

STOE NEWS | December 2019

SEASON'S GREETINGS

SAVE THE DATE:

STOE USER MEETING 2020

Darmstadt, September
3rd & 4th, 2020

Dear STOE user,

be it Christmas, Chanukah, Silvester, Nikolaus, Kwanzaa, Las Posadas, Eid-al-Adha, Diwali, Chinese New Year... it's that time of year when we remember those that are important to us.

Being clearly the highlight in the STOE calendar, we were honored to welcome the participants of the STOE User Meeting 2019 which took place in early September.

We are looking forward to stay in touch with you, at one of next year's conferences or at the **STOE USER MEETING 2020**.

As in recent years, our User Meeting will be a platform for upcoming news and exchange of experiences among STOE users.

It will cover Powder- and Single-Crystal diffraction. In addition to STOE talks about the newest developments, we look forward to welcome guest speakers, which will share insights on their research with us.

The User Meeting 2020 will take place at our company in Darmstadt, Germany (close to Frankfurt Airport). We will start on Thursday, September 3rd, at 10 am and finish on Friday around 1 pm.

Participation fee is just 50 €, including food, drinks & the BBQ on Thursday. Please feel free to already pre-register at info@stoe.com

We hope that 2019 has been a good year for you as well and wish you all the best for the year to come.

Your STOE Team



THREE YEARS AFTER: INTERVIEW WITH SYLVAIN BERNÈS, MEXICO



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

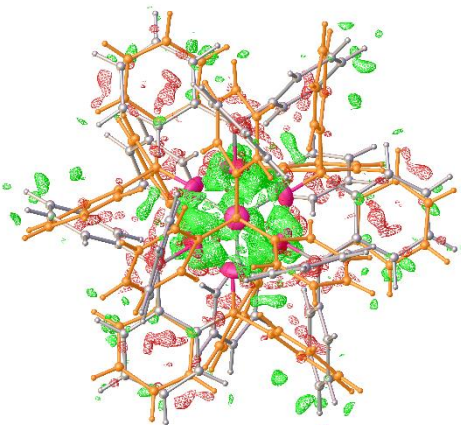


Figure 1: The crystal structure of triphenylmethanol, a small organic molecule, is severely disordered. The figure shows eight molecules, with a difference map locating the eight hydroxy H atoms (green wire), which are involved in a complex set of 24 hydrogen bonds. Diffraction data were collected at $-120\text{ }^{\circ}\text{C}$ 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-K α 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-K α 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 $337\text{ }\text{\AA}^3$, was refined at $0.61\text{ }\text{\AA}$ resolution ($R_{\text{int}} = 2.7\%$, $R_1 = 1.4\%$). At the opposite end of the crystal spectrum, a steroidal compound crystallizing in space group C2 with $Z' = 6$ had a cell volume approaching $20,000\text{ }\text{\AA}^3$, the largest cell parameter being close to $50\text{ }\text{\AA}$. Very small crystals

(all dimensions below $50\text{ }\mu\text{m}$) of lanthanide-containing samples were collected without particular difficulties. Most interesting recent results include the characterization of a large cluster based on a $[\text{Dy}_6\text{Mn}_8]$ core, the discovery of a polymorphic form for a proteinogenic amino acid, 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 $100 - 800\text{ }^{\circ}\text{C}$, 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.

NEW TRANSMISSION CAPSULES FOR EASY STORAGE OF SAMPLES

Cover



+

Socket



=

Closed Capsule



Sample Holder ready for Measurement



TPT Capsule

The TPT capsule complements the traditional sandwich preparation. It can be used for dry or moist powders or pastes and is compatible with the STOE transmission sample holder inserts.

This single-use capsule allows an easy storage of the measured sample for traceability or further analysis, e.g. in pharmaceutical research.

It has been developed in cooperation with F. Hoffmann-La Roche AG by Gimelli Engineering AG and been used for many years.

We are now pleased to bring this development to you, and we included it into the STOE product range.

Usage

1. Preparation:
 - a) Place the socket (underside) on a set mandrel (support the foil)
 - b) Place sample with spatula in mask
 - c) Smooth out sample with stamp
 - d) Snap lid onto pan => TPT capsule is complete
2. Insert TPT capsule in the STOE sample holder insert (special screws for clamping mechanism)
3. Perform measurement.
4. Take the TPT capsule out of the sample holder (just push it out). Capsule can now be discarded according to the appropriate guidelines or retained for further analysis or backup.

Please contact us for further details, samples and your offer.

Variants

The TPT capsule is available in several variants to suit your needs:

Cellulose Acetate Film:

For applications with samples up to class 3B, in which no solvent is present.

Kapton:

For applications with samples up to class 4, in which solvents may also be present. For class 4 specimens, the openings in the snappers must also be sealed by using e.g. nail polish.

Aperture Sizes:

Depending on the substance quantity / hazard class, the aperture can be selected with a diameter of 3 mm (sample quantity approx. 2.8 µl) or 8 mm (sample quantity approx. 20.1 µl).

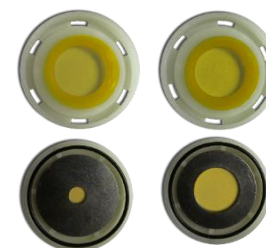
Cellulose Acetate



3 mm

8 mm

Kapton



3 mm

8 mm



MEET STOE

UPCOMING EVENTS

DECEMBER 17-20, 2019
AsCA, SINGAPORE

JANUARY 30-31, 2020
DESY Photon Science Users' Meeting
HAMBURG, GERMANY

FEBRUARY 23-27, 2020
DGK Joint Polish-German Crystallographic
Meeting 2020, WROCLAW, POLAND

MARCH 18-20, 2020
HÄKO, BAYREUTH, GERMANY

MARCH 30-APRIL 1, 2020
CHEMIEDOZENTENTAGUNG
DRESDEN, GERMANY

APRIL 06-09, 2020
BCA, LEEDS, UK

MAY 26-30, 2020
EPDIC17, SIBENIK, CROATIA

JUNE 17-19, 2020
CEMWOQ, TROIS-RIVIÈRES, CANADA

AUGUST 2-7, 2020
ACA Annual Meeting, SAN DIEGO, USA

AUGUST 3-7, 2020
DENVER X-RAY CONFERENCE
ROCKVILLE, MD, USA

AUGUST 22-29, 2020
IUCR, PRAGUE, CZECH REPUBLIC

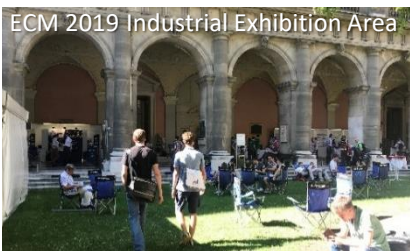
SEPTEMBER 3-4, 2020
STOE USER MEETING
DARMSTADT, GERMANY

SEPTEMBER 9, 2020
SGK, SWITZERLAND

SEPTEMBER 29-OCTOBER 2, 2020
WÖHLER- & GDCH FESTKÖRPERTAGUNG
COLOGNE, GERMANY

OCTOBER 4-6, 2020
2ND JOINT MEETING OF THE YOUNG
CRYSTALLOGRAPHERS (DGK) AND THE
YOUNG CRYSTAL GROWERS (DGKK)
FREIBERG, GERMANY

ECM 2019 Industrial Exhibition Area



REINFORCING OUR SALES TEAM

TOM FASKE

We are pleased to welcome Tom as part of our STOE sales team. He joins us from the Technical University of Darmstadt, where he worked on his PhD in Materials Science in the group of Prof. Wolfgang Donner. Previously, he studied Mineralogy and Materials Science at Leipzig University. His doctoral thesis covers the development of a powder diffractometer with magnet for the investigation of temperature and magnetic field induced phase transitions. He has intensive hands-on



TOM FASKE

experience in Powder and Single Crystal XRD. Feel free to contact Tom at +49 6151-9887-14 or faske@stoe.com.

NEW STADI P CONTROLLER

With the expectation of important electronical components being announced to be discontinued and computer motherboards with PCI slots becoming decreasingly available, we decided to usher our STADI P diffractometers into a new era and present a new SPC-driven interface for our powder goniometers.

The new controller is connected via ethernet to the PC and fully backward compatible for all STADI P / MP goniometers which were able to be operated by the previous interface type.

Feel free to contact us for any further question!

STOE CORP., NORTH AMERICA

LUZIA GERMANN

Luzia Germann has joined STOE North America as scientific advisor in August 2019. She has extensive experience with STOE diffractometers from her PhD at the Max Planck Institute for Solid State Research in Stuttgart, where she was investigating solid state reactions *in situ* and determining the crystal structure of polycrystalline materials. Currently, she is a Postdoctoral Fellow at the McGill University (Montreal). Luzia will represent STOE at North American



LUZIA GERMANN

Conferences and be a point of contact. Feel free to contact Luzia at germann@stoe.com.

YOUR PARTNER IN X-RAY DIFFRACTION | WWW.STOE.COM

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