

Minutes of the July 2019 meeting of the IUPAC Commission I.1 during the 50th IUPAC General Assembly

Times: 13:00 – 17:00 Tuesday 9 July, 09:00 – 12.00 Wednesday 10th July

Location: Palais des Congres, Room 241

Attendees: Jeremy Frey, Jürgen Stohner, Stuart Chalk (? morning of 10th), Roberto Marquardt, Yutaka Kuroda, Jan Kaiser, Martin Quack, Franco Pavese, Jim McQuillan (via Skype), Romeu Rocha (via Skype).

1. General Comments

Roberto Marquardt reported that IUPAC provides a good quality virtual meeting platform (software) named *GoToMeetings*. Fully attended virtual meetings or face-to-face meetings important for communication.

2. Review of Commission membership

Jeremy Frey. Commission membership tenure is limited by IUPAC rules while Task Groups for Green Book (GB) projects do not have such limitations. For the preparation of the Green Book we might have I.1 members and collaborative members. A country cannot have an NR and TM simultaneously in Commission I.1. Financial issues with meetings. More effective to have small meetings of those directly involved in projects.

3. Review of activities since last meeting in Sao Paulo

Roberto Marquardt. Portuguese GB translation handled by professional company and ~3000 USD paid by IUPAC and Brazilian Chemical Society. XML version used a LaTeX -> wiki platform -> LaTeX format again -> pdf version. The pdf version contains funding acknowledgement. XML version hopefully available.

Romeu Rocha explained wiki solution for Brazilian translation and translation to XML version. Layout can be rendered closer to GB format with automatic indexing.

4. Exchange on current status of Gold Book

Stuart Chalk XML version for Gold Book is a dynamically generated XML file. Equations shown nicely and correctly. The source is partially LaTeX. Need to determine the best choice for web representation (MATHJACS). Presently in XML version of Gold Book, LaTeX is used only for fonts and when necessary. Need consistent symbols in GB versions. Whole protocol to be made

available on GITHUB. Experts to have editing access to Gold Book entries. What method LaTeX, outmath, or mathml to be used? Americans with Disabilities Act (ADA) mentioned.

5. Report on Green Book 4th Edition meeting (Jan. 2019 Zurich)

Martin Quack. Assignments for reviewing of the 13 chapters and sections made. Bulk of task to be done by Martin, Jurgen, and Roberto with support from Jeremy, Franco and Yutaka.

6. Report on Green Book abridged version meeting (Jan. 2019 Zurich)

Jurgen Stohner and Roberto Marquardt Abridged version is the most advanced and needs the most urgent attention. Assigned checking tasks listed to Roberto, Martin, Jurgen, Jeremy, Franco, Yutaka, and Stuart.

7. Project proposal for Green Book 5th Edition

Jeremy Frey

a. Application has been reviewed. Need to bring in new people. Biophysics to be included but in what form and how much? Green Book and Gold Book information can be duplicated but must not be contradictory. GB 3rd Edition is latest official IUPAC recommendation (PSE). GB 4th Edition did not add a new recommendation and does not need approval from PSE reviewing.

b. Table compilation? Need feedback from topic experts on what to include.

c. The 5th Edition will be reviewed by Division PSE and ICTNS.

d. Can start with 4 pages "Concise summary of the GB" as for the web version.

e. Content suggestions: NMR, biophysical chemistry, computational chemistry, molecular dynamics, cheminformatics, nano-physical chemistry, surface chemistry, ultrafast, non-equilibrium thermodynamics, uncertainty, chemical engineering.

f. The electronic version of the GB 5th Edition could be a big book, and an abridged version in print would be needed.

8. Release plans for GB abridged and GB 4th Edition

Publisher needs to be kept informed. It is noticed that the 3rd edition is sold out (all three prints), and that around 1200 samples were sold.

9. Next meeting

Formal meeting at Montreal GA 2021 with invitations limited to ~12 people.