THREE YEARS AFTER: INTERVIEW WITH SYLVAIN BERNÈS, MEXICO

Jens Richter, STOE, interviewing Sylvain Bernès, Instituto de Física Luis Rivera Terrazas, BUAP, Puebla, Mexico

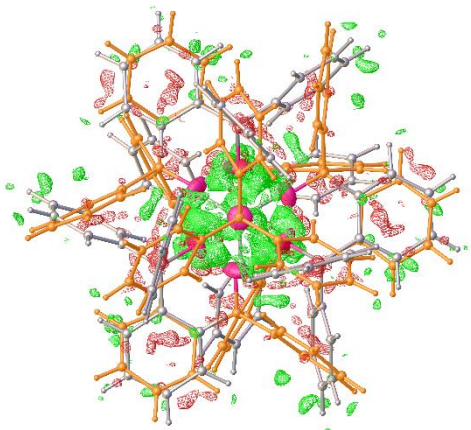

Figure 1: The crystal structure of triphenylmethanol, a small organic molecule, is severely disordered. The figure shows eight molecules, with a difference map locating the eight hydroxy H atoms (green wire), which are involved in a complex set of 24 hydrogen bonds. Diffraction data were collected at -120 °C on the STADIVARI diffractometer in operation at Puebla, Mexico (Doi: 10.1107/S2053229619010714)

JR: The installation of your STADIVARI single crystal diffractometer took place in early 2017. It was the first STOE single-crystal facility accessible in Mexico. Following the installation, how are your experiences up to now?

SB: As we near three years of work, the impression we get is that the outcome is quite satisfactory: the full system revealed to be exceptionally reliable, accumulating so far 20,000 hours of diffraction, which calculates to an impressive average of 20 hours for every day since installation. Data collection was not even interrupted by a strong earthquake shaking the building, in September 2017. Over three years, only a couple of minor issues affected the goniometer, which were solved through remote assistance by the STOE staff, within a matter of days. Both the Axo Ag-Kα X-ray microfocus- source and the Dectris Pilatus detector provided continuous, trouble-free service.

JR: We see an increasing demand for harder wavelengths. Are you satisfied with the results of your Ag source?

SB: Indeed, the Ag-Kα radiation has proven to be a universal tool for chemical crystallography. The only drawback of using such a short wavelength is that about 1-2% of the samples are unstable in the beam, however, this can be addressed by just collecting data at low temperature. Many different crystals were studied, ranging from small to large unit cells, including organic, metal-organic and inorganic materials. For example, the structure of ammonium metavanadate, with a cell volume of 337 Å3, was refined at 0.61 Å resolution (R_{int} = 2.7%, R_1 = 1.4%). At the opposite end of the crystal spectrum, a steroidal compound crystallizing in space group C2 with Z' = 6 had a cell volume approaching 20,000 Å^3, the largest cell parameter being close to 50 Å. Very small crystals (all dimensions below 50 µm) of lanthanide-containing samples were collected without particular difficulties. Most interesting recent results include the characterization of a large cluster based on a [Dy_6Mn_8] core, the discovery of a polymorphic form for a proteinogenic aminoacid, and the elucidation of an unexpected reversible order-disorder phase transition at low temperature for a cycloalkane. Tackling "difficult" problems is also on the agenda, like crystal structure determinations for compounds that are liquids at room temperature, or refinements of strongly disordered systems (see Figure 1).

JR: Given the high utilization, are there multiple users operating the STADIVARI?

SB: It should be emphasized that the STADIVARI in operation at Puebla is part of a shared platform: some researchers and students with no expertise in crystallography just need to address a specific problem, while others, in particular PhD students with a project relying on frequent X-ray determinations, prefer to become independent. After a period of training, they enjoy accessing the laboratory at (almost) any moment, with the hope of making rapid progress on their projects. The remaining 20 % users originate from outside Puebla, including some abroad collaborators, for example colleagues working in Venezuela or Senegal.

JR: So, what are your plans for the future of your instrumentation?

SB: If the circumstances allow, we plan to move soon towards crystallography at non-ambient conditions, that is diffraction experiments at temperatures in the range 100 - 800 °C, and high-pressure single crystal diffraction using a diamond anvil cell.

JR: Thank you for your insights. We are excited to continue to support you going forward.