IUPAC - DIVISION III: Subcommittee on Structural and Mechanistic Chemistry

Virtual Meeting held during July and August 2020

MINUTES

- 1) **Welcome** from the Chair. Since we were unable to meet physically in Hiroshima during the week of 5-10 July 2020, due to Covid-19 restrictions and the postponement of ICPOC25, the idea of a virtual meeting by exchange of emails over a longer period was appreciated by members.
- 2) The minutes from the last SSMC meeting in Paris (6 July 2019) were approved.

3) **ICPOC25**

The same conference site (Grand Prince Hotel Hiroshima) has been booked for July 10-15th, 2022.

venue: https://www.princehotels.com/hiroshima/

conference: https://icpoc25.jp

Manabu Abe will rethink the list of invited, keynote, and plenary speakers in order to ensure that there are new topics and new faces, and that there is an appropriate gender balance; he will write to all the previously invited speakers soon with a carefully worded letter. This suggestion met with general approval, and Manabu was thanked for all his hard work. New topics to be considered might include artificial intelligence and synthetic biology as related to POC.

Action: Manabu Abe

4) **ICPOC26**, 2024, Beijing

Jin-Pei Cheng intends to keep the same venue (Friendship Hotel) for the re-scheduled ICPOC26 in 2024, but he will not confirm this yet; he will also identify an alternative venue, in case one should be needed. Other arrangements will be managed as previously reported. Any suggestions regarding the conference are most welcome. Jin-Pei was thanked for his hard work.

Action: Jin-Pei Cheng

5) Venues for future ICPOCs

There was consensus that there should not be three consecutive conferences in Asia, and that a European venue for ICPOC27 would be desirable, together with considerable support for the possibility of Munich (ICPOC27, 2026) and Mumbai (ICPOC28, 2028), assuming that an acceptable bid would be received for each in due course. European alternatives might include Russia, Czech Republic or Croatia, if suitable organizers could be identified; Igor Alabugin commented that he could help to arrange a conference in Moscow. Presently there does not appear to be any prospect of holding a conference in Latin America. Ulli Siehl pointed out that, in view of the world-wide consequence of the SARS-CoV-2 virus becoming endemic, the days of large live international conferences may be over.

Chair's proposal: It would be good to continue our practice of an open process for inviting competitive bids, with the committee deciding each venue four years in advance. Ian Williams should write to Hendrik Zipse (Munich) and R B Sunoj (Mumbai) to advise them of the situation regarding 2026 and 2028. Igor could investigate the possibility of Moscow as a potential venue for 2026.

Proposed actions: Ian Williams & Igor Alabugin

6) Membership

There was consensus for inviting R B Sunoj to become a member of SSMC. Action: lan Williams

7) Projects:

(a) Charlie Perrin reported that the revised Glossary of Terms in Physical Organic Chemistry had been submitted to *Pure and Applied Chemistry* in June; it now has >53,000 words, including 433 references inserted by Silvia Braslavsky. Publication had been delayed by several reviewers who continued to insist that we must not take logarithms of dimensioned quantities even though physical-organic chemists have been very successful with linear free-energy correlations that do so and that can be

justified as not introducing any error. We have revised the entries to accommodate or address that objection, but the manuscript is still under review.

(b) Aromaticity – update awaited

(c) Suggestions for new projects

Manabu: Open-Shell Molecules in New Reactions and Materials

Igor: Physical Organic Chemistry of Excited States

lan: Online Video Library of POC Topics as an Open Teaching Resource

Ulli commented that a library of authoritative short video presentations would be useful, and he suggested that it would be essential for it to be hosted by an academic or NGO

server and not by a commercial enterprise (e.g. YouTube).

Does anyone have (or know of someone who has) expertise in this area?

Enthusiastic support would be required for any one of these suggestions to become a reality. This does not have to be from within the current SSMC membership. Any ideas for who might be interested?

Action: all members

8) Web pages:

Manabu suggested that a "history of ICPOC" should be created, with a link to appear on websites of future ICPOC meetings. There was a consensus in support of this proposal.

Action: Ian Williams + Manabu Abe with help from Einar Uggerud & Ulli Siehl

9) POC brain drain and

10) POC and research evaluation:

It was recognized that these are long-standing, big and important issues with no simple answers. We need to continue to reflect upon them and perhaps devote time at a future ICPOC to discussing them.

Could we prepare accounts of "ICPOC" to advertise our POC findings?

How can excellent published POC work be brought to the attention of younger people?

Could an online 'student-focused' symposium be arranged? (Jason Harper has ideas and could put together a proposal.)

Igor commented that even the "flagship" journal for POC – the Journal of Physical Organic Chemistry was not in a good shape; perhaps POC is too "fundamental" in our age of applied science and funding priorities?

Manabu asked if we could do exchange programs for PhD students? Despite the time-zone problem, could we hold live-streamed lectures on (say) the last Friday of each month?

11) Election of SSMC Chair:

Given the extraordinary circumstances, lan's offer to remain as Chair until ICPOC25 in Hiroshima (July 2022) was accepted.

12) Any other business.

Matters raised have been incorporated under items 9) and 10) above.

lan Williams 24 August 2020

Action: Henrik Ottosson