

# International Union of Pure and Applied Chemistry

Secretariat: P.O. Box 13757, Research Triangle Park, NC 27709-3757, USA  
TEL: +1-919-485-870 FAX: +1-919-485-8706 EMAIL: secretariat@iupac.org

## Minutes of the ICTNS meeting at the IUPAC GA 2007, Torino, Italy, August 7<sup>th</sup> and August 8<sup>th</sup>, 2007

### 1 Opening

Prof. Bernardo J. HEROLD, secretary of ICTNS, welcomed members and visitors to the meeting of ICTNS at 9:15 on August 7<sup>th</sup>, 2007. Prof. HEROLD forwarded greetings from Prof. J. W. LORIMER, Chair of ICTNS, who was unable to attend the meeting for health reasons. Prof. Anders THOR expressed his wishes for a rapid recovery of Prof. LORIMER, and all present members joined this expression. Prof. HEROLD will be Chair of the Meeting. Prof. MARQUARDT will take charge of recording the minutes.

The following persons signed as present (acronyms used later in this report, as well as acronyms indicating their relation to ICTNS are given in parentheses):

Prof. Bernardo J. HEROLD (*BH*, Secretary ICTNS),  
Dr. Ture DAMHUS (*TD*, TM ICTNS),  
Prof. Roberto MARQUARDT (*RM*, TM ICTNS),  
Dr. Alan MCNAUGHT (*AM*, TM ICTNS),  
Prof. Hiroshi OGINO (*HO*, AM ICTNS),  
Prof. Ron WEIR (*RW*, REP DIV I),  
Prof. John CORISH (*JC*, REP DIV II),  
Prof. Amélia P. RAUTER (*AR*, REP DIV III),  
Dr. Jaroslav KAHOVEC (*JK*, REP DIV IV),  
Prof. Włodzimierz KUTNER (*WK*, REP DIV V),  
Dr. John H. DUFFUS (*JD*, REP DIV VII),  
Prof. Josef NYTRAI (*JN*, REP DIV VIII),

Prof. Anders J. THOR (*AT*, REP ISO/TC 12),  
Mrs. Danièle GIBNEY (*DG*, OBS RSC),  
Prof. Jeremy FREY (*JF*, VISITOR DIV I),  
Prof. Leslie GLASSER (*LG*, VISITOR CPEP),  
Dr. Bedrich KOSATA (*BK*, VISITOR CPEP),  
Dr. Miloslav NIC (*MN*, VISITOR CPEP),  
Dr. Bohumir VALTER (*BV*, VISITOR CPEP).

The Agenda, which had been distributed before the meeting, including annexes can be found at <http://www.iupac.org/web/ins/027> under “Minutes, Torino, Italy, 7-8 Aug 2007, agenda”.

## 2 Minutes of Beijing meeting

The following comments were made with respect to the Minutes of the Beijing meeting:

*AT* has sent a report to Beijing (see item 9 below). *TD* has had comments that were not included in the Beijing minutes, namely with respect to the discussion about the kilogram and with respect to the guidelines for revision of draft manuscripts.

At this point, the meeting was interrupted to receive the visit of the four members of CPEP mentioned above under item 1. A rapid presentation of the current status of the “Gold Book”, the XML version of which is being maintained by CPEP, was made by Dr. KOSATA, who pointed out the occurrence of “small fixes”, and corrections of errors in PDF files. “All corrections were made following consultation with J. LORIMER” (*BK*). After the presentation, the following discussion took place:

*BH* confirmed that there has been an exchange of mails between CPEP and Prof. J. LORIMER. *LG* stresses the position of CPEP that, in the long term, the on-line documents will be the authority documents. *AM* indicates that important revisions are needed in the present version of the “Gold Book”. A discussion of this point is postponed to item 12 of the agenda. *AT* indicates the need for backtracking of corrections and cross-referencing modifications. *AM* answers that previous printed versions of the “Gold Book” allow for backtracking of modifications. *JK* adds to this point that he has experienced problems in the browsing and error processing of the on-line version of the “Gold Book”. *BK* explains that a backtracking system is implemented in the on-line version of the “Gold Book”. *RM* expresses the wish to have a discussion forum and FAQ web page for the on-line version of the “Gold Book”. *BK* answers, pointing out the spam problem and the related management problem of electronic media that would arise. *AM* suggests the implementation of a web page for new terms and an RSS<sup>1</sup> alert related to that. Technical and time delay problems related to this were mentioned. *WK* mentioned that the on-line version of the “Gold Book” should be appropriate for publishers and editors of dictionaries and glossaries.

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<sup>1</sup> RSS stands for "Really Simple Syndication". It is a way to easily distribute a list of headlines, update notices, and sometimes content to a wide number of people. It is used by computer programs that organize those headlines and notices for easy reading.

At this point, the visit from members of CPEP ended.

### **3 Business arising from the Beijing meeting**

As to the proposed series of explanatory articles on IUPAC base units, *RM* mentioned recent email exchanges between Profs. LORIMER, HEROLD, ATKINS and MILLS, and says that Prof. ATKINS would join the project, but not as a leader. *BH* says that P. MAHAFFY from CCE will be contacted in this matter, too.

### **4 Report to IUPAC Council**

*TD* pointed out that comments on the “Green Book” were not included in the report. *JF* said that a report from Commission I.1 is in preparation.

*AT* pointed out that he represents the ISO body “ISO/TC 12”, and not the whole ISO, as given in the report to IUPAC Council.

At this point, *JF* mentioned that many documents arriving from ISO do not reach IUPAC bodies for review. ICTNS is asked to request action from IUPAC secretariat to improve this situation. In this context, *AM* questions the mechanisms for receiving documents on the VIM (“Vocabulaire International de Métrologie”).

*TD* questioned the meaning of the term “conformability” on the 5<sup>th</sup> line of page 2 of the report. Also, it is dangerous to say, following *TD*, that, “the on-line version of the ‘Gold Book’ provides an opportunity for almost continuous update of IUPAC approved terminology, as well as corrections where necessary” (section 2.2 of the report). *RM* added to this remark that ICTNS should be more active in setting up guidelines for the update and correction of the on-line version of the “Gold Book”, as the contents of this book are really interdivisional subjects. This matter will be discussed during the visit of Prof. A. JENKINS, and under item 12.

*TD* questioned a certain ambiguity in the procedure for election of members to ICTNS. *BH* says that the present procedure is appropriate for IUPAC.

*TD* wishes to change the term “ligands” by the term “metals” in reference 21 of section 3.1.2 of the report. *BH* says that all changes should be sent to Prof. LORIMER.

*BH* acknowledges the excellent work ICTNS has done in the past two years, which allowed to reduce the backlog considerably; he thanks in particular all reviewers. In this context *JF* wishes to express his gratitude to ICTNS, in the name of all authors of the 3<sup>rd</sup> edition of the “Green Book”, for the efficient review process.

### **5 Items for PAC Editorial Advisory Board Meeting on 2007-07-08**

*AM* will represent ICTNS at the PAC Editorial Board Meeting and will report on the following:

As to the question of titles on references in PAC, *AM* proposes using a table of titles and references. *TD* always uses titles in references. *DG* says that, following the RSC titles should always be given. *JF* suggests adding the DOI (“Digital Object Identifier”), and *BH* suggests adding the ISBN to the reference, too. *TD* remarks that, depending on how the search algorithm is set up titles should be added.

Regarding the style guide for Conference Reports and Special Issues, *TD* remarked that the guidelines formulated by Division VIII for graphical representations should be used imperatively.

*BH* said that there is general agreement upon the changes made to the Guidelines for authors in the Handbook, but that there is a delay in making the changes in the on-line version.

*BH* finally asked *AM* to draw the attention of the PAC Editorial Board that Divisions have not been paying sufficient care to the scientific contents of submitted manuscripts. He reiterates that ICTNS often receives manuscripts that contain scientific errors, and that it is not the role of ICTNS to review scientific contents. *AM* and *JK* say that Division representatives should be in charge of this task. *BH* replies that not all Division representatives are really put in charge by their Divisions. *JD* remarks that there are difficulties for Division representatives to attend ICTNS meetings. *JC* recalls that these problems did not exist in times when Commissions were fully operative.

After the Editorial Board of PAC had met, *AM*, who had attended that meeting in the mean time reported the following: The Editorial Advisory Board of PAC was informed on the decision about the action to be taken by division presidents; as to the quality of documents, copies should be edited by Cheryl WURZBACHER prior to being downloaded for review; as to titles in PAC references, an exception is made for NMR material; all supplementary material should be made available by IUPAC, and by no other organization; as to the review procedure, it is up to the ICTNS to decide whether reviewed manuscripts are sent again for a second review or not.

## **6 Current status of manuscripts and other documents**

The current status of Technical Reports and Recommendations was discussed under item 4.

A power-point presentation is made of JCGM documents (“Joint Committee on Guidelines for Measurements”) to inform the members of the meeting: the VIM (see above) and GUM (“Guide to the Expression of Uncertainty in Measurement”). *AT* made comments on the presentation. There were no further comments.

The IUPAP and ISO project on terminology and nomenclature in nanotechnology was not discussed.

It was stated that authors must be reminded of their responsibility to watch for of internal consistency, mainly of glossary entries, with existing Recommendations. A specific discussion on this topic with respect to the “Gold Book” is reported under item 12.

Finally, the nomenclature problems between IUPAC and IFCC (the “International Federation of Clinical Chemists”) were treated. A letter from Prof. LORIMER, dated 2007-03-09, was read (agenda item 6.6). *JD* reports on the history of the problems and their origins: misunderstandings, lack of funding (in particular with IFCC), and lack of authority within Division VII. *JD* continued by saying that it is generally agreed now, that the SC-NPU database needs revision, which is an on-going project between DIV VII and SC-NPU, and that the most recent SC-NPU publication (PAC-REP-04-10-25) is already a good result.

*BH* addressed the discussion on safety issues related to toxics: non-IUPAC names should be kept in addition to IUPAC names, which is supported by *AM* (“education goes step by step”); *JD* thanks *JL*, *BH* and *AM* for tolerance; *JK* says that all names should be accompanied by IUPAC names; *BH* says that care must be taken about trivial names that look similar to systematic names.

In this context *JF* asked whether the WHO has agreed upon nomenclature in clinical chemistry; *BH* explained that IUPAC only recommends and that the WHO does not always approve IUPAC names; *AM* explained further that the WHO is advised by authors from the “Blue Book” and by the current president of IUPAC Division VIII. *AM* noted that authority on bio-chemical names is with the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature.

## 7 Publicity for ICTNS

There has been no evolution on this topic since the last ICTNS meeting. Who writes a material for publicity? It is suggested that Mrs. Danièle GIBNEY (*DG*), present at the meeting as an observer for the RSC, should write an appropriate publicity text, describing the nature of ICTNS and its relation to PAC.

## 8 Reports from IUPAC Divisions

Division reports have been added to the agenda.

Div I report was presented by *RW* who underlined the publication of the 3<sup>rd</sup> edition of the “Green Book”. In this context *RM* addressed the question of ownership of documents and materials and pointed out to the necessity for having guidelines ruling this issue.

Div II report was presented by *JC*; on page 44 of the agenda, attachment 8, the year “2006” should be “2005”. A discussion followed about current translation projects of the “Red Book” under the auspices of National Adhering Organizations: *BH* mentioned the existence a team of Portuguese and Brazilian chemists working on a translation which would be acceptable in any of both countries as well as in other countries with Portuguese as an official language; *TD* said that the Spanish translation of the “Red Book” looks similar to the English version; *RM* proposed that quite generally translated work of IUPAC documents should be supervised by IUPAC; *JF* says that the symbol “Rg” must not be used for “real gas”.

Div III report has been prepared and was presented by *AR* who is representing this division without being a member of it. *AM* has notified ICTNS that Div II and Div III seem to have little activity on terminology and recommends that more projects from these groups should be made to serve as inputs to the “Gold Book”. *JN* pointed out to the work on nomenclature for Rotaxanes (PAC-REC-05-12-09).

Div IV report was presented by *JK*; there was no following discussion.

Div V report was presented by *WK*, who commented on the work of project-oriented commissions; no time remained for discussion.

Receipt of Div VI report is acknowledged, but in absence of any representative of this division, a discussion on this report was postponed.

*JD* presented Div VII report. There was no further discussion apart from that mentioned under item 6.

Div VIII report was presented by *JN*. *BH* requested explanations with respect to nomenclature of Rotaxanes and *TD* had a question related to stereochemistry and coordination numbers. Furthermore, *TD* addressed the question on the review of the online version of the “Blue Book”; he stated that there should be a compromise between speed and accuracy.

The presentation of reports from the divisions was interrupted by a **visit of Prof. Aubrey JENKINS**, who reported on the status of the “Gold Book”. It is stated that a new commission should be formed, formally as an ICTNS project that would take care of the “Gold Book”. *AM* underlines the need for such a formal group and points out to three major tasks this group should consider: collection, correction and inclusion of new definitions. As an example for problems appearing in the “Gold Book”, *RM* mentions the entry for “donor number” (see also attachment 12 of the agenda). On behalf of ICTNS, and in contact with Prof. JENKINS, *RM* is asked to write a project for a task group meeting at the next General Assembly in 2009; names of potential members to integrate this group are expected to be sent from the divisions.

## 9 Reports from Other International Organizations

No written reports from other international organizations were available.

Reports not received in time to be discussed at the meeting can be found at <http://www.iupac.org/web/ins/027>, under “Minutes, Torino, Italy, 7-8 Aug 2007, other reports”.

*AT* represents unofficially BIPM (“Bureau International des Poids et Mesures”). He reported on the 8<sup>th</sup> edition of the SI brochure which is published simultaneously in English and French, and on activities of CCU (“Consultative Committee on Units”) related to new definitions of base units, which are currently being discussed at the CGPM (“Conférence Générale des Poids et Mesures”) and the JCGM (as reported

above under item 6). *WK* addressed the question as to the use of the period or the comma as decimal separator. *AT* answered that the CGPM resolution 10 from 2003 establishes the rule, that both are acceptable, the period in publications in English, and the comma elsewhere.

Representing ISO/TC12 (“Technical Committee 12” of the “International Organization for Standardization”) and IEC/TC 25 (“Technical Committee 25” of the “International Electrotechnical Commission”), *AT* reported on the three-step procedure used to define base quantities and base units. In this context, *RM* and *AT* asked to rewrite the following in the middle of page 16 of the Beijing 2005 minutes (attachments items 2 and 3 of the agenda): “... of the ampere to fix, for example, the elementary charge, and of the kelvin to fix the Boltzmann constant...”. In case the kilogram is redefined, *AT* suggested introducing either of the units “gio” or “bes” to represent the currently used kilogram (for Giovanni Giorgi, the founder of the MKSA-system, or besman, the name of a special mass balance; the name of Berzelius has also been mentioned for the unit kilomole).

With respect to IUPAP, it is stated that no concerted interaction has taken place during the preparation of the “Orange Book” and IUPAP. The ICTNS chair is asked to recommend concerted action in future (in connection with Div V).

Present members agreed to follow the suggestion of D. SHAW and proposed to add the following under item 2 of the Recommendations section: “Division Presidents nominate 15 expert referees.”

Furthermore, Fabienne MEYERS will be requested to improve the access to guidelines for the preparation of documents and reports.

## 10 Review of the IUPAC on-line Handbook

The discussion concerns the Procedure for Publication of IUPAC Technical Reports and Recommendations as well as the Guidelines for Drafting IUPAC Recommendations.

*JK* requested that the use of parentheses on chemical names is recalled in the guidelines. While *BH* reminded that the duty of Division Presidents is to oversee changes in terminology. *RW* recalled that he addresses answers of authors to reviewers, including the revised documents. *AM* said reviewers should be asked whether they want to see all reviews.

*TD* asked quite generally: “What is our role as reviewers?”

*BH* asked the members to access the guidelines within the next few weeks, to read them and to send criticism to ICTNS officers before the end of the year.

*TD* also addressed the internal reviewing process within ICTNS: he commented that he has no other written rules for internal reviewing ICTNS procedures than those given in the message from Profs. J. LORIMER and B. HEROLD of 2006-02-01 to all of ICTNS (*doc060201*), and asked whether there are new versions of these guidelines. Although outside the scope of item 10, *TD* asked to include the following to these

minutes. Referring to 2.0.2, item 2 of document *doc060201*: *TD* asked whether it was still true that the system (Manuscript Central) stops sending out reminders after having received three reviews and whether -if yes- this may mean that certain reviewers may end up being ignored by the system (nobody replied). Referring to 2.0.2, item 3(i) of document *doc060201*: *TD* says that the rules are not clear. They state that reviewers should not submit reviews for the AE only, but also that the officers in general will send all reviews to the authors. It should be stated exactly how reviewers are to proceed. Referring to 2.0.3, item 4 of document *doc060201*: It is strongly suggested that at the end of the review period and when the authors have reacted to all reviews, the author's remarks and all reviews are shared with all the ICTNS reviewers. This would enable reviewers to check that their reviews have not been lost and have been taken properly into account. As a further general remark, *TD* suggests being much stricter with respect to the quality of the documents received by ICTNS. If they do not follow the guidelines for authors, it should be the right of ICTNS to return them without any further comment.

## 11 Update on status of “colour” books

*RM* briefly reported on the publication of the 3<sup>rd</sup> edition of the “Green Book”, which takes place timely with the present 44<sup>th</sup> IUPAC General Assembly.

With respect to the “Blue Book”, *AM* recalls that a preliminary version of the manuscript for the new edition was submitted 3 years ago, and that 15 persons have commented on the web board; 8 of 10 chapters are close to completion; the deadline to finish the work is April, 2008; the word processor used is MS-word.

*BH* reported on the history of the “Purple Book”, the list of publications, frictions, and reviewing processes on changes. The manuscript for the 2<sup>nd</sup> edition should be submitted for publication in September using an adopted (customized) reviewing procedure. *TD* suggested that Divs IV and VIII be asked to check the 2002 guidelines for authors with respect to polymer nomenclature on the IUPAC website [www.iupac.org/reports/IV/guide-for-authors.pdf](http://www.iupac.org/reports/IV/guide-for-authors.pdf).

The status of the “Orange Book” was presented by *WK* (see remarks under item 9). A discussion followed on word processing involving *RM*, *JD* and *WK*.

Regarding the “Silver Book”, members were informed that Prof. George FERRARS would be the leading person of the task group.

The “Gold Book” should have special attention at this meeting under item 12. However, due to lack of time, the discussion is rather short, reviewing mainly comments made under items 2, 6 and 8 above. *TD* stressed, however, that glossary entries must be checked for consistency (see item 6 above); furthermore, a list needs to be prepared for internal work using a template from the CPEP group. *RM* asks about the 2001-062-2-027 project; *AM* answered that it will be stopped by the end of 2007. In the context of the discussion on the “Gold Book”, *TD* asked *BH* about two emails sent on 2007-07-26 and 2007-02-15.

## 12 XML Gold Book

Due to lack of time, and because some discussion has already taken place as mentioned above under items 2, 6 and 8, this item was postponed.

## 13 Membership

The list compiled by Paul LE CLAIR contains errors; for instance, Prof. OGINO, AM to ICTNS, is paying by the Research Council of Japan.

The following names have been proposed as new division representatives:

Div I : Dr. John DYMOND  
Div II : void (not Prof. CORISH)  
Div III: void  
Div IV: Dr. Richard JONES  
Div V : Prof. Maciej JAROSZ (from Poland)  
Div VI: Dr. Peter FEDOTOV  
Div VII: Dr. John DUFFUS  
Div VIII: Prof. Josef NYTRAI

Division representatives should be division TM and paid from division funds; if not, an AM should be sent and paid for from division funds as well. ICTNS cannot accept that official members attend its meetings without financial support.

Associate members: *BH* mentioned that Dr. O'HARE cannot be contacted anymore by e-mail and that Prof. HWU, due to his academic duties, had apologized for not being able to attend the ICTNS meeting. *TD* suggested Sven HARNUNG, an associate professor at the University of Copenhagen ([harnung@kiku.dk](mailto:harnung@kiku.dk)). *AM* proposed Prof. Jeremy FREY. *BH* proposes Profs. Amélia RAUTER and Włodzimierz KUTNER as well as Dr. Jaroslav KAHOVEC as new AM or TM. *TD* informed ICTNS that he regrets to need to leave this body because of a too heavy working load. *AM* proposed the name of Jeffrey LEIGH to replace *TD*.

## 14 Future meetings

*TD* suggested that future meetings of this body should leave place and time to discuss experiences with problematic reviews, to be prepared in advance.

## 15 Adjournment

*RM* thanks *BH* for chairing this meeting, all members agree. The meeting was adjourned. On August 8 at 6.00 p. m.

## **Annexes:**

The **Agenda**, which had been distributed before the meeting, including annexes can be found at

<http://www.iupac.org/web/ins/027> under “Minutes, Torino, Italy, 7-8 Aug 2007, agenda”.

Reports of other international organizations not received in time to be discussed under item 9 can be found at <http://www.iupac.org/web/ins/027>, under “Minutes, Torino, Italy, 7-8 Aug 2007, other reports”.