



## 25<sup>th</sup> ASSEMBLY AND CONGRESS OF THE INTERNATIONAL UNION OF CRYSTALLOGRAPHY (IUCr). HYBRID CONGRESS IN THE TIME OF PANDEMIC, AUGUST 2021

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The IUCr organizes its congresses in conjunction with assemblies once every three years. In the meantime, there are conferences of its regional associates, ACA, AsCA, LACA, and ECA. In the Czech Republic the adhering body is the Regional Committee of Czech and Slovak Crystallographers included now in the Crystallographic association (Krystalografická společnost registered in the Czech Republic - international name Czech and Slovak Crystallographic Association (CSCA). Since modern crystallography is very interdisciplinary and no single institution (university, institute) can cover its whole scope, it was just CSCA that took the effort to organize the congress in Prague, and after several attempts we won the bid in 2014 during the congress in Montreal. This was a bid for the organization of the 25th anniversary congress in 2020.

### Congress Peripetia

We were celebrating our victory in 2014 having no idea what we really had. This appeared clear only in 2020. The preparation started well, immediately after the 24th congress in Hyderabad in 2017. In 2017-18, the International Program Committee (IPC) was formed with 35 members, mostly representing IUCr commissions. The IPC meeting was held from 14 to 16 May 2019 in Prague. This meeting related to some kind of workshop called 'Current Trends and Future of Crystallography', where representatives of all commissions presented current problems, trends, and highlights of their fields. During the subsequent two-day meeting that was very effective, the whole programme scheme was agreed on consisting of 3 plenary lectures, 35 keynote lectures, more than 100 standard scientific microsymposia, and several special sessions. In the following months, the basic programme was finalized. For all the sessions, two co-chairs were asked to invite two speakers to their sessions for 30 minutes each assuming that four more speakers will be selected from contributed abstracts. In February 2020 this basic programme was more or less complete. However, this was also the time of the beginning of the pandemic. In the middle of March, an extraordinary meeting of IUCr EC (the first its online meeting) decided to postpone the congress to summer 2021 since it was clear that the organization of classical congress in August 2020 is not very realistic. In the full calendar of the Prague Congress Center one week after August 13 was possible. The prepared programme was fixed, and we could only watch the situation with the pandemic in the world. Unfortunately, this was not good at all. In January 2021, after a short discussion, we concluded that there was no room for further postponing of the congress for several reasons. The possibility of a classical congress remained unrealistic, and the simplest way was to change it to a pure online form. However, we were not bidding for such a congress, and moreover, a significant number of people really looked for-

ward to the congress in Prague. The only possibility was to leave the hybrid form open, i.e. the combination of real and virtual participation. At the beginning of February, we had a chance to see a demonstration of presentation system gCon developed by Prague group T.R.I. that is basically independent on the locations of chairpersons and speakers. We were convinced that hybrid congress should be possible depending on the overall situation, and final decision on the form can be made at relatively short time before the congress. This, of course, would require the maximum flexibility of all involved. It was clear that before about June we would not be able to make this decision simply because earlier anyone would know anything. Then we started communication with all co-chairs and invited speakers, that is, with nearly 500 persons asking them to confirm their participation in any form. Any participation cancelled less than 10% of them. We open the registration for virtual participation with a possibility of upgrading to real one, and we were watching Covid numbers. In the second half of May the situation looked quite optimistic and, moreover, conditions for organization of events in summer were published. According to polls among preregistered people, it seemed that we could expect 700-800 people in Prague. During June, the program of sessions was optimized and completed. Real registration was open. However, Coronavirus did not seem to give up, transformed to the so-called delta form, and destroyed our hopes to the full extent. However, there was no way back. The last weeks before the congress were very hectic. Basically, what is usually prepared 3-4 months before the congress we had to do in about 3-4 weeks. The exhibitors were asking about the number of real participants on site. This was something we also wanted to know. The colors of the counts on the Covid maps changed often. The virus seemed to be able to distinguish citizenship since different conditions were defined for EU citizens living in UK than UK citizens. The latter were simply not allowed to come to Prague regardless of vaccination. However, even worse appeared to be the bans on travel put on travel by institutions. I think this was idealistic in the situation where people could travel easier and visit a risky environment in their cities. The uncertainty was enormous.

### Hybrid Congress

After all, the congress was realized basically as planned in the last months as hybrid and in very nice atmosphere also for online participants as it follows from e-mails received after the congress. A very good quality programme could be prepared. In this aspect, the possibility of online presentation is very positive because for invited speakers this can be quite simple and much cheaper. Only a few approached speakers refused. We have more than 2500 preregistered people, and the total number of final registrations reached

nearly 1700. Less than one-third were able to come to Prague, quite often for a shorter time; they watched the rest online. With respect to restrictions, we had most real participants from Poland and Germany, but others arrived from France, Spain, Sweden, Denmark, Finland, Croatia, Italy, USA and other countries.

### Programme

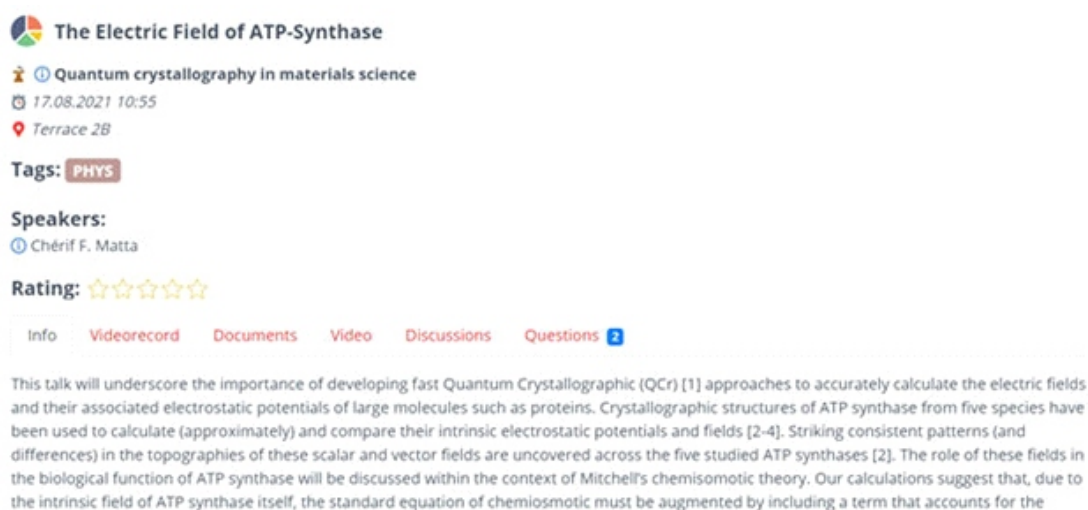
The programme consisted of three plenary lectures, five lectures connected with prizes, 35 keynote lectures, 103 standard sessions, 7 special sessions, Software Fayre – always 9 sessions in parallel, 55 poster sessions and several commercial presentations. In total, 624 lectures and over 550 posters in different forms were presented at the congress.

In this year, two sessions were devoted to the structural biology of coronaviruses and to new methods to combat the pandemic. In biocrystallography, the highest number of abstracts reached the session on the structural biology of enzymes and also on bioinformatics. New W.H. and W. Bragg Prize lectures were also related to biocrystallography – Structure-guided design of next-generation malaria vaccine (Jean-Philippe Julien, Kanada), Targeting COVID-19 viral enzymes in an evolving landscape of publishing and peer review (James Fraser, USA) – as well as one plenary lecture by David Eisenberg The Expanding Amyloid Family: Structure, stability, function, and pathogenesis related, for example, to Alzheimer's disease. The main Ewald prize and one plenary lecture were related to crystallographic data and databasis. The Ewald prize was awarded to Olga Kennard (UK) for the development of Cambridge structure database, and a plenary lecture by Helen Berman (USA) was devoted to protein database PDB. Several sessions and pre-congress school were devoted to electron crystallography (structural studies by electron diffraction). The school was mostly online, but the last day in hybrid form. There were nearly 200 registered participants. In this branch, the Gjonnes medals are awarded. The prize went to Sven Hovmöller (Sweden) and Ute Kolb (Germany). Another significant topic of the con-

gress was quantum crystallography. For both the above topics, relatively many experts were able to come to Prague. Among materials, the highest attention attracted materials for energy conversion and storage, often studied in situ (also plenary lecture by Clare Grey on In situ and ex situ studies of battery materials with magnetic resonance and diffraction methods), nanomaterials, and magnetic materials. The highest number of abstracts was in the session - Complex structure of minerals and inorganic compounds, and in the session of phase transitions in complex materials. Especially interest was also expressed for the session of disordered materials. Despite low advertising of the congress among chemical crystallographers, the highest number of registered people were just from this area, materials important for the pharmaceutical industry, metal-organic frameworks (MOFs), and catalysis. Two sessions were dedicated to application of crystallography in art and many sessions to individual techniques as neutron scattering, small-angle scattering, synchrotron radiation, XAFS etc.

### How the Hybrid Congress Was Working

All presentations were run from local servers in Prague (for details see also <https://www.tri.cz>) and speakers were asked to upload their presentations (pptx, pdf) in advance, which was not accepted by all and caused stressful situations to technical staff, in particular at the beginning of the congress. Files underwent technical control before approval for smooth presentation. If the speakers were online then they had full control of presentation by arrows and mouse motion was mapped and shown (pointer). Remote participants could write questions into tab „Questions“. These questions were visible to all, and co-chairs could select them for live discussion. The questions could be answered later by speakers in the 'Discussion.' As a new feature, the possibility of live entrance by additional participants was included by request "Raise hand". The co-chairs allowed entry and for remote participants, a quick test of their microphone and camera was included before they were connected.



The screenshot shows the gCon interface for a lecture titled "The Electric Field of ATP-Synthase". It includes a color-coded icon, the lecture title, a category "Quantum crystallography in materials science", a timestamp "17.08.2021 10:55", a location "Terrace 2B", a tag "PHYS", a speaker "Chérif F. Matta", and a rating of five stars. Below this is a navigation bar with tabs: Info, Videorecord, Documents, Video, Discussions, and Questions (with a blue indicator). The "Info" tab is active, displaying an abstract that discusses the importance of developing fast Quantum Crystallographic (QCr) approaches to accurately calculate the electric fields and their associated electrostatic potentials of large molecules such as proteins. The abstract mentions that crystallographic structures of ATP synthase from five species have been used to calculate (approximately) and compare their intrinsic electrostatic potentials and fields [2-4]. It also notes that striking consistent patterns (and differences) in the topographies of these scalar and vector fields are uncovered across the five studied ATP synthases [2]. The role of these fields in the biological function of ATP synthase will be discussed within the context of Mitchell's chemiosmotic theory. The abstract concludes by stating that their calculations suggest that, due to the intrinsic field of ATP synthase itself, the standard equation of chemiosmotic must be augmented by including a term that accounts for the

**Figure 1.** gCon page of one lecture – Info: abstract, Videorecord – recording of the lecture, Documents – documents for download, Video – video provided by the author for download, Discussions – active all the time, Questions – active only during the lecture and immediate discussion but visible all the time.



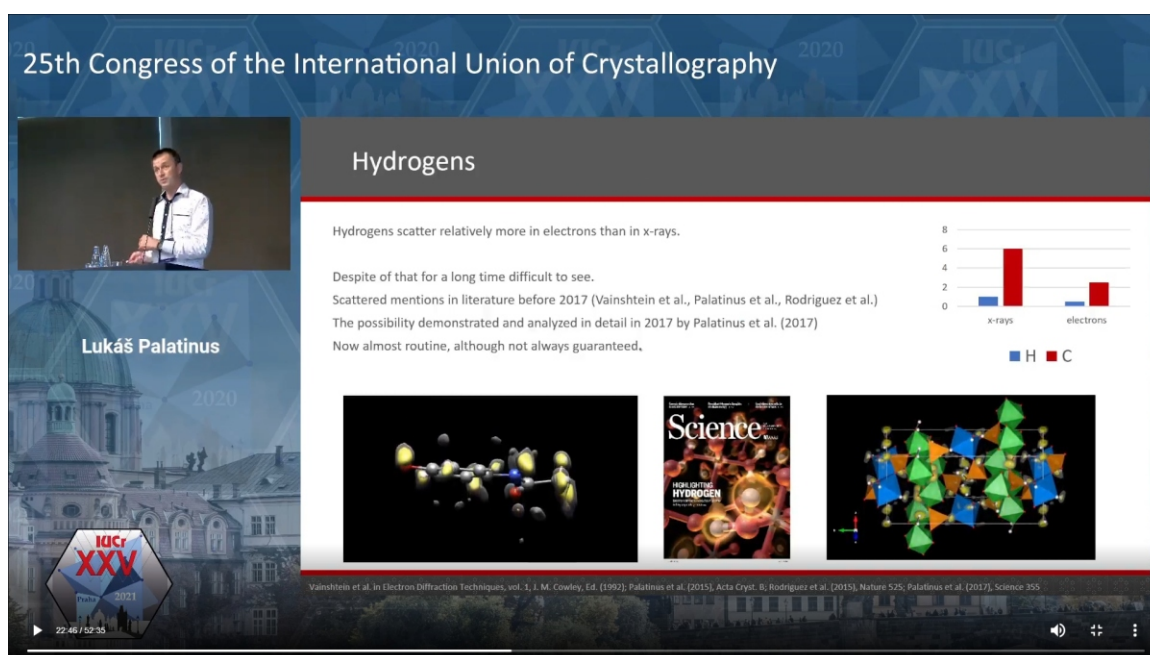
**Figure 2.** gConpage of a poster – the author uploaded more pages and in addition some documents. Virtual room was active only during corresponding virtual session.

Some speakers decided to upload the full lecture as an MP4 video. Especially in case of inconvenient time differences (such as west coast of the USA or Australia). Quite often, they were available live for discussion. The presentation files are not accessible by anyone, but each author could upload files without format restrictions to the tab 'Documents' and these files are available for download for registered participants. During congress, we met all possible combinations of locations of speakers, two cochairs and asking participants, and always everything worked well.

All poster files were available for viewing and download (unlike recordings). It was possible to upload not only posters, pdf but also pptx presentations or MP4 videos according to the needs of the authors. In time of poster sessions for each poster virtual room could be entered. The limit of one room was 25 visitors and the rooms were working for live meeting similarly to, e.g., Zoom with possibility of screen sharing. Of course, in hybrid mode it was

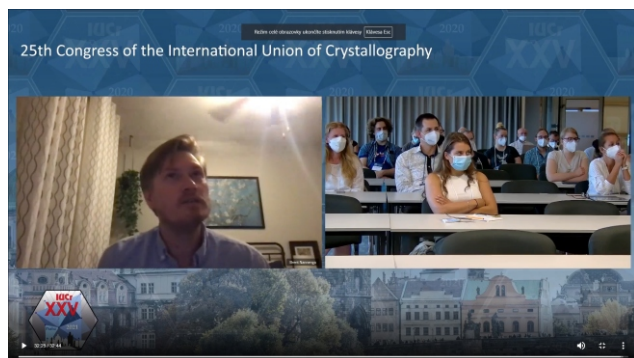
necessary to separate virtual rooms from real poster sessions. In addition to usual poster panels, electronic panels were available too allowing easy search and zooming of details.

All responses of local and remote participants show that the congress was successful in most aspects and was better than expected when a number of people were sceptical to the hybrid form. Perhaps, it can be taken as an example for hybrid congresses. Credits should be given to all those involved in the organization. For the good impression of online participants, probably the greatest credit goes to T.R.I., their system gCon and very professional approach. Namely, the way of streaming and design with views of lecturers, chair persons, asking people, hall that made the congress really live. Online participants also appreciated the streamed concerts. They were simply attracted directly to the action of the congress. Below, there are screens captured from recordings.



**Figure 3.** Typical screen of live lecture in the stream





**Figure 4.** Remote speaker local listeners.



**Figure 6.** Remote chair persons, speaker, local listeners.



**Figure 8.** Concert in stream, watched by about 100 online participants.

The relatively long absence of real events was reflected in positive acceptance by the onsite participants, the work of the staff of the Prague Congress Center and the catering company Zátíší. All were doing their best to ensure the success of the conference. Of course, organizers should be mentioned first: colleagues from the Faculty of Mathematics and Physics - Milan Dopita and other colleagues and students, people from Institute of Organic Chemistry and Biochemistry CAS (Pavlna Řezáčová, chair of local organizing committee), Faculty of Science, University of South Bohemia in České Budějovice (Ivana Kutá Smatanová, chair of international programme committee), from the Institute of Biotechnology (CAS) and very important group Auletris (headed by Martin Haloun) [www.auletris.com](http://www.auletris.com). We were very satisfied with the Conftool registration system (<https://www.conftool.net>) and also presentation system gCon by T.R.I.



**Figure 5.** Remote chair, speaker, local listeners



**Figure 7.** Remote speaker, two local co-chairs

In addition to scientific programme, the Social programme was organized – boat trips on the Vltava River, conference dinner with a Brand new band concert at the National House and a train trip to Pilsen brewery. For more information, see <https://www.iucr25.org>.

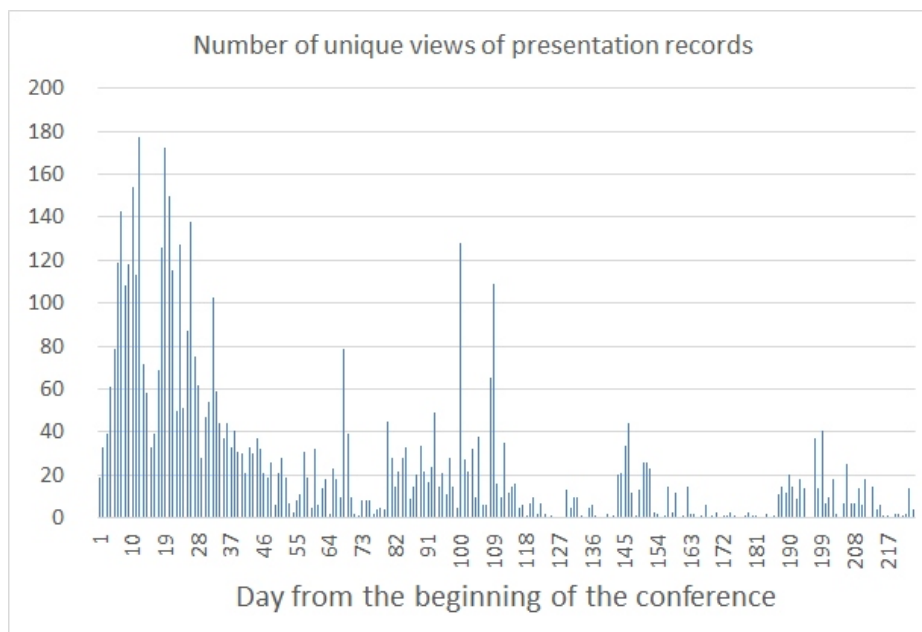
Different conference statistics are available at <https://iucr25.org/hybrid-conference-statistics/>

Photos and short video clips <https://www.xray.cz/iucr/photo/default.htm>.

Finally, the gcon website with all the conference materials was open till the end of March 2022 and during all the time people were watching the materials. About 300 of registered participants never connected to the gcon system but over different 700 people have been watching something since the end of the congress. Most of the days during these 7 months at least one person opened something on the gcon website. The histogram of unique views (i.e. by different persons) can be seen in Figure 9.

The most viewed keynote lectures were by Dyan Jayatilaka on quantum crystallography (277), Lukáš Palatinus on electron crystallography on molecular crystals (246) and Andrew Goodwin on functional materials (227). The five most popular sessions were: Automation in bio-crystallography: tools, perspectives and applications (210 unique views), Crystal structures of pharmaceutical and organic compounds from electron diffraction (208), Total scattering (199), Structural biology against coronavirus/covid-1 (192) and Machine learning in biological and structural sciences (191)

The most on-line visited poster sessions were Powder diffraction (average views – i.e. per poster – 181), Drug design (133), Crystal structure prediction (127), General interest (103) and Structural bioinformatics (94). The most popular posters had over 200 visits while the least number of visits was 12 that is still not that bad.



**Figure 9.** Number of unique views of presentation records

Such a kind of statistics has never been available and hopefully it will help also to organization of next congresses.



**Figure 10.** Last participants and organizers after closing ceremony (photo by Petr Pachl)