INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

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Minutes of the ICTNS meeting at the IUPAC GA 2007, Torino, Italy, August 7th and August 8th, 2007

1 Opening

Prof. Bernardo J. HEROLD, secretary of ICTNS, welcomed members and visitors to the meeting of ICTNS at 9:15 on August 7th, 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. Wlodzimierz 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[1] 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.

[1] 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 5th 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 3rd 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 3rd 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 8th 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 3rd edition of the "Green Book", which takes place timely with the present 44th 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 2nd 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.

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). *AM* proposed Prof. Jeremy FREY. *BH* proposes Profs. Amélia RAUTER and Wlodzimierz 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 reveived 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”.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 5.1

Report to IUPAC Council

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) Biennial Report to IUPAC Council, August, 2007 to August, 2009

Executive Summary

During the biennium August, 2007 to August 2009, ICTNS continued its activities on behalf of IUPAC in reviewing and approving for publication 27 Technical Reports and Recommendations, resulting in 1127 published pages in *Pure and Applied Chemistry*. Three other publications reviewed by ICTNS emanated from international bodies of which IUPAC is a member. In addition, the new "Purple Book" was also reviewed by ICTNS before publication, and updates to the on-line "Gold Book" continued.

Two important changes concerning ICTNS were initiated. The first, to clarify the meaning of "manuscripts containing new experimental data", was suggested to the Secretary General, and new wording was supplied by him and approved by ICTNS. The second, to provide a mechanism for reviewing IUPAC-sponsored books for adherence to IUPAC standards of terminology, symbols, units and nomenclature, was the subject of a submission to the Bureau by ICTNS. The Bureau approved guidelines, and requested ICTNS to provide detailed wording, which is now under review.

ICTNS monitored and was consulted on IUPAC's interactions with international metrological societies on which IUPAC has representation.

ICTNS acted as a resource for the Secretariat in answering many questions received from a wide variety of students and professionals on terminology, symbols, units and general scientific questions.

1. ICTNS Biennial Report, August, 2007 to August, 2009

1.1 Terms of Reference of ICTNS

These include:

(a) To be responsible for submission to the Bureau/Council,…, for publication or otherwise, any IUPAC document concerned with terminology, nomenclature, symbols, and other conventions.

(b) Before recommending any material for publication as an IUPAC document, to ensure that full consultations have taken place, and the widest possible consensus has been reached among all Divisions and other bodies of the Union, and between IUPAC and other ICSU bodies, the international standardizing organizations, and the CGPM and its committees.

ICTNS is thus responsible for editing and approving the content of IUPAC Recommendations and Technical Reports for publication in *Pure and Applied Chemistry*, and also for approving, on behalf of IUPAC, publications emanating from international bodies on which IUPAC has representation. Editing of these publications is carried out by the respective organization.

ICTNS carries out these tasks by very extensive review processes. For IUPAC Recommendations, a Public Comment Period of five months is required, with input from ICTNS members within three months. Both Recommendations and Technical Reports are carefully scrutinized for conformability with

IUPAC-approved terminology and nomenclature, and are also edited carefully for scientific content. For documents whose source lies with international bodies, ICTNS also carries out careful reviews. The overall goal in these activities is to continue and enhance IUPAC's reputation as a source of international standards in chemical terminology and nomenclature through publication of *Pure and Applied Chemistry* and continuing interaction with international organizations.

Publication of 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.

ICTNS maintains up-to-date and detailed instructions of preparation of publications for *Pure and Applied Chemistry*. and also acts as a consulting resource for the Secretariat and other IUPAC bodies in replying to queries from professionals and students on problems in terminology and nomenclature.

The terms of reference require ICTNS to conduct, and advise the Executive Committee accordingly, all negotiations concerned with nomenclature and symbols with other ICSU bodies, with international standardizing organizations, and with CGPM and its committees. This measure ensures that IUPAC views carry the fullest possible weight among other international organizations. In practice, ICTNS maintains contact with IUPAC representatives on these organizations and also through ICTNS members from the Bureau International des Poids et Mesures (BIPM), International Organization for Standardization (ISO), and the International Unions for Biochemistry and Molecular Biology (IUBMB), Crystallography (IUCr), Pharmacology (IUPHAR), and Pure & Applied Physics (IUPAP). For example, in 2007, ICTNS considered the advisability of recommending a proposal from CCU (Consultative Committee on Units of BIPM) re-define the SI base units in terms of atomic quantities.

2.0 Changes to Operating Procedures

ICTNS initiated two changes to operating procedures.

(1) Publication of IUPAC reports in journals other than *PAC,* and publication of reports that contain new experimental data

(2) Review of IUPAC-sponsored Books for Adherence to IUPAC Standards of Nomenclature, Terminology, Symbols and Units

This initiative arose from correspondence with the Executive of the ISCT (International Society for Chemical Thermodynamics). A submission was made to the Bureau to point out that there was no clear mechanism for carrying out this type of review, and to ask for instructions. The Bureau recognized that problem, and replied that the review should be conducted by ICTNS, wand added several instructions, but asked ICTNS to provide the final wording. A draft has been prepared and is under review.

J. W. Lorimer, Chairman

B. J. Herold, Secretary

2009-06-19

APPENDIX

2.0 Summary of Publications in *PAC* for the Period 1 June, 2007 to 31 July, 2009

The previous report covered the period to 31 May, 2007. Following the Manuscript Central reference number and the title, the name of the lead author(s) and the Division or other organization where the project originated are given.

PAC vol.	Total Articles			Technical Reports			Recommendations		
	number	pages	av. Pages	number	pages	av. pages	number	pages	av. Pages
77 (2005)	12	414	35	9	267	30	3	147	49
78 (2006)	13	354	27	8	168	21	5	186	37
79 (2007)	8	466	58	4	135	34	4	331	78
80 (2008)	12	463	39	6	168	28	6	295	48
81 (2009)*	9	353	39	6	148	25	3	205	68

*** to end of June, 2009**

2.1 Publications reviewed, edited and approved by ICTNS for publication in *Pure and Applied Chemistry*
Total Recommendations and Technical Reports: 27
Total pages published June, 2007 to June, 2009: 1120

2.1.1 IUPAC Recommendations
Total number: 13
Total pages published: 776

1. PAC-REC-06-04-02. IUPAC Glossary of Terms Used in Toxicology, 2nd ed. J. H. Duffus, M. Nordberg, D. M. Templeton - VII. . *PAC* **79** [7], 1153-1344 (2007). 192 pp.

2. PAC-REC-06-01-06. IUPAC Explanatory Dictionary of Key Terms in Toxicology. M. Nordberg, J. H. Duffus, D. M. Templeton. - VII). *PAC* **79** [9], 1583-1633 (2007). 51 pp.

3. PAC-REC-06-02-01. Definitions of Terms Related to the Structure and Processing of Inorganic and Polymer Gels and Networks, and Inorganic-polymeric Materials. J. Alemán, A. V. Chadwick, J. He, M. Hess, K. Horie, R. G. Jones, P. Ktatochvil, I. Meisel, I. Mita, G. Moad, S. Penczek, R. F. T,. Stepto. - IV. *PAC* **79** [10], 1801-1829 (2007). 29 pp.

4. PAC-REC-06-12-04. Further Conventions for NMR Chemical Shifts. R. K. Harris, E. D. Becker, S. M. Cabral de Menezes, P. Granger, R. E. Hoffman, K.W. Zilm. - I. *PAC* **80**[1], 59-84 (2008). 26 pp.

5. PAC-REC-06-12-03. Structure-based Nomenclature for Cyclic Macromolecules. W. Mormann, K.-H. Hellwig - IV. *PAC* **80**[2], 201-232 (2008). 32 pp.

6. PAC-REC-07-03-01 Glossary of Terms Related to Solubility. H. Gamsjäger, J. W. Lorimer, P. Scharlin, D. G. Shaw - V. *PAC* **80**[2], 233-276 (2008). 44 pp.

7. PAC-REC-07-02-0. Graphical Representation Standards for Chemical Structure Diagrams. J. Brecher - VIII. *PAC* **80**[2], 277-410 (2008), 134 pp.

8. PAC-REC-05-12-09. Nomenclature of Rotaxanes. A. Yerin, E. S. Wilks, G. P. Moss, A. Harada - VIII. *PAC* **80**[9], 2041-2068 (2008). 28 pp.

9. PAC-REC-07-02-02 Glossary of Terms Related to Kinetics, Thermodynamics and Mechanisms of Polymerization. S. Penczek, G. Moad - IV. *PAC* **80**[10], 2163-2193 (2008). 31 pp.

10. PAC-REC-08-05-02. Dispersity in Polymer Science. R. F. T. Stepto – IV. *PAC* **81**[2], 351-353 (2009) 3 pp.; Erratum *PAC* **81** [4], 779 (2009) (1 p.)

11. PAC-REC-08-07-09 Glossaary of Terms Used in Ecotoxicology. M. Nordberg, D. M. Templeton, O. Andersen, J. H. Duffus – VII. *PAC* **81** [5], 829-970 (2009) (142 pp.)

12. PAC-REC-04-10-14. Compendium of Terms Used in Pharmaceutics. E. Breuer, M. S. Chorgade, J. Fischer, G. Golomb – VI. *PAC* **81**[5], 971-999 (2009); (29 pp.)

13. PAC-REC-08-01-30. Glossary of Class Names of Polymers Based on Chemical Structure and Molecular Architecture. M. Barn, K.-H. Hellwich, M. Hess, K. Horie, A. D. Jenkins, R. G. jones, P. Kratochvil, W. V. Metanomski, W. Mormann, R. F. T. Stepto, J. Vohlidal, E. S. Wilks - IV. *PAC* **81** [6], 1153-1186 (2009) (34 pp.)

2.1.2 IUPAC Technical Reports
Total number: 14
Total pages published: 344

14. PAC-REP-06-04-09. Critically Evaluated Rate Coefficients for Free-radical Polymerization 6: Propagation Rate Coefficient of Methacrylic Acid in Aqueous Solution. S. Beuermann, M. Burbank, P. Hesse, F.-D. Kuchta, I. Lacik, A. M. van Herk - IV. *PAC* **79**[8], 1463-1469 (2007). 7 pp.

15. PAC-REP-06-07-05. Representation of Configuration in Coordination Polyhedra and the Extension of Current Methodology to Coordination Numbers Greater than Six. R. M. Hartshorn, E. hey-Hawkins, R. Kalio, G. J. Leigh - VIII. *PAC* **79**[10], 1779-1799 (2007). 21 pp.

16. PAC-REP-07-03-03 Performance Evaluation Criteria For Preparation and Measurement Of Macro and Microfabricated Ion-Selective Electrodes. E. Lindner, Y. Umezawa - V. *PAC* **80**[1], 85-104 (2008). 20 pp.

17. PAC-REP-06-01-06. Solute Movement if Soils with Potential Rapid By-pass Transport (Pesticide Movement in Soils) Actual title: Transport of Pesticides via Macropores. W. Kördel, H. Egli, M. Klein - VI. *PAC* **80**[1], 105-160 (2008). 56 pp.

18. PAC-REP-07-06-05 Chemists and the “Public”. P. Mahaffy, A. Ashmore, B. Bucat, Choon Do, M. Rosborough - CCE. *PAC* **80**[1], 161-174 (2008). 14 pp.

19. PAC-REP-07-10-04. Impact of Scientific Developments on the Chemical Weapons Convention M. Balali-Mood, P. S. Steyn, L. K. Sydnes, R. Trapp - International Advisory Board. *PAC* **80**[1], 175-200 (2008). 26 pp.

20. PAC-REP-07-07-03. Recommendations on the Measurement and Analysis of Results on Biological Substances with Isothermal Titration Calorimetry. F. P. Schwarz, T. Reinisch, H.-J. Hinz, A. Suratha - I. *PAC* **80**[9], 2025-2040 (2008). 16 pp.

21. PAC-REP- 08-01-12.. Protocols on Safety, Efficacy, Standardization and Documentation of Herbal Medicine. M. Mosihuzzaman, M. I. Choudhary - III. Received 2008-01-16. *PAC* **80**[10], 2195-2230 (2008). 36 pp.

22. PAC-REP-08-04-02. Immunological Effects of Mercury. M. Schwenk, R. Klein, D. M. Templeton – VI). *PAC* **81**[1], 153-167 (2009). 15 pp.

23. PAC-REP-08-05-01. Teaching High-temperature Materials Chemistry at University. G. Balducci, A. Ciccioli, G. de Maria, F. Hoda, G. M. Rosenblatt - II. *PAC* **81**[2], 299-338 (2009). 40 pp.

24. PAC-REP-08-07-22. Guidelines for Rheological Characterization of Polyamide Melts. D. J. Dijkstra – IV. *PAC* **81**[2], 339-349 (2009). 11 pp.

25. PAC-REP-08-06-05. The Use of Countercurrent Chromatography in Analytical Chemistry. A. Berthod, T. Mryutina, B. Spivakov, O. Shpigun, I. A. Sutherland – IV. *PAC* **81**[2], 355-387 (2009). 34 pp.

26. PAC-REP-08-09-21. Thermodynamic and Thermophysical Properties of the Reference Ionic Liquid 1-hexyl-3mrthyl(amidozolium) *bis*[(trifluoromethyl)sulfonyl]amide. Part 1. Experimental Methods and Results. K. N. Marsh, J. F. Brennecke, R. D. Chirico, M. Frenkel, A. Heintz, J. W. Magee, C. J. Peters, L. P. N. Rebelo, K. R. Seddon – I. *PAC* **81**[5], 781-790 (2009). 10 pp.

27. PAC-REP-08-09-22. Thermodynamic and Thermophysical Properties of the Reference Ionic Liquid 1-hexyl-3mrthyl(amidozolium) *bis*[(trifluoromethyl)sulfonyl]amide. Part 2. Critical Evaluation and Recommended property values. R. D. Chirico, V. Diky, J. W. Magee, M. Frenkel, K. N. Marsh – I. *PAC* **81**[5], 791-828 (2009). 38 pp.

2.2 Publications reviewed and approved by ICTNS for publication elsewhere than in PAC (Editing by respective organization)
Total number: 6

28. PAC-REC-04-04-03. IUPAC Recommendations 2005. *Nomenclature of Inorganic Chemistry* (the "Red Book"). Prepared for publication by N. G. Connelly, T. Damhus, R. M. Hartshorn. RSCPublishing, Cambridge, UK (2005).

29. PAC-REC-05-11-10. IUPAC Physical Chemistry Division. *Quantities, Units and Symbols in Physical Chemistry*. 3rd ed. (the "Green Book"). Prepared for publication by E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, A. J. Thor. RSC Publishing, Cambridge, UK (2007).

30. PAC-REC-04-05-02 *International Vocabulary of Metrology*, 3rd ed. (VIM3) BIPM/JCGM (2008). Accepted on behalf of IUPAC 2006-10-16. Available on BIPM web site: www.bipm.org/en/publications/guides/vim.html

31. PAC-REC-04-05-03 *Evaluation of Measurement Data - Supplement 1 to the Guide to the Expression of Uncertainty in Measurement (GUM). Propagation of Distributions Using a Monte Carlo Method.* BIPM/JCGM 100: (2008). Accepted on behalf of IUPAC 2007-04-26. www.bipm.org/en/publications/guides/gum.html

32. PAC-REC-07-08-26. *Evaluation of Measurement Data. An Introduction to the "Guide to the Expression of Uncertainty in Measurement" and Related Documents*. BIPM/JCGM (2008). Accepted on behalf of IUPAC 2007-11-05.

33. PAC-REC-05-10-23. IUPAC Recommendations 2008. *Compendium of Polymer Terminology and Nomenclature*(the "Purple Book"). Prepared for publication by R. G. Jones, J. Kahovec, R. Stepto, E. S. Wilks, M. Hess, T. Kitayama, W. V. Metanomski, with advice from A. Jenkins and P. Kratochvil, RSCPublishing, Cambridge, UK (2008).

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 5.2

Revisions to Terms of Reference and Procedure for Publication of IUPAC Technical Reports and Recommendations

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Revisions to Terms of Reference and Procedure for Publication of IUPAC Technical Reports and Recommendations

TERMS OF REFERENCE OF ICTNS

(i) To be responsible for submission to the Bureau/Council, in accordance with Bylaw 2.11, for publication or otherwise, any IUPAC document concerned with terminology, nomenclature, symbols and other conventions.

(ii) Before recommending any material for publication as an IUPAC document, to ensure that full consultations have taken place, and the widest possible consensus has been reached among all Divisions and other bodies of the Union, and between IUPAC and other ICSU bodies, the international standardizing organizations, and Conférence Générale des Poids et Mesures (CGPM) and its Committees.

(iii) To ensure, via each Division's Titular Member on ICTNS, that all documents for publication emanating from that Division have been subject to a satisfactory level of review of substantive material by the Division Committee.

(iv) To ensure that any considered IUPAC view shall carry the fullest possible weight among other international organizations, all negotiations on matters concerned with nomenclature and symbols with other ICSU bodies, with the international standardizing organizations, and with CGPM and its Committees, shall be conducted through ICTNS, which shall advise the Executive Committee accordingly.

(v) To be responsible, after consultation with all relevant bodies of IUPAC, for the official IUPAC comments on all documents on nomenclature, symbols, terminology and conventions sent to the Union for comment.

(vi) To advise the President and the Executive Committee on suitable persons for appointment as representatives of IUPAC on other bodies concerned with nomenclature, symbols and terminology.

CHANGES TO TERMS OF REFERENCE

1. Manuscripts submitted that contain original experimental work

Revised statement from the Secretary-General

Technical Reports and Recommendations resulting from IUPAC Projects should be published in Pure and Applied Chemistry. The procedure is described at http://www.iupac.org/reports/provisional/procedure.html. The Bureau has established a procedure to allow publication in other journals in exceptional circumstances where it can be demonstrated by the Task Group and the Division or Standing Committee that publication in another journal is in the best interests of IUPAC. Approval for such an exception should be requested by the Division President or Standing Committee Chair from the Secretary General. This request should of course explain why publication in another journal would be preferable to publication in Pure and Applied Chemistry.

One such exceptional instance might be the presentation of new experimental data more suited to publication in primary research journals related to the specific field of chemistry. In such a case, the Chair of ICTNS also has the right to decline publication in Pure and Applied Chemistry. However, IUPAC projects should deal with the standardization of experimental measurement, where reports in Pure and Applied Chemistry are appropriate, and not in the acquisition of new experimental data more suited to publication in primary research journals.

2. Review of IUPAC-sponsored books

From R. Weir: The agenda item that dealt with IUPAC labelled books and the need to ensure IUPAC units and recommendations are followed was discussed. All understood that the weak link in the current process lies only with some of the books (not all) that are produced as projects within Divisions.

The editor(s) of these books is supposed to ensure that the book conforms with IUPAC. Some do this faithfully and some do not. In some cases, the President of the Division may not see the book prior to its appearing in print. It is estimated that no more than three books per year are produced via the projects through the Divisions and some of these may already conform.

The following was decided by the Bureau.

1. The matter is one that is the responsibility of the ICTNS.
2. The protocol and procedures to ensure conformity are to be determined by ICTNS and sent to the Bureau for approval. This process is to be executed by E-mail as soon as possible and Bureau approval will be rendered by E-mail.
3. It was suggested that ICTNS consider tasking the Divisional member on ICTNS from where the book project emanates be tasked with identifying the items that do not conform. (This may have to be done in parallel with the ICTNS Chair). To avoid delays in producing the book, it was suggested that the ICTNS changes be conveyed to the book editor within the same time frame as the final technical editing is done, which does not involve ICTNS.
4. The various ideas all focused on a practical protocol that does not delay matters and does not impose a huge additional workload in the ICTNS.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 5.3.2

Divisional review of manuscripts for *PAC*

GUIDELINES FOR SUBMISSION OF IUPAC TECHNICAL REPORTS AND RECOMMENDATIONS (IUPAC WEB SITE, HANDBOOK):

A "**Technical Report**" is a report on the subject of a specific study, such as:

- compilations and critical evaluations of data, or of parameters and equations
- critical assessments of methods and techniques
- guidelines for the presentation of methods of analysis; or for the calibration of instruments
- determinations of specific elements or compounds in selected samples in special environments
- studies of the biodegradability of materials
- chemical process control aspects
- evaluations of properties of specific materials

A **"Recommendation**" results from studies on nomenclature, symbols, terminology, or conventions, and its purpose is to recommend for a specific field unambiguous, uniform, and consistent nomenclature and terminology, usually presented as:

- glossaries of terms for specific chemical disciplines
- definitions of terms relating to a group of properties
- nomenclature of chemical compounds and their classes
- terminology, symbols, and units in a specific field
- classifications and uses of terms in a specific field

In practice, bullets 1 and 4 are essentially indistinguishable.

Publication of Recommendations and a Technical Report as one paper is not allowed in *PAC*; the two have different DOIs (Digital Object Identifiers, used in electronic indexing).

1.0 Recommendations and Technical Reports Submitted Before 2004-01-01 and Not Published by current date – total 6

1.0.1 Recommendations Submitted Before 2004-01-01 and Not Completed or Accepted, or Abandoned by current date – total 4

67 X-ray emission analysis (Gohshi - V). JWL to Gohshi 2004-03-05 asking for report on status; reply from Gohshi indication revised ms will be supplied. Further reply to K. Powell reporting progress. No further information. Query to Div. IV 2006-04-05. Abandoned 2006-11-05.

1137 Exposure…Logbook Method (Olsen - VII). Comments sent JWL to BJH 2003-11-19. Reminder by BJH 2004-10-07. Another reminder 2005-04-21. Abandoned - notice from Div VII 2006-04-06.

PAC-REC-05-07-04 Use of the Terms "robust" and "rugged" and the Associated Terms "robustness" and "ruggedness" in descriptions of analytical procedures (Burns - V). Received 2005-07-15. Public comment period ends 2006-01-31. ICTNS comments by 2005-12-31. Ms being reconsidered by Div. V. New ms 2006-11-01 to Div. V. Abandoned 2008-02.

PAC-REC-08-09-20. Recommendations for Nomenclature and Databases for Biochemical Thermodynamics. (Albety – I). Received 2008-09-19. Rejected – does not follow requirements for an IUPAC Recommendation. Negative reviewers' reports at Division level.

1.0.2 Technical Reports Submitted Before 2004-01-01 and Not Completed or Accepted, or Abandoned by current date – total 2

81 Melt rheology (Plochocki - IV). 17 pages comments JWL to BJH 2003-11-03. Reminder by BJH 2004-10-07. Query to R. Stepto 2005-04-21. Query to Div. IV 2006-04-05.

878/PAC-REP-04-06-08 IR & Raman at High T, p (Heyns - I). Corrected ms requested 2002-09-04. Comments by BJH, TC, JWL sent 2004-06-22. New ms. sent to Secretariat 2005-10-15 as a pdf file. Author asked how he intends to proceed 2006-04. JWL produced 2 doc files from pdf by 2006-07-17. Abandoned 2008-09-19.

2.0 Recommendations Submitted Between 2004-01-01 and Current Date– total 32

2.0.1 Recommendations Submitted, Accepted and Published in PAC Between 2004-01-01 and Current Date– total 20

PAC-REC-05-08-11 XML-based IUPAC~Standard for Experimental, Predicted and Critically Evaluated Thermodynamic Data Storage and Capture (ThermoML) (Frenkel - CPEP). *PAC* **78**[3], 541-612 (2006). 72 pp.

PAC-REC-05-09-13 JCAMP-DX for EMR (Lancashire-CPEP). *PAC* **78**[3], 613-631 (2006). 19 pp.

PAC-REC-05-03-01 Graphical Representation of Stereochemical Configuration (Brecher - VIII). *PAC* **78**[10], 1897-1970 (2006). 73 pp.

PAC-REC-04-12-04 Terminology of Polymers Containing Ionizable or Ionic Groups and of Polymers Containing Ions (Kubisa - IV). *PAC* **78**[11], 2067-2074 (2006). 8 pp.

PAC-REC-06-01-01. Glossary of Terms Relating to Pesticides (Stephenson - VI). *PAC* **78**[11], 2155-2168 (2006). 14 pp.

PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions. Part A. The Suspension Effect. (Oman - V). *PAC* **79**[1] 67-79 (2007). 11 pp.

PAC-REC-05-10-26 Glossary of Terms Used in Photochemistry (Braslavsky - I, III). *PAC* **79**[3], 293-465 (2007), 173 pp.

PAC-REC-06-04-02. IUPAC Glossary of Terms Used in Toxicology, 2nd ed. (Duffus - VII). *PAC* **79**[6], 1153-1344 (2007). 192 pp.

PAC-REC-06-01-06. IUPAC Explanatory Dictionary of Key Terms in Toxicology (Nordberg - VII). *PAC* **79**[9], 1583-1633 (2007). 51 pp.

PAC-REC-06-02-01. Definitions of Terms Related to the Structure and Processing of Inorganic and Polymer Gels and Networks, and Inorganic-polymeric Materials (Jones - IV). *PAC* **79**[10], 1801-1829 (2007). 29 pp.

PAC-REC-06-12-04. Further Conventions for NMR Chemical Shifts (Harris - I). *PAC* **80**[1], 59-84 (2008). 26 pp.

PAC-REC-06-12-03. Structure-based Nomenclature for Cyclic Macromolecules (Mormann - IV). *PAC* **80**[2], 201-232 (2008). 32 pp.

PAC-REC-07-03-01 Glossary of Terms Related to Solubility (Shaw - V). PAC **80**[2], 233-276 (2008). 44 pp.

PAC-REC-07-02-0. Graphical Representation Standards for Chemical Structure Diagrams. (Brecher - VIII). *PAC* **80**[2], 277-410 (2008), 134 pp.

PAC-REC-05-12-09. Nomenclature of Rotaxanes (Yerin-VIII). *PAC* **80**[9], 2041-68 (2008). 28 pp.

PAC-REC-07-02-02 Glossary of Terms Related to Kinetics, Thermodynamics and Mechanisms of Polymerization (Moad - IV). *PAC* **80**[10], 2163-2193 (2008). 31 pp.

PAC-REC-08-05-02. Dispersity in Polymer Science(Stepto – IV). *PAC* **81**[2], 351-353 (2009) (3 pp.); Erratum *PAC* **81** [4], 779 (2009) (1 p.)

PAC-REC-08-07-09 Glossaary of Terms Used in Ecotoxicology (Nordberg – VII). *PAC* **81** [3], 829-970 (2009). 142 pp.

PAC-REC-04-10-14. Compendium of Terms Used in Pharmaceutics (Breuer – VI). *PAC* **81**[5], 971-999 (2009). (29 pp.)

PAC-REC-08-01-30. Glossary of Class Names of Polymers Based on Chemical Structure and Molecular Architecture (Vohlidal - IV). *PAC* **81** [6], 1153-1186 (2009). 34 pp.

2.0.2 Recommendations Submitted, Accepted and Published Elsewhere Between 2004-01-01 and Current Date-total 6

PAC-REC-04-04-03. Nomenclature of Inorganic Chemistry (Revised Red Book) (Connelly - II). RSCPublishing (2005).

PAC-REC-05-11-10. Quantities, Units and Symbols in Physical Chemistry, 3rd ed. ("Green Book") (Quack - I). RSCPublishing (2007).

PAC-REC-04-05-02 International Vocabulary of Metrology, 3rd ed. (VIM3) BIPM/JCGM (2008). Accepted on behalf of IUPAC 2006-10-16. Available on BIPM web site: www.bipm.org/en/publications/guides/vim.html

PAC-REC-04-05-03 Evaluation of Measurement Data - Supplement 1 to the Guide to the Expression of Uncertainty in Measurement (GUM). Propagation of Distributions Using a Monte Carlo Method. BIPM/JCGM 100: (2008). Accepted on behalf of IUPAC 2007-04-26. www.bipm.org/en/publications/guides/gum.html

PAC-REC-07-08-26. Evaluation of Measurement Data. An Introduction to the "Guide to the Expression of Uncertainty in Measurement" and Related Documents. BIPM/JCGM (2008). Accepted on behalf of IUPAC 2007-11-05.

PAC-REC-05-10-23 Compendium on Macromolecular Terminology and Nomenclature (The Purple Book), 2nd ed. (Jones - IV). RSCPublishing (2008).

2.0.3 Recommendations Submitted and Accepted Between 2004-01-01 and Current Date– total 0

2.0.4 Recommendations Submitted and Accepted, but Awaiting Final Manuscript Between 2004-01-01 and Current Date or Final Review by ICTNS – total 1

PAC-REC-07-09-39. Metrological Traceability of Measurement Results in Chemistry (de Bièvre - V). Manuscript reviewed; additional reviewers invited. Major revision received 2009-07-06.

2.0.5 Recommendations Submitted Between 2004-01-01 and Current Date but Under Review on Current Date– total 9

PAC-REC-04-10-24 Nomenclature of Cyclic Peptides (Moss - VIII). 2 reviews. Public comment period ends 2005-03-31. Asked for major revision, 2005-03-15. Reminded author 2006-10-30.

PAC-REC-04-11-03 Nomenclature of Organic Chemistry ("Blue Book") (Powell - VIII). Public comment period ends 2005-03-31. Complete revision underway.

PAC-REC-06-04-06. Standard Definitions of Terms Relating to Mass Spectroscopy (Murray - V). Submitted 2009-05-01. 5th revision under review.

PAC-REC-09-03-01. Explanatory Dictionary of Key Terms in Toxicology. Part II (Nordberg – VII). Submitted 2009-03-12. Under review.

PAC-REC-08-04-03. Terminology for Reversible-deactivation Radical Polymerization (Jones – IV). Submitted 2009-03-04. 1st revision under review.

PAC-REC-09-01-22. Convention for the Use of Units of Time in Earth and Planetary Sciences (Villa – joint IUPAC-IUGS). Revision received 2009-08-12.

PAC-REC-09-05-03. Glossary of Terms Used in Biomolecular Screening. (Proudfoot – VII). Received 2009-05-05. Under review.

PAC-REC-09-06-05. JCGM 106. Evaluation of Measurement Data. The Role of Measurement Uncertainty in Conformity Assessment. Received 2009-06-24. (JCGM/BIPM). Under review.

PAC-REC-09-07-03. JCGM 102. Evaluation of Measurement Data. Models with Varying Number of Output Quantities. Received 2009-07-10. (JCGM/BIPM). Under review.

3.0 Technical Reports Submitted Between 2004-01-01 and Current Date– total 37

3.0.1 Technical Reports Submitted, Accepted and Published in PAC Between 2004-01-01 and Current Date– total 25

PAC-REP-04-05-06 The International Harmonized Protocol for the Proficiency Testing of Analytical Chemistry Laboratories (Ellison - V). *PAC* **78**[1], 145-196 (2006). 50 pp.

PAC-REP-05-05-03 Guidelines for Calibration in Analytical Chemistry. Part 3. Uncertainty Estimation and Figures of Merit for Multivariate Calibration (Olivieri - V). *PAC* **78**[3], 633-661 (2006). 27 pp.

PAC-REP-04-04-04 NMR for pKs (Popov - V). *PAC* **78**[3], 663-675 (2006). 11 pp.

PAC-REP-05-09-16 (formerly PAC-REC-05-09-16) Guidelines for Terminology for Microtechnology in Clinical Laboratories (Wilding - VII). *PAC* **78**[3] 677-684 (2006). 6 pp.

PAC-REP-04-08-05 Standards, Calibration and Guidelines in Microcalorimetry. Part 2. Calibration Standards for Differential Scanning Calorimetry (Della Gatta-I). *PAC* **78**[7], 1455-76 (2006). 20 pp.

PAC-REP-06-03-01. Atomic Weights of the Elements 2005 (Wieser - II). *PAC* **78**[11], 2051-2066 (2006). 16 pp.

PAC-REP-05-12-12. Cytokine Profiles in Human Exposure to Metals (Templeton - VII). *PAC* **78**[11], 2155-2168 (2006). 14 pp.

PAC-REP-06-05-06. Education, Outreach and Codes of Conduct to Further the Norms and Obligations of the Chemical Weapons Convention (Pearson, Mahaffy - CCE). *PAC* **78**[11], 2169-2192 (2006). 24 pp.

PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions. Part B. Guidelines for Practical pH Measurements in Soil Suspensions. (Oman - V). *PAC* **79** [1] 81-86 (2007). 6 pp.

PAC-REP-04-10-25 Properties and Units in the Clinical Laboratory Sciences. Part XX. Properties and Units in Clinical and Environmental Toxicology (Duffus - VII). *PAC* **79** [1] 87-152 (2007). 66 pp.

PAC-REP-06-05-09. Chemical Speciation of Environmentally Significant Ligands. Part 2. The Cu^{2+} - OH^-, Cl^-, CO_3^{2-}, SO_4^{2-} and PO_4^{3-} Systems (Powell - V). *PAC* **79**[5]**,** 895-950 (2007). 56 pp.

PAC-REP-06-04-09. Critically Evaluated Rate Coefficients for Free-radical Polymerization 6: Propagation Rate Coefficient of Methacrylic Acid in Aqueous Solution (Lacik - IV). *PAC* **79**[8], 1463-1469 (2007). 7 pp.

PAC-REP-06-07-05. Representation of Configuration in Coordination Polyhedra and the Extension of Current Methodology to Coordination Numbers Greater than Six (Leigh - VIII). PAC **79** [10], 1779-1799 (2007). 21 pp.

PAC-REP-07-03-03 Performance Evaluation Criteria For Preparation And Measurement Of Macro and Microfabricated Ion-Selective Electrodes (Lindner, Umezawa - V). *PAC* **80**[1] 85-104 (2008). 20 pp.

PAC-REP-06-01-06. Solute Movement if Soils with Potential Rapid By-pass Transport (Pesticide Movement in Soils) Actual title: Transport of Pesticides via Macropores (Kördel - VI). *PAC* **80**[1] 105-160 (2008). 56 pp.

PAC-REP-07-06-05 Chemists and the “Public” (Mahaffy -CCE). *PAC* **80**[1] 161-174 (2008). 14 pp.

PAC-REP-07-10-04. Impact of Scientific Developments on the Chemical Weapons Convention (Sydnes - International Advisory Board). *PAC* **80**[1], 175-200 (2008). 26 pp.

PAC-REP-07-07-03. Recommendations on the Measurement and Analysis of Results on Biological Substances with Isothermal Titration Calorimetry (Schwarz I). *PAC* **80**[9], 2025-2040 (2008). 16 pp.

PAC-REP- 08-01-12.. Protocols on Safety, Efficacy, Standardization and Documentation of Herbal Medicine. (Mosihuzzaman - III). *PAC* **80**[10], 2195-2230 (2008) 36 pp.

PAC-REP-08-04-02. Immunological Effects of Mercury (Templeton – VI). Submitted 2008-04-02. Accepted with minor revision 2008-05-20. *PAC* **81**[1], 153-167 (2009). 15 pp.

PAC-REP-08-05-01. Teaching High-temperature Materials Chemistry at University (Balducci - II). Submitted 2008-05-01. Minor revision requested 2008-07-14. Further minor revision requested 2008-09-01. Accepted 2008-09. *PAC* **81**[2], 299-338 (2009). 40 pp.

PAC-REP-08-07-22. Guidelines for Rheological Characterization of Polyamide Melts (Dijkstra – IV). *PAC* **81**[2], 339-349 (2009). 11 pp.

PAC-REP-08-06-05. The Use of Countercurrent Chromatography in Analytical chemistry (Spivakov – IV). *PAC* **81**[2], 355-387 (2009). 34 pp.

PAC-REP-08-09-21. Thermodynamic and Thermophysical Properties of the Reference Ionic Liquid 1-hexyl-3mrthyl(amidozolium) *bis*[(trifluoromethyl)sulfonyl]amide. Part 1. Experimental Methods and Results. (Marsh – I). *PAC* **81**[5], 781-790 (2009). 10 pp.

PAC-REP-08-09-22. Thermodynamic and Thermophysical Properties of the Reference Ionic Liquid 1-hexyl-3mrthyl(amidozolium) *bis*[(trifluoromethyl)sulfonyl]amide. Part 2. Critical Evaluation and Recommended property values. (Chirico – I). *PAC* **81**[5], 791-828 (2009). 38 pp.

3.0.2 Technical Reports Submitted, Accepted and Published Elsewhere Between 2004-01-01 and Current Date-total 1

Reference Data for the Density and Viscosity of Liquid Aluminum and Liquid Iron (Assael - I). *JPCRD* **35**, 285-300 (2006). 14 pp.

3.0.3 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Not Published by Current Date– total 3

PAC-REP-07-12-06. Lymphocyte Subpopulations in Human Exposure to Metals (Templeton - VII). Accepted 2007-03-10.

PAC-REP-08-03-05. Discovery of Element 112 (Karol – II). Accepted 2009-

PAC-REP-09-03-02. Towards Definition of Materials Chemistry (Interrante – II). Sumbitted 2009-03-01. Accepted 2009-05-18.

3.0.4 Technical Reports Submitted and Reviewed but Not Accepted for PAC (but acceptable for publication elsewhere) Between 2004-01-01 and Current Date-total 3

PAC-REP-06-01-07. Structure and Properties of Polyester Elastomers Composed of poly(butylenes terephthalate) and poly(ε-caprolactone) (Takigawa - IV). Rejected for PAC, OK for publication elsewhere 2006-10-30.

PAC-REP-06-06-01. Structure and Properties of Polyamide-6 and 6/66 Clay Nanocomposites (Kim - IV). Rejected for PAC, OK for publication elsewhere 2006-11-02.

PAC-REP-07-09-47. Understanding the Compressive Behavior of Linear and Cross-linked Polyvinylchloride Foams (Allstaedt – IV). Rejected for PAC, OK for publication elsewhere.

3.0.5 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Awaiting Final Manuscript or Final Review by ICTNS– total 0

3.0.6 Technical Reports Submitted Between 2004-01-01 and Current Date and Under Review on Current Date– total 5

PAC-REP-008-03-06. Requirements for Specification for AnIML – Version 1.0 (Davies – CPEP). Submitted 2008-03-28.

PAC-REP-08-07-11. Thermochemistry of Chemical Reactions. II. Experimental methods for Determination of Bond Energies (Ribeiro da Silva - I). Div. I waiting for revised manuscript for Divisional approval.

PAC-REP-09-01-05. Correction for the ^{17}O Interference in $\Delta^{13}C$ Measurements when Analyzing CO2 with Stable Isotope mass spectrometry (Brand – II). Submitted 2009-01-10. Under review.

PAC-REP-09-03-04. Metals in Biological Systems and –omics. Guidelines for Terminology and Critical Evaluation of Analytical chemistry Approaches (Lobinski – V). Submitted 2009- Under review.

PAC-REP-09-03-05. Chemical Speciation of Environmentally Significant Metals with Inorganic Ligands. Part 3. The Pb^{2+} + OH^{-}, Cl^{-} , CO_3^{2-}, SO_4^{2-} and PO_4^{3-} Systems (Sjöberg – V). Submitted 2009-05-01. Under review.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 5.4

Current status of manuscripts in the review cycle, completed, published, in preparation

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Current status of manuscripts in the review cycle, completed, published, in preparation by 2009-07-31

The following is a list of the status of all TRs and Recommendations that were:

(a) submitted before 2004-01-05 but not completed by that date;

(b) submitted between 2004-01-05 and current date.

Sponsoring Division(s) or organization in parentheses after name of corresponding author.

Summary

PAC vol.	Total Articles			Technical Reports			Recommendations		
	number	pages	av. pages	number	pages	av. Pages	number	pages	av. Pages
77 (2005)	12	414	35	9	267	30	3	147	49
78 (2006)	13	354	27	8	168	21	5	186	37
79 (2007)	8	466	58	4	135	34	4	331	83
80 (2008)	12	463	39	6	168	28	6	295	48
81 (2009)*	9	353	39	6	148	25	3	205	68

*** up to 2009-06-30**

1.0 Recommendations and Technical Reports Submitted Before 2004-01-01 and Not Published by current date – total 6

1.0.1 Recommendations Submitted Before 2004-01-01 and Not Completed or Accepted, or Abandoned by current date – total 4

67 X-ray emission analysis (Gohshi - V). JWL to Gohshi 2004-03-05 asking for report on status; reply from Gohshi indication revised ms will be supplied. Further reply to K. Powell reporting progress. No further information. Query to Div. IV 2006-04-05. Abandoned 2006-11-05.

1137 Exposure…Logbook Method (Olsen - VII). Comments sent JWL to BJH 2003-11-19. Reminder by BJH 2004-10-07. Another reminder 2005-04-21. Abandoned - notice from Div VII 2006-04-06.

PAC-REC-05-07-04 Use of the Terms "robust" and "rugged" and the Associated Terms "robustness" and "ruggedness" in descriptions of analytical procedures (Burns - V). Received 2005-07-15. Public comment period ends 2006-01-31. ICTNS comments by 2005-12-31. Ms being reconsidered by Div. V. New ms 2006-11-01 to Div. V. Abandoned 2008-02.

PAC-REC-08-09-20. Recommendations for Nomenclature and Databases for Biochemical Thermodynamics. (Albety – I). Received 2008-09-19. Rejected – does not follow requirements for an IUPAC Recommendation. Negative reviewers' reports at Division level.

1.0.2 Technical Reports Submitted Before 2004-01-01 and Not Completed or Accepted, or Abandoned by current date – total 2

81 Melt rheology (Plochocki - IV). 17 pages comments JWL to BJH 2003-11-03. Reminder by BJH 2004-10-07. Query to R. Stepto 2005-04-21. Query to Div. IV 2006-04-05.

878/PAC-REP-04-06-08 IR & Raman at High T, p (Heyns - I). Corrected ms requested 2002-09-04. Comments by BJH, TC, JWL sent 2004-06-22. New ms. sent to Secretariat 2005-10-15 as a pdf file. Author asked how he intends to proceed 2006-04. JWL produced 2 doc files from pdf by 2006-07-17. Abandoned 2008-09-19.

2.0 Recommendations Submitted Between 2004-01-01 and Current Date– total 32

2.0.1 Recommendations Submitted, Accepted and Published in PAC Between 2004-01-01 and Current Date– total 20

PAC-REC-05-08-11 XML-based IUPAC~Standard for Experimental, Predicted and Critically Evaluated Thermodynamic Data Storage and Capture (ThermoML) (Frenkel - CPEP). *PAC* **78**[3], 541-612 (2006). 72 pp.

PAC-REC-05-09-13 JCAMP-DX for EMR (Lancashire-CPEP). *PAC* **78**[3], 613-631 (2006). 19 pp.

PAC-REC-05-03-01 Graphical Representation of Stereochemical Configuration (Brecher - VIII). *PAC* **78**[10], 1897-1970 (2006). 73 pp.

PAC-REC-04-12-04 Terminology of Polymers Containing Ionizable or Ionic Groups and of Polymers Containing Ions (Kubisa - IV). *PAC* **78**[11], 2067-2074 (2006). 8 pp.

PAC-REC-06-01-01. Glossary of Terms Relating to Pesticides (Stephenson - VI). *PAC* **78**[11], 2155-2168 (2006). 14 pp.

PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions. Part A. The Suspension Effect. (Oman - V). *PAC* **79**[1] 67-79 (2007). 11 pp.

PAC-REC-05-10-26 Glossary of Terms Used in Photochemistry (Braslavsky - I, III). *PAC* **79**[3], 293-465 (2007), 173 pp.

PAC-REC-06-04-02. IUPAC Glossary of Terms Used in Toxicology, 2nd ed. (Duffus - VII). *PAC* **79**[6], 1153-1344 (2007). 192 pp.

PAC-REC-06-01-06. IUPAC Explanatory Dictionary of Key Terms in Toxicology (Nordberg - VII). *PAC* **79**[9], 1583-1633 (2007). 51 pp.

PAC-REC-06-02-01. Definitions of Terms Related to the Structure and Processing of Inorganic and Polymer Gels and Networks, and Inorganic-polymeric Materials (Jones - IV). *PAC* **79**[10], 1801-1829 (2007). 29 pp.

PAC-REC-06-12-04. Further Conventions for NMR Chemical Shifts (Harris - I). *PAC* **80**[1], 59-84 (2008). 26 pp.

PAC-REC-06-12-03. Structure-based Nomenclature for Cyclic Macromolecules (Mormann - IV). *PAC* **80**[2], 201-232 (2008). 32 pp.

PAC-REC-07-03-01 Glossary of Terms Related to Solubility (Shaw - V). PAC **80**[2], 233-276 (2008). 44 pp.

PAC-REC-07-02-0. Graphical Representation Standards for Chemical Structure Diagrams. (Brecher - VIII). *PAC* **80**[2], 277-410 (2008), 134 pp.

PAC-REC-05-12-09. Nomenclature of Rotaxanes (Yerin-VIII). *PAC* **80**[9], 2041-68 (2008). 28 pp.

PAC-REC-07-02-02 Glossary of Terms Related to Kinetics, Thermodynamics and Mechanisms of Polymerization (Moad - IV). *PAC* **80**[10], 2163-2193 (2008). 31 pp.

PAC-REC-08-05-02. Dispersity in Polymer Science(Stepto – IV). *PAC* **81**[2], 351-353 (2009) (3 pp.); Erratum *PAC* **81** [4], 779 (2009) (1 p.)

PAC-REC-08-07-09 Glossaary of Terms Used in Ecotoxicology (Nordberg – VII). *PAC* **81** [3], 829-970 (2009). 142 pp.

PAC-REC-04-10-14. Compendium of Terms Used in Pharmaceutics (Breuer – VI). *PAC* **81**[5], 971-999 (2009). (29 pp.)

PAC-REC-08-01-30. Glossary of Class Names of Polymers Based on Chemical Structure and Molecular Architecture (Vohlidal - IV). *PAC* **81** [6], 1153-1186 (2009). 34 pp.

2.0.2 Recommendations Submitted, Accepted and Published Elsewhere Between 2004-01-01 and Current Date-total 6

PAC-REC-04-04-03. Nomenclature of Inorganic Chemistry (Revised Red Book) (Connelly - II). RSCPublishing (2005).

PAC-REC-05-11-10. Quantities, Units and Symbols in Physical Chemistry, 3rd ed. ("Green Book") (Quack - I). RSCPublishing (2007).

PAC-REC-04-05-02 International Vocabulary of Metrology, 3rd ed. (VIM3) BIPM/JCGM (2008). Accepted on behalf of IUPAC 2006-10-16. Available on BIPM web site: www.bipm.org/en/publications/guides/vim.html

PAC-REC-04-05-03 Evaluation of Measurement Data - Supplement 1 to the Guide to the Expression of Uncertainty in Measurement (GUM). Propagation of Distributions Using a Monte Carlo Method. BIPM/JCGM 100: (2008). Accepted on behalf of IUPAC 2007-04-26. www.bipm.org/en/publications/guides/gum.html

PAC-REC-07-08-26. Evaluation of Measurement Data. An Introduction to the "Guide to the Expression of Uncertainty in Measurement" and Related Documents. BIPM/JCGM (2008). Accepted on behalf of IUPAC 2007-11-05.

PAC-REC-05-10-23 Compendium on Macromolecular Terminology and Nomenclature (The Purple Book), 2nd ed. (Jones - IV). RSCPublishing (2008).

2.0.3 Recommendations Submitted and Accepted Between 2004-01-01 and Current Date– total 0

2.0.4 Recommendations Submitted and Accepted, but Awaiting Final Manuscript Between 2004-01-01 and Current Date or Final Review by ICTNS – total 1

PAC-REC-07-09-39. Metrological Traceability of Measurement Results in Chemistry (de Bièvre - V). Manuscript reviewed; additional reviewers invited. Major revision received 2009-07-06.

2.0.5 Recommendations Submitted Between 2004-01-01 and Current Date but Under Review on Current Date– total 9

PAC-REC-04-10-24 Nomenclature of Cyclic Peptides (Moss - VIII). 2 reviews. Public comment period ends 2005-03-31. Asked for major revision, 2005-03-15. Reminded author 2006-10-30.

PAC-REC-04-11-03 Nomenclature of Organic Chemistry ("Blue Book") (Powell - VIII). Public comment period ends 2005-03-31. Complete revision underway.

PAC-REC-06-04-06. Standard Definitions of Terms Relating to Mass Spectroscopy (Murray - V). Submitted 2009-05-01. 5th revision under review.

PAC-REC-09-03-01. Explanatory Dictionary of Key Terms in Toxicology. Part II (Nordberg – VII). Submitted 2009-03-12. Under review.

PAC-REC-08-04-03. Terminology for Reversible-deactivation Radical Polymerization (Jones – IV). Submitted 2009-03-04. 1st revision under review.

PAC-REC-09-01-22. Convention for the Use of Units of Time in Earth and Planetary Sciences (Villa – joint IUPAC-IUGS). Revision received 2009-08-12.

PAC-REC-09-05-03. Glossary of Terms Used in Biomolecular Screening. (Proudfoot – VII). Received 2009-05-05. Under review.

PAC-REC-09-06-05. JCGM 106. Evaluation of Measurement Data. The Role of Measurement Uncertainty in Conformity Assessment. Received 2009-06-24. (JCGM/BIPM). Under review.

PAC-REC-09-07-03. JCGM 102. Evaluation of Measurement Data. Models with Varying Number of Output Quantities. Received 2009-07-10. (JCGM/BIPM). Under review.

3.0 Technical Reports Submitted Between 2004-01-01 and Current Date– total 37

3.0.1 Technical Reports Submitted, Accepted and Published in PAC Between 2004-01-01 and Current Date– total 25

PAC-REP-04-05-06 The International Harmonized Protocol for the Proficiency Testing of Analytical Chemistry Laboratories (Ellison - V). *PAC* **78**[1], 145-196 (2006). 50 pp.

PAC-REP-05-05-03 Guidelines for Calibration in Analytical Chemistry. Part 3. Uncertainty Estimation and Figures of Merit for Multivariate Calibration (Olivieri - V). *PAC* **78**[3], 633-661 (2006). 27 pp.

PAC-REP-04-04-04 NMR for pKs (Popov - V). *PAC* **78**[3], 663-675 (2006). 11 pp.

PAC-REP-05-09-16 (formerly PAC-REC-05-09-16) Guidelines for Terminology for Microtechnology in Clinical Laboratories (Wilding - VII). *PAC* **78**[3] 677-684 (2006). 6 pp.

PAC-REP-04-08-05 Standards, Calibration and Guidelines in Microcalorimetry. Part 2. Calibration Standards for Differential Scanning Calorimetry (Della Gatta-I). *PAC* **78**[7], 1455-76 (2006). 20 pp.

PAC-REP-06-03-01. Atomic Weights of the Elements 2005 (Wieser - II). *PAC* **78**[11], 2051-2066 (2006). 16 pp.

PAC-REP-05-12-12. Cytokine Profiles in Human Exposure to Metals (Templeton - VII). *PAC* **78**[11], 2155-2168 (2006). 14 pp.

PAC-REP-06-05-06. Education, Outreach and Codes of Conduct to Further the Norms and Obligations of the Chemical Weapons Convention (Pearson, Mahaffy - CCE). *PAC* **78**[11], 2169-2192 (2006). 24 pp.

PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions. Part B. Guidelines for Practical pH Measurements in Soil Suspensions. (Oman - V). *PAC* **79** [1] 81-86 (2007). 6 pp.

PAC-REP-04-10-25 Properties and Units in the Clinical Laboratory Sciences. Part XX. Properties and Units in Clinical and Environmental Toxicology (Duffus - VII). *PAC* **79** [1] 87-152 (2007). 66 pp.

PAC-REP-06-05-09. Chemical Speciation of Environmentally Significant Ligands. Part 2. The Cu^{2+} - OH^-, Cl^-, CO_3^{2-}, SO_4^{2-} and PO_4^{3-} Systems (Powell - V). *PAC* **79**[5]**,** 895-950 (2007). 56 pp.

PAC-REP-06-04-09. Critically Evaluated Rate Coefficients for Free-radical Polymerization 6: Propagation Rate Coefficient of Methacrylic Acid in Aqueous Solution (Lacik - IV). *PAC* **79**[8], 1463-1469 (2007). 7 pp.

PAC-REP-06-07-05. Representation of Configuration in Coordination Polyhedra and the Extension of Current Methodology to Coordination Numbers Greater than Six (Leigh - VIII). PAC **79** [10], 1779-1799 (2007). 21 pp.

PAC-REP-07-03-03 Performance Evaluation Criteria For Preparation And Measurement Of Macro and Microfabricated Ion-Selective Electrodes (Lindner, Umezawa - V). *PAC* **80**[1] 85-104 (2008). 20 pp.

PAC-REP-06-01-06. Solute Movement if Soils with Potential Rapid By-pass Transport (Pesticide Movement in Soils) Actual title: Transport of Pesticides via Macropores (Kördel - VI). *PAC* **80**[1] 105-160 (2008). 56 pp.

PAC-REP-07-06-05 Chemists and the “Public” (Mahaffy -CCE). *PAC* **80**[1] 161-174 (2008). 14 pp.

PAC-REP-07-10-04. Impact of Scientific Developments on the Chemical Weapons Convention (Sydnes - International Advisory Board). *PAC* **80**[1], 175-200 (2008). 26 pp.

PAC-REP-07-07-03. Recommendations on the Measurement and Analysis of Results on Biological Substances with Isothermal Titration Calorimetry (Schwarz I). *PAC* **80**[9], 2025-2040 (2008). 16 pp.

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PAC-REP-08-06-05. The Use of Countercurrent Chromatography in Analytical chemistry (Spivakov – IV). *PAC* **81**[2], 355-387 (2009). 34 pp.

PAC-REP-08-09-21. Thermodynamic and Thermophysical Properties of the Reference Ionic Liquid 1-hexyl-3mrthyl(amidozolium) *bis*[(trifluoromethyl)sulfonyl]amide. Part 1. Experimental Methods and Results. (Marsh – I). *PAC* **81**[5], 781-790 (2009). 10 pp.

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3.0.2 Technical Reports Submitted, Accepted and Published Elsewhere Between 2004-01-01 and Current Date-total 1

Reference Data for the Density and Viscosity of Liquid Aluminum and Liquid Iron (Assael - I). *JPCRD* **35**, 285-300 (2006). 14 pp.

3.0.3 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Not Published by Current Date– total 3

PAC-REP-07-12-06. Lymphocyte Subpopulations in Human Exposure to Metals (Templeton - VII). Accepted 2007-03-10.

PAC-REP-08-03-05. Discovery of Element 112 (Karol – II). Accepted 2009-

PAC-REP-09-03-02. Towards Definition of Materials Chemistry (Interrante – II). Sumbitted 2009-03-01. Accepted 2009-05-18.

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PAC-REP-06-01-07. Structure and Properties of Polyester Elastomers Composed of poly(butylenes terephthalate) and poly(ε-caprolactone) (Takigawa - IV). Rejected for PAC, OK for publication elsewhere 2006-10-30.

PAC-REP-06-06-01. Structure and Properties of Polyamide-6 and 6/66 Clay Nanocomposites (Kim - IV). Rejected for PAC, OK for publication elsewhere 2006-11-02.

PAC-REP-07-09-47. Understanding the Compressive Behavior of Linear and Cross-linked Polyvinylchloride Foams (Allstaedt – IV). Rejected for PAC, OK for publication elsewhere.

3.0.5 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Awaiting Final Manuscript or Final Review by ICTNS– total 0

3.0.6 Technical Reports Submitted Between 2004-01-01 and Current Date and Under Review on Current Date– total 5

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PAC-REP-08-07-11. Thermochemistry of Chemical Reactions. II. Experimental methods for Determination of Bond Energies (Ribeiro da Silva - I). Div. I waiting for revised manuscript for Divisional approval.

PAC-REP-09-01-05. Correction for the ^{17}O Interference in $\Delta^{13}C$ Measurements when Analyzing CO2 with Stable Isotope mass spectrometry (Brand – II). Submitted 2009-01-10. Under review.

PAC-REP-09-03-04. Metals in Biological Systems and –omics. Guidelines for Terminology and Critical Evaluation of Analytical chemistry Approaches (Lobinski – V). Submitted 2009- Under review.

PAC-REP-09-03-05. Chemical Speciation of Environmentally Significant Metals with Inorganic Ligands. Part 3. The Pb^{2+} + OH^{-}, Cl^{-} , CO_3^{2-}, SO_4^{2-} and PO_4^{3-} Systems (Sjöberg – V). Submitted 2009-05-01. Under review.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

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Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 6

Discussion of review of manuscripts, with examples

Part 1: Examples of missed items in reviews, J. W. Lorimer
Part 2: Review of nomenclature in manuscripts, B. J. Herold

Part 1

EXAMPLES OF MISSED ITEMS IN REVIEWS

J. W. Lorimer

1. PAC-REC-07-09-39. Metrological Traceability of Measurement Results in Chemistry (de Bièvre - V). Manuscript reviewed; additional reviewers invited. Major revision received 2009-07-06.

- contains many pages that have nothing to do with Recommendations

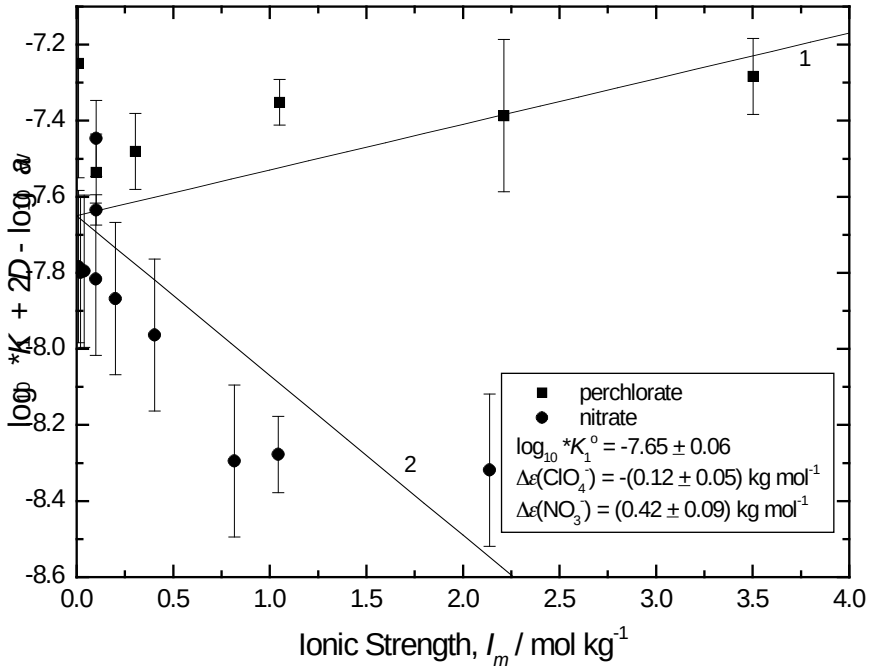
2. PAC-REC-04-10-14. Compendium of Terms Used in Pharmaceutics. E. Breuer, M. S. Chorgade, J. Fischer, G. Golomb – VI. *PAC* **81**[5], 971-999 (2009); (29 pp.)

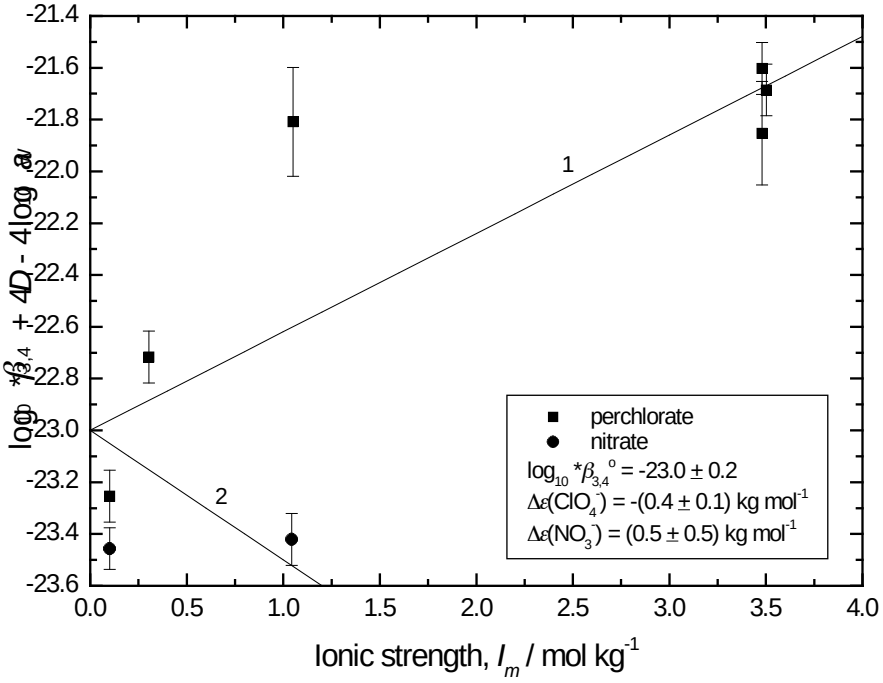
- absence of Abstract missed by all (including Editor)

3. General comments on nomenclature problems. – BJH

4. PAC-REP-09-03-05. Chemical Speciation of Environmentally Significant Metals with Inorganic Ligands. Part 3. The Pb^{2+} + OH^-, Cl^- , CO_3^{2-}, SO_4^{2-} and PO_4^{3-} Systems (Sjöberg – V). Submitted 2009-05-01. Under review.

- serious scientific error in plots

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3.0
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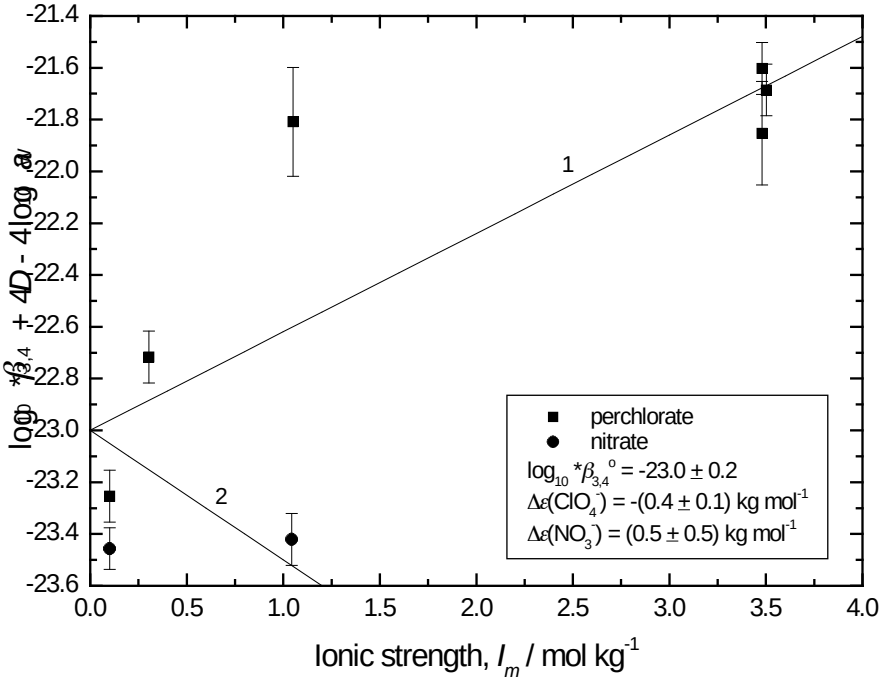
1
2
perchlorate
nitrate
log10 *β3,4° = -23.0 ± 0.2
Δε(ClO4-) = -(0.4 ± 0.1) kg mol-1
Δε(NO3-) = (0.5 ± 0.5) kg mol-1
log10 *β3,4 + 4D - 4log aw
Ionic strength, Im / mol kg-1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-23.2
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-23.6
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
1
2
perchlorate
nitrate
log10 *β3,4° = -23.0 ± 0.2
Δε(ClO4-) = -(0.4 ± 0.1) kg mol-1
Δε(NO3-) = (0.5 ± 0.5) kg mol-1
log10 *β3,4 + 4D - 4log aw
Ionic strength, Im / mol kg-1

Part 2

REVIEW OF NOMENCLATURE IN MANUSCRIPTS

Manuscripts from Divisions I to VII:

Most **recommendations and technical reports** of this origin do not pose any nomenclature problems at all with some rare exceptions. In those few cases where large numbers of compounds are quoted by their names (tables of properties, glossaries), there is however no major problem in replacing them, when necessary, by IUPAC names that are at least acceptable and to add preferred ones (PINs) in square brackets. We have always had competent reviewers to point out what names have to be changed and to make useful suggestions to that purpose.

When certain reviewers just comment that the nomenclature is sloppy, and do not make the corrections themselves, I was also able to suggest to the authors by myself alternative names. Sometimes I had the problem to mediate between “nomenclature fundamentalists” and authors of the polymer, analytical, medical or environmental community. I had then to explain to certain reviewers that common denominations, even if deprecated by IUPAC, sometimes cannot be dropped altogether, if they are widely used e. g. for toxic or otherwise dangerous substances. Safety comes before systematic perfection.

In tables of properties, the compounds often belong to a wide family of compounds. Authors like to use names, in such cases, where the common core of the structures appears in all names of the compounds of that family. This understandable wish leads often to names which are not compatible with certain IUPAC rules for acceptable names and even less so with the new rules for PINs. This can lead to long-winded arguments between authors and reviewers as well as between various reviewers. An editorial ruling can then become the only way to solve such cases eventually.

Manuscripts from Division VIII Nomenclature and Structure Representation:

Nomenclature recommendations for publication in PAC.

Appointment of reviewers: The same procedure as for any other recommendation.

Nomenclature Recommendations from Division VIII usually are impeccable as regards nomenclature itself. Objections from reviewers can be easily rebated. Problems can arise however regarding the terminology used in the wordings of the rules

Regarding terminology in nomenclature recommendations, there was e. g. the case of the use of "unsymmetrical" with a meaning different from that of "asymmetric" and

"dissymmetric", which regrettably already do not have the same meaning. In Romanic languages there would be a translation problem, because there are not enough synonyms for negative prefixes. This led to along discussion in a meeting of Division VIII, which I attended last year in Buedingen (near Frankfurt/Main). No consensus could be found for a replacement of "unsymmetrical" by another term. Andrey Yerin wants to submit a project dealing with the problem of symmetry in 2-dimensional and 3-dimensional structures. It is easy to solve if one uses mathematical terminology or symbols, but risks to lead to terms which are undecipherable for most chemists. The project would also deal with the terminology for symmetrical properties of assemblies of several molecules. The Gold Book forbids applying the definition of "asymmetric" to anything, which is not a molecule, as e.g. rotaxanes.

Another terminology problem, which surfaced recently, was that of "living" polymers. Again, no consensus was possible and an editorial ruling became necessary.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 7.1

Report from Division I
Physical and Biophysical Chemistry

Report by Dr. J.H. Dymond on Activities of the Physical and Biophysical Chemistry Division Committee in the Biennium 2007-2009

The Physical and Biophysical Chemistry Division (PBCD) has continued its activities in both physical and biophysical chemistry according to the charter of the division. For the biennium 2008-09, the Division has 24 projects running, with 8 nearing completion or recently completed, and 7 on-going interdivisional. These projects encompass different areas of physical and biophysical chemistry. They can conveniently be classified as follows:

(1) **"Colour" Book.** Following the publication of the third edition of the Green Book in August 2007, Division I supports two follow-on projects: (a) the underwriting of a student edition of the Green Book (project no. 2007-032-1-100) and (b) the preparation of the translation of the Green Book into six languages (German, French, Italian, Turkish, Japanese, Portuguese) (project no. 2008-007-3-100). IUPAC is supporting only the preparations in order to minimize errors in translation. This guarantees a virtually errorless translation and transcription of the symbols, formulas and units into a foreign language. Other languages into which the Green Book should be translated in high priority would be Spanish, Chinese and Russian. It remains to be seen to what extent the web may be involved in the dissemination of the content of the Green Book, either in its full version or as an abridged version of the forthcoming student edition.

(2) **Technical Reports and Recommendations**

(a) Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies (project no. 120/15/95). Format of final publication to be resolved.

(b) Spectroscopy under extreme conditions of temperature and pressure (project no.150/24/95)

(c) Electrochemical impedance spectroscopy - terminology, nomenclature and data exchange formats (project no. 2001-028-1-100) [main work complete- first draft being prepared]

(d) Thermodynamics and non-equilibrium criteria for development and application of supplemented phase diagrams (project no. 2003-036-2-100) [reports almost ready for submission to IUPAC]

(e) Categorizing hydrogen bonding and other intermolecular interactions (project no. 2004-026-2-100) [a draft report is ready for IUPAC]

(f) Recommendations for nomenclature and databases for biochemical thermodynamics (project no. 2006-023-3-100) [the authors have not yet decided which changes to make to the draft document to make it acceptable to IUPAC. However, it is likely that the draft document will be posted on the IUBMB web-site for public comment.]

(f) Liquid intrusion and alternative methods for the characterization of macroporous solids (project no. 2006-021-2-100)

(g) Wet surface vibrational spectroscopy experiments (project no. 2006-050-3-100) [on-going, progress slower than previously anticipated]

(h) Guidelines for reporting of phase equilibrium measurements (project no. 2007-024-2-100) [expected completion end-2009].

(i) Guidelines for modulated-temperature differential scanning calorimetry (MTDSC) (project no. 2007-002-1-100) [expected completion end-2009].

(j) Assessment of theoretical methods for the study of reactions involving global warming gas species degradation and by-product formation (project no. 2007-048-2-100)

(k) Ultrafast intense laser chemistry (project no. 2007-055-2-100)

1.1 (l) International harmonized protocol for standard preparation, irradiation and measurement for assuring metrological traceable results in neutron activation analysis (project no. 2007-010-2-500)

1.2 (m) Analysis of the usage of nanoscience and technology in chemistry (project no. 2007-040-2-200)

1.3 (n) Extension of ThermoML - the IUPAC standard for thermodynamic data communications (project no. 2007-039-1-024) [a draft on Biomaterials has been prepared]

1.4 ***(3) Critically Evaluated Data and the Creation and Maintenance of Physical and Biophysical Data Bases.*** *Projects include:*

1.5 (a) the Atmospheric Chemistry data base spanning all atmospheric processes except in the liquid phase (cloud and fog chemistry) (project no. 2007-001-2-100),

1.6 (b) the H_2O spectroscopic data base regarding line positions and line strengths of all known isotopomers of H_2O (project no. 2004-035-1-100),

1.7 (c) Continued compilation and critical evaluation of published thermodynamic properties, including the computation of accurate thermochemical data for selected free radicals, that are of importance in atmospheric and combustion chemistry (project no. 2003-024-1-100),

1.8 (d) Standard potentials of free radicals in solution (project no. 2001-015-1-100)

1.9 *(e) Heat capacity of liquids: critical review and recommended values for liquids with data published between 2000 and 2004 (project no. 2004-010-3-100) [completed]*

1.10(f) Critical evaluation of thermodynamic properties of hydrogen storage materials: metal organic frameworks and metal or complex hydrides (project no. 2008-006-3-100) [on-going]

1.11(g) Critical compilation of vapour liquid critical properties (project no. 2000-026-1-100)

[Part 12 in course of production]

1.12(h) A critical evaluation of the viscosity and density of molten copper and tin (project no. 2008-045-2-100)

1.13*(h) Establishing recommended data on thermodynamic properties of hydration for selected organic solutes (project no. 2004-036-1-100) [draft technical report in July 2010]*

1.14 ***(4) Publications of Monographs*** *authored by multiple experts offering detailed views into a field and describing the state-of-the-art provide a rapid and handy entry to complex fields of expertise. Examples are Climate and global change: observed impacts on planet earth (project no. 2007-050-2-600), Experimental Thermodynamics Vol. VIII. Applied Thermodynamics of Fluids (project no. 2008-014-1-100) [expected completion by June 2010] and Heat capacities of liquids and vapours (project no. 2007-059-1-100) [expected completion by end-2009].*

Completed Projects since The General Assembly in 2007:

1.15Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems (project no. 2002-005-1-100). IUPAC Technical Report published in Pure Appl. Chem., *2009, Vol. 81, No. 5, pp. 781-790 (part I) and Vol. 81, No. 5, pp. 791-828 (part 2).*

Future Energy: Improved, sustainable and clean options for our planet (project no. 2007-015-2-100). Elsevier 2008.

1.16Ionic liquids database (project no. 2003-020-2-100)

Kinetic Database (project no. 2005-044-1-100)

Titration Calorimetry (project no. 2001-030-1-100)

1.17NMR chemical shifts: updated conventions (project no. 2003-006-1-100)

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 7.2

Report from Division II
Inorganic Chemistry

Part 1, sent by Prof. Luis Oro

Part 2, presented by Prof. Jan Reedijk

Report on the activities Inorganic Chemistry Division during the biennium 2007 – 2009 related to ICTNS

During this period it has been a considerable discussion in support of retaining Wolfram as an alternative name. Conclusion:

Division II recommends that Division VIII consider going back to the designation tungsten (wolfram) for element 74, that was used in the 1990 edition of the Red Book

Recommendation from Inorganic Chemistry Division (From the Minutes of Committee Meeting in Helsinki, Finland on August 11-12, 2008).

Report on the use of Wolfram as an Alternative Name for Tungsten

As requested when this topic came up for discussion at our meeting in Torino, N. Holden agreed to look up the history of the naming of this element and to prepare a report for our information at the current meeting. This report is attached as Appendix. At our Torino meeting, Oro pointed out that wolfram had been removed as an allowed alternative name for element number 74 from the last edition of the "red book". This has caused some concern/frustration among the Spanish community, homeland of the discovers of this element, as recently described in Goya, P.; Román. P. Wolfram vs. Tungsten. *Chemistry International* 2005, 27 (4), 26–27. After some discussion, it was suggested that we revisit the question at our next Division meeting after seeking advice from experts in Division VIII. Prior to the meeting, Jeff Leigh also provided some background regarding the sequence of events that followed the original discovery of element 74 and the subsequent history of the two names, wolfram and tungsten, that have been used to refer to this element.

After considerable discussion, which included a presentation by Garcia in support of retaining wolfram as an alternative name, a vote was taken on the following motion: "Division II recommends that Division VIII consider going back to the designation tungsten (wolfram) for element 74, that was used in the 1990 edition of the Red Book". This motion was passed by a majority of the Division members present and Secretary Interrante was charged with preparing a letter (or message) to Division VIII to inform them of our recommendation and to ask them to include a discussion on this topic on the agenda of their next meeting. In support of this recommendation, Jan Reedijk and Javier Garcia-Martinez will present new evidence on the tungsten/wolfram naming issue of element 74 to Division VIII .

Appendix

Prepared for the IUPAC BNL-81324-2008-CP
Inorganic Chemistry Division
Committee Meeting in
Helsinki, Finland on
August 11-12, 2008

Element 74, the Wolfram Versus Tungsten Controversy

Norman E. Holden

Abstract

Two and a quarter centuries ago, a heavy mineral ore was found which was thought to contain a new chemical element called heavy stone (or tung-sten in Swedish). A few years later, the metal was separated from its oxide and the new element (Z=74) was called wolfram. Over the years since that time, both the names wolfram and tungsten were attached to this element in various countries. Sixty years ago, IUPAC chose wolfram as the official name for the element. A few years later, under pressure from the press in the USA, the alternative name tungsten was also allowed by IUPAC. Now the original, official name "wolfram" has been deleted by IUPAC as one of the two alternate names for the element. The history of this controversy is described here.

Introduction

Pilar Goya and Pascual Roman had expressed a concern[1] about the revision of the Red Book[2] (Nomenclature of Inorganic Chemistry - IUPAC Recommendations 2005), in which wolfram was deleted as an alternative name for tungsten (element 74). They argued that the case of wolfram, which was recommended by IUPAC with the alternative name of tungsten allowed in the English speaking world, was significantly different from that of other elements where the listed second name referred to the Latin root of that element and which explained the chemical symbol associated with that element.

Luis Oro and Javier Garcia brought up this issue of the deletion of the name wolfram again at the meeting of the Inorganic Chemistry Division Committee during the 44th IUPAC General Assembly in Torino, Italy in August 2007, where Oro and Garcia are Division Committee Titular Members. Following a few initial brief comments on this issue, it was decided to postpone a detailed discussion of this matter until the upcoming "off-year" meeting of the Division II Committee in Helsinki, Finland, which is scheduled for August 2008. This paper addresses some of the basic issues that were involved in the previous history of these disputed names for element 74. Since most of these discussions were held fifty to sixty years ago, many (if not most) of the participants in this present discussion may be completely unaware of the existence of, or any of the details of the earlier decision about the naming controversy and the origin of the use of the two names by IUPAC.

Early History

The early history of element 74 is well established. During the sixteenth century, the mineral wolframite [(Fe, Mn) WO_4] was noted in the literature. The origin of the

name wolframite comes from the fact that the mineral interfered with the reduction of the principal ore of tin, cassiterite, (SnO_2). The mineral was said to devour the tin like a wolf devours a sheep.
Some two centuries later, the Swedish chemist and mineralogist, Axel Fredrik Cronstedt
discovered a heavy mineral that he called heavy stone (or "tung-sten" in Swedish). He thought that this mineral contained a new element. Carl Wilhelm Scheele, who worked as a pharmacistand private tutor in Uppsala, isolated the tri-oxide of the element in 1781. He did not isolate the pure element. This tungsten mineral was later called scheelite, $CaWO_4$.
Torbern Bergman at Uppsala predicted that the acid isolated by Scheele contained a new metal. He thought that it should be possible to prepare the metal by charcoal reduction. During 1782, a Spanish nobleman named Juan Jose de Elhuyar, studied under Bergman at the University of Uppsala. Returning to Spain in 1783, Juan Jose and his brother Fausto de Elhuyar were the first to prepare this metal by reduction with carbon, as suggested by Bergman. They named this element wolfram. The name wolfram was established in Germany and Scandinavia, while the Anglo-Saxon countries preferred Cronstedt's name of tungsten.

The IUPAC Connection

The original International Commission on Atomic Weights preceded the formation of the International Association of Chemical Societies (IACS), in 1911, by more than a decade and the formation of the International Union of Pure and Applied Chemistry (IUPAC), in 1919, by about two decades. The Atomic Weights Commission, which had been part of the IACS, joined IUPAC at its inception. At the first Conference, there did not exist a Commission on Nomenclature within IUPAC, but one was created at the next IUPAC Conference.
The Atomic Weights Commission was reorganized in 1923 within a Commission on the Chemical Elements of IUPAC. In 1930, this Chemical Elements Commission was divided into a number of separate Commissions including one on the Atomic Weights and a Commission on Atoms that was formed to cover the areas of isotopes, atomic structure, physical methods for masses and nuclear chemistry.
The desirability of fixing element names, which could be used with little adaptation in different languages and of facilitating the adoption of universal element symbols in a chemical formula, was of concern to IUPAC. During the first half of the Twentieth Century, there was a particular issue regarding the long-standing controversy over the two chemical names, beryllium and glucinium (with chemical symbols Be and Gl), for element number 4, which were currently used in different groups of countries.
There was no IUPAC Conference (General Assembly) between the years 1938 (the 13th Conference) and 1947 (the 14th Conference) because of World War II. During the 1947 IUPAC Conference in London, the problem of approving a name for a number of new chemical elements that had been discovered in the previous decade, as well as resolving the controversy of the disputed names for other elements was initially referred to the Atoms Commission. Unfortunately, the Atoms Commission was involved in the process of dissolving itself during this 14th IUPAC Conference[3]. As a result, the matter of these element names was referred to two other IUPAC Commissions, the Commission on Nomenclature of Inorganic Chemistry (CNIC) and the Atomic Weights Commission. A joint meeting of these Commissions was planned to take place during the 15th IUPC Conference in Amsterdam, the Netherlands in

1949.

The IUPAC Authority for the Names of the Chemical Elements

At that particular period in time (1947-1949), the situation facing the Commission on Atomic Weights was the following. Most of the Commission members had either died or had withdrawn after the 1947 meeting because of their professional retirement. During early 1949, Edward Wichers (US National Bureau of Standards) was asked by the Union's Executive Committee to serve as chairman and to reorganize the Commission. To acquaint himself with the Commission's past procedures, Wichers wrote to Professor Gregory Baxter (Harvard University), who had been the previous Commission President from 1930 to 1947. In the correspondence, Wichers mentioned the problem of the element names. He noted that the 1947 atomic weight table in French listed "Tu" as a second choice symbol for tungsten.

Baxter replied to Wichers that his procedure in the past was to write and then circulate each report (in English) on the Atomic Weights to Commission members for suggestions or additions. He noted that there was never even a discussion about these disputed names. The procedure in place was that the Commission members would approve the table with all of the chemical names, as they were used in English in this English text of the report. The various members would use the element names favored in their own country, when they translated this table into other languages. Since there had previously never been an occasion for IUPAC to insist on a single name in all languages for each element, Baxter concluded his reply by suggesting to Wichers that he leave the matter of the element names to the Nomenclature Committee and would avoid any possible international trouble[4].

From the above discussion, it can be seen that the Atomic Weights Commission never made an official decision on the names of the elements. However, the names listed in the Table in a particular country corresponded to those, which were commonly used and accepted for the element in that country and to this extent, the appearance of an element in the Atomic Weights Table was an implicit acknowledgment that IUPAC accepted that particular element. The Commission avoided the potential problem of an initially false discovery of an element in the following manner. No element would be listed in the Atomic Weights Table until a measurable amount of that element had been separated and a value measured for its atomic weight. This process usually took a considerable number of years, by which time any potential problems or controversies with the discovery of the element were usually apparent in the scientific literature.

It will be seen that in 1949, the Atomic Weights Commission ceded the responsibility for the names of the chemical elements to the CNIC, where it remained until 2001 when IUPAC was reorganized and when IUPAC terminated the CNIC and almost all of the other IUPAC Commissions. The previous responsibility for the names of the chemical elements was transferred to the Inorganic Chemistry Division Committee (Division II). All of the previous nomenclature and terminology work that was being done in IUPAC was consolidated within a new Division of Chemical Nomenclature and Structure Representation (Division VIII).

The 15th IUPAC Conference

During the 1949 Conference, there was a joint meeting of the two Commissions, CNIC and Atomic Weights, to deal with element names. In addition to the

beryllium/glucinium
controversy, there were other elements for which two separate names were being used Helsinki Minutes - 31internationally. The other elements included niobium/columbium, cassiopeium/lutetium, celtium/hafnium and tungsten/wolfram. The discussion led to a general recommendation (which was subsequently incorporated into the 1957 Rules of the CNIC) that the old custom of allowing the right of naming of a new element to rest with the first discoverer should be abandoned, since it had resulted in many useless controversies and a principle of general acceptability should be used. Some examples of the problems that resulted from this practice of allowing the discoverer to name a new element can be seen from a review of the History of the Chemical Elements[5]. For general acceptability, the issues that were considered in the meeting included which name had the more widespread use in science, the priority of discovery and the number of languages in which the disputed names were used.
One outcome from this meeting was that in the future, the Atomic Weights Commission would withdraw from any further discussion about the names of the chemical elements. A second outcome of the meeting was that names would be recommended for the more recently discovered elements, technetium, promethium, astatine, francium, neptunium, plutonium, americium and curium. In additional, the names of beryllium, niobium, lutetium, hafnium, and wolfram were recommended for the cases of the disputed names, where two or more names were current. For element 91, the name protactinium was recommended to replace the previous name of protoactinium. Finally, the name lutetium from the Latin name of Paris, Lutetia, had been preferred to lutecium, from the French equivalent name of Paris, Lutece.

The Specific Case of Wolfram/Tungsten

During the course of the 1949 discussion, the subject of wolfram versus tungsten was raised, although this case was quite different from that for which the new principle had been enunciated. In this instance, the problem arose because in Scandinavian languages the word tungsten (or local variations) signifies “heavy stone” and this name seemed to be inappropriate for designating an element. Against this statement, it was argued that wolfram had long been accepted as the name of a particular mineral.
It was eventually suggested that the name wolfram should be recommended as the scientific name for the element, while the name tungsten could be retained, where desired, for commercial use, in analogy with the word “steel” for many commercial forms of “iron”. These suggestions from the 1949 meeting were followed by considerable correspondence from many parts of the world, which did not reveal any clear consensus.
These issues were reconsidered again by the CNIC at the 1951 IUPAC Congress. After studying the correspondence, Commission members agreed to leave the suggestions as they stood, with the name wolfram for element 74, in the hope that merit of uniformity in chemical nomenclature would gain recognition when the underlying reasons for the proposed change became generally understood.
Unfortunately, the 1951 Commission meeting of the CNIC was held in conjunction with the American Chemical Society’s (ACS) Centennial celebrations and unlike previous Commission meetings, it received much more attention from the press. Before the CNIC sessions were completed and long before the Commission’s report had been prepared for the IUPAC Council’s approval and its subsequent publication, a report appeared in the press suggesting that the Commission had decreed the

abolition of the name tungsten. This report was completely in error, but it provoked a storm of protest from all over the world. Although efforts were made to correct the error, much harm was done to the standing of the Nomenclature Commission. The CNIC decided to recognize both names. At the 1953 meeting of the CNIC, it was decided to let the whole matter drop until a fresh review of the matter could be made under calmer conditions.

Since 1953, the CNIC Commission has been very fully occupied in dealing with the many nomenclature problems brought about by the rapid and extensive developments in inorganic chemistry and it has not been possible to undertake a fresh look at the wolfram-tungsten question[6]. It could be seen from the 1970 edition of the Nomenclature rules that both forms, wolfram and tungsten, were provided for in the rules as alternative names for the element.

Although the responsibility for the names of the chemical elements in IUPAC passed from the CNIC to the Inorganic Chemistry Division Committee, Division II, the recent change in the element name was made by Division VIII, without notifying or consulting the sole IUPAC authority responsible for the names, the Division II Committee.

Side Note on a Spanish Member of the Atomic Weights Commission

I might note that Enrique Moles, who was a Professor at Madrid University and had been an IUPAC Vice-President during the period of the 1930s, was invited to attend the 1949 reorganization meeting of the Atomic Weight Commission because of his known interest in atomic weights. Professor Moles was elected to the Commission at the meeting and he was chosen as the Secretary-Reporter. At the meeting, Moles proposed a table, which included the element, tungsten, with the symbol W and without any mention of wolfram, since the table for the report was prepared in English. In November 1949, when Wichers sent the final version of the report on atomic weights to the IUPAC Council, it included the element name, wolfram, with the symbol W and a reference to the IUPAC Nomenclature Commission making the change. In the 1949 Report of the Atomic Weight values in the USA[7], the names and symbols adopted by IUPAC were used but as a concession to the fact that the new names were unfamiliar in the United States (and may not find acceptance there), the old names of columbium and tungsten were also given for the elements 41 and 74, respectively. In the 1951 Report of the Atomic Weight values in the USA[8], the name wolfram, as the preferred name of the element more commonly known as tungsten in the English speaking countries has been dropped from the table because it failed to gain acceptance in the United States (see the above note on the uproar in the USA press over the elimination of tungsten). It was noted in the report that IUPAC now recognized both names of tungsten and wolfram.

I might note that some forty years after the decision had been made by the CNIC on the preferred element names, metallurgists in the USA were writing to ask me why the name columbium, which was used by metallurgists throughout the USA, was not listed in the Atomic Weights Table in English.

Conclusions

From the above history of the wolfram-tungsten affair, it can be seen that a special set of circumstances was involved in the resolution of the disputed names for element 74 some sixty years ago. Under these circumstances of bowing to the public pressure of

the press in the USA, the 1970 edition of the Nomenclature rules allowed the use of both of the names, wolfram and tungsten. As the nomenclature rules change with time, the choice of using either name for element 74 as a compromise has now been withdrawn by IUPAC. However, a half-century after the controversy, probably much of this history has been lost and is now forgotten by the people who were involved in making this recent decision.

On the other hand, the thinking involved has also evolved during this period. As Ture Damhus has noted[9], the recommended chemical names are now those names as used in English, which is the one official language of IUPAC[10]. Damhus also noted that there is still the option of using other names in various other national nomenclatures (at least for the time being). Whether this option will remain as rules continue to evolve in the future is not clear.

As a final note, I would also mention that if these present rules had been in place in 1949, the name for element 41 would probably now be columbium and not niobium. However, nomenclature rules evolve over time and one should not try to impose rules from one time era to decisions that were made during another time era. Whether the origin of the dispute over wolfram and tungsten would justify the retention of wolfram as an alternate name for element 74, only time will tell.

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Jan Reedijk, Division II; Date: August 1, 2009

Report from Division II for ICTNS and Division VIII

a) element 112 name and its abbreviation
b) element 74: tungsten name(s)

About element 112: The early (and bad) publicity on Cp and Copernicium is regretted.
The division can agree with the proposed name for the element; the proposed symbol, however, is not accepted, for 2 main reasons, namely: The symbol Cp is a most common and frequently used ligand abbreviation. Moreover, the abbreviation Cp was once proposed and used (and rejected by IUPAC). An IUPAC decision from 2002 was that once rejected, a symbol (or name) cannot be proposed for another element. (W.H. Koppenol, Pure Appl. Chem., **74**, 787–791, 2002). This will be communicated to the proposer using the official route. ***N.B.*** The Division has discussed possible alternative abbreviations, but is not allowed to make suggestions for alternatives to the proposers.

About a possible allowed second name for element 74, W:
Division II had asked division VIII to reconsider their earlier decision (2005 Red Book) on one or two names for W. The 2008 motion was: *"Division*

II recommends that Division VIII consider going back to the designation tungsten (wolfram) for element #74, that was used in the 1990 edition of the Red Book"

This item has been discussed in detail by Division VIII (July 31, 2009), and the outcome was evaluated in Division II on August 1. It was concluded and agreed that:

1. The 2005 paper in Chem. International (Damhus et al.) is still valid in its entirety.
2. The text in the old red book was primarily meant as a service to the reader that also "Wolfram" occurs; (but in documents on polyoxometallates CNIC was not always so clear in the past)
3. The 6-page 2008 memo on the history of naming elements written by Norman Holden was well received and highly agreed with.
4. No new convincing arguments in favour of allowing also wolfram were presented.
5. As before, in other languages one is free to use names based on wolfram; (like for K, Na, Hg…)

Additional comments:

6. The accepted PIN system (Preferred IUPAC Names for compounds) would NOT allow a name for W different from tungsten.
7. The use of wolfram in Mexico appears as not occurring.

8. The use of wolfram(ate) in and outside of Spain is also very limited, as shown from a July 31, 2009 search on Web Of Science (covering papers from the period 2000-2009): Only 1 paper written in English was found using wolframate in title, abstract or keywords.

Details:

Tungsten or tungstate: yields 19416 hits (2000-2009)

Wolfram or wolframate :yields 598 hits (most of which are NOT chemistry, and deal with medicinal aspects, like "wolfram syndrome"), or have "Wolfram" as part of a person's name in the text.

Wolfram or wolframate (and a Spanish address): yields only **21 hits** (from which only 3 are about chemistry: 2 from a journal written in Spanish, Revista de Metallurgia; only one paper was in English: Journal of Physical Chemistry A **111** (2007), 9969-9977 *Mixed-valence polyoxometalates: Spin-coupling and electron distribution in the decawolframate anion reduced by two electrons).*

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 7.3

Report from Division III
Organic and Biomolecular Chemistry

Report to ICTNS
Organic and Biomolecular Division (III)
(2008 – 2009)
Based on the information sent by Prof Mary Garson Division III Secretary)

Amélia Pilar Rauter, Associate Member ICTNS, representative of Division III and National Representative on Division III

INTRODUCTION

The Division operates through six sub-committees, namely:

Organic Synthesis (Prof F. MacDonald, USA)
BIomolecular Chemistry (Prof G.M. Blackburn, UK)
Green Chemistry (Prof B. Han, China)
Photochemistry (Prof S. Braslavsky, Germany)
Structural and Mechanistic Chemistry (Prof E. Uggerud, Norway)
Biotechnology (Prof F. Nicotra, Italy)

Division III activities for this biennium are mainly based on the organization of conferences and projects, summarized as follows:

Projects

Current projects include:

- P.Tundo, **"Making the on-line journal of green chemistry: green rapid Internet communications; feasibility study (2008-016-1)"**; running.
- C.L. Perrin, "Update of IUPAC Glossary of Physical Organic Chemistry." (2008-002-100); approved.
- L. Mammino: "Biomass burning in Sub-Saharan Africa (2007-025-1)"; workshop to be held in 2009 followed by a book.
- A. Pascariu: "Translation in Romanian and Dissemination of a Monograph for Universities and Secondary Schools on "Global Climate Change" (2007-035-1)"; completed. (Note that previous IUPAC projects have involved the translation of this book from first Italian into English, and then into Arabic)
- M. Mozihuzamann: "Workshop for finalising project proposal documents for setting up of an International Centre for Natural Product Research (2005-034-1-300 and 2007-051)"; in progress.
- M. Isobe: "Strategic planning for a new East Asian Network for Organic Chemistry (2005-039-2-300)"; completed.
- M. Isobe: "Strategic planning for a new East and South East Asian Network for organic Chemistry" (2008-026-1); running.
- Sun et al. "Thermodynamic Study on Hydrogen Storage Materials: Metal Organic Frameworks and Metal or Complex Hydrides". (2008-006-3-100); joint project with Div.I and III, approved.

Projects currently under review include:
- V. Lunin: "Green Chemistry: creation and implementation of international cooperation in teaching and investigations" (2008-017-2)
- Axel Griesbeck, " Standard Photochemical Processes." (2008-037-1)

- Stefano Raccanelli et al., "Evaluation of measurement methods and QA/QC for PCDD/F, PCB and PAHs in environmental matrices used in estimation of global pollution" (2008-007-1);
-Patricia Vasquez et al. "Green Chemistry: sustainable education and environmental development (SEED) in Latin America." (2008-014-1); currently under review within Division III.

From these listings, it can be seen that a number of Divisional projects, particularly those within the area of Green Chemistry, have an educational focus. The Division will administer the CHEMRAWN VII Prize for Atmospheric and Green Chemistry, awarded every two years to a young investigator (<45 yrs) from a developing country, beginning in 2010.

Conferences

a. Organic Synthesis. ICOS-17 (Daejeon, Korea: June 22-27, 2008). This is a large and well-recognised meeting that is traditionally attended by many postgraduate students. ICOS-18 will be held in Bergen, Sweden 2-5 August 2010 and ICOS-19 in Melbourne, Australia in July 2012.

b. Biomolecular Chemistry. The CHEMBIOTECH meeting held at the IUPAC Congress in Torino (August 2007) and ISCNP26/ICOB6 in Charlottetown, PEI, Canada (July 13-18 2008) both attracted strong scientific programs. ISNCP27/ICOB7 to be held in Brisbane July 10-14 2011.

c. Green Chemistry. ICGC-2; Moscow, Russia: September 14-20, 2008; a special issue of Pure Appl. Chem. was linked to this meeting. ICGC-3 will be held in Ottawa, Canada 15-19 August 2010.

d. Photochemistry. 22nd IUPAC Symposium on Photochemistry (Gothenburg, Sweden: July 28-1 August 2008; 24th International Conference on Photochemistry will be held in Toledo July 19-24 2009)

e. Structural and Mechanistic Chemistry. International Symposium on Physical Organic Chemistry ICPOC-19, held at Santiago de Compostella, Spain: July 13-18, 2008.

f. Biotechnology. 13-IBS; Dalian, China: October 12-17, 2008. This meeting held a special session addressing professional training and education in the Asian region. More than 2000 delegates attended, representing >80 countries. A Young Scientist and Students Award was established, to showcase the best of the next generation biotechnology research leaders and their research endeavours. The 14-IBS will take place in Rimini, Italy from 15-19 September 2010.

Amélia Pilar Rauter
Representative of Division III to ICTNS
16 July 2009

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

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Report from Division IV
Polymer

Division IV Report to ICTNS for the Biennium 2008-09

Amongst the divers aims and objectives of the Polymer Division, that of principal concern to ICTNS is the definition of terminology in macromolecular and polymer science and technology. This work is conducted under the auspices of the Sub-committee on Polymer Terminology (SPT) to which Division VIII delegates the additional responsibility for guiding the progress of projects in polymer nomenclature. There are activities within other sub-committees of the Division that result in the publication of methodologies, standards and data for polymer science and education, but these topics do not fall within the terms of reference of ICTNS.

The means by which the SPT fulfils its responsibilities include the development of position papers on issues of importance to the international polymer community and the provision of financial support for approved projects in polymer terminology and polymer nomenclature. Since its inception in 2001, the following statistics place its activities in context:

- 12 peer-reviewed publications in Pure & Applied Chemistry;
- 5 translations of PAC output into either German or Japanese;
- 1st edition of the 'Purple Book' translated into Japanese;
- publication of a new edition of the 'Purple Book';
- 19 active projects, 7 of which are concerned with polymer nomenclature or are nomenclature-related.

Output 2008-09 post-Torino GA

1. The publication of the new edition of the 'Purple Book' under the name *Compendium of Polymer Terminology and Nomenclature* (project number 2002-048-1-400), the previous edition having been called the *Compendium of Macromolecular Nomenclature*. Thus, though we can speak of the 2nd edition of the 'Purple Book', strictly speaking it is not a second edition.

The compendium comprises 13 chapters of terminology and 9 chapters related to nomenclature, all of which are based on documents previously published in PAC. An introduction reviews the history of terminology and nomenclature activities within the Polymer Division. An appendix presents a bibliography of bio-polymer nomenclature.

2. The publication of the following projects:

- 2000-007-1-400: Glossary of terms relating to polymeric gels and networks, hybrid inorganic polymeric materials and the processing thereof;
- 2002-016-1-400: Terminology for the kinetics, thermodynamics, and mechanism of polymerization;
- 2002-014-1-400: Glossary of class names of polymers based on their chemical structure and molecular architecture;
- 2008-022-1-400: Dispersity;
  This is a single-term recommendation that is considered to be of the utmost importance to the polymer community and which has been accepted for re-publication by *Polymer International*.
- 2001-082-1-800: Terminology and nomenclature of macromolecules with cyclic structures.*

* Division VIII projects pursued under the auspices of SPT.

Future output

1. The following project has undergone public review, been accepted for publication in PAC and is in the final stages of consideration by ICTNS:

    - 2002-006-2-400: Terminology for radical polymerizations with minimal termination - the so-called "living" and/or "controlled" radical polymerization (at publication, these recommendations are expected to be called,'Terminology for reversible-deactivation radical polymerization previously called 'controlled' radical or 'living' radical polymerization');

2. The following projects are nearing completion with submission predicted within the period 2010-11 as indicated:

    - 2002-017-1-400: Polymerization processes and polymers in dispersed systems (late 2009);
    - 1999-051-1-800: Nomenclature for Chemically Modified Polymers (late 2009/early2010); *
    - 2003-019-2-400: Definitions of terms relating to crystalline polymers - revision of IUPAC Recommendations 1988 (2010);
    - 2005-005-2-400: Definitions of terms relating to individual macromolecules, their assemblies, and dilute polymer solutions (2010);
    - 2006-004-1-400: Recommendations on the Abbreviated Terms of Polymers (2010);
    - 2001-081-1-800: Terminology and structure-based nomenclature of dendritic and hyperbranched polymers (2010);*
    - 2004-043-1-400: Terminology Relevant to Bio-related Polymer Science and Applications (2011);
    - 2005-043-2-400: Terminology for self-assembly and aggregation of polymers (2011).

3. The following projects are still in preparation with end-dates expected beyond mid-2011:

    - 2003-060-2-400: Terminology on separation of macromolecules;
    - 2000-037-1-800: Nomenclature for macromolecular rotaxanes (revised title); *
    - 2003-042-1-800: Source-based nomenclature of single-strand linear and graft polymers; *
    - 2006-028-1-400: Terminology for stimulus-responsive polymers (revised title);
    - 2006-041-1-400: Glossary of thermal and thermomechanical properties of polymers;
    - 2007-008-1-400: Development of a multilingual encyclopaedia of polymer terminology;
    - 2008-015-1-400: Preferred names for polymers;
    - 2008-020-1-400: Revision of "IUPAC Recommendations on Macromolecular Nomenclature – Guide for Authors of Papers and Reports in Polymer Science and Technology";
    - 2008-032-1-400: Basic guidelines to polymer nomenclature.

R G Jones - July 1, 2009

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* Division VIII projects pursued under the auspices of SPT.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

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Item 7.5

Report from Division V
Analytical Chemistry

Report to ICTNS
Analytical Chemistry Division (V)
(January 2008 – June 2009)

Maciej Jarosz, Associate Member ICTNS, ACD

based on

Report to Council 2009 (period covered 2008 - 2009)
IUPAC Analytical Chemistry Division (V), prepared by Aleš Fajgelj, ACD President

Content

1. Activities performed in frames of the Goals of the IUPAC Strategic Plan

1.1. Providing leadership as a worldwide scientific organization that objectively addresses global issues involving the chemical sciences

For the biennium 2008-2009 the following interest groups were created: *Communication, Critical evaluation of data, Electronic resources, Emerging analytical issues, Metrology and the Analytical potential of nuclear techniques*. They are expected to reflect the current core interests of the Division and to foster creation of new projects.

1.2. Facilitating the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion

The main Division tools of general interest for analytical chemistry community is the Compendium of Analytical Nomenclature - Orange Book, the Solubility Database and the Stability Constants Database, the k_0-NAA database

the Compendium of Analytical Nomenclature - Orange Book. Review of Orange Book revealed a need of complete revision of this document; this will be the most important activity for the near future with the involvement of all Division Committee Members. A dedicated one day workshop on Orange Book revision is planned during the IUPAC GA in Glasgow.

the IUPAC Stability Constant Database (SCDB). In 2007 Academic Software, developer of the database, has indicated that it wishes to transfer the responsibility for management and maintenance of SCDB to IUPAC. Division V formed a consultative team to work with Academic Software to achieve a successful transition. The work of the Secretary-General's *ad hoc* committee that had as its Terms of Reference: "To explore requirements to achieve a modernized interactive IUPAC web site and an ability for IUPAC to provide large databases of value to chemists" led to the current developing arrangements with FIZ-Chemie. It can be reported now that agreement was reached with the IUPAC Bureau that the database will be frozen as soon as collection of literature data for 2006 is completed. For the future the

database will be made available to users through IUPAC as a frozen compilation. Division V is ready to support further work compilations if such a need will be identified in the future.

the k_0*-NAA Database* - contacts were established with the BIPM Consultative Committee for Ionizing Radiation (CCRI) and the International Atomic Energy Agency (IAEA) regarding future updates and developments. The Division expressed interest for further cooperation and for further hosting this database.

1.3 Assisting chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement in the quality of life

In understanding the role measurement results produced by analytical chemists play in international trade and in helping lowering barriers to trade, the following projects of Analytical Chemistry Division deserve special attention:

Metrological Traceability of Measurement Results in Chemistry is aimed to establish common understanding of metrological traceability and to describe common concepts as prerequisite for comparability of measurement results

Comparable pH Measurements by Metrological Traceability (interdivisional project) utilizes already given concepts and applies them to the most frequent chemical measurement – measurement of pH

Investigating out-of-Specification Test Results of Chemical Composition Based on Metrological Concepts is aimed in developing a guide for identification of root causes of out–of-specification (OOS) test results of chemical composition based on metrological concepts

Trace Element Analysis – Role of Particle Size Distribution in Solid Reference Materials (WPHQA project) of crucial importance for reference materials production in assuring "commutability" of reference materials

1.4 Fostering communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries

Members of the Analytical Chemistry Division have been actively involved and have cooperated with the following organizations and bodies:

International Committee on Weights and Measures/Consultative Committee on the Amount of Substance (BIMP/CCQM)

ISO-Committee on Reference Materials (ISO/REMCO)

International Committee on Weights and Measures/Joint Committee for Guides in Metrology (BIPM/JCGM) Working Group1 and Working Group 2

Joint Committee on Traceability in Laboratory Medicine (JCTLM)

Cooperation on International Traceability in Analytical Chemistry (CITAC), etc.

One of the most important documents published during this biennium in which Division members were actively involved is the 3rd Edition of the *International vocabulary of metrology — Basic and general concepts and associated terms (VIM).* IUPAC was together with BIPM, IEC, IFCC, ILAC, ISO, IUPAP and OIML one of eight international organizations, which worked together in producing this document under the coordination of the Working Group 2 of the Joint Committee for Guides in Metrology (JCGM/WG 2).

2. Attachment I

Projects, recommendations, technical reports, books, conferences, symposia

Current projects

2008-031-1-500: Methods of measurement and evaluation of natural antioxidant capacity/activity
2008-025-1-500: Humic-metal binding constants database
2008-030-1-500: Investigating out-of-specification test results of chemical composition based on metrological concepts
2008-008-1-500: An introduction to the IUPAC-NIST Solubility Data Series: Preparation and use of compilations and evaluations
2008-002-1-500: A glossary of concepts and terms in chemometrics
2007-039-1-024: Extension of ThermoML - the IUPAC standard for thermodynamic data communications
2007-041-1-500: Mechanistic aspects of chemical vapor generation of volatile hydrides for trace element determination
2007-044-1-500: Solubility data related to industrial processes. Solubility in systems with lithium and/or sodium nitrates
2007-047-1-500: Solubility data related to industrial processes. Nitriles C+3: binary and multicomponent systems
2007-046-1-500: Solubility data related to industrial processes. Mutual solubility of esters with water
2007-045-1-500: Solubility data related to industrial processes. Solubility of higher alkynes in liquids
2007-010-2-500: International harmonized protocol for standard preparation, irradiation and measurement for assuring metrological traceable results in neutron activation analysis
2006-026-1-500: Electrochemical DNA-based biosensors: terms and methodology
2006-039-2-600: Extraction and fractionation methods for exposure assessment related to trace metals, metalloids and hazardous organic compounds in terrestrial environments
2006-037-1-500: Metal-focused -omics: guidelines for terminology and critical evaluation of analytical approaches
2006-034-1-500: The solubility of oxygen in all solvents (update of SDS vol 7. 1981)
2006-033-1-500: Solubility data related to industrial processes. Rare earth metal chlorides (Sc, Y, lanthanoids) in water and aqueous systems
2006-032-1-500: Solubility data related to industrial processes. Mutual solubility of ethers and ketones with water
2006-022-1-500: Spectrochemical Analysis - Conversion of Orange Book Chapter 10 to Glossary Format
2006-016-1-200: Recommendations for isotope data in geosciences
2006-010-1-500: Adjustment, estimation and uses of equilibrium reaction constants in aqueous solution
2005-041-2-500: Determination of selenomethionine in selenized yeast supplements
2005-035-2-500: Trace elements analysis: role of grain size distribution in solid reference materials
2005-048-2-100: Solubility and thermodynamic properties related to environmental issues
2005-033-1-500: Transition and 12 to 14 main group metals, lanthanide, actinide and ammonium halates Series: Solubility Data Series; editor-in-chief: Mark Salomon
2005-024-2-600: Establishment of guidelines for the validation of qualitative and semi-quantitative (screening) methods by collaborative trial: a harmonized protocol
2005-019-2-500: Selection and use of proficiency testing schemes for limited number of participants (chemical analytical laboratories)
2005-017-1-500: Glossary of terms related to solubility - updates and revisions to the Orange Book
2005-014-1-500: IUPAC Stability Constants Database - completion of data collection up to 2006
2004-005-2-500: Comparable pH measurements by metrological traceability
2004-017-1-500: Standardization of analytical approaches and analytical capacity-building in Africa
2003-056-2-500: Standard definitions of terms relating to mass spectrometry

2003-015-2-500: Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry
2002-058-1-500: Definitions and fields of application of the terms robust and rugged and the characteristics or qualities of robustness and ruggedness in analytical chemistry
2002-044-1-500: Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions
2002-038-1-500: Solubility data of compounds relevant to human health. Antibiotics: peptide antibiotics and macrocyclic lactone antibiotics
2002-037-1-500: Solubility data of compounds relevant to human health. Solubility of halogenated aromatic hydrocarbons Series: Solubility Data Series; editor-in-chief: Mark Salomon
2002-036-1-500: Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates
2002-035-1-500: Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis
2002-032-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb)
2002-031-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates
2002-025-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Inorganic actinide compounds
2002-009-2-500: Optical spectrochemical analysis using waveguides and optical fibers
2001-072-1-500: Low activation materials for fusion technology: state and prospects
2001-063-1-500: Revision of terminology of separation science
2001-010-3-500: Metrological traceability of measurement results in chemistry (revised title)
1999-050-1-500: Chemical Speciation of Environmentally Significant Heavy Metals and Inorganic Ligands

Recommendations and Technical Reports

Performance evaluation criteria for preparation and measurement of macro and microfabricated ion-selective electrodes (IUPAC Technical Report), *Pure Appl. Chem.*, Vol. 80, No. 1, pp. 85–104, 2008.

Glossary of terms related to solubility (IUPAC Recommendations 2008), *Pure Appl. Chem.*, Vol. 80, No. 2, pp. 233–276, 2008.

Countercurrent chromatography in Analytical chemistry (IUPAC Technical Report), *Pure Appl. Chem*., Vol. 81, No. 2, pp. 355–387, 2009.

Books, conference proceedings

D. B. Hibbert, Quality Assurance for the Analytical Chemistry Laboratory, Oxford University Press, 2007

30th International Conference on Solution Chemistry (ICSC 30), Perth, Australia, 16–20 July 2007 2008, (E. Königsberger, editor), *Pure Appl. Chem.* Vol. 80, No. 6 (dedicated issue)

International Symposium on Metallomics 2007 (ISM 2007), Nagoya, Japan, 28 November–1 December 2007, (H. Haraguchi, editor), *Pure Appl. Chem.*, Vol. 80, Issue 12, 2008 (dedicated issue)

Challenges to metallomics and analytical chemistry solutions (S. Mounicou and R. Lobinski), *Pure Appl. Chem*., 2008, Vol. 80, No. 12, pp. 2565-2575, 2008

Conferences/symposia/workshops

The 13th International Symposium on Solubility Phenomena and Related Equilibrium Processes (13th ISSP) was held at Trinity College Dublin, Ireland, from July 27th to 31st, 2008. This was the latest in a successful series of biennial meetings that bring together scientists from diverse areas where solubility and associated equilibria play important roles. The 13th ISSP continued the tradition of ultidisciplinarity with contributions ranging from theory and modelling, biological systems, industrial processes, environmental chemistry and geochemistry among others

IUPAC-SSED Workshop on Metrological Traceability of Solubility Data, 28 February 2008, Rome, Italy. Lecturers: D. B. Hibbert, H. Gamsjäger, M. Costa-Gomez, and D. Knox.

IUPAC-WPHQA Workshop on Trace Element Analysis: Role of Particle Size Distribution in Solid Reference Materials, 29 February 2008, Rome, Italy. Lecturers: M. Belli, A. Sahuquillo, P. de Zorzi, Z. Mester, U. Sansone, and A. Fajgelj

IUPAC Workshop on Metrology, Chinese Academy of Metrology Science (CAMS), Beijing, China, 21 November 2008. Lecturers: A. Fajgelj, B. Hibbert, W. Lund, and Hongmei Li

Lectures and seminars

Seminars on the new International Vocabulary of Metrology (VIM 3) were given by P. De Bièvre in:

Gaithersburg, USA, National Institute for Standards and Technology, 24 October 2008;

Helsinki, Finland, National Institute for Metrology of Finland (MIKES) on 3 February 2009, and Labquality Days on 25 February 2009;

Bangkok, National Metrology Institute of Thailand, 24 to 27 March 2009;

Singapore, Health Science Authority, 30 March 2009.

Lectures on the redefinition of the kilogram and the mole were given by P. De Bièvre in:

Bangkok, Kasetsart University, 27 March 2009; and

Singapore, National University of Singapore, 31 March 2009.

Seminar 'Traceability in Chemistry', 26 February 2008, Rome, Italy. Lecturers: R. Dybkaer, P. De Bièvre, and M. Sega

Lecture on Introduction to IUPAC and other relevant guidance documents was given by A. Fajgelj at the APLAC Workshop on Reference Materials Producers Assessors Training Workshop, Hong Kong. 17 to 19 November 2008.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

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Supplement to the report from Division V

Analytical Chemistry

on recent activities of JCGM-WG1 (GUM Guide to the Expression of Uncertainty in Measurement)

Report to ICTNS on recent activities of JCGM-WG1 (Guide to the Expression of Uncertainty in Measurement)

D Brynn Hibbert (IUPAC representative)

The JCGM has representatives from IUPAC, IUPAP, BIPM, IFCC, ILAC, OIML, ISO, and IEC. The committee meets twice each year, often at the BIPM in Sèvres, France.

1. The latest meeting of WG1 was 2009-04-07 to 10, at BIPM, Sèvres.
2. Dr Rene Dybkaer was confirmed as an IUPAC representative, and Dr Rűdiger Kessel as a technical expert on behalf of IUPAC.
3. Supplement 104 published and sent to member organizations. Note that the two published Supplements (104 – introduction to the GUM; and 101 – use of Monte Carlo methods) are both available on the BIPM web site: http://www.bipm.org/en/publications/guides/gum.html .
4. DBH gave a presentation on uncertainty of "Qualitative identifications" from a chemistry perspective.
5. The GUM is freely available on the BIPM web site, see http://www.bipm.org/en/publications/guides/gum.html .
6. There was a question about copyright of the "free vision". The statement accompanying this, "cannot use on - line" is interpreted as that the on-line version cannot be re-published. An hyperlink to the official vision is the only way to promulgate the GUM.
7. A proposal has been made for the establishment of WG3 as an ad-hoc committee on software for metrology.
8. Discussions continued on the revision of the GUM. It will be a revision of the present edition, but will include material from the supplements where possible and appropriate.
9. At present the following documents and supplements are in existence or preparation:

JCGM 101:2008. Evaluation of measurement data — Supplement 1 to the “Guide to the expression of uncertainty in measurement” — Propagation of distributions using a Monte Carlo method
JCGM 102. Evaluation of measurement data — Supplement 2 to the “Guide to the expression of uncertainty in measurement” — Models with any number of output quantities
JCGM 104:2009. Evaluation of measurement data — An introduction to the “Guide to the expression of uncertainty in measurement” and related documents
JCGM 105. Evaluation of measurement data — Concepts and basic principles
JCGM 106. Evaluation of measurement data — The role of measurement uncertainty in conformity assessment
The following documents are at an earlier stage of preparation:
Evaluation of measurement data — Supplement 3 to the “Guide to the expression of uncertainty in measurement” — Modelling
Evaluation of measurement data — Applications of the least-squares method

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

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Item 7.6

Report from Division VI
Chemistry and the Environment

IUPAC Division of Chemistry and the Environment (DCE)

(DCE President - **Prof. N. Senesi**, also has been recently elected President of the European Confederation of Soil Science Societies (ECSSS) for the quadrennial 2008-2012, and assigned the organization of the next EUROSOIL-2012 Congress in Bari, Italy, in 2012)

Through its internationally recognised membership, DCE provides unbiased and authoritative views regarding environmental and human health aspects of chemistry. Through its timely projects, publications, and outreach activities the Division seeks to advance research aimed at understanding fundamental chemical mechanisms of environmental processes and promote protection and stewardship of the environment.

Apart from the Division Committee, DCE has subcommittees (on biophysical/chemical processes in environmental systems, on crop protection, and on environmental compartments). Each subcommittee involves about 15 members.

About thirty DCE projects are in progress at the moment. Progress of projects is in general most satisfactorily. The following recently completed and ongoing projects may be of interest for ICNTS.

2001-022-1-600 (Unsworth) **Global availability of information on agrochemicals**. The initial phase of this project is now complete with the major goal of the project, i.e. to ensure that there is easy access to a definitive and reliable source of information on agrochemicals and issues relating to their use, being achieved with the preparation of an internet webpage. This webpage is hosted on the IUPAC website (http://old.iupac.org project 2001-022-1-600). It includes information on 22 topics related to agrochemicals, together with a direct link to the FOOTPRINT database which contains data on the physicochemical, ecotoxicological and toxicological properties of approximately 650 active substances and 200 metabolites. This database is currently being extended to include formulation adjuvants.

2003-011-3-600 (Wauchope-Shaw) **A critical compendium of pesticide physical chemistry data**. Project finished.

2004-015-1-600 (Wilkinson) **Environmental Colloids: Behaviour, Structure and Characterisation.** A book edited by J. R. Lead and K. J. Wilkinson was the main output from this project. The book has been published by John Wiley and Sons, Chichester, UK, as Vol. 10 of the UPAC Series on Analytical and Physical Chemistry of Environmental Systems.

2003-014-2 (Senesi) **Fractal Structures and Processes in the Environment.** A book edited by N. Senesi and K. J. Wilkinson was the main output from this project. The book has been published by John Wiley and Sons, Chichester, UK, as Vol. 11 of the IUPAC Series on Analytical and Physical Chemistry of Environmental Systems

2004-003-3-600 (Violante) **Biophysico-Chemical Processes of Heavy Metals and Metalloids in Soil Environments.** A book edited by A. Violante, P. M. Huang, and G. Gadd was the main output from this project. The book has been published by John Wiley and Sons, Hoboken, NJ, USA, as Vol. 1 of the New IUPAC-Sponsored Wiley Series edited by P.M. Huang and N. Senesi.

2006-014-1-600 (Senesi) **Biophysico-Chemical Processes Involving Natural Nonliving Organic Matter in Environmental Systems.** The project is in advanced stage. In 2010, a book edited by N. Senesi, B.Xing, and P.M. Huang is to be published by John Wiley and Sons, Hoboken, NJ, USA, as Vol. 2 of the New IUPAC-Sponsored Wiley Series edited by P.M. Huang and N. Senesi.

As a Representative of Chemistry and the Environment Division to ICTNS, in 2008-2009 Petr Fedotov has been asked to review a few technical reports submitted for publication in Pure and Applied Chemistry. As an example: GLOSSARY OF TERMS USED IN ECOTOXICOLOGY (IUPAC Recommendations 2008) by Monica Nordberg, Douglas M. Templeton, Ole Andersen, John H. Duffus is of special interest for Division VI since the glossary is very impressive and may be very helpful not only for ecotoxicologists themselves and researchers working in the fields of environmental chemistry, medical chemistry, soil science etc. but as well as for risk assessors and regulators. However, terms related to the environmental impact of chemicals could be more clearly defined.

In general, it seems reasonable if in future Division VI finds possibilities to collaborate more actively with other Division Committees and ICNTS. Such a joint work may promote elaborating comprehensive interdisciplinary approaches to terminology that is used in different fields. This may help to avoid numerous mutual misunderstandings that often occur until now.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

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Item 7.7

Report from Division VII
Chemistry and Human Health

Chemistry and Human Health Division (VII)

IUPAC General Assembly Report to ICTNS

(August 2009)

Summarised from the Division VII (DVII) Report and submitted by Monica Nordberg

OVERVIEW

Division VII is organized with three Subcommittees showing the diversity of the Division, namely *Medicinal Chemistry and Drug Development* (MC), *Nomenclature, Properties and Units in Laboratory Medicine* (NPU), and *Toxicology and Risk Assessment* (TRA). The activities of the given subcommittees relevant to ICTNS are listed below.

The TRA´s "*Explanatory Dictionary of Terms in Toxicology" part 2 is under review* on the IUPAC website.

Several MC-sponsored glossaries are nearing completion: "*Combinatorial Chemistry Terms;" "Drug Metabolism Terms;" "Pharmaceutical Technology;" "Pharmaceutical Process Chemistry;" "Biomolecular Screening;"* and, an all encompassing "*Compendium of Glossaries."*

DETAILS OF INDIVIDUAL PROJECTS

SC Medicinal Chemistry and Drug Development
2003-044-1-700: Glossary of Combinatorial Chemistry Terms.
The project leader has been changed because of his work commitments (from D. Maclean to A. Ganesan). Derek stays on as a team member.

2000-009-1-700: Glossary of Drug Metabolism Terms. (P. Erhardt)
Definitions are being adjusted to IUPAC format.

2000-009-1-700: Metabolism terms P. Erhardt

2000-010-1-700: P.Erhardt Human drug metabolism database

2002-001-1-700: Compendium of Glossaries. Compendium of terms associated with drug discovery and development (R. Ganellin)

The Glossary of Terms in Pharmaceutical Process Chemistry was split into two separate Glossaries. One of these has now been published as Breuer E., Chorghade M.S., Fischer J., and Golomb G., Glossary of terms Related to Pharmaceutics, (IUPAC Recommendations 2009) *Pure Appl. Chem.*, Vol. 81 (5) 971–999 (2009).

2001-048-2-700: Research and training in medicinal chemistry in India, Pakistan and Sri Lanka: A comprehensive survey to ascertain status and sophistication of faculties,

doctorate programs, etc. - Recommendations for a standardized curriculum (M. Chorghade)

2001-049-2-700: Glossary of Terms in Pharmaceutical Process Chemistry. (M. Chorghade/ E. Breuer) Ongoing definitions are being adjusted to IUPAC format.

2005-050-1-700: Prototype Analysis of Molecular Biomarkers in Cancer. (M. Liebman)
Molecular Biomarkers have become a major focus of disease management and drug development, particularly in oncology. This prototypic study will identify the existing biomarkers in breast cancer and classify them in terms of disease progression and also as to their clinical vs. research use. The project is underway.

2004-019-3-700: Glossary of Terms for Biomolecular Screening. (J. Proudfoot)
Glossary sections were prepared by three sub-teams and recompiled into one document.
This is undergoing internal review by the team members and contains draft definitions of approximately 150 terms related to biomolecular screening. A manuscript has been submitted to Pure and Applied chemistry.

2005-049-1-700: Biological Context by Data Mining. (M. Liebman)
To extend the usefulness and applicability of the glossaries, it would be worthwhile to explore methods for identifying the various contexts in which the terms appear in the scientific literature. In the ideal situation, this project can transcend the three Subcommittees of the Division to incorporate activities of each.

2007-006-1-700: An introduction to computer assisted drug design (Y. Martin)

2008-010-1-700: Update of glossary of terms used in medicinal chemistry (D. Buckle)

2008-013-1-700: Analogue-based Drug Discovery II (J. Fischer)

The SC-NPU generic database
The SC-NPU generic database is, as of 2004-09-01, published on the net under the URL:
<http://dior.imt.liu.se/cnpu/>. The database is published on the IFCC homepage (Scientific division) and IUPAC (Division of Chemistry and Human Health) homepage
with a link to the server Dior, and to the Danish National Board of Health server. As it was decided that the NPU generic database should be managed by its owners (IFCC and IUPAC), these two organizations were contacted to study their possibilities of managing this database daily. The IUPAC denied this possibility but he IFCC SD and Executive Board has thus proposed that the database be hosted on the IFCC website. The cost of such a management has been communicated to IFCC officers, so that IFCC SD could finalize its decision. A meeting in Amsterdam, at Euromedlab(2007) IFCC-FESCC congress and a second one in Antalya, at the IFCC General Conference in April 2008 settled the project. The IFCC Publication Division Chair announced at

the Antalya meeting that the generic NPU database was planned to be managed by an IFCC employee at the Milan headquarters, starting in October 2009.

Ongoing projects of SC-NPU

1. Properties and units for function examinations (IUPAC: 2001-067-1-700). An updating has been undertaken.

2. Properties and units for urinary calculi (IUPAC: 2001-070-1-700). A full reformatting of the manuscript is being done.

3. Internationally agreed terminology for observations in scientific communication. (IUPAC 2004-023-1-700, extended as 2008-019-1-700) Chair : F. Pontet. Two drafts have been circulated and discussed during the last Sub-Committee meetings.

4. Mapping of IFCC-IUPAC laboratory coding system to SNOMED CT (IUPAC 2006-008-1-700) Chair : U.Magdal. The objective has been widened to include the LOINC terminology in the mapping, under the “umbrella” of the International Health Terminology Standards Development Organisation (IHTSDO), which manages SNOMED CT.

5. Securing and structural updating of information in the NPU coding system and its environment (IUPAC 2006-012-1-700) Chair : U. Magdal. A user’s guide is being written.

6. Recent advances in Nomenclature, Properties and Units: strategy for promoting SCNPU achievements (IUPAC 2006-048-1-700) Chair : F.Pontet. A poster was presented at the IFCC-FESCC Euromedlab 2007 Congress in Amsterdam. A poster was presented and a symposium organized in Turin IUPAC Congress (2007).

7. Revision of the “Silver Book” (IUPAC 2007-033-3-700) Chair : Georges Férard. A preparatory meeting was held in Antalya, 2007, and the first technical meeting was held in Paris, in November 2008.

8. Demonstration of NPU-SNOMED CT mapping/harmonization of terms used in Clinical Laboratory Sciences (IUPAC 2009-005-1-700) Chair : Urban Forsum. To test the feasibility of mapping both NPU and LOINC terminologies to SNOMED CT, a trial period of 6 months is ongoing until October 1st, with the IHTSDO and LOINC Committee.

9. The Portuguese translation of the SC-NPU data base has been updated in 2005. Ongoing

10. Paper on IFCC WG-HbA1c name and units (G. Nordin). This manuscript on the impact of systematic nomenclature on the naming of this particular important property has been agreed on by a ballot in IFCC and published in Clinical Chemistry and Laboratory Medicine.

11. Revision of ENV 1614 has been done in collaboration with CENT C 251. It is now published.

12. 2007-033-3-700: Revision of the "Silver Book": Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences (G. Ferard)

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SC Toxicology and Risk

1999-047-1-700: The project has generated two publications in Pure and Applied Chemistry 2008/2009 1) Schwenk, M., Klein, R. and Templeton, D.M., Lymphocyte subpopulations in human exposure to metals', *Pure Appl. Chem.* 80(6), 1349-1364, (2008). 2) Schwenk, M., Klein, R. and Templeton, D.M., Immunological effects of mercury, *Pure Appl. Chem.* 81(1), 153-167, (2009).

The project has also initiated a new project 2007-053-1-700 (D. Templeton) Glossary of terms used in immunotoxicology. The aim is to prepare a glossary defining terms in the specialized field of immunotoxicology, to supplement the recently published Glossary of Terms Used in Toxicology (2nd ed.), and aid chemists in the interpretation of the output of project #1999-047-1-700, Immunochemistry of Metals. Work has just started.

2005-047-1-700: has generated a publication in Pure and Applied Chemistry; Nordberg M., Templeton D.M., Andersen O., and Duffus J.H., Glossary of Terms Used in Ecotoxicology, (IUPAC Recommendations 2009) *Pure Appl. Chem. 81(5)* 829-970 (2009).

2003-028-1-700: has generated two publications; 1) Duffus JH., Nordberg M., and Templeton DM., Glossary of Terms used in Toxicology, 2nd edition (IUPAC Recommendations 2007) *Pure Appl. Chem.*, 79 (7), 1153–1341 (2007), 2) Duffus JH., Nordberg M., and Templeton DM., Glossary of Terms used in Toxicology, 2nd edition (IUPAC Recommendations 2007) Chemistry International Sep-Oct Vol 29, No 5, 21 (2007).

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2004-045-1-700: Training of school children on pesticides and health - "Toxicology in the classroom" (W. Temple)). The prototype for the Toxiclaro project is available on the web at www.prn2.usm.my/toxicology2009. The working group held a teleconference in late March 2009 and subsequently members have been working slowly through the website making corrections and submitting these to Professor Rahmat and his team at USM. This is a slow process dependent both on the time group members have to review the material and for the Malaysian team to make the necessary changes. The project completion is therefore dependent on this last phase.

2006-020-1-700: is reported in CI as Nordberg M., Duffus JH., and Templeton DM., IUPAC Explanatory Dictionary of Key Terms in Toxicology (IUPAC Recommendations 2007) Chemistry International Nov-Dec 29, 6, 27 (2007).

2006-020-1-700: Explanatory dictionary of key terms in toxicology, part II. A project proposal was funded in 2007. Terms have been defined and the manuscript is under review for publication in PAC as IUPAC Recommendation. A final document is submitted for public review and comments until 31 August 2009.

A book, “Concepts in Toxicology” based on Explanatory Dictionary of Key Terms in Toxicology, parts 1 and 2, is in press with the Royal Society of Chemistry.

Duffus JH., Nordberg M., and Templeton DM.(2009) Glossary of Terms used in Toxicology, 2nd edition (IUPAC Recommendations 2007) has been incorporated as Annex II in In Information Resources in Toxicology, 4th edition Wexler P.(Ed)

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 7.8

Report from Division VIII
Chemical Nomenclature and Structure Representation

IUPAC
CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION (DIVISION VIII)

Report to ICTNS for 2007 – 2009

Structure of Report

1. Division meeting in 2008
2. Projects
3. Publications
4. Division Election

1. Division meeting in 2008

The Division had meetings in Büdingen (Germany) between July 31 Aug. 1 2008. Before the plenary meeting several task groups meetings were held:

1.1 The inorganic (2006-038-1-800) (Richard M. Hartshorn), PINs (preferred IUPAC names) group and the organic PINs (Blue Book) (2001-043-1-800) (Warren H.Powell) team had met in the days before the Division VIII meeting, both separately and together. The main issues dealt with had been:
- The idea of having several levels of PINs according to the degree of detail one wants to communicate with the PINs, including whether there should be a fixed or variable number of levels of PINs for various classes of compounds.
- Defining the borderline between organic and inorganic PINs when it comes to organometallic compounds.
-No decision was taken

1.2 Second edition of *Principles of Chemical Nomenclature, A Guide to IUPAC Recommendations* (2006-029-1-800) (G. Jeffrey Leigh).

The Principles group had held a meeting the day before the Division Committee meeting. GJL reported that the project plan had largely worked in that about 90 % of the material was in, but said there were differences of opinion regarding the style of the book.

Plenary meeting topics:

1.1 The IUPAC International Chemical Identifier (InChI) (2007-052-1-800)

Stephen R. Heller reported that the InChI has now been widely adopted by databases (*e.g.* Beilstein, EBI) and publishers (*e.g.* RSC). Version 1.0.2 of the InChI was to be launched later in 2008.

1.2 Preferred names in the nomenclature of organic compounds (Blue Book) (2001-043-1-800)

Warren H. Powell gave a detailed report about the status of this project**.** Since than Chapters 1,2,3,7 and 8 are on the Division web board. Chapters 4,5,6,9,10 will be finished by the GA in Glasgow.

1.3 Nomenclature for rotaxanes and pseudorotaxanes (2002-007-1-800)

A status report was given by Andrey Yerin. The recommendations resulting from what Andrey Yerin now called the first part of the project (no consideration of stereoisomerism) had been accepted for publication in PAC [See: Publications 3.5]

Stereoisomerism of rotaxanes had turned out to present some fundamental problems for nomenclature and terminology. These were discussed separately with colleagues who were involved in rotaxane project. The discussion had brought forth some suggestions for the description of symmetry properties of rotaxane components, in particular, but no firm decisions were made.

1.4 Nomenclature of phosphorus-containing compounds of biochemical importance (2006-019-1-800)

It was promised to be posted on the web board.

1.5 Comparison of procedures for naming hydro derivatives of fused ring systems

It was discussed whether the document is properly classified as a technical report or a recommendation. Warren Powell will submit it as a recommendation.

1.6 Second edition of *Principles of Chemical Nomenclature, A Guide to IUPAC Recommendations* (2006-029-1-800)

By the end of November all chapters were rewritten, the reviewers have provided their remarks. They had a meeting in Cambridge (April 24, 2009), and the final version of all chapters is now on the Division web board.

1.7 Preferred names for inorganic compounds (2006-038-1-800)

Richard M. Hartshorn summarised some main hurdles that still lay ahead:

- Delocalised anions as ligands.
- More work on κ, η, and μ, including the 'κ_L device' used for distinguishing kappas referring to ligation to central atoms within a ligand or on a higher level within a coordination complex containing that ligand. In principle, μ is superfluous, but nevertheless it is planned to include it in PINs for clarity.
- When to use rings and chains – a decision tree is being worked out.
- Preparing a list of retained names.

1.8 Nomenclature for rotaxane polymers (2007-009-1-800)

This project had been taken over by Jiři Vohlídal from Ted Wilks and had been waiting for the rotaxanes document (from project 2002-007-1-800). In the meantime, Jiři Vohlídal and Andrey Yerin had revised and shortened the project document. Working group members had provided feedback, and the document was mostly in the polishing stage, however with issues remaining in the overlap area between nomenclature for regular polymers and the new recommendations.

1.9 Preferred names for polymers – list of preferred, acceptable (other IUPAC-approved) and not acceptable (wrong or outdated) names for polymers (2008-015-1-400)

Karl-Heinz Hellwich has initiated this project. The intention is to produce a table-like database of constitutional repeating units and common polymers with

specification and classification for each name (ever) used for them in any IUPAC document

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2. Projects

Project No. 2008-035-1-800: IUPAC International Chemical Identifier (InChI) Symposium
Project No. 2008-033-1-800: InChI and InChIKey: Further Promotion
Project No. 2008-034-1-800: IUPAC International Chemical Identifier (InChI): Further Development
Project No. 2008-020-1-400: Revision of "IUPAC Recommendations on Macromolecular Nomenclature – Guide for Authors of Papers and Reports in Polymer Science and Technology"
Project No. 2007-009-1-800: Nomenclature for Rotaxane Polymers
Project No. 2006-038-1-800: Preferred IUPAC Names (PINs) for Inorganic Compounds
Project No. 2006-029-1-800: Revision of "Principles of Chemical Nomenclature"
Project No. 2006-019-1-800: Nomenclature of phosphorus-containing compounds of biochemical importance
Project No. 2004-039-1-800: IUPAC International Chemical Identifier (InChI): Promotion and Extension
Project No. 2004-024-1-800: Nomenclature of cyclic peptides
Project No. 2003-033-1-200: Determination of atomic weights using new analytical techniques
Project No. 2003-045-3-800: Graphical representation standards for chemical structure diagrams
Project No. 2003-034-1-200: Classification, terminology and nomenclature of borophosphates
Project No. 2003-031-2-200: Isotopic compositions of selected elements
Project No. 2003-042-1-800: Source-based Nomenclature of Single-strand Organic Polymers
Project No. 2003-025-1-800: Extension of IUPAC rules for stereo descriptors to include coordination numbers 7-12
Project No. 2002-007-1-800: Nomenclature of rotaxanes and pseudorotaxanes (revised title)
Project No. 2001-043-1-800: Preferred names in the nomenclature of organic compounds

3. Publications

3.1 Representation of configuration in coordination polyhedra and the extension of current methodology to coordination numbers greater than six (IUPAC Technical Report), R. M. Hartshorn, E. Hey-Hawkins, R. Kalio, and G. Jeffery Leigh, *Pure Appl. Chem.* **79**(10) 1779-1799 (2007); doi:10.1351/ pac200779101779

3.2 Structure-based nomenclature for cyclic organic macromolecules (IUPAC Recommendations 2008), W. Mormann and K.-H. Hellwich, *Pure Appl. Chem.* **80**(2) 201-232 (2008); doi:10.1351/ pac200880020201

3.3 Graphical representation standards for chemical structure diagrams (IUPAC Recommendations 2008), J. Brecher, *Pure Appl. Chem.* **80**(2) 277-410 (2008); doi:10.1351/pac200880020277

3.4 Corrections to *Red Book* 2005 [see www.chem.qmul.ac.uk/iupac/bibliog/RBcorrect.html

3.5 Nomenclature for rotaxanes and pseudorotaxanes (IUPAC Recommendations 2008), A. Yerin, E. S. Wilks, G. P. Moss and A. Harada, *Pure Appl. Chem*. **80**(9), 2041-2068, 2008].

4. Division Election

Division VIII Committee membership as of July 2008	**Division VIII Committee membership after GA 2009**
Gerard P. Moss (United Kingdom)	Richard Hartshorn (New Zealand)
President	*President*
Richard Hartshorn (New Zealand)	Gerard P. Moss (United Kingdom)
Vice President	*Past President*
Ture Damhus (Denmark)	Ture Damhus (Denmark)
Secrectary	*Secrectary*
Titular Members	***Titular Members***
Jonathan Brecher (United States)	Jonathan Brecher (United States)
Kirill Degtyarenko (United Kingdom)	Kirill Degtyarenko (United Kingdom)
Stephen R. Heller (United States)	Andrey Yerin (Russia)
Karl-Heinz Hellwich (Germany)	Philip Hodge (United Kingdom)
Philip Hodge (United Kingdom)	Alan T. Hutton (South Africa)
Alan T. Hutton (South Africa)	G. Jeffery Leigh (United Kingdom)
G. Jeffery Leigh (United Kingdom)	Jeffrey Wilson (United States)
Jeffrey Wilson (United States)	
Associate Members	***Associate Members***
Jaroslav Kahovec (Czech Republic)	Warren H. Powell (United States)
Alexander Lawson (Germany)	Ebbe Nordlander (Sweden)
Ebbe Nordlander (Sweden)	Karl-Heinz Hellwich (Germany)

József Nyitrai (Hungary)

Warren H. Powell (United States)

Andrey Yerin (Russia)

Jaroslav Kahovec (Czech Republic)

József Nyitrai (Hungary)

Jan Reedijk (Netherlands)

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 8.2.1
Report from BIPM

45 th IUPAC GENERAL ASSEMBLY (AUGUST 2009)

KEY POINTS TO BE REPORTED BY THE INTERNATIONAL BUREAU OF WEIGHTS AND MEASURES (BIPM)

The main issues of interest to the ICTNS are that:

1. Joint Committee for Guides in Metrology (JCGM)

1.1The 3rd edition of the **International Vocabulary of Metrology (VIM**) is available for downloading on the BIPM web site:

http://www.bipm.org/en/publications/guides/vim.html

It is also published as ISO Guide 99 by ISO (ISO/IEC Guide 99-12:2007 International Vocabulary of Metrology – Basic and General Concepts and Associated Terms, VIM).

1.2 The "GUM" *Evaluation of measurement data – Guide to the expression of uncertainty in measurement*
JCGM 100:2008 (GUM 1995 with minor corrections) is available on the BIPM web site for downloading at:

http://www.bipm.org/en/publications/guides/gum.html

1.3 The JCGM Working Group 1 is also preparing the following documents

Evaluation of measurement data – Supplement 1 to the "Guide to the expression of uncertainty in measurement" – Propagation of distributions using a Monte Carlo method
JCGM 101:2008. This is now available on the BIPM web site at:

http://www.bipm.org/utils/common/documents/jcgm/JCGM_101_2008_E.pdf

The following documents are at an early stage of preparation:

- *Evaluation of measurement data – An introduction to the "Guide to the expression of uncertainty in measurement" and related documents*
  JCGM 104:2009

- *Evaluation of measurement data – Supplement 3 to the "Guide to the expression of uncertainty in measurement" – Modelling*

- *Evaluation of measurement data – Applications of the least-squares method*

2. Membership of the BIPM has now increased to 53 from (in 2008) 51 Member States with 17 "Associates".

3. A redefinition of four base units of the "International System of Units" (the SI) is still a reality. The current considerations are the base units for mass, electricity, temperature and the amount of substance. Whether this will be achieved at the meeting of the General Conference on Weights and Measures in 2011 remains to be seen. The current view is that a redefined kilogram unit will be based on a fixed value of the Planck Constant and here one needs resolution of experimental differences in the result of various experiments either using "watt balances" or an approach based on a measurement of the Avogadro Number in pure silicon.

Andrew Wallard

23 June 2009

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 8.2.2
Report from ISO/TC12

TC 12, Quantities and units

2009-06-30 ISO/TC 12

Handled by Anders J Thor, +46 8 555 521 59

E-mail anders.j.thor@sis.se

Report on activities in ISO /TC 12, 2007/2009

ISO/TC 12 has, in close cooperation with IEC/TC 25, Quantities and units, continued the work with harmonized ISO/IEC 80000-series on *Quantities and units*. 11 parts of 14 have now been published. The remaining 3 parts are: Part 1: *General*; Part 2: *Mathematical signs and symbols to be used in natural sciences and technology*; and Part 10: *Atomic and nuclear physics*. These 3 parts are now at the FDIS-stage (Final Draft International Standard).

ISO/TC 12 and IEC/TC 25 have recently decided to develop a new series, i.e. ISO/IEC 80003, *Quantities and their units used in physiology*. These 6 parts are now at the WD-stage (Working Draft). Part 3, with the subtitle *Chemistry*, should be of special interest for IUPAC.

The Secretary of ISO/TC 12 has been active in several International organizations such as IUPAC (Com. I.1, ICTNS, and the ad hoc WG on a light version of the Green Book), BIPM (CCU), JCGM (WG 2, VIM), and IEC (TC 1, *Terminology* and TC 25, *Quantities and units*).

Anders J Thor
Secretary of ISO/TC 12

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 8.2.3
Report from IUPAP

Report to the International Union of Pure and Applied Chemistry Interdivisional Committee on Terminology, Nomenclature and Symbols from the International Union of Pure and Applied Physics Commission C2 – SUNAMCO

Commission on Symbols, Units, Nomenclature, Fundamental Constants and Atomic Masses

27 July 2009

The membership of IUPAP C2 for the period 2008 – 2011, as confirmed at the 26th General Assembly of IUPAP (Tsukuba, Japan, October 2008), is

Chair:	Peter Mohr (USA)
Vice-chair:	Christian Bordé (France)
Secretary:	Stephen Lea (UK)
Members:	Juha Äystö (Finland)
	Jens Dilling (Canada)
	Bodil Holst (Norway)
	Alexander Ivanchik (Russia)
	Koit Mauring (Estonia)
	Kazumoto Hosaka (Japan)
	Andrew Wallard (BIPM)
	Jörn Stenger (Germany)
	Filippo Levi (Italy)
	Amitava Sen Gupta (India)

It is C2's intention to co-opt as Associate Members former members Jeffrey Flowers (UK), Savely Karshenboim (Russia) and Wolfgang Wöger (Germany).

Part of the mandate of IUPAP C2 [http://www.iupap.org/commissions/c2/mandate.html] is to promote the exchange of information and views among the members of the international scientific community in the general field of Fundamental Constants including:

(a) physical measurements
(b) pure and applied metrology
(c) nomenclature and symbols for physical quantities and units;
(d) encouragement of work contributing towards improved recommended values of atomic masses and fundamental physical constants and facilitation of their adoption.

In the light of this, IUPAP reports the following activities of C2 to ICTNS
(see also the report from C2 to the IUPAP General Assembly, October 2008, available at http://www.iupap.org/commissions/c2/reports/ga-08.pdf):

Recommendation of IUPAP to the Consultative Committee for Units (CCU)

Following up on the IUPAP Resolution on Redefinitions of SI Units, a submission was made to the CCU to provide the recommendation of IUPAP and was reviewed at the meeting of the CCU held on 26–28 May 2009. At this meeting, the consensus was to redefine the SI simply by stating that it is the unit system scaled such that certain fundamental constants have certain exact values. This was an unexpectedly progressive change, which changes the concept of a unit system.

Red Book

An update of IUPAP-25 "Symbols, Units, Nomenclature and Fundamental Constants in Physics" (the "Red Book") is being considered by C2. This book has been widely distributed since its latest revision in 1987 and is now available on-line[1]. It includes recommended values of fundamental constants that are now out of date. A revision will be of particular importance when the redefinitions of SI Units are implemented. The "Red Book" overlaps with IUPAC's "Colour Books", in particular the "Orange Book" so coordination with IUPAC would be desirable.

Supported Conferences

Conference on Precision Electromagnetic Measurements (CPEM).

C2 supported CPEM 2008 (Broomfield CO, USA, June 2008), at which an IUPAP Young Scientist Prize in Fundamental Metrology was awarded to Sébastien Bize (LNE-SYRTE, France). C2 expects to continue to recommend support of this series, which is widely attended by members of C2 involved in precision measurements. The next conference is to be held 13–18 June 2010, in Daejeon, Korea.

International Conference on Exotic Nuclei and Atomic Masses (ENAM).

C2 supported ENAM'08 (Ryn, Poland, September 2008), at which an IUPAP Young Scientist Prixe in Fundamental Metrology was awarded to Frank Herfurth (GSI, Germany) and IUPAP SUNAMCO Senior Scientist Medals were awarded to Heinz-Jürgen Kluge (GSI, Germany) and Georg Bollen (Michigan State, USA). This series is widely attended by members of C2 involved in precision atomic mass measurments but the date of the next meeting is not known at present.

The next meeting of Commission C2 is expected to be held in conjunction with CPEM 2010, in June of 2010.

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http://www.npl.co.uk/server.php?show=nav.772

[1] http://www-v2.sp.se/metrology/IUPAP_SUNAMCO/IUPAP%20SUNAMCO%20Commission_files/IUPAP_Red_book_1987/introduction_red_book_iupap_sunamco_1987.htm - note that this is C2's old website. It is hoped that the UK Institute of Physics will host a revised C2 website alongside the IUPAP website http://www.iupap.org/index.html.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 8.2.4
Revised definitions of SI base units

To Jack Lorimer

From Ian Mills
9 July 2009

Dear Jack,

I am planning to come to Glasgow specifically to attend the ICTNS meeting, because I would like ICTNS to be aware of the proposal from the CCU to redefine four of the SI base units, and in particular the mole. I would like to hear opinions from members of your committee. I certainly wish ICTNS to be aware of this proposal, and I would really like to come away with some expression of support for the proposal – or perhaps of opposition, if that should be the case. I believe that you discussed this at your meeting in Beijing two years ago and expressed support for the proposed change, but I would like to hear a repeat discussion to confirm how people feel about this matter.

I am flying up on Easyjet flight 83 that arrives in Glasgow at 12:00 on Sunday 2 August, and after checking into my room at the Crowne Plaza I shall endeavour to find my way to your ICTNS meeting. I shall be there for the remainder of Sunday and all day Monday, returning south on Easyjet flight 78 departing Glasgow at 19:45 on Monday evening.

Briefly, the issue is as follows. The present definition of the mole is made to fix the molar mass of carbon 12, $M(^{12}\mathrm{C})$, to be exactly 12 g/mol; the value of the Avogadro constant N_A then has to be determined experimentally, either from the silicon crystal density experiment (XRCD) or from watt balance measurements (WB), and the value of N_A is at present (June 2009) known with a relative standard uncertainty of about 5 parts in 10^8. The proposal is to redefine the mole to fix the value of the Avogadro constant exactly to its best estimate at the time of making the change; then the value of the molar mass of carbon 12 will have to be determined experimentally, and it will actually be known with an uncertainty of a few parts in 10^8. This is based on our present knowledge of the fundamental constants.

I shall try to explain this, in an objective way, to ICTNS. I attach some papers that various people have written on the subject, and I shall bring a PowerPoint display of a few slides to help the explanation.

The CCU strongly supports making the change to fix the value of N_A. However some French chemists, championed by Yves Jeannin (a former president of IUPAC), are strongly opposed to making this change – they wish to retain the present definition of the mole. The CCQM (Consultative Committee for Amount of Substance, Quantité de Matiere) support the CCU in proposing this change, as do a number of other groups. I will try to summarise the situation objectively when I am with you.

I look forward to seeing you!

With my kind regards, Ian

(I attach various documents on the subject that I would be happy for you to circulate to members of ICTNS in advance of the meeting

Fixer le nombre d'Avogadro ou la masse molaire du carbone-12 Quelle option choisir ?

De nombreuses discussions sont en cours qui visent à donner des valeurs fixes sans unité à des constantes fondamentales afin de réduire le nombre d'unités de base et celui des étalons qui y sont attachés.

La mole pose une question particulière car il faut choisir entre fixer le nombre d'Avogadro ou fixer la masse molaire du carbone-12.

A partir de la relation connue : $h = \alpha^2 c m_e / 2R_\infty$
où h est la constante de Planck, α la constante de structure fine, c la vitesse de la lumière, m_e la masse absolue d'un électron, R_∞ la constante de Rydberg, on peut écrire :

$$h.N_A = [\alpha^2 c m_e / 2R_\infty m(^{12}C)].M(^{12}C)$$

avec $m(^{12}C)$ masse absolue d'un atome de l'isotope 12 du carbone, et $M(^{12}C)$ la masse molaire de l'isotope 12 du carbone ;

$$\text{soit} \quad h.N_A = K.M(^{12}C)$$

Cette relation montre qu'il y a trois possibilités de fixer les constantes :

1- fixer la constante de Planck h et le nombre d'Avogadro N_A, la masse molaire du carbone-12 $M(^{12}C)$ est calculée ;

2- fixer la constante de Planck h et la masse molaire $M(^{12}C)$ du carbone-12, le nombre d'Avogadro N_A est calculé ;

3- fixer le nombre d'Avogadro N_A et la masse molaire $M(^{12}C)$ du carbone-12, la constante de Planck h est calculée.

Le choix de la constante de Planck s'impose du fait de sa position centrale en physique quantique. Les avantages sont décrits dans une note « On the possible redefinition of the kilogram » préparée par Taylor et Mohr pour le 14th meeting du CCU in 2001.

Quelles raisons peut-on invoquer pour choisir entre N_A et $M(^{12}C)$?

Aujourd'hui la définition de la mole retenue par l'IUPAC repose sur une valeur 12 exacte pour la masse molaire de l'isotope 12 :

La mole est la quantité de matière d'un système qui renferme autant d'entités élémentaires qu'il y a d'atomes dans 0,012 kilogramme de carbone-12.

La table des masses atomiques relatives des isotopes et par voie de conséquence la table des masses molaires des éléments sont établies sur la base de cette valeur.

Dans la définition de la mole, le kilogramme est impliqué. L'unité de base « mole » se définit avec l'aide d'une autre unité de base « le kilogramme » définie au préalable. Ce cas n'est pas unique ; l'actuelle définition du mètre implique une autre unité de base, la seconde.

Une conséquence de cette définition est que le nombre d'Avogadro est ensuite déterminé expérimentalement.

Il a été proposé de choisir un nombre d'Avogadro fixé. De la sorte une nouvelle définition de la mole pourrait être :

La mole est la quantité de matière qui contient un nombre d'entités élémentaires égal à $6{,}0221415.10^{23}$.

Cette proposition exige d'être regardée avec le plus grand soin.

La première remarque que l'on peut faire est que la masse atomique du carbone-12 ne sera plus constante. Elle variera au gré de l'amélioration des mesures expérimentales ; de même toutes les masses molaires des éléments varieront. De telles modifications dans le futur resteront certes mineures, mais c'est tout aussi vrai si l'on fixe $M(^{12}C)$ et si on laisse N_A flotter. Néanmoins c'est un changement de philosophie majeur par rapport à la situation actuelle, changement qui risque fort d'être incompris des chimistes qui utilisent la table des masses molaires tous les jours.

Une seconde remarque vient de la considération simultanée des trois constantes, la vitesse de la lumière, la constante de Planck, le nombre d'Avogadro. La physique implique tout un ensemble de constantes qui se rattachent à des phénomènes ou à des propriétés de la matière. Mentionnons, la charge de l'électron, la perméabilité du vide, la masse de l'électron, la constante de structure fine et bien d'autres encore. Certaines d'entre elles ont déjà des valeurs fixées par convention internationale.

La situation de N_A est complètement différente ; c'est une constante de proportionnalité. Quand Dalton a construit sa table des « poids atomiques » dont l'intérêt pratique et historique est considérable, il a choisi 1 pour l'hydrogène, le plus léger de tous les éléments. Ceci a conduit à la valeur 16 pour l'oxygène. Quelque temps après, Berzelius a proposé la valeur 100 pour le poids atomique de l'oxygène : ceci venait du fait que l'oxygène donne naissance à un nombre bien plus grand de combinaisons stables et faciles à obtenir avec les autres éléments, le passage obligé pour la détermination des masses molaires des éléments. La communauté des chimistes n'a pas retenu sa proposition. Si elle avait été adoptée, le nombre d'Avogadro eut été bien différent. La signification physique au plan fondamental du nombre d'Avogadro ne saurait donc être comparée avec celle de la vitesse de la lumière ou celle de la constante de Planck.

Un nombre d'Avogadro fixé conduit à une mole définie sans faire référence à une autre unité de base. La mole est donc si indépendante de toute autre unité qu'il s'avère nécessaire de la considérer comme une unité de base. Si $M(^{12}C)$ est pris égal à 12 exactement, ce qui est le cas aujourd'hui, la mole implique une autre unité le kilogramme. Supposons que le kilogramme se définisse avec l'aide d'une constante de Planck fixée en impliquant la seule seconde et s'il perd de ce fait son statut d'unité de base, la mole perd aussi son statut d'unité de base. Ce choix diminue donc le nombre d'unités de base de un. C'est séduisant.

Si N_A est fixé, la relation $h.N_A = K.M(^{12}C)$ donne $M(^{12}C)$; la méthode de la sphère de silicium donne la masse molaire de l'élément M(Si). On se retrouve avec deux façons indépendantes de définir le point de départ de la table des masses molaires des éléments. Ce n'est pas la situation la plus favorable. La détermination des abondances isotopiques demeure le maillon faible. Des efforts considérables sont faits pour s'en affranchir en enrichissant le silicium en ^{28}Si pour résoudre ce problème. Cependant il reste deux entrées, l'une est calculée, l'autre est mesurée. La situation idéale serait d'avoir le même isotope dans les deux cas, mais est-ce possible ?

Reste le problème de l'étalon. La définition avec un nombre d'Avogadro fixé ne suggère pas d'étalonnage. En se plaçant sur un plan très pratique, on observe que le mètre se mesure avec une règle, que la durée se mesure avec un chronomètre, que la tension se mesure avec un voltmètre, que le kilogramme se mesure avec une balance, que la température se mesure avec un thermomètre. Et la quantité de matière ? Il faut une balance et le nombre de moles s'en déduit à l'aide des masses molaires. Qu'on le veuille ou non, si le nombre d'Avogadro fixé évite d'impliquer le kilogramme dans la définition, la détermination du nombre de moles passe par le kilogramme.

Pour toutes ces raisons, le choix d'une masse molaire $M(^{12}C)$ fixée paraît plus judicieux.

Yves Jeannin

Mars 2009

A fixed Avogadro constant or a fixed carbon-12 molar mass
Which one to choose ?

Yves Jeannin
Emeritus Professor, Pierre and Marie Curie University
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In a recent issue of Chemistry International, Ian Mills and Martin Milton suggested a new definition for the mole, one of the seven base units.(1) This matter is controversial and needs a careful examination.

The Green Book (2) describes the seven base units and gives their definitions. They are the length unit, the meter, the time unit, the second, the mass unit, the kilogram, the current unit, the ampere, the temperature unit, the kelvin, the amount of substance unit, the mole, and the luminous intensity unit, the candela. Some of them require the help of another base unit : for instance, the time unit involves the length unit, the current unit involves the length unit, the amount of substance unit involves the mass unit.

Historically, the first standard for the meter was based upon the earth so that it was accessible to everybody at any time. Later on Johnstone-Stoney and Planck had a completely different view and recommended to use fundamental constants of theoretical physics for defining units. In the mean time and independently base units and corresponding standards have been defined on an purely experimental basis. Although it provides a set of clearly defined units, this set is not very consistent. Moreover progresses of modern physics led to fundamental constants known with a great accuracy.(3) This suggests to think again about base unit definitions with the help of fundamental constants, all the more as it would allow to reduce the number of base units.

Presently, discussions are in progress about this subject. As an example, let us take the case of the speed of light c. It has already been decided to choose a fixed value equal to 299,792,458 $m.s^{-1}$. Indeed the speed of light is a fundamental constant of physics, the value of which is independent of the galilean referential in which it is measured ; it allows a clear definition for the unit of length. Now considering the well known formula $\lambda=c/\nu$, in which wave length λ is bound to frequency ν through c, it appears that it is no longer necessary to define two base units, meter and second, if the speed of light is arbitrarely considered as a constant without unit. If the length is chosen as a base unit, the time is expressed in m^{-1}. If the

second is chosen as as a base unit, the length is expressed in s^{-1}. Let us underline that this is a metrology approach. For practical purposes, speed should keep its traditional unit. This view has the great advantage for metrologists to reduce the number of base units by one.

Exploring the development of this idea, Mills, Mohr, Quinn, Taylor, and Williams (4) presented a choice of four constants to be fixed as the speed of light ; the Planck constant, the electron charge constant, the Boltzmann constant, and the Avogadro constant. As a consequence of a fixed Avogadro constant, Mills and Milton introduced a new definition of the mole :

The mole is the amount of substance of a system which corresponds to 6.0221415 x 10^{23} elementary entities.

The present definition is :

The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon-12. *(14th CGPM, 1971)*

This mole definition implies a fixed carbon-12 molar mass $M(^{12}C)$ equal to 12 exactly and the use of another base unit the kilogram. Therefore, the mass unit has to be defined prior to the mole unit. The definition proposed by Mills and Martin disconnects the mole unit from the kilogram, hence the advantage of this definition.

From the known relation : $h = \alpha^2 c m_e / 2R_\infty$ **(1)**
with h Planck constant, α fine structure constant, c speed of light, m_e mass of one electron, R_∞ Rydberg constant, one can deduce :

$$h.N_A = [\alpha^2 c m_e / 2R_\infty].[M(^{12}C)/m(^{12}C)]$$

with $m(^{12}C)$ mass of one atom of carbon-12 isotope and $M(^{12}C)$ molar mass of carbon-12 ; this formula can be shortened as :

$$h.N_A = K.M(^{12}C)$$

If fixed values are assigned to the Planck constant, and/or to the carbon-12 molar mass, and/or to the Avogadro constant, there are three possibilities :

1- a fixed Planck constant h and a fixed Avogadro constant N_A, the carbon-12 molar mass $M(^{12}C)$ is computed ;

2- a fixed Planck constant h and a fixed carbon-12 molar mass $M(^{12}C)$, the Avogadro constant N_A is computed ;

3- a fixed Avogadro constant N_A and a fixed carbon-12 molar mass $M(^{12}C)$, the Planck constant h is computed.

The choice of a fixed Planck constant seems obvious because of its central position in quantum physics. The advantages have been detailed in a note « On the possible redefinition of the kilogram » written by Taylor and Mohr.(5)

What about N_A or $M(^{12}C)$? Which one to choose ?

Let us look at the consequences of a new mole definition.

The first remark to be made is that the molar mass of carbon-12 is no longer constant if N_A is fixed. Increasing the accuracy of experimental methods in the future will consequently yield a better $M(^{12}C)$ value ; any improvement will introduce changes on the whole table of element molar masses. Such modifications will indeed remain minor, by the way as well as this one on N_A if a fixed $M(^{12}C)$ is chosen as it is today. From a practical point of view, every chemist concerned with synthetic chemistry will not troubled by those changes. Nevertheless it is a major modification with respect to the actual situation of stable values for all molar masses ; it will raise some feeling of unstability.

Let us consider together the speed of light, the Planck constant, and the Avogadro constant. Physics meets quite a number of such constants which relate to phenomena or to the properties of matter. One might mention the electron charge, the electron mass, the fine structure constant, the permeability of vacuum, and so on. Each of them has a deep physical meaning. Some of them have already fixed values by international agreement.

The nature of N_A is completely different. It is nothing but a proportionnality constant. When Dalton thought about atomic weights and set up his famous table which has a considerable historical and practical value, he took 1 for the lightest element, hydrogen.(6) It led to the value 16 for oxygen and 12 for carbon. At his time nobody really had any idea about the mass of a single atom. Later on, Berzelius proposed to use oxygen atomic weight as a starting value because he noted that oxygen reacts with many more elements than hydrogen to yield compounds, a mandatory step to determine atomic weights. He chose 100.(7) The chemical community did not follow his proposal. If this value had been retained, the Avogadro

constant would have been different. The physics laying behind the Avogadro constant cannot be compared with this one of the speed of light or of the Planck constant.

A fixed Avogadro constant leads to a definition of the mole without reference to any other unit. The mole becomes independent of any other unit so that it gets the statute of base unit. If $M(^{12}C)$ is kept equal to 12 exactly as it is today, the mole definition implies another unit, the kilogram. The kilogram definition is presently based upon the standard kept at the Pavillon de Breteuil where the Bureau International des Poids et Mesures is located. Unfortunately, this standard weight slightly changes over the years without any clear explanation : this is not very satisfactory. It seems possible to get a new definition for the mass unit with a fixed Planck constant without unit. By comparing a mechanical power and an electrical power, mass is found to be proportional to frequency.(8) The kilogram mass unit would be defined with the only help of the time unit. Then it is no longer necessary to consider the mass unit as a base unit. Consequently the mole would also loose its statute of base unit. The choice of a fixed carbon-12 molar mass would decrease the number of base units by one. It is attractive from a metrology point of view.

If N_A is fixed, the relation $h.N_A = K.M(^{12}C)$ provides $M(^{12}C)$ by computation. The silicon sphere method compares experimentally the macroscopical volume of a sphere and the microscopical one of a single atom.(9) A fixed N_A yields M(Si) which in turn yields $M(^{12}C)$. There are thus two independent entries to the molar mass table. This is not the most favourable situation. The isotopic abundance determination remains a weak step in the silicon sphere method. One should point out that there are considerable efforts going on to enrich silicon into its most abondant natural isotope so that difficulties with isotopic abundances will be overcome. One may also note that any other isotope could be introduced in place of carbon-12 in relation (1), particularly this one of an element having a single stable isotope which could also be used in place of silicon for the experimental volume comparison. However is it possible ?

The exact number 12 is designed by A_r and called carbon-12 « atomic weight » ; it has no unit. Although it is not strictly speaking a weight, this word is accepted by IUPAC due to its long traditional use and as a tribute to Dalton. By definition the « molar mass » M_r is this number expressed with a unit which is the kilogram. One can write :

$M_r = A_r \cdot M_u$ with $M_u = 0.001$ kg

M_u is called « molar mass constant ». All the other atomic weights are determined relatively to carbon-12 atomic weight, so that they are called « relative atomic weights ». In the present SI, atomic weight and molar mass of carbon-12 have exact values, M_u is exactly 0.001 kg.

With the new proposal of a fixed N_A, molar mass $M(^{12}C)$ is known with a standard deviation ; it is no longer fixed and will slightly fluctuate at the rythm of the accuracy improvement of experimental methods. Consequently the molar mass constant M_u will also fluctuate so that the value 12 for carbon-12 atomic weight will remain constant. However this situation seems rather unfortunate. To use a unit conversion factor which is not really a constant is disturbing. Moreover Martin and Mills recommend a larger use of M_u especially in teaching ;(1) the need of a new constant M_u if fluctuating will be difficult to understand for pupils and even students. Finally if a chemist wants to compute a number of mole, he will use a balance and the weight of the substance is known with a mass unit : this result will then be divided by the molar mass also expressed with a mass unit, not by the relative atomic weight which has no unit. Then it is important that element molar masses are constant.

A good definition for a base unit is supposed to provide at the same time a standard which can be easily used by anybody anywhere in the world. The definition proposed by Mills and Martin means that one has to count atoms. It does not seem possible to get a standard by this method. A weighing balance is the tool used by a chemist to measure an amount of substance with the help of molar masses. While the kilogram is needed in the present definition, it disappears from the new definition but it has to be used to measure an amount of substance. Thus why not to keep a mass unit in the mole definition and to maintain the present definition.

For these reasons, the choices of a fixed $M(^{12}C)$ and of the actual definition are favoured.

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3- C.J.Bordé, Phil. Trans. Roy. Soc. A, 363, 2177 (2005)

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5- B.N.Taylor, P.J.Mohr, On the possible redefinition of the kilogram, document prepared for the 14th CCU meeting (2001)

6- A New System of Chemical Philosophy, J.Dalton (1808)

7- Théorie des proportions chimiques et table analytique des poids atomiques des corps simples et de leurs combinaisons les plus importantes, J.J.Berzelius (1835)

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An open letter to Yves Jeannin from Ian Mills

- in reply to Jeannin's letter of 18 November 08

- copied to other members of the Academie Science et Métrology WG

(slightly revised) 1 March 2009

Dear Yves,

I have some sympathy with your desire to retain the present definition of the mole, rather than to revise the definition in the manner that is now being considered by the CCU. I was personally opposed to the proposed change when it was first suggested, but I have been converted to thinking that it may be a good way to go.

However I have to say that I think you slightly miss-understand the proposal. There is no suggestion that the present atomic mass scale, giving the masses of the atoms relative to the mass of the carbon 12 atom, would change. The present atomic mass scale would remain exactly as it is at present.

Note that what are commonly called "atomic weights" and "molecular weights" are actually *relative* atomic and molecular masses, relative to carbon 12 as exactly 12. They are not either weights or masses; they are dimensionless numbers. Denoting the atomic weight of X as $A_r(X)$, as in the Green Book, the equations are:

atomic mass of carbon 12 $= m(^{12}C) = 12\, m_u$

unified atomic mass unit $= m_u = 1\ u = 1\ Da = m(^{12}C)/12$

atomic weight of carbon 12 $= A_r(^{12}C) = 12$

atomic weight or molecular weight of X $= A_r(X) = m(X)/m(^{12}C) = m(X)/12m_u$

where X denotes any atom or molecule or entity.

For example for the fluorine atom,

atomic mass of fluorine $= m(F) = 18.998\ 403\ 22\ (15)\ m_u = 18.998\ 403\ 22\ (15)$ u

atomic weight of fluorine $= A_r(F) = 18.998\ 403\ 22\ (15) = 12\, m(F)/m(^{12}C) = m(F)/m_u$

All these relations are exact in the current SI, and **they will all remain exactly true in the new SI** as at present proposed, except that the number 18.998 403 22 (15) is an experimentally determined number with a standard uncertainty of 15 in the last two digits. With the exception of carbon 12 whose atomic weight is exactly 12 by definition, the atomic weights of all other elements are determined experimentally by sophisticated mass spectrometry. For many of the atoms early in the periodic table their atomic weight is known with a relative uncertainty of a few parts in 10^8, as for fluorine; for many of the heavier elements the uncertainty is a few parts in 10^7.

The proposed new definition of the mole, which – for convenience – I shall call "the new SI", would fix the value of the Avogadro constant, but the molar mass of carbon 12 would become a quantity to be determined experimentally. By contrast the present definition of the mole fixes the value of the molar mass of carbon 12, but the value of the Avogadro constant is a quantity to be determined experimentally. If we adopt the new definition, then it is possible that future measurements might lead us to revise the molar mass of carbon 12 slightly, so that it would no longer be exactly 12 g/mol, but the value of the Avogadro constant would never change. The possible future changes that might occur in $M(^{12}\mathrm{C})$ and $M(\mathrm{X})$ will be (at the most) a few parts in 10^9. If however we stay with the present definition of the mole, then it is possible that future measurements might lead us to revise the value of the Avogadro constant slightly, but the molar mass of carbon 12 would never change from exactly 12 g/mol.

Note however, in particular, that the atomic weight of carbon 12 will remain exactly 12, by definition, $A_r(^{12}\mathrm{C}) = 12$.

Experimentally determined quantities always have an associated uncertainty, whereas for exactly defined quantities the uncertainty is always zero.

The situation is similar to that when we changed the definition of the meter in 1983, to fix the speed of light. The previous definition of the metre fixed the wavelength of the red krypton line, whereas the new definition fixes the speed of light in vacuum. Using the old definition, it was possible that the speed of light would have to have been revised as a result of new experiments, but the wavelength of the red krypton line would never have changed. Using the new definition, it is possible that the wavelength of the red krypton line may have to be revised as a result of new measurements, but the speed of light will never change.

I have tried to summarise the situation in the table below, in which I also use the molar mass constant , M_u, which is defined as one twelfth of the molar mass of carbon 12. M_u has not been used very much in the chemical literature up to now, but we believe it could be used more with advantage in teaching chemistry, because of the fact that it provides a simple route to calculating molar masses in general, through the relation (which holds true in the current SI and in the new SI):

$$\text{molar mass} = \text{molecular weight} \times M_u$$

quantity	in current SI: value	in current SI: uncertainty	in new SI: value	in new SI: uncertainty
$M(^{12}\mathrm{C})$:	12 g/mol	0.0	$12\times(1 \pm 3\times10^{-9})$ g/mol	3×10^{-9}
$A_r(^{12}\mathrm{C})$	12	0.0	12	0.0
$M_u = M(^{12}\mathrm{C})/12$:	1 g/mol	0.0	$1\times(1 \pm 3\times10^{-9})$ g/mol	3×10^{-9}
molar mass of X:	$A_r(\mathrm{X})$ g/mol	$u_r(A_r(\mathrm{X}))$ g/mol	$A_r(\mathrm{X})\ M_u$	$u_r(A_r(\mathrm{X}))\ M_u$
Avogadro constant:	N_A	$u_r(N_A)$	N_A	0.0

I use the symbol $u_r(Q)$ to denote the value of the relative standard uncertainty in the value of a quantity Q. Notice that although the molar mass of carbon 12 is known exactly in the current SI, by definition, to be 12 g/mol, the molar mass of other atoms and molecules is not known exactly but is subject to uncertainties due to the uncertainties in the relative masses of the atoms. These relative uncertainties in the atomic weights vary from about 10^{-8} (for those that are best known) to about 10^{-5} or 10^{-6} as you work up the atomic mass scale. Thus although the molar mass of carbon 12 will no longer be known exactly in the new SI, its relative standard uncertainty of about 3×10^{-9} will be much smaller than the relative uncertainty in the atomic weight of any of the other atoms.

The following relations hold among these quantities. **These relations hold true in both the current SI and the new SI.**

$$M_u = N_A \times m_u$$

$$M(^{12}\mathrm{C}) = N_A \times m(^{12}\mathrm{C}) = 12\ M_u$$

$$M(\mathrm{X}) = N_A \times m(\mathrm{X}) = A_r(\mathrm{X})\ M_u$$

Thus the Avogadro constant is the conversion factor from atomic to molar quantities. Multiplying by the Avogadro constant converts the unified atomic mass unit into the molar mass constant, or the mass of an atom or molecule X into the molar mass of X.

I now write those same three equations, and I put **in red** those quantities whose values are exactly known, by definition, in the current SI:

$$M_u = N_A \times m_u$$

$M(^{12}\mathrm{C}) = N_\mathrm{A} \times m(^{12}\mathrm{C})$

$M(\mathrm{X}) = N_\mathrm{A} \times m(\mathrm{X}) = A_\mathrm{r}(\mathrm{X})\, M_\mathrm{u} = A_\mathrm{r}(\mathrm{X})\ (1\ \mathrm{g/mol})$

and now I put in red those quantities whose values would be known exactly, by definition, in the new SI:

$M_\mathrm{u} = N_\mathrm{A} \times m_\mathrm{u}$

$M(^{12}\mathrm{C}) = N_\mathrm{A} \times m(^{12}\mathrm{C})$

$M(\mathrm{X}) = N_\mathrm{A} \times m(\mathrm{X}) = A_\mathrm{r}(\mathrm{X})\, M_\mathrm{u}$

The quantities in black have to be determined by experiment.

For example, in the current SI the value of the Avogadro constant is known to be

$N_\mathrm{A} = 6.022\ 141\ 79\ (30) \times 10^{23}\ \mathrm{mol}^{-1}$ with $u_\mathrm{r} = 50 \times 10^{-9}$ (CODATA, 2006)

In the new SI it would have the value

$N_\mathrm{A} = 6.022\ 141\ 79 \times 10^{23}\ \mathrm{mol}^{-1}$ exactly, with $u_\mathrm{r} = 0$

In the current SI the molar mass of carbon 12 has the exact value

$M(^{12}\mathrm{C}) = 12\ \mathrm{g/mol}$ exactly, with $u_\mathrm{r} = 0$

In the new SI it would initially have the same value

$M(^{12}\mathrm{C}) = 12\ \mathrm{g/mol}$ but with an experimental uncertainty, $u_\mathrm{r} = 3 \times 10^{-9}$.

It is possible that the best estimate of $m(^{12}\mathrm{C})$ may have to be slightly revised as the years go by, due to small revisions in the values of other constants, but any change from 12 g/mol is ulikely to be greater than a relative change of 3 parts in 10^9.

I attach copy of a paper that I hope will further help to explain these things. It is a short note that Martin Milton and I wrote a month ago for Chemistry International, on *Amount of substance and the mole*. It is at present with Fabienne (editor of CI), and will appear in CI in the new year (I believe).

The advantage of the new definition of the mole is that it would be conceptually simpler, and easier for students to understand. Also it would detach the definition of the mole from the definition of the kilogram, so that the mole would not reflect the present uncertainty in the mass of the International Prototype of the kilogram. The advantage of the current definition of the mole is that it enables one to calculate the molar mass of any molecule without knowing or making use of the value of the Avogadro constant, which was the reason for the defining the mole as it is defined in the current SI – because the value of the Avogadro constant was not known as well as the atomic weights of the atoms at that time.

However we now know the value of the Avogadro constant to better than a part in 10^7, and this reason no longer applies.

On balance I prefer the proposed new definition. I do hope all this helps! Do challenge me with further questions if you think I can help.

Kind regards, Ian Mills 25 November 2008, revised and extended 1 March 2009

Why the mole should be redefined in term of an exact value of the Avogadro constant N_A: A reply to document CCQM/09-06 by Andres *et al*.

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Introduction. **Andres *et al*., in document CCQM/09-06, have expressed some concerns about the CCU recommendation to the CIPM and CGPM that the mole should be redefined in terms of an exact value of the Avogadro constant N_A when the kilogram, ampere, and kelvin are redefined in terms of exact values of the Planck constant *h*, elementary charge *e*, and Boltzmann constant *k*, respectively. The purpose of this note is to indicate why we believe these concerns are unfounded and to once again point out the many benefits of redefining the mole in terms of an exact value of N_A.**

Problem with current definition. **It is our collective personal experience that the current definition of the mole is in fact poorly understood. This view is based on many decades of teaching physics and chemistry to students at all levels, working closely with researchers and technologists in diverse fields, including fundamental metrology, promoting the SI in non-metric countries, working closely with industry of all kinds and at different levels of sophistication, and writing numerous papers on the SI and the fundamental constants. Invariably, people do not understand that the SI base quantity amount of substance is independent of the SI base quantity mass and that its unit mole is not a measure of mass but rather of the "number of things" (entities). The proposed new definition of the mole in terms of N_A will end this confusion, as the following definition being considered by the CCU clearly shows (the formal definition is given in sans serif type, while the accompanying explanatory text, which is not part of the formal definition, is in serif type):**

mole:

> **The mole, unit of amount of substance of a specified elementary entity, which may be an atom, molecule, ion, electron, any other particle or a specified group of such particles, is such that the Avogadro constant is equal to exactly 6.022 141 79 $\times 10^{23}$ per mole.**
>
> **Thus we have the exact relation $N_A = 6.022\ 141\ 79 \times 10^{23}$ mol^{-1}. The effect of this definition is that the mole is the amount of substance of a system that contains 6.022 141 79 $\times 10^{23}$ specified elementary entities.**

Independence of ISQ from definition of the mole. Although not discussed by Andres *et al*., we take this opportunity to emphasize that defining the mole in terms of an exact value of N_A has no impact whatsoever on the system of quantities, which

includes the equations among them, on which the SI is based. This system, as discussed in Sec. 1.2 of the 8th edition of the BIPM SI Brochure [1], has recently been given the name "International System of Quantities," abbreviated ISQ. The following examples of quantities and equations relevant to the quantity amount of substance are part of the ISQ and do not depend on the definition of any SI unit [2]:

$$A_{\mathrm{r}}(X) = \frac{m(X)}{m_{\mathrm{u}}} \quad \textbf{with} \quad m_{\mathrm{u}} = \frac{m(^{12}\mathrm{C})}{12} \tag{1a}$$

$$M(X) = A_{\mathrm{r}}(X) M_{\mathrm{u}} \quad \textbf{with} \quad M_{\mathrm{u}} = N_{\mathrm{A}} m_{\mathrm{u}} = N_{\mathrm{A}} \frac{m(^{12}\mathrm{C})}{12} = \frac{M(^{12}\mathrm{C})}{12} = \frac{2R_{\infty} N_{\mathrm{A}} h}{\alpha^2 c A_{\mathrm{r}}(\mathrm{e})}. \tag{1b}$$

Here $A_r(X)$ is the relative atomic mass of entity X, $m(X)$ is the mass of entity X, m_u is the atomic mass constant, $m(^{12}C)$ is the mass of the carbon 12 atom, $M(X)$ is the molar mass of X, M_u is the molar mass constant, $M(^{12}C)$ is the molar mass of the carbon 12 atom, R_∞ is the Rydberg constant, α is the fine-structure constant, c is the speed of light in vacuum, and $A_r(e)$ is the relative atomic mass of the electron.

In the current SI, *the value* of M_u is 1 g/mol exactly due to the definition of the mole, while in the New SI in which the kilogram, ampere, kelvin, and mole are defined in terms of exact values of h, e, k, and N_A, *the value* of M_u is calculated from the far right-hand-side of Eq. (1b). However, since the constants entering that expression are either exactly known or have extremely small relative standard uncertainties (i.e., less than one part in 10^9), the uncertainty of M_u and its difference from 1 g/mol will be so small that they will have no practical consequences. (The words "the value" are in italic type to emphasize the difference between quantities and the equations among them and values of those quantities; only the latter require the introduction of units—the ISQ does not.) It should also be understood that the periodic IUPAC compilations of relative atomic masses of the elements (commonly called the atomic weights of the elements), and the periodic Atomic Mass Data Center compilations of the relative atomic masses of the nuclides, are not affected in any way by redefining the mole in terms of an exact value of N_A.

Connection of mole to mass. **Andres *et al*. are correct that by defining the mole in terms of an exact value of N_A rather than in terms of the number of entities in a body of a particular mass as is currently the case (i.e., 0.012 kg of carbon 12), the current explicit connection of the mole to the kilogram is severed. We view this as a significant advantage, because the explicit connection in the current definition is the source of confusion concerning the real meaning of the quantity amount of substance and its unit mole. However, this connection is not severed in practice, as the discussion in the previous two paragraphs clearly shows. The molar mass of an entity remains a very useful quantity that can be readily calculated from the relative atomic mass of the entity and employed in the determination of amount of substance in the unit mole.**

***N_A is* a fundamental constant.** We see no utility in either trying to prioritize the relative importance of different fundamental constants or to decide if a particular constant is a "true" constant of nature. Many of the constants are simply a consequence of how we have chosen to formulate the equations of physics that we use

to describe nature. A different formulation would lead to different constants in our equations, and in some cases they would have never appeared. If one looks at the 200 year history of the Avogadro constant, one sees that it invariably has been viewed as a constant of nature; many famous scientists have spent many years of their lives elucidating and determining N_A. Thus in our view, even though in some sense it is simply an arbitrary reference number that enables us to avoid dealing with very large numbers in the field of chemistry, there is no reason whatsoever for removing it from its current place of honor in the Pantheon of fundamental constants along side *h*, *e*, *k* and many others.

Indeed, although one might argue that N_A is a constant that we may choose at our convenience to determine the size of the unit mole, it being simply the conversion factor from the unit "entity" to the unit mole, an exactly similar comment may be applied to *k*. Thus the Boltzmann constant is the conversion factor from energy to thermodynamic temperature through the relation $E = kT$, and may be chosen at our convenience to determine the size of the unit of temperature in terms of the unit of energy.

Benefits for the SI of redefining the mole in terms of an exact value of N_A. Such a definition together with the redefinitions of the kilogram, ampere, and kelvin in terms of exact values *h*, *e*, and *k* will mean that five of the seven SI base units are directly linked to exact values of well recognized fundamental constants. Although the remaining two base units are not so linked, each is directly linked to an exact value of an invariant of nature—the ground state hyperfine splitting frequency of the cesium 133 atom, $\Delta(^{133}\mathrm{Cs})_{\mathrm{hfs}}$, for the second; and the spectral luminous efficacy of monochromatic radiation of frequency 540×10^{12} Hz, $K(\lambda_{555})$, for the candela. For example, the explicit-constant form of the definitions of the meter, second, and candela (with accompanying explanatory text) would read as follows, with similar definitions for the kilogram, ampere, and kelvin (the similar definition of the mole is given above):

meter:

> The meter, unit of length, is such that the speed of light in vacuum is equal to exactly 299 792 458 meters per second.
>
> Thus we have the exact relation c = 299 792 458 m/s. The effect of this definition is that the meter is the length of the path travelled by light in vacuum during a time interval of 1/299 792 458 of a second.

second:

> The second, unit of time, is such that the ground state hyperfine splitting frequency of the caesium 133 atom is equal to exactly 9 192 631 770 hertz.
>
> Thus we have the exact relation $\Delta\nu(^{133}\mathrm{Cs})_{\mathrm{hfs}}$ = 9 192 631 770 Hz. The effect of this definition is that the second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium 133 atom.

candela:

> The candela, unit of luminous intensity in a given direction, is such that the spectral luminous efficacy of monochromatic radiation of frequency 540×10^{12} hertz is equal to exactly 683 lumens per watt.

> Thus we have the exact relation $K(\lambda_{555}) = 683$ lm/W. The effect of this definition is that the candela is the luminous intensity, in a given direction, of a source that emits monochromatic radiation of frequency 540×10^{12} hertz and that has a radiant intensity in that direction of 1/683 watt per steradian.

As these three examples show, the definitions of all seven base units can be written in a common explicit-constant form, thereby bringing to the SI base-unit definitions a simplicity, uniformity, understandability—and yes, elegance and beauty—never before imagined.

Benefits for the fundamental constants of redefining the mole in terms of an exact value of N_A. As discussed in Sec. 4.2 of Ref. [3], the impact on our knowledge of the values of the constants of redefining the kilogram, ampere, kelvin, and mole in terms of exact values of h, e, k, and N_A will be extraordinary. In addition to these four constants being exactly known, many other constants and energy equivalency factors will also be exactly known or will have significantly reduced uncertainties. Those constants whose "exactness" depends on N_A being exact include the Faraday constant $F = N_A e$, molar Planck constant $N_A h$, molar gas constant $R = kN_A$, and molar volume of an ideal gas at temperature T and pressure p, $V_m = RT/p$. Moreover, with a significant number of fundamental constants and energy equivalency factors having exact values or much reduced uncertainties, the changes in the recommended values of the constants and factors from one CODATA least-squares adjustment to the next will be significantly reduced—the surprisingly large fluctuations in the recommended values over time will be a thing of the past and for many constants it will be completely eliminated. This advance will be of major benefit to many scientists, engineers, and students who regularly use these values.

Further, the elimination or reduction in uncertainty of many of the constants resulting from fixing the values of h, e, k, and N_A will significantly clarify the links among the constants as well as highlight those areas of physics where important advances can be made through improved theory and experiment [3].

Conclusion. For all of the reasons given above, it is the NIST view that ***not*** redefining the mole in terms of an exact value of N_A would miss an opportunity to improve the SI and our knowledge of the constants and could well be seen as a disservice to all of science and technology.

References

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[2] B. N. Taylor, Metrologia **46**, L16 (2009).
[3] I. M. Mills, T. J. Quinn, P. J. Mohr, B. N. Taylor, and E. R. Williams, Metrologia **43**, 227 (2006).

Remarks based on discussions at the Committee on science and metrology of the French Academy of Sciences

By Jean Kovalevsky and Christian Bordé
Joint presidents of the Committee
May 2009

The Committee estimated it necessary to consider simultaneously the definitions of all the seven base units because of their mutual connections and because of the non-univocal (one to one) relations that link them to the fundamental constants. For instance, the quantum of action h is between mass and proper time because it is the product of these two quantities that provide the action, and therefore the phase for a massive object in quantum mechanics. A priori, the Planck constant could be used to define one or the other of these units. Similarly, let us remember the link between mass and the amount of substance, between time and length, between time and temperature, between electromagnetic field and luminous intensity.

The new definitions should, therefore, state explicitly the constants in question as well as the associated physics, provided however that it remains understandable to non-specialists.

The Committee confirms the conclusions of the Working Group (Annex 1) other than for the **mole**. The chemists of the Academy unanimously advise keeping a molar mass equal to 12 grams of carbon 12 (see the joint letter of Christian Amatore and the arguments by Yves Jeannin in Annex 2). The present definition of the Avogadro constant implies the mass of an atom of carbon which is a true physical constant as opposed to an arbitrary number of elementary entities. Furthermore, the "mise en pratique" of the mole with a balance seems to be much easier than counting atoms.

As regards **the unit of mass**, there was agreement to use the Planck constant. But how one can formulate a definition of the kilogram fixing the Planck constant in such a way that a layman can understand it? At macroscopic scale of a kilogram, the de Broglie-Compton frequency of an object is enormous, and its meaning appears to some as being only formal. However, this is what is measured by a watt balance. The other pitfall is that one must use a quantum mechanical concept in the macroscopic domain, where its validity may be questioned, particularly because of decoherence. Nevertheless, the BIPM watt balance will indeed involve a quantum phase at this scale thanks to the super-conductivity of its coil. Taking advantage of the additivity of masses, this double difficulty could be resolved by defining a macroscopic mass as a very large number (to be chosen) of microscopic entities (hypothetical massive particles) without mutual interactions and having a fixed de Broglie-Compton frequency. But these massive particles cannot correspond to real particles without re-defining the unit of time, nor can they be photons. Let us remember that mass is a Lorentz scalar. The energy of a particle is the time component of a 4-vector and is transformed as such by a Lorentz transformation. A mass can be defined by the energy of a massless particle only if it is put in a box with a privileged reference frame, and this is utterly artificial.

As far as **electrical units** are concerned, a majority of physicists of the Committee are still in favour of maintaining fixed the properties of light in vacuum: speed and impedance. The charge of the electron is easily deduced with a very good accuracy (some 10^{-10}) with the fine-structure constant. The uncertainty on the theoretical values of R_K and K_J will be reduced to the same level. This choice would thus satisfy both opticians and electricians.

Concerning **the unit of temperature** (the kelvin), there is general agreement to fix the Boltzmann constant as soon as its value is confirmed by independent methods at the level of 10^{-6}. However, it is suggested rather to fix the ratio between the Boltzmann and the Planck constants in order to set the link with the unit of time. It is indeed this ratio, which enters in the Planck black body law and in formulæ where temperature is associated with an atomic mass (as, for instance, the formula giving the Doppler width of spectral lines).

The question of the re-definition of **the unit of time** was widely discussed and highlighted in view of the spectacular progress of optical clocks. The second has been defined since 1967 as the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium 133 atom. At that time, the realisation of this definition was made with an uncertainty of some parts in 10^{11}. Since then, progress reached parts in 10^{15} or, possibly a few parts in 10^{16}. It will be very difficult to improve this performance because of an ensemble of fundamental effects (black body radiation, recoil effect, sensitivity to collisions and to residual fields, etc…). The most evident way to improve this situation is to increase the frequency of the clock.

The appearance of femtosecond lasers has led to the development of several types of clocks using optical frequencies in the visible domain up to ultra-violet. Several clocks using various neutral atoms or ions exist in the world and many others are under construction. Potentially, levels of relative uncertainty smaller than 10^{-17} are accessible now. Optical clocks have now largely overtaken caesium clocks in reproducibility and stability.

The inconvenience of this situation is that optical clocks can no longer be compared to caesium clocks and, consequently, to the SI second. They are now compared among themselves which amounts to the use of a system parallel to the SI. This is legitimate as long as this is done only in order to perfect instruments and to compare their properties. But, as soon as industrial applications need such high frequencies, such as clocks embarked on satellites, one will be in the same situation as are now electricians: a non-SI system will be used.

This is why we consider that it is urgent to reflect seriously on a new definition of the second using a suitably chosen atomic transition in the optical domain. As is the case for caesium, their frequencies cannot be expressed explicitly with a sufficient accuracy as functions of fundamental constants. We reach here the limits of the concept aiming at defining the units using only fundamental constants: the corrections to be applied to theoretical expressions are not known to the level of the reproducibility of the phenomenon used to define the unit or its realization. This may be a generic property of any system of units. One must chose one atomic transition, but on what criterion?

We expect soon to get results on several types of clocks built in different laboratories, to compare them and, from the results obtained, make a choice. Other types of clocks may be used as secondary realisations of the second to a given level of accuracy. Of course, it is not possible to finalize such a programme for the 2011 CGPM, but one should be prepared for the next General Conference.

We should note that a definition to such a level of accuracy will set problems that were not known in 1967. At that time, nothing was said on the conditions for obtaining the second, but it was implicitly acknowledged that it was a proper time in an environment, which does not perturb the clock. Until now, a global description of the Earth's potential was sufficient for the comparison of distant clocks. This will no longer be possible because, at this accuracy, the frequency depends on the fluctuating potential of the site (Earth tides, underground waters, etc…). It seems to us that a concrete definition should be given without reference to General Relativity, applying it to a non-perturbed atom on its world line. It is by postulate that we consider that an atomic transition can be a measure of the proper time of the theory. It is an incorrect usage to confound "proper time" with "local time" provided by a physical property. The definition of the second must be distinguished from its realization (which is modifiable) so that it can be applied in the context of General Relativity or some other theory (see document CCU/09-17).
Let us note that it is only proper time that is measurable. The problem of time scales, which are systems of time pointers, must be considered because they are used in practice to measure durations. As long as this measure is performed locally with the same clock in proper time, there is no difficulty. But additional texts will have to be written to indicate how a second should be used to measure durations within a non-local time scale. This poses complex problems on the Earth as well as in space and for this we draw the attention of the CCU to the document CCC/09-02-2 by Klioner *et al.*.

The definition of **the metre** is not brought into question now, but its realization involves lasers set on frequencies of atomic transitions with fixed conventional values. Considering the present evolution of clocks toward high frequencies, we strongly recommend the merging of the lists of frequencies used to realize the definition of the metre with those which serve as secondary representation of the second.
For measurements in space, which are implemented either by time interval measurements or by measuring the Doppler effect of waves emitted by an object, it is desirable that the definition of the astronomical unit of length in the solar system be strictly tied to the SI (see the note CCU/09-02-1.

The **candela** could be re-defined on the basis of a number of photons, but the link beween the creation/annihilation operators of photons and the electric field operator must be carefully taken into account because it involves the permittivity of vacuum. In other words, the electromagnetic energy density in a light beam can also be expressed from the electric field by means of the permittivity of vacuum. So, there are two ways to express the energy carried by the beam: one using the flux of photons, the other from the electric field of the wave and it is desirable not to introduce an uncertainty due to the permittivity of the vacuum between the two representations.

ANNEX 1

Report of the Working Group of the Académie des Sciences on base units and fundamental constants

by *Jean Kovalevsky, President of the Group*[1]
October 2007

A Working Group on base units and fundamental constants was created by the Académie des Sciences in 2002. It has already presented to the CCU in 2005 a first Report on the choice of a unit of mass in which it recommended the adoption of the Compton-de Broglie frequency as the reference for the kilogram. This in fact comes down to fixing the Planck constant. For two years now, the Group has examined what could be the new definitions of the electrical units having *mise-en-pratiques* that would allow a better accuracy than those that result from the present definitions.

1 - Theoretical considerations

At the outset, it was well understood that this discussion should take place in the context of local physics and the Einstein equivalence principle, which suffices for metrologists, the vacuum being that which comes into the interpretation of laboratory experiments and not the vacuum of cosmology.

The Working Group examined the possibility of choosing this or that reference to define electrical units. Two possibilities were studied by the Working Group:

- Define electrical units starting from the charge on the positron, e. The ampere would be defined by a certain number of charges, $-e$, per second.
- Take as the base the Planck charge $q_p = (2\varepsilon_0 hc)^{1/2}$. In this expression, c and h are fixed by the definitions of the metre and the kilogram whereas ε_0 is the permittivity of free space which would be thereby fixed.

The second option can also be expressed as a function of the vacuum impedance

$$Z_0 = \sqrt{(\mu_0/\varepsilon_0)} = 1/c\varepsilon_0 \qquad (1)$$

from which we deduce

[1] English translation of the original French text by T.J. Quinn

$$q_P = \sqrt{(2h/Z_0)} \quad (2)$$

From a theoretical point of view, we note that since the fine structure constant α is given by

$$\alpha = \sqrt{\frac{\mu_0}{\varepsilon_0}} \frac{e^2}{2h} \quad (3)$$

we have the following relation between e and q_P

$$q_P = e/\sqrt{\alpha} \quad (4)$$

To sum up the discussion, it comes fundamentally to choosing between two versions of physics:

1. α is a property of the vacuum, in which case we choose e as the base for the electrical units. Such a choice would accord with those who predict, in the long term, the most advanced string theory. It should also be noted that in this case the force between two charges or two currents would no longer be fixed, and this represents a significant difference from the present system. Finally, this would allow the subsequent fixing of the constants R_K and K_J, on the condition of course that the equations that link them to e be confirmed or completed, which is not the case at present.
2. α represents a property of the electron, which justifies the choice of q_P. In this case, ε_0, μ_0 and Z_0 are fixed. The constant R_K being linked in a simple way to Z_0, ($Z_0 = 2\alpha R_K$), we would directly have its value and the watt balance gives access to K_J. We note by the way that the values of μ_0 and ε_0 are already linked in the SI by the relation $c^2 = \mu_0\varepsilon_0$. Choosing q_P also fixes the ratio μ_0/ε_0, which renders the definitions of the metre and the electrical units coherent.

It appears that there is no crucial experiment that allows us to choose between these two visions that each have supporters within the Working Group.

The Working Group also considered the consequences of a possible time variation of α. The choice of e leads to an easier formulation of gauge invariance and its normalization, particularly if we consider electromagnetism as being a part of electroweak theory. However, laboratory experiments (the atomic fountain) give an upper limit to the annual variation of α that is below 10^{-15}. The Working Group has thus concluded that under these conditions this should not be a consideration in the choice of SI units. In fact, we are not looking for definitions that should rest unchanged for centuries. By then progress in physics would have led to new opportunities perhaps in quite unexpected directions.

For this reason the Working Group has decided, in establishing the conclusions of this Report, to ignore all considerations based on a possible variation of α and to consider that it is a constant.

2- Practical considerations

In order to give criteria for the choice, the Working Group has considered the practical consequences of each. We note, however, that since $q_p = e/\sqrt{\alpha}$, the two proposals have, as far as metrologists are concerned, certain consequences that are similar.

In the same way, the problems concerning R_K and K_J are the same in the two cases (we can equally use either the metrological triangle, the watt balance or the calculable capacitor, not forgetting the measurement of α). Each of these two quantities will be determined independently, without making any assumption as to the exactness of the relations linking them to e.

There are also different practical consequences that can be summarised as follows:

1. The simplicity of the definition works in favour of e, since the Planck charge or even the vacuum impedance seem more difficult to explain to the man in the street and to put in legislation than does the charge on the electron.
2. The choice of q_p has the advantage of not modifying the basic hypothesis of the present definition by keeping fixed the values of μ_0 , ε_0 and Z_0. But of course the definitions would be changed.
3. The danger of the choice of e is to be tempted to link, in practice, the definition of the charge of the positron to value of R_K and K_J whereas it has not be demonstrated that there are not corrective terms to the simple equations ($R_K = h/e^2$ and $K_J = 2e/h$). While the definition using e does not presuppose these equations, the temptation to use them will be great.
4. Taking into account the more esoteric nature of q_p, it would be preferable to give the definition in terms of the vacuum impedance Z_0.
5. The danger of the choice of q_p stems from the fact that the charge of the electron would be a quantity to be determined. Its uncertainty would be equal to half that of α, that is to say of the order of 10^{-9}. But, measurements of voltage are made with relative reproducibilities of 10^{-10} to 10^{-11} and one fears that the electrical community would adopt another conventional value for e for use with J_K as is done today when K_J is known in terms of SI to only parts in 10^7.

We thus note that the two definitions present advantages and disadvantages as well as dangers of interpretation. The Working Group was divided on this issue but a majority preferred to propose the value of the Planck charge, q_p or, better still, that of the vacuum impedance Z_0 for the definition of the new electrical base unit. In this case, for the definition of the electrical base unit we could:

- Either define the coulomb by fixing the numerical value of the Planck charge q_p with $\mu_0 = 4\pi\ 10^{-7}$ H m^{-1}. In which case the ampere would be the current corresponding to the flow of one coulomb per second.
- Or, take the ohm as the base unit of the SI which would be defined by fixing the numerical value of the vacuum impedance, $Z_0 = \mu_0 c$. In this case the primary realization of the definition would be by means of the Thompson-Lampard calculable capacitor which is the best realization of the vacuum impedance. R_K would then be determined by direct comparison with Z_0, and then K_J with the watt balance taking Z_0 instead of R_K without making any hypothesis as to the equations relating these constants to e, h or α.

Anyway, regardless of which solution is retained (e or q_p), even outside any possible variation of α, the underlying problem of either one of these fundamental approaches to physics will remain.

3 – Other recommendations on the new units of the SI

The Working Group has in addition made the following recommendations:

1. If e should be taken as the base for the new electrical units, it is recommended that the present relations between R_K and K_J should not be assumed to be exact.
2. In the same way, it is desirable not to proceed to a change in the present definition of the kilogram until the inconsistency between the determinations of the Planck constant h and the Avogadro number N_A have been resolved.
3. The Working Group recommends fixing the value of the Boltzmann constant k_B for the new definition of the kelvin. In any case, regardless of the form of this definition, it must be consistent with the value of 273.16 K for the thermodynamic temperature of the triple point of water with an uncertainty of 0.46 mK.
4. With the exception of one member in favour of the *status quo*, the Working Group recommends a new definition of the mole based on the Avogadro number N_A independent of the new definition of the unit of mass.
5. Taking account of the current use of the CGS Gaussian system among theoretical physicists, notably because it explicitly includes the symmetries of modern physics and thus gives access to a better physical understanding of electromagnetism, it is desirable that it also be given in detail in the BIPM SI Brochure and be taught in university courses alongside the SI.

ANNEX 2

A fixed Avogadro number or a fixed carbon-12 molar mass?

Many discussions are in progress about giving fixed values to some universal constants in order to reduce the number of base units and of related standards.

In this context, the case of the mole raises a particular question since one may choose either a fixed Avogadro constant N_A or a fixed carbon-12 molar mass $M(^{12}C)$.

From the known relation : $h = \alpha^2 c m_e / 2R_\infty$

with h Planck constant, α fine structure constant, c speed of light, m_e absolute mass of one electron, R_∞ Rydberg constant, one can easily deduce :

$$h N_A = [\alpha^2 c m_e / 2R_\infty m(^{12}C)]\, M(^{12}C) \qquad (1)$$

with $m(^{12}C)$ being the absolute mass of one atom of carbon-12 isotope ;

or $\quad h N_A = K.M(^{12}C)$

There are three possibilities to assign fixed values to h, and/or to N_A, and/or to $M(^{12}C)$:

1- the Planck constant h and the Avogadro constant N_A are fixed, the carbon-12 molar mass $M(^{12}C)$ is computed ;

2- the Planck constant h and the carbon-12 molar mass $M(^{12}C)$ are fixed, the Avogadro constant N_A is computed ;

3- the Avogadro constant N_A and the carbon-12 molar mass $M(^{12}C)$ are fixed, the Planck constant h is computed.

The choice of a fixed Planck constant seems obvious because of its central position in quantum physics. The advantages have been detailed in a note « On the possible redefinition of the kilogram » prepared by Taylor and Mohr for the 14th meeting of the CCU in 2001.

What about N_A and $M(^{12}C)$?

Today the IUPAC definition of the mole is based upon the exact value 12 given to the isotope ^{12}C molar mass :

The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon-12.

The table of element molar masses is built upon this value given to carbon-12.

The base unit « mole » is defined with the help of another base unit « the kilogram ». This is not a unique case ; the actual definition of the metre involves another base unit, the second. As a consequence of this mole definition, the Avogadro constant has to be determined experimentally.

Mills et al., have proposed to choose a fixed value for the Avogadro constant. Consequently a new definition of the mole might be :

The mole is the amount of substance which contains a number of elementary entities equal to 6.0221415×10^{23}.

This proposal requires to be considered in detail.

The first remark to be made is that the molar mass of carbon-12 is no longer a constant. Improving the accuracy of experimental methods in the future will consequently improve $M(^{12}C)$ value ; then it will introduce changes on the whole tables of element molar masses. Such modifications will indeed remain minor, as well as that on N_A if a fixed $M(^{12}C)$ was chosen. Nevertheless it is a major change with respect to the actual situation of stable values for molar masses, which may give the idea of a permanent instability.

A second remark comes from considering together the three constants, speed of light, Planck constant, Avogadro constant. Physics meets quite a number of such constants, which relate to phenomena or to the properties of matter. One might mention the electron charge, the electron mass, the fine structure constant, the permeability of vacuum, and so on. Each of them has a deep physical meaning. Some of them have already fixed values by international agreement.

The nature of N_A is completely different. It is a proportionality constant. When Dalton thought about atomic weights and set up his table of atomic weights, which has a considerable historical and practical value, he took 1 for the lightest element, hydrogen. This led to the value 16 for oxygen and 12 for carbon. In his time, nobody really had any idea about the absolute mass of a single atom. Later on, Berzelius proposed to use oxygen atomic weight as a starting value for the atomic weight table because he noted that oxygen reacted with many more elements than hydrogen to yield compounds, a mandatory step to determine atomic weights. He chose 100. The chemical community did not follow his proposal. Had this value were retained, the Avogadro number would have been different. Its physical meaning cannot be compared with that of the speed of light or of the Planck constant, one could even say that N_A has no particular physical meaning being just a number of atoms arbitrarily chosen to get an easy to use unit.

A fixed Avogadro constant leads to a definition of the mole without reference to the kilogram. The mole becomes then independent of any other unit so that it gets the statute of base unit. If $M(^{12}C)$ is kept equal to 12 exactly as it is today, the mole definition implies another unit, the kilogram. If the kilogram looses its statute of base unit because it is defined with the help of a fixed Planck constant and of the watt balance, the mole would loose as well its statute of base unit. It would decrease the number of base units by one.

If h are N_A are fixed, the relation $h.N_A = K.M(^{12}C)$ provides $M(^{12}C)$; the method of the silicon sphere provides $M(Si)$. There are thus two independent entries to build up the molar mass table.

This is not the most favourable situation. The isotopic abundance determination remains a weak step in the silicon sphere method. One may note that there are considerable efforts going on to enrich silicon into its most abundant natural isotope so that difficulties with isotopic abundances will be overcome. One may also note that any other isotope could be used in relation (1) in place of carbon-12, particularly an element having a single stable isotope. The ideal situation would be to have the same element for both determinations, but is it possible ?

A fixed N_A allows conceiving a new definition for the mole. However it does not provide any method to get a standard. The definition suggests counting atoms. A chemist who desires to measure an amount of substance uses a weighing balance. With such a new definition, the mole indeed appears disconnected from the kilogram; in practice, the kilogram is needed to determine a number of moles. Where is the advantage to have a definition not mentioning the use of the kilogram if the measurement of a number of moles implies the use of the kilogram ?

For these reasons, the choice of a fixed $M(^{12}C)$ is undisputedly favored by the Chemistry Section of the Académie des Sciences.

Professor Yves Jeannin
on the behalf of
The Chemistry Section of
Académie des Sciences

CCU09-24

ECOLE NORMALE SUPÉRIEURE

DÉPARTEMENT DE CHIMIE

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Professor Jean Kovalevsky
Académie des Sciences
23, quai de Conti
75270 Paris Cedex 05

Paris, May 7th, 2009.

Mon Cher Jean,

I am writing on the behalf of the Chemistry Section of the Académie des Sciences, acting as its Delegate in charge of the section. I am writing in English so that you will be able to make further use of this letter.

Following the current discussions about giving fixed values to some universal constants in order to reduce the number of base units and of related standards, the Section of Chemistry felt extremely concerned by the possibility that the scale of atomic masses based on carbon 12 mass may be modified following the choice of a fixed value for the Avogadro number. Beyond historical and cultural reasons, the Chemistry Section has undisputedly decided that the choice of keeping ^{12}C at a mass of 12g, hence allowing the Avogadro number to fluctuate according to future increase in precision, was a better solution since this will have less consequences on exchange of chemical data and their processing. For example in proteomics, the determination of protein fragments isotopic mass with a high precision is required for the direct identification of their raw chemical formula, a basic element for the algorithmic reconstruction of proteins sequences. Many other examples of this kind militate for keeping a common atomic mass reference, viz., ^{12}C at a mass of 12g.

The attached text written by Professor Yves Jeanin on the behalf of our Chemistry Section has been agreed upon undisputedly and summarizes its views. I hope that you will be able to convey our views to the CCU Members so that a positive decision will be recommended.

Très amicalement,

Christian Amatore
Membre de l'Institut
Délégué de la Section des Chimistes de
l'Académie des Sciences

The CCU is considering new definitions for four of the base units of the SI, and a new format for all the definitions

- new definitions for the kilogram, ampere, kelvin and mole

to fix the values of h, e, k, and N_A respectively,

- and a new format for the formal definitions

of the base units of the SI

We solicit the views of ICTNS in particular on the proposed new definition of the mole, but also on all the other changes under consideration.

Who decides to change the definition of a base unit?

CGPM has to take the ultimate decision

(Conference Generale des Poids et Mesures)

Conference of ca. 200, 4 or 5 delegates from each of 52 nations

last met in 2007, will next meet in October 2011

⇑

CIPM has to recommend action to the CGPM

(Comité Internationale des Poids et Mesures)

Committee of 18, from 18 different nations,

meets in October each year

⇑

the CIPM receives advice from 10 Consultative Committees,

composed of experts in each field, generally drawn from NMIs

⇑

CCTF (for Time and Frequency); **CCM** (for Mass); **CCL** (for length);

CCQM (for amount of substance - quantité de matiere); etc.

CCU (CC for Units) responsible for advising on changes to the SI

Desirable qualities for the definition of a base unit

- We should chose reference standards that we believe to be stable under translation in space and time, on an astronomical scale, i.e. that are related to an invariant of nature
- We must be able to realise the definition as accurately as the best practical measurements require
- We should chose definitions that may be experimentally realised by anyone, anywhere, at anytime.
- It is desirable to choose simple definitions, both to comprehend and to realise, using apparatus that is neither too expensive nor too complex. However it is the nature of modern science that this may be difficult to achieve.

"Yet, after all, the dimensions of our earth and its time of rotation, though, relative to our present means of comparison, very permanent, are not so by physical necessity. The earth might contract by cooling, or it might be enlarged by a layer of meteorites falling on it, or its rate of revolution might slowly slacken, and yet it would continue to be as much a planet as before.

But a molecule, say of hydrogen, if either its mass or its time of vibration were to be altered in the least, would no longer be a molecule of hydrogen.

If, then, we wish to obtain standards of length, time and mass which shall be absolutely permanent, we must seek them not in the dimensions, or the motion, or the mass of our planet, but in the wavelength, the period of vibration, and the absolute mass of these imperishable and unalterable and perfectly similar molecules."

James Clerk Maxwell, 1870

Any definition of a base unit fixes the value of the reference constant used in the definition

Example:

> **The second, unit of time, is the duration of 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the caesium 133 atom.**

This fixes the specified transition frequency as 9 192 631 770 Hz.
An exactly equivalent statement of the definition would be:

> **The second, unit of time, is such that the ground state hyperfine splitting frequency of the caesium 133 atom is equal to exactly 9 192 631 770 hertz.**

The CCU is recommending draft words for the definition of the base units using a common explicit constant format, as illustrated below:

The second, unit of time, is such that the ground state hyperfine splitting frequency of the caesium 133 atom is equal to exactly 9 192 631 770 hertz.

Thus we have the exact relation $\Delta\nu(^{133}\mathrm{Cs})_{\mathrm{hfs}} = 9\ 192\ 631\ 770$ Hz. The effect of this definition is that the second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium 133 atom.

The metre, unit of length, is such that the speed of light in vacuum is equal to exactly 299 792 458 metres per second.

Thus we have the exact relation $c = 299\ 792\ 458$ m/s. The effect of this definition is that the metre is the length of the path travelled by light in vacuum during a time interval of 1/299 792 458 of a second.

The value of any quantity is the product of a number and a unit: $Q = \{Q\}\,[Q]$

The ***value*** of the speed of a bicycle is $V = 5.0$ m/s $= 18$ km/h. **The value of the speed is the same in these two statements**. Although the number has changed, and the unit has changed, the value of the speed (which is the product of the number and the unit) remains the same.

When we talk of fixing the value of a fundamental constant to define a unit, such as fixing the hyperfine splitting of the caesium atom to define the second, or fixing the speed of light to define the metre, or fixing the elementary charge to define the ampere, it is always the ***numerical value*** of the fundamental constant that we choose to fix … the actual ***value*** of the fundamental constant remains unchanged. It is not for us to choose.

I hesitate to say that the value of the speed of light is chosen by God, because I do not wish to get into an argument with humanists. However if I were a serious believer I might say that. Instead I prefer to say that the value of the speed of light is a **constant of nature**.

Redefining the kilogram

First alternative:

The kilogram, unit of mass, is the mass of exactly $5.018\ 451\ 66 \times 10^{25}$ free carbon 12 atoms at rest and in their ground state

or:

The kilogram, unit of mass, is such that the mass of a free carbon 12 atom in the ground state is exactly $1.967\ 941\ 58 \times 10^{-26}$ kg

- this fixes the value of the mass of a carbon 12 atom.

Second alternative:

The kilogram, unit of mass, is such that the value of the Planck constant is $6.626\ 0693 \times 10^{-34}$ kg m^2 s^{-1}

- this fixes the value of the Planck constant.

Redefining the kilogram

The second alternative is preferred for two reasons.

1. The Planck constant h and the speed of light c are the fundamental constants of quantum mechanics and relativity respectively. Theoretical physics would be well served if they both had exactly known values.

2. Precise electrical measurements are made using the Josephson and the quantum Hall effect, which depend on the Josephson constant $K_J = 2e/h$, and the von Klitzing constant $R_K = h/e^2$, respectively. It would bring electrical metrology within the SI if we knew exact values for these two constants.

Realising the kilogram

The realisation of the definition of the kilogram would be achieved by maintaining a number of kilogram prototypes which would be used as secondary standards, in exactly the same way as is done today.

However these would be calibrated at intervals against the definition in terms of the Planck constant *h*, using a watt balance, or any other experiment that could be used to measure the value of *h*, such as the XRCD experiment. This procedure would replace the calibration of secondary standard prototypes against the international prototype K, as happens today.

Initially it is likely that the international prototype would be calibrated against the Planck constant using a watt balance, so that it could continue to be used as a reference standard. However any laboratory equipped with a watt balance could maintain their own reference standard of mass.

The Planck constant h and the mass of a carbon 12 atom $m(12C)$ are related through the equation

$$m_u = \frac{m(^{12}\mathrm{C})}{12} = \frac{2R_\infty h}{\alpha^2 c\, A_r(\mathrm{e})}$$

All of the constants in this relation are known with a relative standard uncertainty of less than 10^{-9}, except for $m(^{12}C)$ and h. The best recent XRCD estimate of $m(^{12}C)$ (International Avogadro project 2009, preliminary result) is now in agreement with the the best watt balance estimate of h (CODATA 2006), with relative standard uncertainties approaching 5×10^{-8}, so that the two alternative definitions are almost equivalent. Improved XRCD results using 99.995 % pure silicon 28 are also expected within the next year and preliminary results show that these are also in agreement.

Redefining the ampere

The current definition:

> the ampere, unit of electric current, is such that the value of the magnetic constant μ_0 is exactly $4\pi \times 10^{-7}$ henries per metre

Possible new alternative definition:

> the ampere, unit of electric current, is such that the value of the elementary charge e (charge on a proton) is exactly $1.602\,176\,487 \times 10^{-19}$ coulomb

Which definition should we choose?

CCU prefer the new alternative definition: To fix *e*

Two reasons:

1. If we fix the value of both *h* and *e,* then both the Josephson constant and the von Klitzing constant, $K_J = 2e/h$ and $R_K = h/e^2$, will have exactly defined values.

This would be a significant advance in electrical metrology, because at present precise electrical measurements are made using the conventional non-SI values of $K_{J\text{-}90}$ and $R_{K\text{-}90}$. This is strongly supported by the CCEM.

2. The elementary charge *e* is a simpler and more fundamental concept, based on the quantisation of charge, rather than the magnetic constant μ_0 based on classical electrodynamics.

Redefining the kelvin:

Current definition:

The kelvin, unit of thermodynamic temperature, is such that the value of the triple point temperature of water is exactly 273.16 kelvin.

Possible new alternative definition:

The kelvin, unit of thermodynamic temperature, is such that the value of the Boltzmann constant is

k = 1.380 6504 joules per kelvin exactly.

The new definition would be in terms of the fundamental constant k rather than the properties of a particular material at a particular temperature that is difficult to realise.

The CCU strongly support redefining the kelvin to fix *k*.

Redefining the mole

Current definition:

The mole, unit of amount of substance, is such that the molar mass of carbon 12 is exactly 12 grams per mole.

Possible alternative simpler definition:

The mole is that amount of substance that contains exactly 6.022 141 79 x10^{23} elementary entities.

or

The mole, unit of amount of substance, is such that the Avogadro constant is equal to exactly 6.022 141 79 x10^{23} mole^{-1}

The current definition fixes the value of the molar mass of carbon 12. The alternative fixes the value of the Avogadro constant N_A.

The CCU recommend changing to the new simpler definition.

Draft re-definition of the mole

The mole, unit of amount of substance, is such that the Avogadro constant is equal to exactly 6.022 141 79 x10^{23} mole^{-1}

Thus we have the exact relation N_A = 6.022 141 79 ×10^{23} mol^{-1}. The effect of this definition is that the mole is that amount of substance that contains exactly 6.022 141 79 x10^{23} elementary entities, which may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.

To summarise:

- The CCU advise that we should redefine the kilogram, ampere, kelvin and mole to fix the values of the Planck constant *h*, the elementary charge *e*, the Boltzmann constant *k*, and the Avogadro constant N_A, respectively;
- The changes should be made simultaneously, and should be based on the latest values of the fundamental constants to preserve continuity;
- The words for each new definition should be considered carefully over the next 18 months, along with the *mises en pratique* to go with each definition. CCU favour “explicit constant” definitions, in a standard format.

To define the second, we fix $\Delta\nu_{hfs}(Cs)$:

$$\Delta\nu_{hfs}(Cs) = 9\,192\,631\,770 \text{ Hz}$$

value of $\Delta\nu$ = numerical value × unit

The value of $\Delta\nu_{hfs}(Cs)$ is a constant of nature.

1. If we define the unit s, and hence the Hz, independently, then we must determine the numerical value of $\Delta\nu$ by experiment, and it will have an uncertainty. This was the situation before 1967, when the second was independently defined from the tropical year 1900.

2. If we fix the numerical value, then the effect is to define the Hz and hence the second s. This is the current definition of the second, since the change in 1967. The numerical value now has zero uncertainty.

NOTE: The *value* of $\Delta\nu_{hfs}(Cs)$ has not changed, only the numerical value and the unit have changed.

To define the metre, we fix *c*:

$$c = 299\ 792\ 458\ \text{m/s}$$

value of *c* = numerical value × unit

The value of *c* is a constant of nature.

1. If we define the units independently, then we must determine the numerical value by experiment, and it will have an uncertainty. This was the situation before 1983, when both the metre and the second were independently defined.

2. If the second is independently defined in terms of the frequency of the caesium transition, and we choose to fix the numerical value of *c*, then the effect is to define the metre. This is the current definition of the metre, since the change in 1983. The numerical value now has zero uncertainty.

NOTE: The *value* of *c* has not changed, only the numerical value and the unit have changed.

To define the kilogram we fix *h* :

$$h = 6.626\ 0693 \times 10^{-34}\ \mathrm{m^2\ kg\ s^{-1}}$$

value of *h* = numerical value × unit

The value of *h* is a constant of nature.

1. If we define the unit $\mathrm{m^2\ kg\ s^{-1}}$ independently, then we must determine the numerical value by experiment, and it will have an uncertainty. That is the present situation.

2. If the metre and the second are already independently defined, and we choose to fix the numerical value, then the effect is to define the kilogram. This is the proposed new definition of the kilogram. The numerical value will have zero uncertainty.

   NOTE that the *value* of *h* is unchanged by the new definition, only the numerical value and the unit have been changed.

$$\mathrm{J\ s = m^2\ kg\ s^{-1}}$$

To define the ampere, we fix *e*:

$$e = 1.602\,176\,487 \times 10^{-19}\ \mathrm{A\,s}$$

value of *e* = numerical value × unit

The value of the elementary charge *e* is a constant of nature.

1. If we define the ampere *A* and the second *s* independently, where the ampere is defined to fix the value of μ_0 and the second to fix the caesium transition, then we must determine the numerical value of *e* by experiment, and it will have an uncertainty. That is the present situation.
2. If however we choose to fix the numerical value of *e*, then the effect is to define the coulomb *C*, and hence the ampere through the relation *A* = *C*/*s*. This is the proposed new definition of the ampere. The numerical value will have zero uncertainty.

   NOTE that the *value* of *e* has not changed; only the numerical value and the unit have changed, such that the product is unchanged.

Note: A = C/s, C = A s

To define the kelvin, we fix the value of *k* :

$$k = 1.380\,6504 \times 10^{-23}\ \mathrm{J/K}$$

value of *k* = numerical value × unit

The unit J = kg m^2 s^{-1} is already defined,
but for the unit K we have a choice.

1. If we define the unit K independently, such that T_{TPW} = 273.16 K, then we must determine the numerical value of the Botzmann constant by experiment, and it will have an uncertainty. That is the present situation.

2. If the however we choose to fix the numerical value of the Boltzmann constant, then the effect is to define the kelvin, K. This is the proposed new definition of the kelvin. The numerical value will have zero uncertainty.

   NOTE that the *value* of *k* has not changed; only the numerical value and the unit have changed such that the product, which is the value of *k,* has not changed. The value of *k* is a constant of nature.

To define the mole, we fix the value of N_A:

$$N_A = 6.022\,141\,79 \times 10^{-34}\ \text{mol}^{-1}$$

value of N_A = numerical value × unit

The Avogaro constant, N_A, is the conversion factor between number of entities N and amount of substance n.

1. If we define the unit mol independently, as that amount of substance in 12 g of carbon 12, then we must determine the numerical value by experiment, and it will have an uncertainty. That is the present situation.

2. If the however we choose to fix the numerical value, then the effect is to define the unit mole. This is the proposed new definition of the mole. The numerical value will have zero uncertainty.

   NOTE that the *value* of N_A has not changed; only the numerical value and the unit have changed, such that the product, which is the value of N_A, has not changed. The value of N_A is a constant of nature.

unit	*constant used as reference*	*symbol*	*uncertainty in the current SI*		*uncertainty in the new SI*	
kg	**mass of IPK**	$m(\mathcal{K})$	**exact**	**0**	**exptl**	5.0×10^{-8}
	Planck const	h	**exptl**	5.0×10^{-8}	**exact**	**0**
A	**magnetic const**	μ_0	**exact**	**0**	**exptl**	6.8×10^{-10}
	elementary charge	e	**exptl**	2.5×10^{-8}	**exact**	**0**
K	**temp of TPW**	T_{TPW}	**exact**	**0**	**exptl**	1.7×10^{-6}
	Boltzmann const	k	**exptl**	1.7×10^{-6}	**exact**	**0**
mol	**molar mass ^{12}C**	$M(^{12}\mathrm{C})$	**exact**	**0**	**exptl**	1.4×10^{-9}
	Avogadro const	N_{A}	**exptl**	5.0×10^{-8}	**exact**	**0**

Relative standard uncertainties for a selection of fundamental constants multiplied by 10^8 (i.e. in parts per hundred million)

constant	current SI	new SI
$m(\mathcal{K})$	0	**5.0**
h	5.0	**0**
e	2.5	**0**
k_B	170	**0**
N_A	5.0	**0**
R	170	**0**
F	2.5	**0**
σ	700	**0**
m_e	5.0	**0.14**
m_u	5.0	**0.14**
$m(^{12}C)$	5.0	**0.14**
$M(^{12}C)$	0	**0.14**

constant	current SI	new SI
α	0.068	**0.068**
K_J	2.5	**0**
R_K	0.068	**0**
μ_0	0	**0.068**
ε_0	0	**0.068**
Z_0	0	**0.068**
q_P	2.5	**0.034**
J↔kg	0	**0**
J↔m^{-1}	5.0	**0**
J↔Hz	5.0	**0**
J↔K	170	**0**
J↔eV	2.5	**0**

imm Aug 09

The Si single crystal approach to the Avogadro constant and the redefinition of the SI units kilogram and mole

Paul De Bièvre

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SNAFU / SIAM / CIAAW
2009-07-20/30
WIEN (AT)

ACDC / ICTNS
2009-07-31 / -08-02
GLASGOW

The Avogadro number {N_A}

via the Si single crystal approach (XRDDMM)

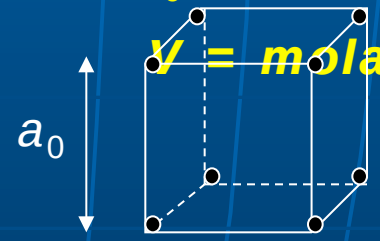
$$M(\mathrm{Si}) = \sum x\,(^{i}\mathrm{E}) \,.\, M\,(^{i}\mathrm{E}) = [\Sigma x\,(^{i}\mathrm{E}) \,/\, \Sigma x(^{i}\mathrm{E})] \cdot M(^{i}\mathrm{E}) = [\Sigma R_{i/28} \cdot M(^{i}\mathrm{E})] \,/\, \Sigma\, R_{i/28}$$

$N_A = M(\mathrm{Si}) \,/\, [\rho\, a_0^3 / 8 \quad]$ $\quad$ $m(\mathrm{Si})$ = mass of a Si atom

$\underline{N_A = M(\mathrm{Si}) \,/\, m(\mathrm{Si})}$ $\quad$ V_0 = volume of unit cell

a_0 = lattice parameter

V = molar volume of Si



$N_A = M(\mathrm{Si}) \,/\, [\rho\, a_0^3 / 8]$

$N_A = [M(\mathrm{Si}) / \rho] \,/\, (a_0^3 / 8)$

$\underline{N_A = V \,/\, V_0}$

PDB99204

A ‘near-perfect’ 1 kg Si single crystal.

Since ‘near-perfect’, it acts as a ‘near-perfect’ mirror for IMGC’s Anna Peuto (degree-of-’unroundness’: ‘hills’ of < 1 m if sphere is enlarged to earth globe)

PDB03053

The Avogadro constant N_A

$$M(\mathrm{Si}) = \Sigma\, M(^{i}\mathrm{Si}).R_{i/j} \;/\; \Sigma\, R_{i/j}$$

in SiF_4 gas measurements, ion current ratios

$I(^{29}SiF_3^+) \;/\; I(^{28}SiF_3^+)$ and $I(^{30}SiF_3^+) \;/\; I(^{28}SiF_3^+)$

are calibrated by synthetic isotope number ratios, prepared from enriched Si isotope amounts:

$$R_{i/j} = N(^{29}\mathrm{Si}) \;/\; N(^{28}\mathrm{Si}) = K_{cal} \cdot I(^{29}SiF_3^+) \;/\; I(^{28}SiF_3^+)$$

K_{cal} = is derived from measurements of synthetic isotope mixtures

PDB01152

The balance, used in early chemistry, compares amounts of substance by comparing mass or "weights"

From early times, mass (or weights) were compared by a single instrument:

the balance

Recognising its status, science gave this measuring process a base (SI) unit:

the kg

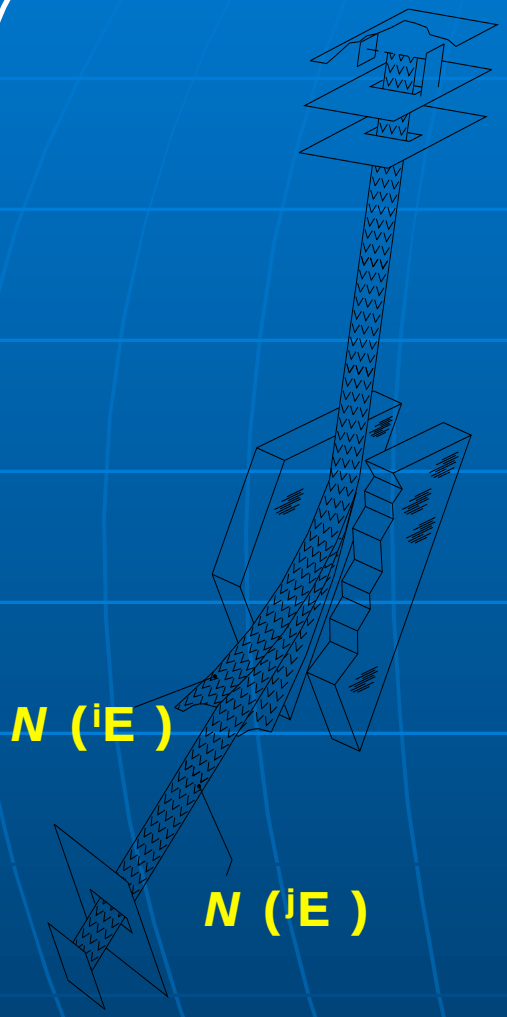
But science and technology discovered the fact that atoms combine in simple numbers, so chemists cannot use the balance directly to compare amounts of substance.

They must divide mass values by "atomic weights" to get what they need.

The balance does not take into account the particulate nature of matter.

PDB03049

Source: P De Bièvre, Fresenius J Anal Chem 337 (1990) 766 – 771 (amended)



THE (ISOTOPE) MASS SPECTROMETER (IMS) :THE MODERN CHEMISTS'S BALANCE

What chemists need is given by the IMS!

it directly compares numbers of isotopic entities (atoms or molecules)

$$R_B = \frac{N\,(^iE)}{N\,(^jE)}$$

In IDMS the IMS sorts, then counts, then compares

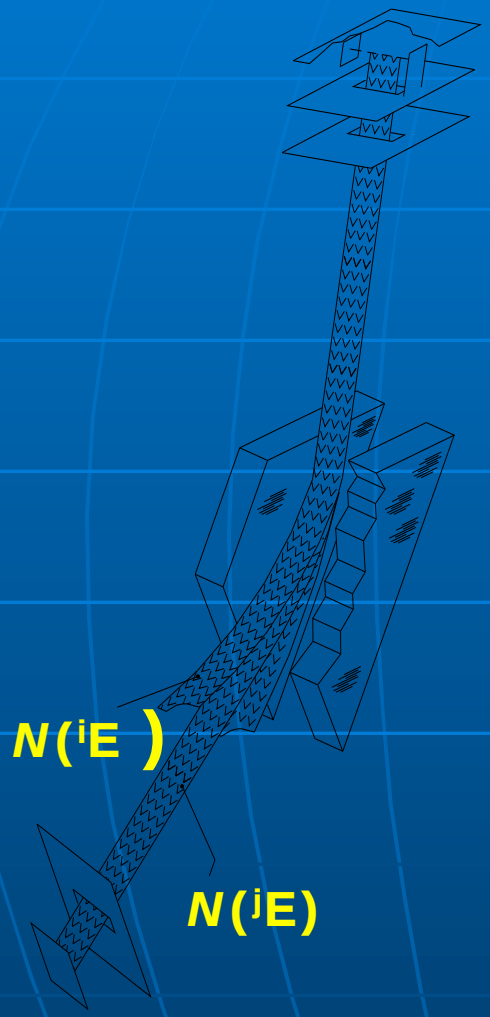
an unknown number $N(^jE)$ of isotopic entities (atoms , molecules) to

a known number $N(^jE)$ of isotopic entities (an "internal standard" added) through a measurement of a number ratio

PDB03048

Source: P De Bièvre, Fresenius J Anal Chem 337 (1990) 766 – 771 (amended)

THE (ISOTOPE) MASS SPECTROMETER: THE CHEMISTS'S AMOUNT COMPARATOR



the IMS directly compares

numbers of isotopic atoms: $R_B = \frac{N(^iE)}{N(^jE)}$

thus measuring
in the natural unit one (symbol "1") or
in the SI unit mole (a multiple of 1)

the IMS sorts, then counts, then measures a 'number ratio' of isotopic atoms

this leads to an atomic weight:

$$A_r(Si) = \Sigma A_r(^iSi).R_{i/j} \; / \; \Sigma R_{i/j}$$

PDB03048

Source: P De Bièvre, Fresenius J Anal Chem 337 (1990) 766 – 771 (amended)

The Avogadro constant N_A

is determined

1.using a quantity equation

(measurement function – VIM3)

2. using the concepts

‘molar volume’, M (Si) = f (ρ) and

‘interatomic distance of Si atoms’

as (sufficiently) invariant concepts

to serve as references for our thinking, rather than using the concept of a ‘perfect Si single crystal’ which was proven to be sometimes wrong

PDB99208

To measure in mol, one does not need to know the number of molecules in a sample;

one does not even have to know the Avogadro constant;

one only has to measure their number ratio

PDB00063

Possible new definition of the kg

The unit for mass measurements is the kilogram, symbol 'kg'.
It is the mass of 6,022 14x yz ·10²³ atoms of ^{12}C in their nuclear ground state multiplied by 1000/12

Notes:
1. **This definition is transparant , hence easy to teach**
2. **It can borrow the actual value for N_A from the interrelationship of fundamental constants**

PDB06006a

A redefinition of the unit mole and decoupling it from the kilogram,

enables to define the mole considerably simpler than is the case at present;

the value of N_A can be borrowed from the (impressive) interrelationship of the fundamental constants

Possible new definition of the mole

***The unit for amount(-of-substance) measurements is the mole, symbol* 'mol'.**

It is an amount-of-substance containing 6,022 14x yz ·10²³ entities.

The entities must be identical and specified.

Notes:

1. **This definition is transparant , hence easy to teach**
2. **It can borrow the actual value N_A from the interrelationship of fundamental constants**

PDB06006a

with

sincere wishes

for

a good discussion

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 9.1
Review of sections of the *IUPAC on-line Handbook*
Current status

The IUPAC Compendium of Chemical Terminology (The Gold Book)

Report on progress in updating since the General Assembly in Torino, 2007.

Introduction

The addition of terms to the Gold Book has continued

1.1 Procedure

Since the meeting in Beijing 2005, the XML web-site has come into operation under the supervision of a group in Prague, my contact there being Beda Kosata.

New terms are now submitted in WORD format, rather than .pdf. New files are sent to both Fabienne Meyers in IUPAC and to Beda Kosata in Prague.

1.2 Progress

As before, the terms to be added to the Gold Book web-site have been chosen so as to spread the coverage across documents from all the IUPAC Divisions. There is a great variation in the amount of relevant material emanating from the Divisions, with some very active in terminology and others producing little.

The total number of terms that have been processed since the present exercise began, following the General Assembly in Ottawa, 2003, is 1014.

1.3 Acknowledgment

It is pleasure to express my gratitude to Fabienne Meyers, Alan McNaught, Míla Nič and Beda Kosata for their friendly and efficient cooperation over the years.

Aubrey Jenkins

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Glasgow 2009-08-02 and 03

Attachment to Minutes
Item 11

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