

IUCr Commission on High Pressure Online Meeting

9 September 2021 (3:00 pm CEST, concluded at 4:10 pm CEST)

Present: Members: Kamil Dziubek (Chair), Boris Zakharov (Secretary), Natalia Dubrovinskaia, Nandini Garg, Kazuki Komatsu, Amy Lazicki, Stephen Moggach, Guoyin Shen. Consultants: Ross Angel, Agnès Dewaele, Giovanni Hearne, Stefan Klotz, Haozhe Liu, Malcolm McMahon, Timothy Strobel.

1. Welcome and apologies for absence

Kamil Dziubek welcomed everyone to the meeting. Apologies received from Narcizo Souza-Neto and Andrzej Katrusiak due to other commitments were announced. The Chair reminded that the new term is shortened to two years as a result of the postponement of the 25th IUCr Congress and General Assembly, and that the term will finish at the 26th IUCr Congress in Melbourne in August 2023.

2. Voting system in the 2021-2023 biennium

Kamil Dziubek suggested the following voting rules in the new biennium:

- Voting can be held in a virtual meeting or by email. In case of email voting, ballots must be emailed either to the internal CHP mailing list or directly to the Chair of the CHP.
- Time limits for email voting is established as one week from the voting start date.
- The voting is valid if more than a half of the CHP Members is present at the virtual meeting or, in case of email voting, cast email ballots before the poll closing time. Both Members and Consultants are eligible to vote and all votes have equal power. Decisions are taken by majority vote.

Ross Angel raised the question if the Consultants should vote or should they just offer the consultation and leave the vote to the Commission Members. In particular, he asked what the IUCr rules are in this regard. Haozhe Liu pointed out that the CHP has maintained the equal voting power of the Members and the Consultants since 2008. Stefan Klotz noted that the pivotal question is what is the role of the Consultants and what rights do they have in light of the IUCr regulations. Kamil Dziubek was thereafter tasked to contact the IUCr Executive Committee in order to clarify this issue.

3. Discussion on the venue of the 2022 IUCr High Pressure Workshop

After previous IUCr High Pressure Workshops: 2021 in Novosibirsk (Asia) and 2019 in Vienna (Europe), the next event is planned to be held in the Americas. Kamil Dziubek presented the suggested venues of the next HP Workshop:

- NSLS-II (Brookhaven National Laboratory). Stony Brook University faculties could be potential local organizers and the local HP groups are quite strong.
- LLNL would be the first dynamic compression lab hosting. Cons:
(1) background checks required to get onsite are quite heavy and
(2) lodging and conference facilities are scarce and expensive.
- Alternative locations outside of the US. There are HP teams in Argentina, but the number of researchers is small and they lack manpower, besides the economic situation in the country may be a problem. Mexico is an option with a strong crystallographic community, but no HP-dedicated groups.

Amy Lazicki commented on possibility of holding the workshop at Livermore, confirming that it would be probably too complicated. However, she mentioned several other institutions in the area that have high pressure groups, including Berkeley, Stanford and LCLS. Timothy Strobel asked when in 2022 is the target date and what is the expected number of participants. Kamil Dziubek responded that the Workshop is held usually in the second half of September to avoid overlaps with other international events and that it usually gathered 50-80 participants before the outbreak of the Covid-19 pandemic. Haozhe Liu emphasized that the Stony Brook group could be considered a potential host. Stefan Klotz suggested that the Workshop can be held in a place outside the LLNL lab, but still close to the facility and organized by the Livermore team.

The CHP Chair and the American Members and Consultants were tasked to collect the suggestions of the local organizers, approach the potential local organizing committees and present the bids to the CHP before the end of October.

4. Status of high pressure research in Africa and perspectives for the future High Pressure Workshop in the African continent

Giovanni Hearne commented on the possibility of organizing the Workshop in Africa after the Melbourne Congress in 2023. Currently there is not many people who would be potentially ready to organize it, as there are just a few groups in Africa working in the field of high pressure crystallography. Ross Angel suggested to organize a tutorial-oriented workshop in order to increase interest in high pressure crystallography and attract participants from the continent. More detailed feedback will be provided by Giovanni

Hearne at the end of the year after his discussion with the colleagues at Stellenbosch University, Len Barbour and Delia Haynes.

5. Identifying CHP representation to the International Program Committee of the 2023 IUCr Congress in Melbourne

Kamil Dziubek was nominated to act as the representative to IPC. Approved unanimously.

6. Progress on the high pressure data management requirements and metadata standards

Kamil Dziubek presented the current situation in this field:

- “Data deposition and validation: state of the art” round table discussion has been organized at the 2021 IUCr High Pressure Workshop in Novosibirsk, February 2021.
- Working group dealing with “standardizing” high pressure data in chemical crystallography was established (R. J. Angel and K. F. Dziubek — CHP; S. Coles, J. Helliwell, A. Sarjeant — CommDat; J. Hester — COMCIFS; D. Allan — DLS; M. Meyer — Rigaku).
- K. F. Dziubek talk "Using raw data to improve the interpretation of high-pressure diffraction experiments" was presented at the “When should small molecule crystallographers publish raw diffraction data?” satellite workshop to the IUCr Congress in Prague, August 2021.
- Article to the Journal of Applied Crystallography on the importance of raw data in high pressure crystallography is to be prepared.

Ross Angel mentioned that the draft version of proposal regarding the HP-related data and metadata descriptors is almost ready. One of the pivotal issues that remains to be resolved by the working group is describing the orientation of a DAC on a diffractometer.

7. Collaboration with other IUCr Commissions and Committees

Kamil Dziubek commented on ongoing collaborations with other IUCr Commissions and Committees including:

- CommDat and Commission on Biological Macromolecules — Standardizing high-pressure descriptors in the macromolecular CIF dictionary and relevant annotations in the PDB.
- Commission on Diffraction Microstructure Imaging (future initiatives on multigrain crystallography in high pressure research in liaison with the CDMI member Sébastien Merkel).

8. Development of CHP website and e-resources (past events and CHP archive, software list, social media)

Boris Zakharov presented current situation on the e-resources:

- A Google drive was set up to store, share and edit files related to the CHP activity.
- A preliminary list of software related to high pressure research was created with the intention of being included at the CHP website.
- The opportunity of creation Twitter account was discussed. Suggestions on possible ways of arranging the CHP Twitter account will be proposed to the CHP in the nearest future.
- The need to collect information (documents, photos etc.) regarding previous Commission activity and the CHP Workshops was expressed.

Kamil Dziubek commented on the possible ways of arranging the software list.

9. CHP logo and the website appearance

Kamil Dziubek presented expectations concerning the appearance of the CHP website. The Commission members were asked to contribute with their ideas of the logo and the “banner” pictures for the CHP home page. Haozhe Liu suggested to organize the “Logo Competition” with the results announced at the next CHP Workshop.

10. Liaison with the IUCr Commission on Crystallographic Nomenclature concerning the production of the Online Dictionary of Crystallography

Kamil Dziubek pointed out the possibility to contribute to the Online Dictionary of Crystallography and encouraged Commission Members, Consultants and their colleagues to send him their suggestions for the Online Dictionary entries.