

**Minutes of the ICTNS Meeting  
Lisbon, 2012-May-05 to 2012-May-06**

1. Opening Remarks and Introduction of the Participants

Prof. Ron Weir called the meeting in order at 9 am, participants were welcomed and introduced themselves. The following persons were present:

Chair:  
Prof. Ron Weir (RDW)

Secretary:  
Prof. Jürgen Stohner (TM) (JS)  
*Chair Commission I.1 on Physicochemical Terminology,  
Symbols, and Units*

Titular members:  
Dr. Gerry Moss (TM) (GM)  
*Division VIII on Chemical Nomenclature and Structure  
Representation*  
Dr. Juris Meija (TM) (JM)  
*Division II.1 Commission on Isotopic Abundances and  
Atomic Weights (CIAAW)*

Associate Members:  
Prof. Amélia Pilar Rauter (APR)  
*Division VIII on Chemical Nomenclature and Structure  
Representation*  
Dr. Robert Wielgosz (RW)  
*Bureau International des Poids et Mesures (BIPM)*  
Prof. Bernardo J. Herold (BH)  
*Division VIII Advisory Subcommittee*

The following members presented their regrets in writing not being able to attend the meeting: Prof. Monica Nordberg (TM), Dr. Andrey Yerin (TM), Anthony Goodwin (TM), Stephen N. Mea (SUNAMCO), Jan Kaiser (AM)

2. Agenda

The Agenda was distributed by email to the ICTNS members prior to the meeting. RW recalled the Agenda was named “provisional” as there is space for additional items in Section 8. None was added at this stage. The participants agreed with the Agenda as set.

### 3. Minutes of the San Juan 2011 Meeting

RW asked to change his statement in the Minutes in the Section “Summary of the Joint Meeting of ICTNS and Division I.1 Commission on Physicochemical Symbols, Terminology, and Units at 16:00 31 July 2011”, last but one paragraph and replace “criticized” by “commented”. The minutes of the San Juan Meeting 2011 were then approved unanimously and sent out for publication on the IUPAC webpage on 10 May 2012 in electronic form by BH.

### 4. Chair’s Report on Business Arising from the San Juan Meeting

4.1. Attention was drawn to item 8.1, where Ales Fajgelj (Past President Division V) expressed his wish to propose an interdivisional project about the consequences of the new definition of the mole. RDW reports that no such proposal has been submitted prior to the Bureau Meeting which was held in Leiden (NL) from 13 to 15 April 2012. APR remarked that Division VIII will meet in July, she will check later.

4.2. RDW noted that item 9.1 on new developments of the Gold Book will be discussed in our Agenda 6.1 below.

4.3. Concerning item 9.2, about the non-searchable PDF of the Green Book, the Chair commented that this is also on our Agenda 8.1. JS remarked that the problem with the PDF of the 3<sup>rd</sup> Edition and 2<sup>nd</sup> Printing of the Green Book (2008) not being searchable still persists. It was suggested to buy some software to transform the non-searchable to a searchable PDF file and ICTNS budgets would cover the costs on the order of a few hundred USD.

*Note added upon writing the Minutes (JS): The problem is solved, the pictures included in the Green Book caused the problems; upon redrawing all the pictures allows creation of a searchable PDF without additional software requirements.*

4.4. RDW comments on item 11 about memberships 2012-2013. Bridging the gap between Commission II.1 (Atomic Weights) and Commission I.1 (Green Book), both JM as Secretary of II.1 and JS as Chair of I.1 are now in ICTNS, and it is to be expected that troubles caused by a couple of individuals will be resolved this way. RDW mentions that he talked to the current Chair of II.1 as well as to the past Secretary of II.1 and both seem to be supportive. A faster kind of way in which individuals can make proposals for changes and get changes introduced into the Green Book without getting the whole book printed is sought; this is why the online version is important. Agenda 9.2 brings this up.

### 5. Report from the IUPAC Bureau Meeting, 13 to 15 April 2012 in Leiden (NL)

Twenty eight individuals were present at the Meeting, representing a total of 18 countries.

Item 6 on their agenda was the President’s report with focus where he is hoping to take IUPAC within the next two years. His focus is about relevance and credibility of IUPAC, being related to IYC2011 which was very positive, but IUPAC was rather disconnected to this event. Each division was required to report to the Bureau.

## Division I

President of Division I indicated told that the Green Book abridged version will be published in 2012. JS commented that getting it out for review in 2012 is more realistic and with completion within the current biennium 2012 to 2013.

JS remarks that the Green Book 3<sup>rd</sup> Edition 2008 translation into Italian is finished, the Japanese translation is already published in book form, the French version is close to being finalized and the German and Turkish editions are in progress. RDW remarks that one has a kind of interim version available prior to the printed one with hardcover that gets amended. We want a system where people can access the latest version (online searchable PDF). Commission II.1 has not been able to access the latest version online. JS comments that there is no continuously updated online version, the latest version is always the latest printed version. No progress has been made from the side of IUPAC to collect all updates/typos/corrections of the various colour books although this has been suggested several times. RDW makes an analogy to the Bird world where every six to seven years, a printed updated version of the bird taxonomy handbook appears; each year the ornithological unions publish an update. JS says that this was exactly the idea of having a prominent place for lists of updates. GM comments that the Red and Blue Books have such lists, although on GM's private webpage and some have even been published in PAC. He finds the title of the Green Book wrong since a date is missing. JS remarks that the 3<sup>rd</sup> Edition has three printings with different dates: 2007 (1<sup>st</sup> printing), 2008 (2<sup>nd</sup> and corrected printing), 2011 (3<sup>rd</sup> printing). This should appear documented at the IUPAC webpage. JM asks for a change to the title, say, 'Green Book 2011 Edition' or similar. JS notes that the printed book should be the reference with the year as given there in the *bibliography*. RDW asks how is the GB3 updated, say, every year prior to preparing a printed new hardcopy? He supposes that the GBWP has regular meetings twice a year or so. JS responds that there are no meetings because of no funding, except between some local people (RM, JS) to finalize currently the Abridged Version. RM asks what is the procedure if some proposal arrives regarding changes/updates of the GB? JS replies that this is noted, and discussed at the next meeting of the GBWP; this will probably occur be for the 4<sup>th</sup> Edition and changes will be implemented when the GBWP agrees with the suggestions. RDW asks about the procedure for minor things, ppm etc.? JS remarks that minor things, when no extensive discussions within GBWP is expected, are handled immediately and included in the next (re)printing issued by the publisher. RDW asks about a publisher independent mechanism, say, every year or twice a year in an online version. JS states that what we see with the Gold Book is not the way we want to go with the GB; many ways of an online publication can be thought of (*e.g.* similar to CRC). Another possibility is to have online the complete PDF version after some time after the hardcopy has been published, and this is the current mechanism with the GB3. Preparing a constantly updated version of the complete PDF would destroy the possibility to have a publisher printing a hardcopy version of the document. GM says that he can find the PDF of the 2<sup>nd</sup> printing of GB3 on the IUPAC webpage. A simple page of changes would also be helpful. JS again suggests that it is IUPAC's business to maintain a webpage where corrections to (all) colour books are collected. It should not be a need to know that GM maintains a correction section of the Blue Book on his webpage in order to find newest corrections. Some discussions went on concerning the incomplete list of bodies or missing entries in IUPAC's members address lists; it was noticed that the updated list of ICTNS members was found on the old IUPAC webpage, but not on the new webpage. JS will approach the Secretariat for corrections if not already done so. RW comments that IUPAC's

business is about publications. The discussion of publishing should be on a higher level. ISO sells its publications. JS suggests that many problems with publications could be solved if IUPAC would be its own publisher. GM notes that RSC publishes on behalf of IUPAC, therefore, marketing is not RSC's business if not otherwise agreed upon in a contract. He suggests that every IUPAC sponsored conference should publicize the colour books by some insert. IUPAC should play a more active role in advertising its colour books. RW asks about the number of copies sold of the GB? JS: About 1000 before the 3<sup>rd</sup> printing was released, but no information about the number of downloads is available. RW: if we want the GB spread, one should have it totally freely on the web. JS: The 2<sup>nd</sup> Printing of the 3<sup>rd</sup> Edition is on the web. The question about searching the PDF is currently unsolved. The fact that the GB3 is not at a prominent position and it is not widely cited – even within IUPAC, is not related to the document not being searchable. Searching for the GB on the internet often still points to the second edition. CPEP is a standing committee responsible for publications. RDW will contact CPEP (chair) and the Secretariat (secretary general) on that matter.

### **Division V**

Maria Camoes (President Division V) raised questions and objections against the IUPAC position on the new definition of the mole; this is also a separate point on our Agenda 7. RW summarizes three current arguments around the mole: (1) keep the mole as it is, linked to carbon-12, (2) the new proposal with a link to a fixed Avogadro constant and shifts uncertainties around, and (3) a large body of discussion whether the mole is a great quantity with a unit mol or whether one should have just a number because one is counting. At the last CCQM with Nicole Moreau (Past President IUPAC) being present, IUPAC's position was reiterated and confirmed. RDW stated that Division V representatives were present at the Glasgow meeting, giving their input and agreed with the consensus. ICTNS followed the formal process with consultation and with representatives of the divisions at the Glasgow meeting. Following the discussions, the position was agreed. If A. Fajgelj wishes to reconsider the decision he should make a formal presentation to the President.

Referring to Agenda 8.1, A. Fajgelj wished to propose a project, but nothing has happened as of this ICTNS meeting. RW noted that he contacted Fajgelj several times asking about the progress of the project, but no definitive answer has been received. If a project materialises, M. Camoes would eventually lead the project. The time schedule for next CGPM congress is 2014, meaning that papers have to go out by the end of 2013. Any document for reconsideration of that matter must therefore be completed no later than mid-2013, about a year from now. The proposal for the General Conference has gone out and consulting takes place. Nothing would change this process except strong opinions from large bodies.

### **Division VIII**

The Blue Book, with between 1500 and 2000 pages in a totally new approach to offer an IUPAC preferred name, is making progress, but very slowly. A revision process continues, but is slowly progressing because people come back to older issues they are not happy with and this has consequences for many places within the document.

About two people do the work and it is disturbing that they are distracted from proceeding in a speedy and efficient way. GM explains and emphasizes the difficulty of the project and the very importance of it. IUPAC preferred names are demanded for drugs registered with WHO and are important for custom authorities.

APR suggests to draw Editors of Organic Chemistry journals attention to IUPAC names and rules, although it seems that many already do. RW asks whether other UN

and EU agencies have in their directives a formulation requiring that IUPAC names and nomenclature rules should be followed. This would mean that IUPAC gains automatically a higher status than CAS. BJH explains that in Portugal, the Portuguese Chemical Society in fact has the authority to translate names into Portuguese. It is already difficult in projects between Portugal and Brazil to get agreement, because there is no authority by law but only by mutual agreement and this turns out to be responsible for major delays and friction while translating the inorganic IUPAC book. CAS and IUPAC rules for naming are different; translations cause problems when a system relies on alphabetical order. CAS rules are less flexible. They might use the Blue Book, once it is finished. It seems that IUPAC is still the recognized authority for naming.

RDW asks who within UN, WHO, UNESCO, EU and customs authorities and their potential bodies should be contacted by IUPAC's President to advocate IUPAC's rules as the standard? JM remarks that probably ISO would be such a place. RW says that as far as legislation is concerned, in Europe this is the European Standardization Body (SEN?) and legislation works with harmonized standards and one should get the IUPAC names into these harmonized standards. Another field are patents and one should find a way that patent authorities require the use of IUPAC preferred names, once the Blue Book is printed. RW shows a REACH document for consultation and there, IUPAC is mentioned; it is IUPAC's task to be more insisting on its role (see [http://www.reachonline.eu/REACH/EN/REACH\\_EN/kw-iupac.html](http://www.reachonline.eu/REACH/EN/REACH_EN/kw-iupac.html)). The really hard question is: What is IUPAC's business model? APR suggests writing a letter to the President with some queries and offering already some solutions as to what one might do here to increase IUPAC's visibility. IUPAC could probably name some delegate who looks for or establishes relevant contacts to international organizations. Some additional organizations being interested in IUPAC preferred names: dealing with chemical warfare, misuse of drugs in sports, food and nutrition, forensics, MSDS (?) sheets. Memorandum of understanding should be sent to as many organizations as possible to have an IUPAC representative present at the meetings. As far as legislation is concerned, for example, every EU member state has a local representative who might be contacted. Probably John Jost might know whether or not any contact person exists between IUPAC and these bodies. We have to get organizations to state officially that IUPAC will be their standard.

For more information, see Minutes from the Bureau Meeting.

### **Important Dates**

The 47<sup>th</sup> General Assembly and 49<sup>th</sup> Congress in Istanbul, are set for 9 to 15 August 2013; this is the time for a full ICTNS Meeting; 48<sup>th</sup> GA and 50<sup>th</sup> Congress in South Korea 2015, 49<sup>th</sup> GA in Australia, Brazil or Nigeria 2017 and 50<sup>th</sup> GA in China or France 2019 (100 years of IUPAC), no decision has been made yet.

### **New Elements**

Symbols and names of element 114 and 116 are out (Flerovium, symbol Fl and Livermorium, symbol Lv); it is to be noted that the symbol Fl was used for fluorine in the 19<sup>th</sup> century. Does this have consequences for the naming proposed element (and actually accepted)? IUPAC recommendation 1979 states that a name may not be 'recycled', in the same spirit and this should also apply to the symbols. ICTNS should respond depending on the reports on the paper; give information to RDW.

## 6. The Gold Book

The Gold Book (GoB) has top priority for the Secretary General René Deplanque. A content management system will be offered by a publisher for a new electronic version. BH emphasizes that the GoB is a collection of recommendations and the question arises as whether or not we can make changes without going through a proper process via the divisions. JS remarks that the GoB also quotes from all editions of the GB, partly wrong contents. In addition, maintaining is a real problem in view of future developments. For the GB, an online version, based on the large and extensive index of the GB is explored by Jeremy Frey and his research team in Southampton. One should think about this concept to apply to other colour books. GM notes that many glossaries appear as recommendations each year, the newest entry in the GoB as far as recommendations are concerned is from early 2008. How to incorporate this into the GoB? RDW says that ICTNS's task is to get the GoB forward. Each Division President offered financial support for the GoB. Someone is needed to update all glossaries, which is certainly a multi-year task; caring about the update with new recommendations is one thing. Checking the update of current entries is another thing. A task group should be installed to: set-up rules for changing, modifying and formatting entries, deliver task description, collect current-future-unpublished process entries and bring recommendations up to date (hire someone with expert knowledge to do this on a more 'mechanical' way). Therefore, the task group should define the process for dealing with current entries, the back-log of unpublished entries and the future process for making entries to the GoB, based upon the future back-office structure of the GoB. It is suggested to ask McLaren (Vice President CIPM, could represent Division II and V) or McNaught to serve as Chair. RDW collects names for Division representatives to join the task group GoB on an advisory basis (BH representing Division III, Pavese or Goodwin representing Division I, xxx representing Division II, Nordberg representing Division VII); the task group should also get involved in discussions between the Secretary General and the publisher. The task group defines the work and cares about funding for meetings (*e.g.*, stage I: defining process, stage II: implementing procedure).

Another point came up: some universities do not support voluntary work of their staff for IUPAC. IUPAC papers are about recommendations; this has a high impact on the community and being invited to be on that board recognizes that members have a high knowledge of that area. JS suggests that after the end of IUPAC member's term, the President should write a short letter thanking for the effort and dedication; this letter can then be shown to the head of department.

## 7. Status of the SI System Regarding the Mole

RDW emphasizes that the position of IUPAC is unchanged; it was reconfirmed at the Bureau Meeting in April 2012. There is a formal and proper way to re-launch a process when someone has the feeling that the decision was not good. Nothing in this regard has been started.

RW said that BIPM organized a workshop with representatives from IUPAC (Moreau, Mills). Its aim was to find out the level of consultation and report on progress on re-measuring the Avogadro constant via the Si sphere work (giving a new value for the Planck constant and which allows the redefinition of the kilogram) at NRC Canada, NIST, in China, and at the PTB; PTB is leading the work and rechecks the data. The

issue about the name 'amount of substance' is still going on, but it is IUPAC business and not of direct BIPM or ISO concern.

RDW emphasized that at the Glasgow meeting a statement regarding the amount-of-substance was issued. Renaming was discussed, but no-one came up with a better idea. It is IUPAC's business to change when feeling this is necessary. Redefinition of the mole earliest in 2015: people should be made aware of this (especially those involved in teaching and responsible for education), 2018 might probably be a bit more realistic. A public relation joint paper should be put forward by the end of this year. The BIPM *ad hoc* working group (RW part of it) is preparing a paper to introduce the background of the proposal some time later this year. PTB will publish a joint paper on the scientific work, after that introductory paper appeared, public relation work will start.

Some proposals have been made in the past for replacing the name of the quantity  $n$ , 'amount of substance', JM suggested collecting them as a base for potential discussions or consultations.

#### **Outlook for the Discussion on the Last Day:**

RW and RDW remarked that VIM3 is not a glossary but rather a self-consistent vocabulary. A supplement is being produced as a means of an easier document to use than VIM3 and to bridge the gap between the vocabulary and current usage in the community. There is a questionnaire on the BIPM website which seems to be rather complicated to use (it has been produced by the VIM committee). How can one incorporate the VIM recommendations into a rather established terminology/nomenclature system?

GM and BH added concerning the GoB: 3 to 4 new glossaries need to be considered in the GoB. This is rather straightforward. More difficult are Technical Reports, which do not enter the GoB as they are not recommendations. JM mentions that the documents on isotopic compositions are named Technical Reports but are on the level of a recommendation (see discussion below).

## 8. Other Items of Business

### **Green Book**

The issue on the searchable PDF is under consideration with probably use of some specialized software (JS). RDW needs to contact Bryan Pearson to ask about the number of downloads of the GB; GM has tools to log the number of web accesses to certain parts of the webpage.

### **Colour Books on the IUPAC Website**

RW reports that BIPM is to redo their website, with major changes (refresh). There should be mainly one database where all the information is kept that finally goes on to the website. A questionnaire is to be prepared asking about the needs of the users. Redesigning with specialized software can easily amount up to 120 k€. The major problem with IUPAC is that currently two websites are maintained in a parallel fashion. IUPAC's webpage does not present the colour books prominently and coherently, JS prepared a summary list of the online access status for various colour books. Some of the colour books reside on non-IUPAC websites (for example, see GM's own website under <http://www.chem.qmul.ac.uk/iupac/>): orange on old IUPAC

site, purple on RSC, red on old site, silver nowhere, white on GM's own website. RW remarks that no BIPM document is on any other website except BIPM. IUPAC needs a policy on the future management of its electronic documents. A discussion went on regarding electronic versions of (colour) books whether they should be produced free or not, about readability in the distant future, distribution through libraries *etc.* Why not produce the 'book' in a purely electronic version and distribute it freely? It is a matter of taste whether or not the authors would agree in producing free online versions without going through a printed version produced by a publisher. IUPAC could create its own publishing business; one would be free to distribute an online version and at the same time fulfil potential requirements for the authors' bibliography. AM prefers both, a printed as well as an online version. Again, what's IUPAC's policy? Web statistics would be very helpful. PAC recommendations are often downloaded, used, but not cited. We are suggesting a policy of maximum publicity and usage of IUPAC publications, especially the colour books.

*Note added by JS after the meeting:* An inquiry among the current authors of the Green Book shows that almost all prefer the current system of having both, a printed version and after delay a freely accessible online version.

### **Chemistry International**

Two years ago, Fabienne Meyers asked to include contributions in CI from topics of the GB. This should be taken up again. It would be a good idea to focus on particular items from the Green Book to help educate the community. One example is 'ppm', being of some issue with some people. Suggested topics showing how to solve problems are:

1.	ppm, ppt, ppb	I. Mills, C. Thomas (BIPM), 2012
2.	axis in graphs	JS, M. Quack, 2013
3.	naming of elements	JM, JS, 2012
4.	(optical) spectroscopy	JS, M. Quack, 2013
5.	atomic weights, isotopic composition	JM, JS, 2013
6.	<i>m/z</i> in mass spectra	JM, JS, 2013
7.	translating names	BH, ?, 2013
8.	story on aluminum/aluminium, sulfur/sulphur <i>etc</i>	GM, ?, late 2013

More ideas are welcomed by email. RDW will contact Ian Mills and Claudine Thomas. Format and style will be discussed together with Fabienne Meyers.

### **Additional information from RDW:**

From one of the projects of Division I, three books on experimental thermodynamics will come out. They carry IUPAC labels but are prepared through a commercial publisher. ICTNS is in charge to make sure they all follow IUPAC recommendations and policies. Tony Goodwin volunteered to take the responsibility and make sure that IUPAC recommendations, nomenclature and symbol's rules are followed. We agreed to share between Tony Goodwin as the primary responsible person and RDW.

### **Atomic Weights**

Technical Reports seem not to be distributed to all ICTNS members, as GM remarks. RDW explains that for Recommendations, 15 members are needed for reviewing after the public review period. All members of ICTNS get the invitation to review.

Technical Reports needs a minimum of 3 reviewers after divisional approval; not all ICTNS members are asked but rather a limited number. Some of the ICTNS members would like to see also the Technical Reports prior to publication. JM asks why the publication of atomic weight and isotopic abundances are Technical Reports rather than Recommendations. It is suggested to make them a Recommendation, especially in view of the fact that the new compilation shows intervals for certain elements rather than a single value. For practical use, an additional recommended single value is given, as exemplified with the conventional atomic weight values (see Table 6, Atomic Weights 2009 report). A 2011 report is currently in preparation and it should be submitted as a recommendation, the format is probably different from a Technical report; RDW checks about the requirements.

GM asks whether NRO's representatives are invited for reviewing, especially in view of language issues (example: "*Sulphur or sulfur? A tale of two spellings*", British Medical Journal 297(6664), 1697 (1988)).

### **VIM**

The questionnaire was motivated by user's comments. It is suggested to have someone in WG2 who has detailed knowledge of the Green Book. How consistent is the terminology with the Green Book should be checked as VIM is to be adopted by IUPAC:

- a) Does it define terms that are used in chemical measurement?
  - b) Is the terminology consistent with IUPAC's recommendations?
  - c) Can we readily implement necessary changes or are the changes too numerous and therefore require a major change?
  - d) What should be done in the future (IUPAC's representative?) for further developments? Might a similar document like EURACHEM/CITAC be useful?
- VIM is on the way to become a vocabulary above any other used to define measurements in chemistry. If IUPAC does not agree with that, VIM should not be published under the name of IUPAC. RDW checks with N. Moreau who is representing IUPAC on WG2 (probably JS?) and immediate action is needed.

The meeting ended 2012-May-06 at 12:45.  
Next meeting is in Istanbul.