

Concise minutes of a virtual meeting of IUPAC Commission I.1

January 6, 2022 12:00-13:00 CEST

Attendees: Martin Quack, Roberto Marquardt, Jim McQuillan, Jan Kaiser, Stuart Chalk, Yutaka Kuroda.

1. Change of Chairmanship

Jim invites Yutaka to take over Chairmanship. Yutaka thanks Jim and all for work on the virtual meetings and the GBav.

Roberto thanks Jim for taking Division Chair one year ago. He asks Yutaka to review committee membership.

2. Approval of minutes of 22 October 2021 meeting

Minor changes then minutes are accepted.

3. Discussion "Numerical representation of units and algebraic expressions containing units" (Stuart)

Presentation of "What's the Future of Digital Chemical Units?" ACS meeting, Fall 2021.

Attention drawn to CIPM activities and metrological issues of digital representations of units and mentions complicated cross-linked interests.

BIPM is working on an exchangeable, authoritative, dependable, and unambiguous data set on the basis of the SI.

Pain points (see CCU): dimensionless units, example of mole fraction (amount of substance (aos) fraction) and mass fraction; these need special conversion factors that carry no unit; how does the computer know that?

Some units cannot be represented by the computer! See

<https://umis.stuchalk.domains.unf.edu/units/view/000001>

C34 is the code for the mole by UN Economic Commission for Europe.

Discussion points:

Computers must identify the quantity by the symbol

Symbols are not the best option (see later)

Limited number of units that you can create to map all seven base units

One can do that; also dimensions, powers, etc.. so as to generate unique strings identifiable by the computer

What is the sense of the discussion?

GB 5th edition will be digital, needs to be machine readable

Publishing and processing challenges, eg problems with molar volume. Different usages might need different representations. Eg cube per mole.

Discussion points:

One should use cm^3 and not m^3 , as former is well used in the GB

Quantity calculus solves this problem uniquely. In literature, people do not put powers in the right place

Quantity calculus solves for humans, but not for machines

One should avoid encodings that are too long, such as in INCHI

Does Stuart have a proposal to make for one specific representation?

DRUM is a CODATA working group on this topic, Stuart and Jeremy are members. DRUM a 4 y program, starts November 2022, asks what chemistry needs.

Roberto asks Stuart to prepare working document on one example for a machine-readable representation for committee discussion (pros and cons) at the next meeting on this topic.

4. General matters

Jan asks the committee to discuss GBav. Martin recalls that decision was made in 2019 at the Paris I.1 meeting, that GBav was accepted with its present contents.

Next meeting scheduled for March 11, 12:00 CET.

Topic: units for angles. Roberto to prepare pdf file.

Subsequent meeting scheduled for April 8, 12:00 CET.

Topic: Sorption, revisited.