

IUPAC – DIVISION III: Subcommittee on Structural and Mechanistic Chemistry

Meeting held on Monday 2nd July 2018 at 18:30, University of the Algarve,
during the 24th International Conference on Physical Organic Chemistry

MINUTES

Present: Manabu Abe (Japan), Igor Alabugin (USA), Maria Cristiano (Portugal), Jason Harper (Australia), Eduardo Humeres (Brazil), Miroslav Ludwig (Czech Republic), Charles Perrin (USA), Hans-Ullrich Siehl (Germany), Einar Uggerud (Norway) and Ian Williams (UK, Chair).

- 1) Apologies for absence had been received from Heidi Muchall (Canada) and Pietro Tundo (Italy), and subsequently from Henrik Ottosson (Sweden).
- 2) The previously circulated agenda was approved.
- 3) Minutes from the SSMOC meetings in Sydney (5 July 2016) and Durham (4 September 2017) were approved without amendment.
- 4) Chair's business.
The "What is SSMOC?" statement circulated in January 2018 was noted and agreed.
- 5) Membership
Noting that no responses to successive emails had been received from Mark Cesa or Ivo Leito, it was agreed to remove these names from the membership listed on the SSMOC webpage (http://iupac.org/who-we-are/divisions/division-details/?body_code=305) along with those whose retirement from the committee had already been noted (Maksić and Radom). In discussion of possible new members, several names were suggested. It was agreed to invite Jin-Pei Cheng (China) and that conversations should be had with certain other people during the ICPOC meeting. (*Note: subsequently Moises Canle (Spain) and Anat Milo (Israel) have accepted invitations to join SSMOC.*) The SSMOC webpage should be updated accordingly. **Action: IW**
- 6) Maria Cristiano reported on ICPOC24: along with many positives (healthy attendance, with about 30 countries represented, and a very strong participation by younger scientists) some disappointments were expressed (*e.g.* not all hoped-for speakers had been able to attend).
- 7) Manabu Abe provided a brief update on ICPOC25, 5 – 10 July 2020, Hiroshima: an informative flyer had been distributed to ICPOC24 participants, and the conference webpage was active (<https://icpoc25.jp>).
- 8) Venues for future ICPOCs
In addition to the previously mentioned possibility of a bid from South America, informal expressions of interest had been received by the Chair from China, India and Russia to host ICPOC26 in 2022. It was agreed that an open and fair process for invitation and consideration of formal bids should be announced. (*Note: An announcement was made by the Chair during the closing ceremony and by email for expressions of interest by 31 July 2018 and formal bids by 31 October 2018 in accordance with guidelines to be provided.*) A decision would be made by SSMOC (excluding anyone themselves involved in a bid) before the end of 2018. **Action: IW**
- 9) Projects:
 - (a) Charlie Perrin reported that significant progress had been made on the Glossary of Physical Organic Chemistry, and that the Task Force would meet on 6-7 July 2018 in Faro to discuss remaining issues before completion of this long-standing project.
 - (b) It was agreed that the previous suggestion of an acid-base project should be considered as closed.
 - (c) *Note: Henrik Ottosson provided a written progress report on the proposed aromaticity project, as follows.*

Together with Miquel Solà (Girona, Spain) and Gabriel Merino (Merida, Mexico), I am co-organizing the conference Aromaticity 2018 on Nov 28 - Dec 1 (www.theochemmerida.org/aromaticity2018). This is by invitation only with 60 speakers (among them Roald Hoffmann); from SSMOC, Igor will also participate. The purpose is to bridge recent theoretical and experimental research on (anti)aromaticity and to discuss how these research findings can extend the description (definition) of the concept. Thus there will be round-table discussions about the present IUPAC description of aromaticity and how it can be updated.

I am also in the process of putting together a work group for the aromaticity project. I would like a group of 12 people: 6 experimentalists and 6 theoreticians, all with different research profiles and with a broad international representation. I would in particular like to have one (or two) organic chemistry textbook writers among the members in the work group. The plan is to apply for some economic support from IUPAC (I will do when back in Uppsala at the end of July). In my view the work group should have two tasks:

(i) to work out an updated IUPAC description (definition) of the aromaticity concept which is equally short and easily understood as the present one. I have been in contact with Charlie and Einar on this matter as it relates to the update of the glossary.

(ii) to compose a (somewhat) longer description of the concept which we can refer to in the IUPAC description.

The work group will in part consist of participants at Aromaticity 2018 so that we can bring in what comes up at the conference. I estimate that the project on aromaticity will be finished late next spring.

- (d) Eduardo Humeres' suggestion for a project to standardize the formatting of literature references in journals was discussed but did not receive support from other members of the committee.
 - (e) Charlie Perrin floated the idea of a possible project on the "transition state".
- 10) Other business: Ian gave warning that, depending upon his personal circumstances beyond 2020, SSMOC might need to appoint a new Chair at its meeting in Hiroshima at ICPOC25.

Ian Williams (26 July 2018)