

**Minutes of the ICTNS Meeting  
Istanbul, 2013-August-11 to 2013-August-12**

**1. Opening remarks and introduction of the participants**

Prof. Ron D. Weir called the meeting in order at 9:06 am. Participants were welcomed and introduced themselves. The following persons were present:

Chair:

Prof. Ron D. Weir (RDW)

Secretary:

Prof. Jürgen Stohner (TM) (JS)  
*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)  
*Secretary Division II.1 Commission on Isotopic Abundances and  
Atomic Weights (CIAAW)*

Prof. Brynn Hibbert (TM) (BH)  
*Division V*

Dr. Anthony R. H. Goodwin (AG)  
*Division I and Commission I.1*

Associate Members:

Prof. Amélia Pilar Rauter (APR)  
*Division VIII on Chemical Nomenclature and Structure  
Representation*

Dr. Andrey Yerin (AY)  
*Division VIII*

Prof. Norman E. Holden (NH)  
*Division II*

Dr. Graeme Moad (GRM)  
*Division IV*

Dr. Bert de Jong (BJ)  
*Young Observer*

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

## 2. **Introductory remarks and responsibilities of ICTNS**

We have two full days. We made a minor change in the Agenda: We switched the joint meeting with Division I scheduled for Monday afternoon to today afternoon and the scheduled meeting with Commission I.1 from today to tomorrow afternoon. We have representatives from Divisions I, II, IV, V and VIII as well as a young observer. As part of RDW's report, a document about the responsibilities of ICTNS has been circulated in advance (Agenda 2.0 Responsibilities of ICTNS.docx) to remind us of what we are supposed to do. As RDW was not invited to yesterday's meeting of Division I, II and V, some misunderstandings persist – as could be anticipated from the briefing by Prof Marquardt (Secretary Div. I). UN, EU and UNESCO take the IUPAC and ICTNS position on nomenclature, terminology, units and symbols as the official legal position which puts pressure on us to get things right. We must recommend up through the Bureau and the Council and let them decide what to do with the recommendations we put forward.

## 3. **Agenda**

The Agenda was distributed by email to the ICTNS members prior to the meeting. RDW recalled the Agenda was named “provisional” as there is space for additional items. The participants approved the Agenda as set.

## 4. **Minutes of the San Juan 2011 meeting**

No changes. The minutes from the San Juan 2011 meeting were approved.

## 5. **Minutes of the Lisbon 2012 meeting**

JM asked for a minor change to the Lisbon minutes: On page 9, replace “It is suggested to make them a Recommendation, ...” by “ICTNS would have no objection, in principle, to make them a Recommendation, ...”. The corrected minutes of the Lisbon 2012 meeting were approved.

### Action item 1

Change minutes accordingly and resend to the Secretariat.

## 6. **Business arising from the San Juan and Lisbon meetings**

In the minutes to the San Juan meeting, there is reference to the Gold Book. We want to discuss the Gold Book later under Agenda item 11.

With the Lisbon minutes item 4.1, Ales Fajgelj said that he would propose a project to be launched dealing with the definition of the mole. Jack Lorimer was Chair of ICTNS at that time and was involved in the handling of this business. A joint meeting between Divisions I, II and V was held yesterday at 16:15. It is unclear whether minutes were taken. One must make sure that the history is correct and no wrong information gets into the minutes. This group will come forward with a project proposal.

BH said that soon after Fajgelj's suggestions 2 years ago, it was realized that there was not enough time to do anything sensible. The meeting yesterday arose because of the decision to defer any decision on redefining SI units. IUPAC has a time window to re-evaluate what has happened since Glasgow and to have a better understanding of the

implications of a redefinition and take a different position or not. There might be no definitive minutes from the meeting yesterday. The Presidents of the three Divisions present yesterday get together today and scope the project. RDW said that he needs to be present at that meeting to make sure no incorrect information is distributed. BH said that he was very positive about the meeting yesterday.

RDW continued with other business item arising from the Lisbon meeting, namely on the Green Book abridged version. This is another item on our Agenda.

Division VIII Blue Book revision was handled (over 1000 pages) and should be in the publishing process with RSC.

Another open business item concerns the agreement of some of us to prepare contributions to *Chemistry International* (see list of contributions, item 8 in the Lisbon minutes). Commitments were re-affirmed by the respective volunteers.

Next we moved to Agenda item 8.0 since Mark Cesa (new President of IUPAC) will come later and RDW wants him to hear the biennial report to the Council since the executive of IUPAC must understand the enormous amount of work handled by ICTNS.

## 7. **Biennial report to the Council**

RDW introduced the current Vice President of IUPAC, Mark Cesa (MC); the attendees of the meeting introduced themselves.

RDW noted that he tries to built cooperation between various commissions and divisions to minimize friction and facilitate cross discussions. He explained the responsibility of ICTNS and mentioned the huge amount of work done by ICTNS's members. RECs are submitted to the Bureau through the Executive Committee and they do with the RECs what they wish. This is relevant because of the 'mole' and the potential change in the SI by BIPM. ICTNS has gone through the motions and made a recommendation to the Bureau two years ago and this has been presented to BIPM as the official IUPAC position. However, commission CIAAW independently sent a message to BIPM representing their own position which was not the same as the one officially communicated to BIPM by IUPAC. This opinion expressed by CIAAW confused the BIPM which corresponded by asking the IUPAC President what is the official position of IUPAC given the CIAAW statement and the associated inconsistency. The Bureau reaffirmed explicitly the procedure followed by ICTNS. Presidents of Division I, II and V met yesterday (the Chair of ICTNS was not invited) but the minutes of this meeting are not published. There are some individuals unhappy with the idea to change the SI, especially the definition of the mole.

Table 1 showing "Volume of Technical Reports and Recommendations processed by ICTNS" of the distributed document (Agenda item 7.0 ICTNS Biennial Report to Council 2011-13.Istanbul.16 July 2013) is projected on the screen and discussed, similarly with the IUPAC books; the data are summarized in Table 2 "Books processed by ICTNS" of the same document.

RDW raised the question whether IUPAC can make money with the royalties for IUPAC sponsored books. This might be a potential source of revenue for IUPAC.

AG mentioned that when *Experimental Thermodynamics* was completed and a contract with a publisher was signed around 2000, the President of IUPAC ensured that IUPAC got royalties. For other books, the contract did provide a royalty to individuals. The strategy must be that IUPAC gets the royalties for IUPAC books and not some individuals.

The rest of the report summarized all details about the work ICTNS members did in reviewing. RDW assured members that all the recommendations from the reviewers are addressed by the authors. The formal Recommendations and the Technical Reports are sent to ICTNS once they have passed internal reviewing within the Divisions.

JS mentions that once in a while corrections asked for in the review are not fully implemented and the final printed version appearing in PAC contains errors. As RDW explained, it might happen by accident but usually he makes sure that all requests of reviewers are implemented. JM confirmed that this happened also in one case known to him and the already published online version was taken off the internet. Probably the proofs should also be checked.

BH remarked that there are various levels of comments. One should probably mark those comments which are very important and must be taken into account. One can mark comments as mandatory (M) or optional (O). This would be very helpful for the Editor.

Before moving to the new Agenda item 9.0, RDW raised the question to MC about the formal Recommendations and Technical Reports which were freely accessible with PAC and can be reproduced freely. What is the policy under the new publisher de Gruyter? MC explained that the contracts are still being negotiated and representatives of de Gruyter are present at the CPEP meeting during this afternoon. It was again noted that IUPAC sponsored books are a potential source for revenues. JS raised concern that it might be difficult on one hand to ask for royalties and on the other hand demand free online access and the right to distribute a PDF version after one year free of charge (as was the agreement with RSC for the Green Book). Commission I.1 responsible for the Green Book is happy with RSC; they also appear at GAs and the Congress to advertise the colour books. NH reported continuous problems with the new website to find minutes, reports *etc.* MC explained that the server will be relocated to North Carolina close to the Secretariat. Bryan Pearson is the person to be contacted in case of difficulties with the webpage and he will take care of them.

## 8. Chair's report from the Bureau meeting Frankfurt 19 to 21 April 2013

A few words from RDW about the Bureau for those attendees not familiar with internal IUPAC structures: The Bureau is composed of Division Presidents, Standing Committee Chairs, a few individuals usually from industry, senior academics and the Officers. They meet every year. Recommendations put forward by ICTNS are sent to the Bureau which decides whether the recommendations are accepted or not.

The minutes of the Bureau meeting are public. Just a few highlights of that April meeting:

- A strategic review of IUPAC's operations was done, particularly due to the drop of financial revenues. PAC subscriptions in university libraries have dropped dramatically. This year, IUPAC will not recover its production costs from the subscriptions. This is dramatic for the organization since there are currently no

other ways to earn money. The Executive Committee seeks another way for PAC to be published. A contract has been signed with de Gruyter (a German publisher) to take over PAC and CI effective 2014, January 1. The colour books are at the moment not part of that contract.

GM noted that there are only individual contracts for the colour books with no presumption that this must be the case in the future. RDW suggested a discussion about what should happen with the colour books and inform the executive committee accordingly. The contracts of the two individuals currently handling PAC will end by December 2013. De Gruyter will absorb all production costs and will not interfere with the editorial and scientific matters that come from IUPAC. Earnings for at least the first year of PAC with de Gruyter will be split 50:50 between IUPAC and the publisher.

- The colour books were not part of the discussion at the Bureau meeting. GM raised the point that Technical Reports (TR) and Recommendations (REC) were open access IUPAC documents and this must be also the case in the future with de Gruyter. RDW replied that a contract has been signed but he has not seen that document. BH made the point that RECs and TRs are essential to IUPAC and public free access must be guaranteed. Otherwise, these documents should be published solely on IUPAC's webpage outside PAC. RDW noted that the Secretary-General would like to see PAC more as a regular journal of scientific articles. Shall we formulate a proposal in case de Gruyter does not guarantee free access to RECs and TRs? JS suggested to consult the contract first; if open access is not guaranteed, we would be forced to disentangle RECs and TRs from PAC. JM suggested to request a look at the contract.

AG pointed out that for a number of books they did in 2013, an effort was made to ensure that contracts explicitly state that royalties go to IUPAC, however, it seems that this process is not formalized within IUPAC. A formal procedure must be established. With PAC it is a bit different because IUPAC needs to publish definitions, recommendations *etc.* and wants the public to have access without paying for it. It is a different issue with IUPAC books.

It was agreed that RDW look into the contracts and check the issue regarding RECs and TRs. RDW will write to Rene Deplanque with a formal request to look after the issue with the IUPAC sponsored books.

RDW informed members that the 48<sup>th</sup> General Assembly has been moved from Seoul to Busan in the south of Korea. The 49<sup>th</sup> will be either Australia or Brazil, the decision has not yet been made by the Bureau. The 50<sup>th</sup> in 2019 will be the 100<sup>th</sup> anniversary of IUPAC and will be held in Paris.

Some serious troubles within the Secretariat needed immediate action and Terry Renner stepped in on short notice. He did an excellent job despite all the difficulties that he faced.

A short break occurred until Mark Cesa arrived at 10 am (the Agenda then continued with Agenda item 7.0 and the Agenda item 9.0).

#### Action item 2

RDW is to contact R. Deplanque about the issues related to TRs and RECs by changing to a new publisher.

## 9. Reports from IUPAC Division representatives

### 9.1. Division I – Physical and Biophysical Chemistry (AG)

The Green Book is dealt separately under Agenda item 11.2. Other important issues are standards of vapour-liquid equilibria for binary mixtures that could be used as calibrants for apparatus. This project could be finished by the end of 2014 (Task Group Chair is R. Chirico). Another comment referred to the deceased M. de Silva; the manuscript on terminology and methods of thermal chemistry has been in the pipeline for seven years. It should be revisited at some point within this committee. It was first suggested to split the manuscript in two parts, one Recommendation and one Technical Report; when this was done initially, it was suggested to reverse and revert to one manuscript. RDW said that as far as he recalls, the problems arose within Division I and not ICTNS. RDW will inquire about this and discuss with M. de Silva's wife (who is also active in this field). He may inform Roberto Marquardt as the next President of Division I to take action.

#### Action item 3

RDW will contact Mrs. De Silva and RM (next President of Division I).

### 9.2. Division II – Inorganic Chemistry including CIAAW (NH)

New elements names for element 114 and 116 were approved. Information for 113, 115, 117 and 118 received and the report from the working party is awaited. Interdivisional Subcommittee on Materials Chemistry discussed various project proposals, especially preparing a report in numbering system option (strongly needed) and a nano-material definition project. CIAAW is close to complete Project 2007-038-3-200 on the Periodic Table of the Isotopes. A 2011 report with changed recommended atomic weights for Ge, In, Hg and intervals for Mg and Br has been published in PAC (2013). The Pie-chart of the periodic table was explained and demonstrated with the various information offered. A serious issue is how to prevent publishers/companies *etc.* from using the IUPAC periodic table and make money with it (for example with an iPhone App)? More information on projects of 'isotopes' and implications in science and beyond, on the evaluation of decay constants as well as on the definition of the year can be found in a report which has been submitted and is attached as *Attachment Agenda item 9.2*. The Chair RDW thanked Mark Cesa for participating and listening.

RDW resumed the discussion on the amount of substance, as CIAAW is recommending 'number of entities' whereas the IUPAC position (and the Green Book) favours 'amount of substance'. Does CIAAW dislike the GB flexibility, for example with the Dalton because of the biochemical community? JM replies that the GB gives two options (Da and u) and CIAAW can pick the one most convenient to their work, namely the Da. RDW noted that this can be discussed when ICTNS meets with Commission I.1 in the afternoon. The GB shows flexibility which helps eliminate much of the emotional discussions between different communities.

BH recalled that in 2009 IUPAC was asked by Ian Mills when he gave his presentation on the change of the SI to offer any alternative names for the quantity 'amount of substance'. There was no reply to CCQM from IUPAC on that issue of the name. This discussion will now start with the meeting of the three Division presidents today at lunch time to launch a project looking into the quantity and the unit, since IUPAC is uniquely positioned to offer an opinion on the unit and quantity

that chemists are worried about. Division V has agreed with the position of the Commission and believe in the 'number of entities'. The project must look into the quantity as well as into redefining the SI units.

JM stated that the letter that was sent to BIPM on the amount of substance did not refer to IUPAC's position but just wanted to make sure that the CIAAW's position was heard at BIPM. Whether or not it is allowed for commissions or divisions to state their opinion outside IUPAC should be regulated by some written policy statement of the Executive Committee. RDW asked the members to imagine the effect to the outside when the Bureau sends its official opinion as the legal representation of IUPAC, signed by the President and then a commission sends out such a letter to an outside body! Bob Loss reiterated that this occurred during his tenure and as President of Division II, he was unable to control CIAAW. Contrary to CIAAW's opinion, there was consultation but apparently CIAAW was unaware. It is hoped that with new people these issues can be resolved and avoided in the future.

### 9.3. **Division III – Organic and Biomolecular Chemistry**

No report received.

### 9.4. **Division IV – Polymer**

A report has been received and is attached as *Attachment Agenda item 9.4*.

### 9.5. **Division V – Analytical Chemistry (BH)**

A report has been received and is attached as *Attachment Agenda item 9.5*. An ongoing IUPAC key-project is a major revision of the Orange Book. It was mentioned by BH that at the 2009 IUPAC meeting in Glasgow, neither the resolution nor Ian Mill's presentation on the new SI and the mole was sent to the Divisions. It was emphasized that the Analytical Chemistry Division supported CIAAW's point of view and resolved in Istanbul that "*In particular we support a definition of the Avogadro number that recognises it as a scaling factor of individual entities*". BH will report on the Orange Book separately. Other active projects are mentioned (quality assurance, metrology, human error in measurement, solubility data). It is not yet clear whether joint projects with NIST are seen by ICTNS. BH will send a list of projects out of Division V together with NIST to RDW. Additional projects mentioned are on metrological traceability and mass spectrometry (which took about eight years and sometimes one gets inconsistent reviewer's reports).

### 9.6. **Division VI – Chemistry and the Environment**

Petr Fedotov (PF) reported planned close collaborations with Division VII and launch a project. PF wanted to send a detailed email on this to RDW, this has not occurred.

### 9.7. **Division VII – Chemistry and Human Health**

No report received. Yvonne Martin (YM) is to send the report to JS. BH mentioned that there is a joint project between IUPAC and IFCC for a vocabulary of terms used in nominal properties which has been reviewed. A 4-volume book is being prepared and shall be published with Wiley (bearing the IUPAC label on it), but this has not gone through ICTNS yet.

### 9.8. **Division VIII – Chemical Nomenclature and Structure Representation**

GM reported briefly that a document on flavonoids has been finally reviewed by the Division and should arrive at ICTNS in October 2013. A document on macro-

molecular rotaxanes is in preparation. Essentials/brief guides of polymer nomenclature are published in CI as a supplementary. The division works on similar documents on inorganic and organic nomenclature. An InChI project is under way with software as output. Other projects concern inorganic compounds, polymers and tautomers. Some projects in a much earlier stage are on revision/extension of indicated hydrogen and added hydrogen, as well as on comparing IUPAC procedure, Chemical Abstracts and Beilstein producing different names. The InChI system is unambiguous because it starts from a structure. Another project deals with graphical representation of reactions. A project on boron nomenclature just started today. JS mentioned that in a meeting with Division II (inorganic) a project is planned to start for labelling hydrogens (Ha, Hb vs. H1, H2 *etc.*), Some contact should be established between Division VIII and Division II on that matter.

## 10. Reports from representatives of other international organizations and from delegates of IUPAC on the same organizations

### 10.1. BIPM

No report received.

### 10.2. ISO/TC 12

No report received.

### 10.3. IUBMB

The basic job of IUBMB is documentation of enzymes. This is the only body that assigns EC numbers. GM reported on current activities on enzyme numbering for database usage (about 5000 enzymes listed, in electronic form only, the last printed version is from 1992); until 2009 about 80 new enzyme entries were added each year. It expands rapidly (currently up to 400 per year). Updating and reclassification are sometimes needed which sums to about 500 cases per year.

### 10.4. IUCr

No report received.

### 10.5. IUNS

No report received.

### 10.6. IUPHAR

No report received.

### 10.7. IUPAP/SUNAMCO

A report was prepared and mailed by S. Lea and is attached as *Attachment Agenda item 10.7*. JS as a representative of Division I on SUNAMCO should contact the Chair S. Lea.

### 10.8. JCGM-WG1&2

BH is the representative of WG1 and PdB of WG2. JCGM essentially looks after two documents. One is the international vocabulary of metrology (VIM) and the other is the guide to the expression of uncertainty in measurement (GUM). Both used to be ISO documents but because of the importance it was disentangled from ISO. Revision of the GUM (JCGM 100) is proceeding. A response to IUPAC/ CIAAW on uncertainties of atomic weights for elements described by an atomic weight interval



was presented (*Attachment Agenda item 10.8.A*). A new Supplement (JCGM 105) on concepts, principles, and methods for the evaluation of measurement uncertainty is to be published with the revised GUM. Supplement JCGM 106 on “Evaluation of Measurement Data: The Role of Measurement Uncertainty in Conformity Assessment” is published. WG2 launched a FAQ to improve the public understanding of the VIM. VIM is a series of definitions, terms and concepts used in metrology. IUPAC has adopted VIM and GUM and must follow it. BH stated that the Green Book should follow VIM. JS clarified this statement in that the GB follows VIM/GUM as far as uncertainty is concerned but not in writing symbols or using fonts *etc.* An annotated VIM is being prepared to improve the use of the VIM in the lab. Discussions on a general VIN (for nominal properties like diagnosis in health sciences) and discussions on the VIM4 are taking place. A report was presented as power-point and is attached as *Attachment Agenda item 10.8.B*.

In August 2009, PdB who is the delegate of IUPAC to JCGM wrote to BH as the delegate of IUPAC to WG1 (GUM committee) on a request by CIAAW to JCGM-WG1 about uncertainty evaluation of atomic weights (when an interval of atomic weights is given in square brackets). The given interval of atomic weights is fine. What one should not do, however, is to take the middle part of the interval, divide the interval by two and give this number as the uncertainty. Without any additional information, other than the values at the ends of the interval, it would be acceptable to adopt a rectangular ‘state-of-knowledge’ distribution with the value in the middle and the standard deviation given by half the interval divided by square root of 3. As far as conventional atomic weights are concerned, one cannot say that the elements with a range of values have no uncertainty. A report was presented as power-point and is attached as *Attachment Agenda item 10.8.C*.

## 11. Update on status of colour books

### 11.1. Gold Book

It seems that there has been no progress for several years. RDW will see what action can be taken. BH notes that unlike the other colour books, the Gold Book should always be evolving as new recommendations come out. New recommendations should automatically go into the Gold Book. Care should be taken, however, since not always does a new recommendation completely replaces an old one, it could also be a revision and so the ‘old’ recommendation should not be simply replaced. To keep the Gold Book up to date, someone should be employed, because this is a really a significant task. JS raised the questions whether or not it was a wise decision to have only an electronic version of the Gold Book and not a printed one. BH noted that ICTNS can or could decide how we want to have the database and how the process of updating should happen. An IUPAC project named “digital IUPAC” (CPEP) pushed by J. Frey is running. M. Kinnan (a young observer) has a similar project on solubility data. RDW should emphasize that anything that happens should go through ICTNS. A clear process should be defined that facilitates the updating of the database. PdB remarked that he ignores the Gold Book because of its internal inconsistencies and inconsistencies with other IUPAC documents or documents IUPAC has subscribed to and are not implemented in the Gold Book (and some others as well).

### 11.2. Green Book

(Has been dealt with in Agenda item 18.1.)

### 11.3. **Blue Book**

RDW reported that he edited the final version on behalf of ICTNS. GM said that the Blue Book is a camera-ready word document of 1456 pages + preliminaries + index. Indexing is not solved yet. It is unclear what the contract indicates. This might cause a delay.

### 11.4. **Purple Book**

GM reported that the contract for the 2009 edition of the Purple Book with RSC expires. There is an intention of the Division to make the chapters available online from that time onwards. There is also an intention to augment that with recommendations that appeared since that time. There seems to be no intention to publish a new version of the Purple Book at this time. JS added that with the Green Book, it has been negotiated that the copyright is not transferred to RSC Publishing but rather stays with IUPAC.

### 11.5. **Orange Book (BH)**

BH says that he will send minutes of their Orange Book meetings to ICTNS on a regular basis to make sure that ICTNS knows what is going on. The last available edition is the 3<sup>rd</sup> Edition from 1997. Currently there are 19 chapters of various sizes from 10 to 60 pages and in various formats including glossaries, diagrams *etc.* The new Orange Book becomes a vocabulary in glossary format (like the Gold Book) and requires a complete rewrite. A presentation was shown about the details related to this important IUPAC project (see *Attachment Agenda item 11.5*). Eleven chapters are planned with a task group Chair for each chapter and with separate funding. JS remarked referring to an example presented that a cross reference is – according to PAC style – written in italic font. This, however, is against IUPAC rules when for example  $\ln K_a$  is involved because  $\ln$  as a mathematical symbol must be in roman font. This might cause inconsistencies and should be resolved somehow (similar problems exist using bold faced typing to indicate cross references). GM suggested that colour is probably the best choice to resolve this and might be discussed with de Gruyter.

Many new terms will be created that have not (yet) been approved. It is suggested to review chapter by chapter to resolve those issues first. In some cases, even a recommendation must be formulated and submitted. It is unlikely that the Orange Book will be completed by the next GA in South Korea but a first version should be available. The project should be finished by the GA in 2017. BH informed members that he started a new project with M. Kinnan to database the OB to show and explore how to do this. The question was raised by BH whether we can in some cases adopt ISO standards and what about the copyright. What if we want to change the definitions? JS explained the case made by ISO about the greek 'kappa' where ISO does not accept all the different writings shown in the Green Book. When there is disagreement between IUPAC (GB) and ISO recommendations, this is stated explicitly in a footnote. It is therefore suggested to go ahead and do what fits the needs of the OB.

### 11.6. **Silver Book**

No report received.

### 11.7. **Red Book**

GM commented that they looked into the document and the task group can learn from the experience of organising the update and revision of the Blue Book. A project on PINs is running (preferred IUPAC names) for inorganic compounds. The Red Book provides often more than one name for the same compound. Revision of the Red Book is in a very early stage and time of completion is not yet clear.

### 11.8. **White Book**

The White Book is more like a compendium of biochemical nomenclature and produced by IUPAC and IUBMB. GM believes it is a quite useful source. There is no clear procedure on how to produce and update the White Book. It is unclear what happens to it.

### 12. **Update on status of IUPAC approved books published outside IUPAC**

RDW will check what books are there by scanning the IUPAC projects. GM commented that these books must use IUPAC nomenclature when the book carries the IUPAC seal. Division VIII was particularly disturbed when a Technical Report from Division III came through to PAC and was published without using IUPAC names; *PAC* **85**(1), 307 (2013) was published without being reviewed by the organic nomenclature group. APR noted that she saw an early version of the manuscript but it was not clear at that time whether it was a TR or a REC. APR shall mark the incorrect statements and pass it on to RDW. He will approach the corresponding Division president. A prompt erratum must be published.

#### Action item 4

RDW is to prepare an erratum based on APR's corrections of *PAC* **85**, 307 (2013).

AG states that Manuscript Central can be used in a much better way. When a recommendation is submitted, it should be routed to all Division Presidents who approve or deny on the basis of the submitted reviews. The responsibility is with the Division. In the final stage of review it goes to ICTNS. MC should grant access to all members of the Division where the manuscript has been prepared and to all Division presidents. JS remarked that sometimes he suggests sending the manuscript to another Division feeling that there might be some inconsistencies, but this should not happen because all Division presidents should see the manuscript prior to publication and prior to submission to ICTNS. ICTNS is the final stage of reviewing.

It should be noted that the manuscripts should also go through the full reviewing process and also involve BH or PdB to check against VIM, for example. PdB commented that the implementation of IUPAC signed documents like VIM and GUM is poor. Is a project needed to define how to implement such documents? RDW recalled that the Bureau informed all the Division Presidents in written form (and it is in the minutes) that they must follow the rules. JS suggested a 4-page version (brochure) of the Orange Book, the VIM, the GUM, similarly to the GB Brochure and some others. JM remarked that some of the papers (for example the traceability) are too complex to understand. BH stated there is a document called the "annotated VIM" which tackles these problems and a short summary might be a good project. PdB, BH, JS are volunteering to prepare such a document. Until GA 2015 in Busan, PdB will send an annotated VIM, which is already drafted. RDW suggested a first draft/layout by the off-year meeting next year in Zurich. JS will send an electronic version of the GB 4-page Brochure to BH, PdB, AG *etc.* RDW will attempt to arrange emergency funding for a project on a 4-page Brochure of the VIM and/or GUM. JM offered to be a reviewer for this project.

#### Action item 5

RDW will try to receive funding for a project on a 4-page Brochure of VIM/GUM.

### 13. **Membership 2014 to 2015**

Terms of TMs: JM (agreed), GM (agreed), JS (agreed), RDW (agreed). The term for Monica Nordberg ends 31 Dec 2013. Therefore one position is open as TM. RDW to ask

Jeremy Frey to fill vacancy.

Terms of AMs: Three positions permitted as AM: J. Kaiser, Hiroshi's term ends, Amelia Rauter will become Division VIII representative on ICTNS. Two AM positions are open, should be someone with funds available (Ingbar Johansson, Sweden; Rene Dybkaer; Rita Cornelis, Belgium; Milan Drabik, Slovakia ) RDW is to invite individuals and clear with Paul Leclair.

#### 14. Other business

##### 14.1. Note on the definitions of concepts in science (JM)

Division V Secretary approached JM to write a document about what to do and what not to do upon writing a manuscript for PAC. Such a kind of document (see *Attachment Agenda item 14.1.*) might be useful for ICTNS as guidance to authors before they start writing for PAC and other members of Division V (for example BH) are prepared to help.

##### 14.2. Comments on TRs and RECs (NH)

It is in the minutes from the Lisbon meeting that JS sent around seemed to indicate that the Committee was in favour of making the atomic weight report and the report on isotopic composition into recommendations. NH consulted the IUPAC guidelines which state that documentation and critical evaluation of data constitute a technical report (see *Attachment Agenda item 14.2.*).

##### 14.3. Comment by JM

JM referred to a paper just appeared in Nature Chemistry (Thornton, Burdette (2013) "The ends of elements", Nature Chemistry 5: 350-352 [doi:10.1038/nchem.1610]) which might be important when new elements 117 and 118 will be named soon. We should know and read it.

##### 14.4. Comment by GM

Having several hats on, GM would like to come back to Agenda item 10.3 for completion.

#### 15. Chair initiated discussion: Overview of ICTNS

Nothing to be added. Concerning the special responsibilities of ICTNS, see Agenda item 2.0 and the referred document circulated in advance of this meeting. The increased responsibilities should be reflected in the financial funds available to ICTNS.

#### 16. Adjournment

The Chair RDW thanked the attendees for the lively and extensive discussions. An off-year meeting will probably be held in Zürich 2014. Some discussion needs to be held about the rather inadequate funding for ICTNS (ca. 4000 USD), perhaps with permission to overdraw.

## **Joint Meeting between ICTNS and Commission I.1 (IUPAC Green Book)**

### **17. Opening remarks and introduction of participants**

Members present were JM, BH, APR, GM, RDW, JS, BJ, AG, and new members joint for this meeting Roberto Marquardt (RM), Yvonne C. Martin (YM) as AM of Division VII, Jim McQuillan (JMQ), Robert Hinde (RH) and Yutaka Kuroda (YK).

### **18. Approval of Agenda**

The Agenda was approved. RDW informed members about a suggestion by JM concerning the appropriateness of having a statement within the IUPAC rules and guidelines that if anyone has an official role to play in IUPAC, we must not to go outside IUPAC and communicate with the press or online if we disagree with a policy matter. This has already been discussed with the Secretary-General R. Deplanque and RDW will prepare a short paragraph that will go to the Executive Committee this week. Another item concerned a meeting between the Presidents of Division I, II and V regarding a new project. The Guidelines were agreed and laid out and the project would launch a Technical Report about the *mole*, the *kilogram*, the *number of entities* and the *amount of substance* to see what the membership has to say. No TR or REC has been prepared by IUPAC on this issue in the past. ICTNS never addressed the issue of *amount of substance* although asked to do that. The President of Division I will take that item to the Bureau and RDW will prepare a supporting statement on behalf of ICTNS to the Bureau. A conclusion should be reached and presented at the Busan IUPAC GA in 2015.

#### **18.1. Green Book**

RDW informed members that some additional pressure has been put on Commission I.1 and on ICTNS. The UN, UNESCO and EU have adopted the IUPAC system of nomenclature, terminology and units as their official legal position. Customs documents must conform to IUPAC standards. We therefore need extensive consultation and as much flexibility as we can afford under these circumstances. JS asked about the costs caused by the potential additional work needed to provide the GB as a legal document. RDW commented that there are no additional costs. We continue to do our work as we did in the past. RM added that great care has been put into the GB in incorporating IUPAC recommendations published in PAC. This also places additional responsibility to any task group within IUPAC working on recommendations. If a request from outside (for example a custom authority) requires some additional work by Commission I.1 or other task groups, the Secretary-General should make sure that financial compensation is granted to IUPAC by the authority. JS summarized the current status of the GB: the first printing of the 3<sup>rd</sup> Edition was published in 2007, the second corrected printing of the 3<sup>rd</sup> Edition appeared in 2008 and a third printing was published in 2011 without any further corrections beyond the 2008 printing; this was decided by RSC without consultation so no corrections could be applied. The second printing is also available as a downloadable searchable PDF version from IUPAC webpage. A project proposal for the fourth printing of the 3<sup>rd</sup> Edition was prepared and submitted; it is expected to have this version available by the end of 2013. Since no major changes are applied, no reviewing process is needed. There are other suggestions to extend the Green Book with various chapters or

sections by various Divisions requiring major changes and this will be done in a 4<sup>th</sup> Edition. A task group has been assembled and a meeting is planned around the time we meet to finalize the fourth printing and a corresponding project has been submitted. A project proposal for the 4<sup>th</sup> Edition should be formulated with provisional end in about four years after project start. It was reported that there are difficulties finding the proper electronic version of the Green Book. RM noted a CPEP meeting this morning; it is desirable to have someone from each committee look into the website regularly and report troubles *etc.* to Bryan Pearson at the Secretariat (with cc to Fabienne Meyers) who is in charge for changes of the website. For Commission I.1, it is the Secretary RH who will do this for example. Technical difficulties with the IUPAC website arose because the data were located on many servers around the world and they will now be merged at one commercial location in the US. This should make it easier to maintain the website. RDW quoted from the Bureau meeting of spring 2013: "... the entire process (of moving the website to the US) should be completed by June 2013. ... The action from that action was for CPEP to develop a website development plan and invite CPEP Chair to present the development plan." This has not yet been done.

JS noted that the off-year meeting of Commission I.1 will be held in Zürich by the time when Division I meets in Zürich. RDW suggested to check whether one can combine this also with an ICTNS off-year meeting.

RDW explained the case of a Recommendation and a Technical Report that are now in the system. JS explained that he met with R. Guidelli and showed him the equations which do not show the correct units. RG could not answer the queries and resolve the issues immediately. The first draft of the manuscript suggested that the GB contained an incorrect equation defining the transfer coefficient and removing the old equation (as appeared in the 2<sup>nd</sup> Edition) which was correct. It was explained that all changes in the GB, especially in the section dealing with electrochemistry, were made by the former Electrochemical Commission and not by the GB responsible authors. Potential inconsistencies are therefore inconsistencies caused by the respective community. However, it is believed that this can be sorted out in due course.

Jim McQuillan advised the author when he approached Division I that the scope of the task group was to resolve confusion in the literature about this fundamental quantity in electro-kinetics. JS replied that the GB would have solved this problem by offering both equations (according to an opposing referee, the equation currently shown in the GB does not cause confusion when properly applied) and stating that there is no complete agreement providing corresponding references.

18.2. **PAC-REC-12-08-01R1**: Defining the transfer coefficient  
(see below)

18.3. **PAC-REC-12-08-03R1**: Defining the transfer coefficient: Assessment of IUPAC. Both manuscripts have been reviewed and two reviewers are very critical about the content blaming the Green Book for having changed the definition of the transfer coefficient in an inconsistent way.

It was mentioned by JS that all the changes from the 2<sup>nd</sup> Edition to the 3<sup>rd</sup> Edition were in accordance with the former Electrochemical Commission and no objections were raised. One reviewer from the electrochemical community did not see any problem with the current definition in the GB and recommended against publication. After revision, he changed his mind and supported the publication. The second

negative reviewer referred to inconsistencies with the units and JS will resolve this problem with the leading author of the two publications. JS suggested formulation of an example where the major difference between the current definition and the definition put forward by the new recommendation are highlighted. Concerns were raised about the long review process and action should be taken to speed up the publication.

#### 18.4. **Periodic Table**

Details about the periodic table were presented under Agenda item 9.2. JS noted that the CI publication 2011 (July-August issue) on the periodic table is erroneous in the examples given: “The atomic weight of an element is calculated from the sum of the products of the atomic mass and the isotopic abundance of each stable isotope of that element ...  $^{12}\text{C} = 12$  and  $^{13}\text{C} = 13$  ... The approximate atomic weight for ... would be  $12 \times 0.99 + 13 \times 0.01 = 12.01$ .”

This section violates many IUPAC rules: (a) The first part shows clearly that the sum of masses weighted by isotope abundances gives a mass; (b) An element symbol,  $^{12}\text{C}$ , must not appear in a mathematical equation; (c) The last example sums relative atomic masses (also called atomic weight). JS will contact NH and suggest a correction. It is to be noted that this publication was not reviewed by ICTNS. JM suggested that articles appearing in CI should also go through ICTNS reviewing.

#### 18.5. **Other**

RDW restated that one must make sure that the technical matters (formatting, fonts *etc.*) are untouched by the new publisher in all IUPAC publications. In view of the change in publisher, great care must be taken concerning the colour book contracts, the respective Commissions should be involved when new contracts with de Gruyter are discussed/formulated. For example, Commission I.1 (Green Book) is happy with RSC and the special contract allowing it to distribute a PDF freely one year after publication of the printed book. RSC published the Green Book in camera-ready form, just the title page and the cover were redone by RSC Publishing. AG recalls difficulties when trying to publish IUPAC documents with Elsevier, refusing to use italics font for physical quantities. They insisted on typesetting from scratch. RM reported from the CPEP meeting where he made the point of negotiating an ideal contract with RSC. Martensen (Chair CPEP) stated that no change of the Publisher would be done without consulting the Commissions. Currently they are looking into a better platform from de Gruyter for web versions of books.

PAC will receive a new Editor and will be published with de Gruyter, similarly CI where Fabienne Meyers keeps responsibility.

RDW closed the session between ICTNS and Commission I.1. ICTNS members will reconvene after a short break and continue with Agenda item 9.4.