the cell dimensions and symmetry data and an hkl-file with the structure factors. We deliberately do not use the current version SHELXT [5] for structure solution, but the charge-flipping method in OLEX2 [3] or the direct methods of SHELXS [6] in ShelXle [4], because here it is necessary to assign the correct atom types (based on chemical criteria). During the step-by-step optimisation of the structural model with the measurement data (refinement), the students apply basic structural chemistry concepts, such as bonding states on atoms or typical geometries of certain types of atoms or functional groups. The comparison with the experimentally determined electron density always provides an opportunity to confirm or correct their own considerations. The final result is a structural model in the form of a 3D molecular model (Fig. 1) or a short video of the rotating molecule. The students then receive a library of data sets of everyday substances which they can work on independently.

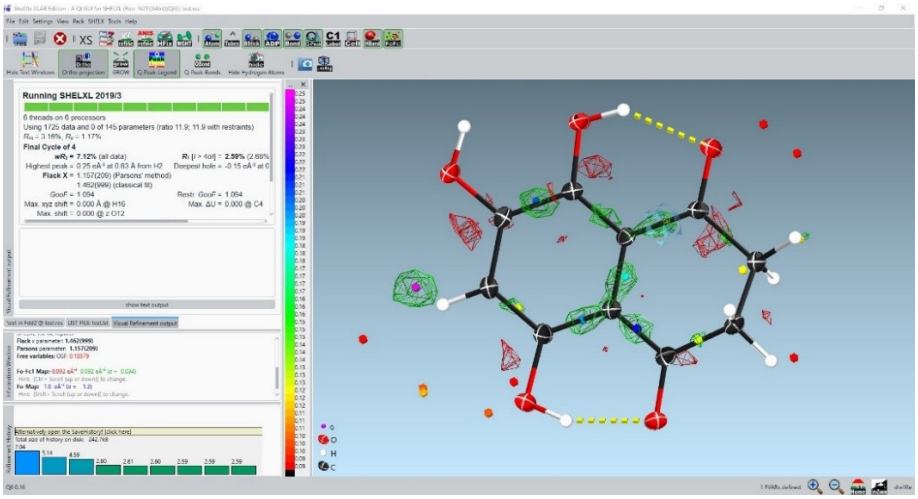

Figure 1. Screenshot of the final result of the structure determination of the tutorial structure with the XLAB Edition of ShelXle

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