INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisonal Committee on Terminology, Nomenclature and Symbols (ICTNS)

Meeting in Beijing, China
16 and 17 August 2005

ATTACHMENTS TO THE MINUTES

List of Attachments

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Attachment 1

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Beijing, China 2005-08-16 and 17
09:00 – 13:00 and 14:00 – 18:00

AGENDA

1. Opening remarks and introduction of participants.
2. Minutes of Ottawa meeting
3. Minutes of meeting of core Titular Members, Lisbon
4. Business arising from the Ottawa meeting not covered in Lisbon
5. Business arising from the Lisbon meeting. Ratification of decisions
   - 5.1. Nomenclature in Technical Reports
   - 5.2. Freeman polemic on the mole
   - 5.3. Inclusion of Chairman and Secretary as editors of PAC
   - 5.4. Request to Bureau and Council in time to change Bylaw B2.11 to shorten the period of public review of Recommendations to three months.
6. Workshop on *Pure Appl. Chem.*, RTP, 2004-11-21
   - 6.1. Editorial positions on Pure Appl. Chem.
   - 6.2. Establishment of Editorial Advisory Board (EAB) for *Pure Appl. Chem.*
   - 6.3. Review of Manuscript Central
7. Report to IUPAC Council
8. Current status of manuscripts: in the review cycle, completed, published
   - 8.1. Technical Reports
   - 8.2. Recommendations
9. Procedures for processing Technical Reports and Recommendations
   - 9.1. Manuscript Central
   - 9.2. Procedures for reviewing TRs and Recommendations
10. Reports from IUPAC Division Representatives
    10.1 to 10.8
11. Reports from Representatives of Other International Organizations
12. Report of June meeting of BIPM/CCU
    Redefinition of the kilogram – pros and cons
13. New IUPAC Periodic Table
14. Review of sections of the *IUPAC Handbook 2004-2005*:
    - 14.1. Procedure for Publication of IUPAC Technical Reports and Recommendations (2004)
    - 14.2. Guidelines for Drafting IUPAC Technical Reports and Recommendations (2004)
15. Update on status of 'color' books
    - 15.1. Red Book
    - 15.2. Orange Book
    - 15.3. Green Book

15.4. Blue Book
15.5. Silver Book
15.6. Gold Book and XML Data Dictionaries
15.7. Purple Book

16. Meeting of JCGM (Joint Committee for guides in Metrology)
17. Membership
18. Plans for future meetings: question of even-year meetings of the core TMs between GAs: available funds, more frequent face-to-face meetings, exclusion of Divisional representatives, etc.
19. Adjournment

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Minutes of the meeting of "Core" Titular Members in Lisbon, Portugal
21 – 22 July 2004

In attendance: J. W. Lorimer (chairman)
B. J. Herold (secretary)

W. V. Metanomski
T. Damhus
R. Marquardt

1. Opening remarks and introduction of participants

Prof Lorimer called the meeting to order.

Prof. Lorimer drew the attention of the participants to the uniqueness of this meeting of only "core" titular members of ICTNS, and proposed to discuss among the titular members present the issue whether to recommend to have in future plenary meetings again every year. Dr. Metanomski reminded the attendees that traditionally in IDCNS, in spite of IUPAC reimbursing only titular members, these would include also those titular members who represent the IUPAC Divisions. He remarked that the latter could have been invited to the present meeting, as well as associate members and representatives of other organizations, under the condition that they paid for themselves the travel and subsistence costs.

Prof. Lorimer recalled the importance of the Sèvres meeting of IDCNS in 2000, (an even year, where there was no IUPAC General Assembly) at the invitation of BIPM for acquainting the members of IDCNS with the work of BIPM, and the very substantial nature of the decisions made at that meeting.

Prof. Lorimer stressed that the urgency of the budgetary implications of holding full meetings every year demand the Bureau to be informed as early as possible, and well before the Beijing meeting.

No decision was however reached whether to propose or not to the Bureau to hold plenary ICTNS meetings every year.

Prof. Lorimer considered, and it was agreed, that the present meeting will act merely as an executive committee.

Prof. Marquardt expressed his concern that it is necessary to decide in the first place which kind of subjects may be decided at the present meeting, and considered that, for those subjects which required a broader basis in order to be decided in a binding way, further discussion among all members of ICTNS might be continued by e-mail.

Prof. Herold considered that any decisions made at the present meeting should be communicated as soon as possible to the absent ICTNS members for consultation. In case that any member should disagree with a given decision, the item concerned should be placed on the agenda of the next plenary meeting to be held on the occasion of the General Assembly of IUPAC in Beijing in the year 2005.

The agenda, which had been circulated previously to the participants was approved under these conditions.

The attendees introduced themselves stating their affiliations with IUPAC or other organizations.

2. Minutes of Ottawa meeting.

The minutes of the ICTNS meeting in Ottawa 12–13 August 2003 (attachment 1) were discussed.

The following corrections were considered to be necessary:

Pg. 4, heading of last para,

instead of "5.4 Macromolecular Chemistry Division"

should read "5.4 Macromolecular Division".

Pg. 4, last line,

instead of "Division VIII would be responsible in future for all nomenclature problems"

should read "Division VIII would be responsible in future for all nomenclature projects".

Pg. 7, para 9, line 3,

Instead of "Dalton"

should read "dalton".

Pg. 10, right column, line 4,

instead of "Dr. Anders Thor"

should read "Mr. Anders Thor".

The minutes were approved only tentatively after these corrections, because the final approval can only be decided in a plenary meeting, and therefore in Beijing 2005.*

3. Business arising from the Ottawa minutes.

* After conclusion of the meeting it was noted that on the front page in the second title line one has to replace:
Interdivisional Committee Nomenclature and Symbols (IDCNS)
by
Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

3.1 Reply to Prof. Freeman on new definition of 'amount of substance'.

Prof. Herold informed that Prof. Cvitas had written as agreed to Prof. Freeman soon after the Ottawa meeting of ICTNS explaining the position of ICTNS as regards his proposal on a new definition of 'amount of substance'. See attachment 2, as well as attachments 3 and 4 for the ensuing correspondence.

4. Procedures for processing Technical Reports and Recommendations

4.1 Implementation by IUPAC of Manuscript Central (MC) manuscript tracking software.

4.2 Editorial positions for PAC and MC.

The positions of the Chairman and Secretary of ICTNS with respect to PAC and to MC (Manuscript Central) were discussed. The points at issue were:

- The Chairman and Secretary of ICTNS have the ultimate responsibility for approval of both Technical Reports and Recommendations in PAC, but their role is not recognized on the inside front cover of issues of PAC.
- In MC, the Chairman of ICTNS is listed as the Editor-in-Chief, the Secretary is listed as the Associate Editor, and their responsibilities are clear to authors, reviewers and other members of ICTNS.
- While the perceived conflicts between the named positions listed in IUPAC publications (Chairman and Secretary) and in MC (Editor-in-Chief and Associate Editor) are not of overwhelming concern to the current incumbents, the TMs of ICTNS recommended that specific recognition be given in PAC to their roles. The TMs pointed out that ICTNS will be faced with nomination of a new Chairman and Secretary, possibly as soon as late 2004 or early 2005 for appointment commencing in January, 2006. The rather heavy duties of these positions are known, and incentives are desirable in order to attract suitable candidates. Better recognition of the roles of the officers of ICTNS would certainly be one desirable incentive.
- The officers of ICTNS have other duties in addition to preparing publications for PAC, such as maintaining cooperation with other bodies like BIPM, so their role relative to PAC can be identified clearly.

The proposal, therefore, is to make the following changes to the inside front cover of issues of PAC:

1. Retain the position of Scientific Editor of PAC (present incumbent James R. Bull).
2. Add the following positions (with present incumbents):
   Editor-in-Chief, Special Issues and Conference Reports: James R. Bull
   Editor-in-Chief, Technical Reports and Recommendations: John W. Lorimer
   Associate Editor, Technical Reports and Recommendations: Bernardo J. Herold

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After conclusion of the meeting Dr. Metanomski sent to the Secretary ICTNS a memo with additional information (see attachment 5).

It was recognized that other designations for the editorial positions are possible, but it is suggested that the above covers the desirable changes in a brief but clear way. While the changes should take place as soon as possible, it was recognized that approval by CPEP and by the Bureau may be necessary.

4.3 Practical procedures for members. Reviewing procedures.

The reviewing procedures were discussed at length, both under the point of view of how to achieve maximum quality, as well as speediness and smoothness. It was also felt that there should be a more precise definition of the responsibilities of the ICTNS officers, "core" titular members, titular members representing divisions, associate members, as well as division presidents and the secretariat. The need to make these procedures compatible with the now existing MC manuscript handling system was also a major concern.

Along the discussion numerous comments were made by the participants, which are summarized as follows:

Prof. Lorimer explained that manuscripts of Technical Reports and Recommendations are sent by the Divisions to the Secretariat, who introduces them in MC. MC then asks automatically core titular members to review. There is no obligation for these members to review every manuscript, but they should notify if they do not wish to comment. Due to the way MC is set up they should nevertheless always reply in the dialogue box that they accept, and either introduce the comments they wish to make or not. MC works on the basis of the following four centers: One called by MC "Editor-in-Chief", which means the Chairman of ICTNS, a second one called "Associate Editor", which means the Secretary of ICTNS, a third one called "Review Center", which means core titular members, as well as all those who have accepted to be reviewers of a given manuscript, and a fourth one called "Author Center", the only one where the designation given by MC corresponds with reality. As to the dates for entering a review, Prof. Lorimer would like to see three weeks as the ideal comment period, but recognized that the size of manuscripts is sometimes too large or they need so many changes that three weeks may not be sufficient.

Prof. Marquardt pointed out that Division Presidents seem sometimes not to be aware of the fact that they are responsible for the quality of the scientific content of manuscripts submitted to ICTNS. He suggested to remind them of that responsibility.

Dr. Metanomski suggested that Titular Members representing Divisions in ICTNS should be asked by the Division President to review papers submitted by that Division. He also considered that Technical Reports and Recommendations should not be sent by the Divisions to the Secretary ICTNS directly but through the Secretariat, a wish seconded by Prof. Herold.

Prof. Marquardt expressed the opinion that whenever ICTNS considers that a manuscript needs further scientific review, in spite of having been approved by the Division, ICTNS should appoint other reviewers. Prof. Lorimer replied that

this has already happened several times. He has selected indeed several times reviewers for special subjects in addition to the Titular Members.

Dr. Damhus suggested that ICTNS should have a kind of webboard like Division VIII, where members should be notified if contributions in their field of interest have been entered.

Prof. Lorimer asked the Titular Members present not to use MC for sending comments directly to authors. This facility is built into the MC system but should not be used.[*]

Dr. Metanomski returned to the problem of insufficient review by the Divisions. He suggested that if neither the Division ICTNS Titular Members nor Division Presidents wish to review a given manuscript to suggest to them to nominate another reviewer.

Prof. Lorimer asked the participants to consider and comment his draft memo for Division Presidents (attachment 6) of February 2004, concerning the 2nd and 3d paragraphs of the "Guidelines for Drafting Technical Reports and Recommendations" in the Handbook.[**]

Dr. Metanomski reminded Prof. Lorimer to ask the Bureau and the Council in time to change Bylaw B 2.11 to shorten the period of public review of Recommendations to three months. He also stressed that comments of ICTNS on manuscripts should be sent to authors and Division Presidents through the Secretariat.

Prof. Herold stressed again his wish that Recommendations should not be sent to the Secretary of ICTNS directly but always through the Secretariat (contrary to paragraph 1 of "Procedure for Publication of IUPAC Recommendations" in the Handbook).

On the subject of selecting additional reviewers for special subjects, Dr. Metanomski advocated to approach individually representatives of other organizations in ICTNS, asking for their participation. Prof. Lorimer, in replying, noted that there was also a problem in restricting the review process within a limited time.

Dr. Damhus expressed his views about deadlines in stressing that there should be only one deadline for the review of Recommendations instead of two: One mentioned in MC and another one "one month before the end of public review." Once the 5 months' period has been reduced to three months, ICTNS review of Recommendations should be 2 months (consistent with "one month before end of public review".

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[*] In a subsequent meeting with the Secretariat it was found that that this facility in fact does not exist.

[**] The updated version resulting from this discussion was circulated to all ICTNS members on 2004-09-08.

About the same problem Dr. Metanomski suggested to approach informally Division Presidents asking them to proceed differently from the "Procedure for Publication of IUPAC Recommendations" as published in the Handbook.

Prof. Lorimer expressed his preference for the following procedure: Authors submit their drafts of Recommendations through the Secretariat to the Division President concerned. After the approval by the Division President the Secretariat places the manuscript on MC This initiates a thorough review by ICTNS at the end of which the authors are asked to present revised manuscript. Simultaneously the Division President selects 15 outside reviewers. This is followed by the 3 months for public review. The comments from public review should be addressed to both the authors and the Secretariat. The Secretariat would send then the comments to the Division President and simultaneously to ICTNS, who would send them to the Divisional Representative Titular Member of ICTNS.*

In addition to this discussion the following two remarks were made:

Dr. Metanomski considered that in spite of Divisions I, II and III having to be involved in Recommendations that originate with Division VIII, this would not be the case for the Macromolecular Division (IV), as he would explain later under the item "Purple Book" (item 12.4).

Dr. Damhus suggested that, as regards the ICTNS review of the new Red Book, it might be helpful for ICTNS reviewers to obtain from Division VIII an assessment, more detailed than its preface, regarding the changes and additions as compared to the older version of the Red Book and other Recommendations on Inorganic Nomenclature. He took the opportunity to point out also in this context that MC does not allow him to see the comments of other reviewers than himself.

5. Current status of outstanding TRs and Recommendations.

5.1 Technical reports

See attachment 7 for a status review on Technical Reports as to December 31, 2003 and attachment 8 for an updated summary as to July 14, 2004.

5.2 Recommendations

See attachment 9 for a status review on Recommendations as to December 31, 2003 and attachment 8 for an updated summary as to July 14, 2004.

The participants expressed their satisfaction regarding the progress made with working up the extensive backlog.

* These procedures have been revised November 2004-11-20 to 21 in a meeting of the Chairman and Secretary ICTNS at the Secretariat of IUPAC. The information is expected to be made available to ICTNS members during December 2004.

Prof. Herold explained the difficulties he found in presenting updated status reviews using the traditional format of preceding years. Due to the extensive use of e-mail it can happen that a given manuscript involves up to 40 messages exchanged between authors, Executive Director, Division Presidents and ICTNS members, which renders the task of reporting about this correspondence in the traditional an extremely heavy task. This was the reason for discontinuing this kind of reports by December 31, 2003 and using a simplified kind of summary for the status as to July 14, 2004.

6. Report from I. Mills on May meeting of CCU. Implications for ICTNS.

It was verified that no report of the May 2004 meeting of the Consultative Committee on Units (CCU) of the International Bureau of Weights and Measures (BIPM) has yet been received by ICTNS. The report of the 2003 CCU meeting had been distributed to ICTNS members in November 2003, and it was verified that there are no implications for the practices of IUPAC. The only issue, which might have had implications (on decimal markers), does not affect the usage in English documents, English being the only language used in IUPAC publications.

7. Review of Appendices III and IV in Handbook and on web site.

It was pointed out that the Appendices III and IV had at the date of the present meeting undergone already substantial changes, which have the approval of ICTNS. Further changes can only be made after the Beijing General Assembly in August 2005.

It was suggested to add, at the top of page 8[8] of the "Guidelines for Drafting IUPAC Technical Reports and Recommendations", instructions on how to introduce a thin space in Latex, because there are many authors who do not use MS Word.

Other issues had been already discussed under item 4.3.

8. Nomenclature (Names of Chemical Substances in IUPAC Technical Reports published in Pure and Applied Chemistry)

The participants expressed their thanks to Dr. Metanomski for submitting a discussion paper on this item (attachment 10). Attachment 10 includes also comments of Prof. Lorimer and Prof. Herold (see also attachment 11) on that paper. In the ensuing discussion several points were raised on how to apply the criteria to specific cases which had occurred during the review of several manuscripts. This allowed some decisions to be reached on what to write to some authors on the position of ICTNS more quickly than would have been possible by correspondence.

[8] This page number refers to a version of the Handbook which could be accessed on the IUPAC homepage on 2004-07-20, but has later been replaced as a consequence of a reorganization of the website.

The problem on capitalization of initial letters of chemical names was raised, and it was pointed out that the usages differ between the Blue and the Red Books, as well as from other IUPAC Recommendations, e. g. Carbohydrate Nomenclature, and that one might consult with Division VIII on that subject.

9. Quantity calculus and empirical correlations

Prof. Herold asked the participants to comment the entries in the Gold Book concerning "acceptor number (AN)" and "donor number (DN)". The general opinion was that the symbols for these physical quantities as quoted in the Gold Book would have to be changed, regardless of the way they were originally defined in the literature. The authors of the revised edition of the Gold Book should be informed.

10. The correct use of arrows

Prof. Lorimer informed the participants about a message he had received from Dr. John Zdysiewicz (see attachment 12) on the use of arrows in manuscripts, pointing out the existing confusion and misuses. The participants asked Prof. Lorimer to invite Dr. Zdysiewicz to propose a project on that subject and to chair the task group.

11. Communications with Division Presidents and Divisional TMs

11.1. Revised front matter.

The text of Prof. Lorimer's draft memo to Division Presidents (attachment 6) was discussed and suggestions were made for redrafting it as regards some minor points.

11.2. Appendices III and IV

The matter had been dealt with in sufficient depth under item 4

12. Update on status of 'color' books

11.1. 'Green Book'

Prof. Marquardt informed that Prof. Martin Quack and Dr. Jürgen Stohner are in charge of the last preparations for editing, and that the final version of some chapters are still missing, as well as the glossary.

11.2 'Red Book'

Dr. Damhus reported about the history of the new edition of the Red Book.. He informed that the correspondence with Dr.Jonathan Brecher recorded on the Division VIII webboard had become irrelevant at the present stage of the draft. The New Red Book will incorporate and revise the 1999 Recommendations on the Nomenclature of Organometallic compounds, as well as earlier recommendations on radical names, which in spite of having been approved by CNIC, had been considered as debatable by some of its members. The draft of the Red Book is already available on MC for ICTNS review.

11.3 'Gold Book'

The participants were informed that Prof. Aubrey Jenkins is working on the updating of the Gold Book. It will become available online along with the production. Concerns were expressed about what would be the procedure if errors have to be corrected, which can be either errors in the transcription from Recommendations or errors in the original Recommendations.

11.4 Others

Concerning the Purple Book, Dr. Metanomski informed that the first edition had not been subject to public review, and that Division IV considers that the second edition should have the same treatment. This seems to be justified because transcriptions from older Recommendations will not be changed. It is expected to be ready for publication by 2006.

Concerning the New Blue Book, it has not yet reached the stage of a Provisional Recommendation. The April 2003 draft is available on the Division VIII webboard for comments. Dr. Metanomski considers that it will not be ready for publication before 2006.

About the Orange Book, the 3d edition dates from 1998 and no plans for revision are known so far.

12. Recommendations on update of 'Silver Book'

ICTNS would wish the Silver Book to be updated if possible. Prof. Lorimer will write to Prof. Urban Forsum, asking if there are plans to rewrite the Silver Book. If this is the case, it is felt that there should be appointed external referees from other Divisions than VII to achieve a higher degree of consistency with other IUPAC Recommendations.

13. Recommendation to IUPAC on use of SI dates

It was considered that IUPAC should use SI dates. Prof. Lorimer proposed to write an article for Chemistry International and a letter to the Bureau.

14. Membership

The terms of Prof. Herold, Prof. Cvitas, Dr. Damhus and Dr. Metanomski finish 2005. Prof. Lorimer and Prof. Marquardt have been elected for a period finishing 2007.

15. Next meeting

The next meeting of ICTNS will be a plenary meeting and will take place during the IUPAC General Assembly in Beijing in August 2005. The exact schedule is not yet known to the participants.

17. Adjournment

The meeting was adjourned on July 22nd 2004 at about 6.00 p. m.

List of Attachments:

1. Minutes of the meeting in Ottawa, Canada, 12 – 13 August 2003
2. Letter to Prof. Freeman 2003 – 08 - 25
3. Reply of Prof. Freeman 2003 – 09 – 07
4. Response to Prof. Freeman 2003 – 09 – 15
5. Memo by Dr. Metanomski on Freeman polemic
6. Draft Memo for Division Presidents
7. IUPAC Technical Reports – ICTNS Review – Status December 31, 2003
8. IUPAC Recommendations – ICTNS Review – Status December 31, 2003
9. Updated summary of TRs and Recommendations, 2004 – 07 – 14
10. Discussion paper by W. V. Metanomski on Item 8
11. Annex to attachment 10
12. Message of Dr. John Zdyziewicz

Attachment 3
Re Item 6

Workshops on Manuscript Central (MC) and Pure & Applied Chemistry (PAC)

At IUPAC Secretariat
Research Triangle Park
North Carolina

20 – 21 November 2004

Prof J W Lorimer and Prof B J Herold attended workshops on Manuscript Central (MC) and Pure & Applied Chemistry (PAC) organized by Dr John W Jost, Executive Director, on 20 and 21 November 2004, at the IUPAC Secretariat, Research Triangle Park, North Carolina.

The workshops were also attended by

Prof David StC. Black, Secretary General
Prof James Bull, Scientific Editor PAC
Dr David Martinsen, Committee on Printed and Electronic Publications (CPEP)

and the following staff of the Secretariat :

Dr Fabienne Meyers, Electronic Publishing Manager, Editor Chemistry International (CI)
Mr Paul T LeClair, Database Specialist
Ms Erin M Slagle, Communications Specialist

The MC Workshop consisted of a review in detail of operations of MC. Dr John Jost went through the successive steps of manuscript submission and review. The operations could be observed on a large projector screen by all participants. All steps were presented separately for each role in MC: Author, Reviewer, Associate Editor, Editor-in-Chief, Administrator, and Production Editor, involved in the submission, review and publication of a manuscript. In spite of the focus having been on MC in its state at that time, some desirable changes to the system were discussed. Since the system is designed for a "normal" peer-reviewed scientific journal, and ICTNS review has its own procedures, which are substantially different, the discussion on the best way how to use it for the review of Technical Reports and Recommendations was not a trivial one.

The goal of the PAC Workshop was to discuss and to clarify the roles and responsibilities of all those involved in the process that leads to a manuscript appearing in PAC. The following subjects were covered:

1. Introduction
2. Operational Roles
3. Planning and Execution
4. Organizational Relationships
5. Communications and Reporting

Item 3 was mostly focussed on Conference Reports, starting with the application procedure for an IUPAC Sponsorship of a Conference and covering the successive steps until the publication of the respective report in PAC.

Item 4 included the relationship of PAC with CPEP and ICTNS and the terms of reference for the Editorial Advisory Board (EAB) of PAC, where ICTNS is represented by its Chairman.

Prof J W Lorimer presented the position of ICTNS as decided at the Lisbon meeting of the Titular "Core" Members regarding the roles as editors of the Chairman and Secretary of ICTNS. This view was immediately accepted on the spot by Prof David StC. Black.

Attachment 4
Re Item 7

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

INTERDIVISIONAL COMMITTEE ON TERMINOLOGY, NOMENCLATURE AND SYMBOLS (ICTNS)

REPORT TO IUPAC COUNCIL, 2005

Activities of ICTNS during the biennium 2004-2005 included the following:

1.01 Technical Reports and Recommendations; total accepted or under review: 48.

- 1.1 Technical Reports reviewed and published in Pure and Applied Chemistry: 19 (list attached)
- 1.2 Recommendations reviewed and published in Pure and Applied Chemistry: 7 (list attached)
- 1.3 Recommendations reviewed and published elsewhere: 1 (*Nomenclature of Inorganic Chemistry*, in press RSC).
- 1.4 Recommendations accepted for publication elsewhere: 2 - Revisions of the VIM (*International Vocabulary of Metrology*) and Supplement 1 of the GUM (*Guide to Uncertainty in Measurement*) for BIPM-ISO.
- 1.5 Technical Reports accepted as of 2005-06-20: 3
- 1.6 Recommendations accepted as of 2005-06-20: 0
- 1.7 Technical Reports under review as of 2005-06 20: 11
- 1.8 Recommendations under review as of 2005-06-20: 5

1.02 New duties for Chairman and Secretary of ICTNS

The holders of these positions are now also Editors, Technical Reports and Recommendations, for *Pure and Applied Chemistry*.

1.03 Revision of *IUPAC Handbook*

The *Handbook 2004-2005*, sections *Procedures for Publication of IUPAC Technical Reports and Recommendations; Guidelines for Drafting IUPAC Technical Reports and Recommendations* are completely revised versions based on extensive discussions within ICTNS.

1.04 Interactions with the International Scientific Community

ICTNS has: (a) answered a number of queries concerning terminology, nomenclature and symbols submitted to IUPAC either by individual scientists or organizations; (b) served as one of IUPAC's active contacts with BIPM and ISO; (c) served as advisors on preparation of reports on a number of extensive IUPAC projects.

J. W. Lorimer
Chairman, ICTNS
2005-06-20

Date: 2005-08-05
To: All Members, ICTNS
From: Jack Lorimer
Re: Updated Summary of TRs and Recommendations (E&OE)

The following is a list of the status of all TRs and Recommendations that were:
(a) submitted before 2004-01-01 but not completed by that date;
(b) approved since that date;
(c) submitted and/or approved after 2004-01-01.

Summary

3.0 Recommendations or Technical Reports listed here and published in *PAC* to June, 2005: 28.
Pages published 2004: 414
Pages published 2005: 254.
Average length of Recommendations in published form: 32 pages (max. 81, min. 5 pages).
Average length of TRs in published form: 26 pages (max. 62, min. 3 pages).

1.0 Technical Reports and Recommendations under Review on 2004-01-01 – total 29 (18 accepted)

1.0.1 Technical Reports Abandoned or Under Reconsideration or Published Elsewhere (numbers are "old" IUPAC numbers) – total 3

563 Radiochem. & Nuclear Chem. Techniques (Karol). D. Moore to K. Powell & JWL 2004-02-10 – Division V requires extensive revisions, possibly through new task group. Notice from Division that project abandoned 2004-05-04.

859 Protecting Groups (Black). Extensive comments from ICTNS being reviewed by authors for possible resubmission.

1354 Commercial Polymers (Moore, Laun). Not an ICTNS document (neither a TR nor Recommendations). Published in *CI* July-August 2004.

1.0.2 Recommendations Accepted since 2004-01-01 ("old" IUPAC number/MC number – total 5

REC 1176 Definitions of Terms Relating to Reactions of Polymers and to Functional Polymeric Materials (Horie). Accepted 2004-02-06. Pub. *PAC* **76**, 889-906 (2004).

REC 034 Glossary of Terms Used in Toxicokinetics (Nordberg). Accepted 2004-01-11. Pub. *PAC* **76**, 1033-1082 (2004).

REC 877 Quantities, Terminology, and Symbols in Photothermal and Related Spectroscopies (Hirota). Accepted 2004-02-23. Pub. *PAC* **76**, 1083-1118 (2004).

974/PAC-REC-04-06-05 Definitions of Terms related to Polymer Blends, Composites, and Multiphase Polymeric Materials (Work). Accepted 2004-06-16. Pub. *PAC* **76**, 1985-2007 (2004).

PAC-REC-04-03-04 Terminology Used in Soil Sampling (Fajgelj). 3 reviews by 2004-06-23. Public comment ended 2004-11-30, ICTNS 2004-08-30. Accepted 2005-03-10. Pub. *PAC* **77**, 827-841 (2005).

1.0.3 Technical Reports Accepted since 2004-01-01 ("old" IUPAC number/MC number.) – total 14

1402 Electrochemical Detection on Liquid Flow Analytical Techniques: Charcterization and Classification (Toth, Lindner). Accepted 2004-02-22. Pub. *PAC* **76**, 1119-1138 (2004).

1227 Critical Evaluation of the State of the Art of the Analysis of Light Elements in Thin Films, Demonstrated Using the Examples of SiO_xN_y and AlO_xN_y Films (Dreer). Accepted 2004-02-22. Pub. *PAC* **76**, 1161-1214 (2004).

1142 Guidelines for Calibration in Analytical Chemistry. Part 2. Multicomponent Calibration (Danzer). Accepted 2004-01-17. Pub. *PAC* **76**, 1215-1240 (2004).

1148 Aerosol Pollution in some Chinese Cities (Zhang). Accepted 2004-06-04. Pub. *PAC* **76**, 1227-1240 (2004).

1147 Aerosols: Connection between Regional Climatic change and Air Quality (Slanina). Accepted 2004-06-03. Pub. *PAC* **76**, 1241-1254 (2004).

PAC-REP-04-05-10 Mechanisms of Immunosensitization by Metals (Templeton). Accepted 2004-06-16. Pub. *PAC* **76**, 1255-1268 (2004).

1172 Diagnostic Relevance of the Lymphocyte Transformation Test for Sensitization to Beryllium and Other Metals (Klein). Accepted 2004-06-16. Pub. *PAC* **76**, 1269-1282 (2004).

1432 Properties and Units in the Clinical Laboratory. Part VIII. Properties and Units in Clinical Molecular Biology (Araujo). Accepted 2004-05-05. Pub. *PAC* **76**, 1799-1807 (2004).

1358 Compilation of k_0 and Related Data for Neutron-activation Analysis (NAA) in the Form of an Electronic Database (Kolotov). Accepted 2004-07-13. Published *PAC* **76**, 1921-1925 (2004).

968 Characterization of Polyamides 6, 11, and 12; Determination of Molecular Weight by Size Exclusion Chromatography (Robert). Accepted 2004-05-07; final ms 2004-05-21. Pub. *PAC* **76**, 2009-2025 (2004).

72 Rheological Properties and Associated Structural Characteristics of Some Aromatic Polycondensates Including Liquid-Crystalline Polyesters and Cellulose Derivatives.(White, Laun). Accepted 2004-06-07. Pub. *PAC* **76**, 2027-2049 (2004).

1357/PAC-REP-04-03-02 Chemical Actinometry (Braslavsky). Accepted 2004-06-16. Pub. *PAC* **76**, 2105-2146 (2004).

1406 Post-genomic Chemistry (Varfolomeyev). Accepted initially 2004-06-25. Publication questioned because of overlap with a previous publication 2004-11-08. Revised changes to ms 2005-04 incorporated and ms returned to author for checking 2005-04-13. Accepted 2005-05-31.

1403/PAC-REP-04-04-06 Cyclic Olefin Copolymers (Kim). Accepted 2004-10-04. Pub. *PAC* **77**, 801-814 (2005).

1407/PAC-REP-04-05-04 High-Temperature Mass Spectrometry (Chatillon, Drowart). Accepted 2004-10-29. Pub. *PAC* **77**, 683-737 (2005).

1355/PAC-REP-04-03-03 Non-specific Sensor Arrays ('Electronic Tongue) (Vlasov). Revised ms. received 2004-11-23; 2nd revision sent to author 2005-02-01. Reply 2005-03-24. Final version sent to author for checking 2005-04-04. Accepted 2005-07-11.

1.0.4 Technical Reports Awaiting Final Revision by Authors or by ICTNS ("old" IUPAC number/MC number) – total 0

1.0.5 Technical Reports Awaiting Reply from Authors to Comments from ICTNS or awaiting final comments from ICTNS ("old" IUPAC number/MC number) – total 3

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

878/PAC-REP-04-06-08 IR & Raman at High T, p (Heyns). Corrected ms requested 2002-09-04. Comments by BJH, TC, JWL sent 2004-06-22. Author preparing new ms.

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

1.0.6 Reports and Recommendations Awaiting Revised Manuscript from Authors ("old" IUPAC number/MC number) – total 2

67 X-ray emission analysis (Gohshi). 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.

877 Thermochemistry (da Silva). New ms being prepared. Reminder by JWL 2004-05-07. Author will prepare revision in September, 2005.

2.0 Technical Reports and Recommendations Received since 2004-01-01 – total 22

2.0.1 Recommendations Accepted – total 5

PAC-REC-04-04-03 Red Book (Connelly). Accepted with minor revisions consisting of individual comments from ICTNS members 2004-08-03. Public comment period ended 2004-08-31. In press (RSC) 2005-04.

PAC-REC-04-04-05 Name for Element 111 (Corish). 4 reviews by 2004-06-23. Public comment ends 2004-10-31. Accepted 2004-09-06. Pub. *PAC* **76**, 2101-2103 (2004).

PAC-REC-04-05-03 Guide to Expression of Uncertainty (GUM), Supplement 1 (ISO/BIPM). 1 review by 2004-06-23. Public comment ends 2004-09-30, ICTNS 2004-08-31. Accepted on behalf of IUPAC with minor editorial revisions to IUPAC and Wallard 2004-09-27. ISO Document JCGM-WG1-SC1-N10. Status queried with A. Thor 2005-04-21 – reply not yet pub.

PAC-REC-04-05-02 International Vocabulary…Metrology (VIM) (ISO/BIPM). Accepted on behalf of IUPAC with minor editorial changes to Wallard 2004-10-05. Status queried with A. Thor 2005-04-21 – reply not yet pub.

PAC-REC-04-03-01 Nomenclature of Fullerenes (W. Powell). Revised ms accepted 2004-10-13. Pub. *PAC* **77**, 843-923 (2005).

2.0.2 Technical Reports Accepted – total 9

961/PAC-REP-04-04-08 Electrochemistry at the Interface Between Two Immiscible Electrolyte Solutions (Samec). Accepted 2004-07-06. Pub. *PAC* **76**, 2147-2180 (2004).

1356/PAC-REP-04-06-06 Chemical Speciation Part I (K. Powell). Accepted 2004-08-15. Pub. *PAC* **77**, 739-800 (2005).

PAC-REP-04-05-07 Polyaniline (Stejskal). Revised ms accepted 2004-10-13. Pub. *PAC* **77**, 815-826 (2005).

PAC-REP-04-05-14 Practical Guide to the Interpretation of Magnetic Measurements (Lueken). Revised ms accepted 2004-10-17. Pub. *PAC* **77**, 497-511 (2005).

PAC-REP-04-04-09 Electrokinetic Phenomena (Delgado). 2 reviews (1 ICTNS). Accepted 2005-03-10.

Project (to be submitted to JPCRD) Reference Data for the Density and Viscosity of Liquid Aluminum and Liquid Iron (Assael). ICTNS review (JWL, R. Weir) sent to author 2005-04-24; final version approved (with minor corrections) 2005-04-25.

PAC-REP-04-04-07 Critical evaluation of metal complexes of complexones (Anderegg, now Popov, now Delgado). Revised ms reviewed by BJH, JWL. Final revision 2005-04-21 waiting for final acceptance from K. Powell. Accepted 2005-05-11.

PAC-REP-04-07-02 Atomic Force Microscopy and Direct Surface Force Measurement (Ralston). 3 reviews (none ICTNS). Revised to IUPAC standards 2005-01; letter of acceptance (minor revision) 2005-04-23. Revised ms 2005-06-05; minor corrections sent to author 2005-06-11. Accepted 2005-07-06.

2.0.3 Technical Reports and Recommendations Reviewed, Waiting for Reply from Authors, or Waiting for Review by ICTNS of Revised Manuscript – total 3

PAC-REP-04-04-04 NMR for pKs (Popov). Revised ms received 2005-07-28.

PAC-REP-04-08-05 Standards, Calibration and Guidelines in Microcalorimetry. Part 2. Calibration Standards for Differential Scanning Calorimetry (Della Gatta). 4 reviews (3 ICTNS). Returned to author for minor revision 2004-11-25. Reminder 2005-04-21.

PAC-REP-04-10-25 Properties and Units in the Clinical Laboratory Sciences. Part XX. Properties and Units in Clinical and Environmental Toxicology (Duffus). Request for revised ms. showing what materials are to be archived on web site 2004-11-20, expanded 2005-01-25.

PAC-REC-04-12-04 Terminology of Polymers Containing Ionizable or Ionic Groups and of Polymers Containing Ions (Kubisa). 9 reviews. Public comment period ends 2005-05-31. Letter 2005-04-20 major revision. Author (2005-04-21) notes final review by Division will be done in Beijing in August.

2.0.4 Recommendations Waiting for Review by ICTNS or Final Review by Officers– total 3

PAC-REC-04-10-24 Nomenclature of Cyclic Peptides (Moss). 2 reviews. Public comment period ends 2005-03-31. Letter asking for major revision, 2005-03-15.

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

PAC-REC-05-03-01 Graphical Representation of Configuration (Brecher). Public comment period ends 2005-07-31. Letter of acceptance with minor revision (revised ms required) 2005-08-04.

PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions (Oman). Received 2005-07-18. Public comment period ends 2006-01-31.

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). Received 2005-07-15. Public comment period ends 2006-01-31.

2.0.5 Technical Reports Waiting for Review by ICTNS or Final Review by Officers– total 2

PAC-REP-04-05-06 International Harmonization Protocol (Fajgelj). Two more reviews requested 2004-10-07 (one received) to confirm adherence to BIPM standards. Reviews sent to author 2004-12-09. Revised ms received, returned for minor correction of symbols 2005-07-11.

PAC-REP-05-05-03 Guidelines for Calibration in Analytical Chemistry. Part 3. Uncertainty Estimation and Figures of Merit for Multivariate Calibration (Olivieri). Last rev. due 2005-05-03. JWL review complete. 2005-06-11: major revision & reviewers' comments sent. Author will prepare revision in September, 2005.

Technical Reports and Recommendations: 2004-5
Output from Manuscript Central on 2005-05-27

Manuscript ID	Title	Date Submitted	Submitting Author	Status
PAC-REC-04-10-14	Compendium of Terms Used in Pharmaceutics	13-Oct-04	Chorghade, Mukund	AE: Ganellin, C. Awaiting Reviewer Scores 2 invited; 2 agreed; 0 declined; 0 returned Erhardt, Paul Forsum, Urban
PAC-REC-04-10-15	Compendium of Terms in Process Chemistry And Manufacturing	13-Oct-04	Chorghade, Mukund	AE: Ganellin, C. Awaiting Reviewer Scores 2 invited; 2 agreed; 0 declined; 0 returned Erhardt, Paul Forsum, Urban
draft	Glossary of Terms Used in Photochemistry		Braslavsky, Silvia	Awaiting Author Submission
PAC-REC-05-07-04	Use of the terms robust" and "rugged" and the associated characteristics "robustness" and "ruggedness" in descriptions of analytical procedures"	15-Jul-05	Burns, Duncan	Awaiting Reviewer Scores 11 invited; 4 agreed; 2 declined; 1 returned
PAC-REP-04-04-04.R1	Recommendations for NMR Measurements for Determination of High and Low pK Values	22-Apr-04	Popov, Konstantin	Awaiting Reviewer Scores 2 invited; 2 agreed; 0 returned
PAC-REC-05-03-06	Recommendations for the use of microtechnology in clinical laboratories	24-Mar-05	Wilding, Peter	Awaiting Reviewer Scores 2 invited; 2 agreed; 0 declined; 1 returned

Technical Reports and Recommendations: 2004-5

Manuscript ID	Title	Date Submitted	Submitting Author	Status
PAC-REC-05-03-01	Graphical Representation of Configuration	3-Mar-05	Brecher, Jonathan	Awaiting Reviewer Scores 21 invited; 10 agreed; 5 declined; 9 returned
PAC-REC-05-07-05	Guidelines for Potentiometric Measurements in Suspensions	18-Jul-05	Oman, Srecko F.	Awaiting Reviewer Scores 4 invited; 3 agreed; 0 declined; 0 returned
PAC-REP-05-03-03.R1	Guidelines for calibration in analytical chemistry, Part 3: Uncertainty estimation and figures of merit for multivariate calibration	7-Jul-05	Olivieri, Alejandro	Invite Reviewers 0 invited; 0 agreed; 0 declined; 0 returned
PAC-REP-04-10-13	Chemical, pharmacological aspects of natural products with medicinal and nutritive value	13-Oct-04	Chorghade, Mukund	Major Revision
PAC-REC-04-10-24	Nomenclature of Cyclic Peptides	26-Oct-04	Moss, Gerard	Major Revision
PAC-REC-04-12-04	Terminology of Polymers Containing Ionizable or Ionic Groups and of Polymers Containing Ions	7-Dec-04	Kubisa, Przemyslaw	Major Revision
PAC-REP-04-08-05	Standards, Calibration and Guidelines in Microcalorimetry Part 2. Calibration Standards for Differential Scanning Calorimetry	9-Aug-04	Della Gatta, Giuseppe	Minor Revision
PAC-REP-04-05-06.R1	International Harmonized Protocol for the Proficiency Testing of (Chemical) Analytical Laboratories	11-Jul-05	Fajgelj, Ales	Select Reviewers
PAC-REP-04-10-25	Properties and Units in the Clinical Laboratory Sciences Part XX. Properties and Units in Clinical and Environmental Human Toxicology (Technical Report)	26-Oct-04	Duffus, John	Select Reviewers 1 invited; 1 agreed; 0 declined; 0 returned
PAC-REP-04-05-08	Electrochemical Detection in Liquid Flow Analytical Techniques: Characterization and Classification	26-May-04	Lindner, Erno	vol:76 iss:06

Technical Reports and Recommendations: 2004-5

Manuscript ID	Title	Date Submitted	Submitting Author	Status
PAC-REP-04-05-09	Piezoelectric Chemical Sensors	26-May-04	Lindner, Erno	vol:76 iss:06
PAC-REP-04-05-10	Mechanisms of Immunosensitization to Metals	26-May-04	Templeton, Douglas	vol:76 iss:06
PAC-REC-04-05-12	Revised Section F: Natural Products and Related Compounds	27-May-04	Moss, Gerard	vol:76 iss:06
PAC-REP-04-05-13	Critical Evaluation of the State of the Art of the Analysis of Light Elements in Thin Films	28-May-04	Dreer, Sabine	vol:76 iss:06
PAC-REP-04-05-11.R1	Diagnostic relevance of the lymphocyte transformation test for sensitization to Beryllium and other metals	1-Jun-04	Klein, Reinhild	vol:76 iss:06
PAC-REP-04-06-01	Aerosol Pollution in Some Cities of China	2-Jun-04	Zhang, Yuanhang	vol:76 iss:06
PAC-REP-04-06-02	Aerosols: Connection between Regional Climatic Change and Air Quality	2-Jun-04	Slanina, Sjaak	vol:76 iss:06
PAC-REP-04-06-07	Guidelines for Calibration in Analytical Chemistry: Part 2. Multispecies Calibration	17-Jun-04	Danzer, Klaus	vol:76 iss:06
PAC-REP-04-06-04	Properties and Units in the Clinical Laboratory Sciences Part XVIII. Properties and Units in Clinical Molecular Biology	14-Jun-04	de Araujo, Pedro	vol:76 iss:09
PAC-REP-04-07-03	Compilation of k0 and related data for NAA in the form of an electronic database	19-Jul-04	Kolotov, Vladimir	vol:76 iss:10
PAC-REP-04-03-05.R1	Characterization of Polyamides 6, 11 and 12; Determination of molecular weight by Size Exclusion Chromatography	25-May-04	Robert, Eric	vol:76 iss:11
PAC-REP-04-06-03	The rheological properties and associated structural characteristics of some aromatic polycondensates including liquid crystalline polyesters and cellulose derivatives	8-Jun-04	Laun, H. Martin	vol:76 iss:11
PAC-REC-04-06-05	Definitions of Terms Related to Polymer Blends, Composites and Multiphase Polymeric Materials	16-Jun-04	Work, William	vol:76 iss:11

Technical Reports and Recommendations: 2004-5

Manuscript ID	Title	Date Submitted	Submitting Author	Status
PAC-REC-04-05-05	Name and Symbol of the Element With Atomic Number 111	24-May-04	Corish, John	vol:76 iss:12
PAC-REP-04-04-08.R1	Electrochemistry at the interface between two immiscible electrolyte solutions	25-May-04	Samec, Zdenek	vol:76 iss:12
PAC-REP-04-03-02.R1	Chemical Actinometry	14-Jun-04	Braslavsky, Silvia	vol:76 iss:12
PAC-REP-04-05-14.R1	Practical guide to measurement and interpretation of magnetic properties	16-Aug-04	Lueken, Heiko	vol:77 iss:02
PAC-REP-04-05-04	High Temperature Mass Spectrometry: Instrumental Techniques, Ionization Cross Sections, Pressure Measurements and Thermodynamic Data	11-May-04	Drowart, Jean	vol:77 iss:04
PAC-REP-04-06-06.R1	Chemical Speciation of Environmentally Significant Heavy Metals With Inorganic Ligands Part 1: The Hg2+ - Cl-, OH-, CO32-, SO42- AND PO43- Aqueous Systems	16-Aug-04	Powell, H. Kipton	vol:77 iss:04
PAC-REP-04-04-06.R1	Chemical Structure and Physical Properties of Cyclic Olefin Copolymers	16-Jun-04	Kim, Sung	vol:77 iss:05
PAC-REC-04-03-01.R1	Numbering of Fullerenes, Recommendations 2004	11-Oct-04	Powell, Warren	vol:77 iss:05
PAC-REP-04-05-07.R1	Polyaniline. Thin Films and Colloidal Dispersions	13-Oct-04	Stejskal, Jaroslav	vol:77 iss:05
PAC-REC-04-03-04.R1	Terminology in Soil Sampling	25-Jan-05	Fajgelj, Ales	vol:77 iss:05
PAC-REP-04-04-07.R1	Critical Evaluation of Stability Constants of Metal Complexes of Complexones for Biomedical and Environmental Applications	29-Dec-04	Delgado, Rita	vol:77 iss:08
PAC-REP-04-06-09	Post-Genomic Chemistry	22-Jun-04	Varfolomeyev, Sergey	vol:77 iss:09
PAC-REP-04-04-09.R1	Measurement and Interpretation of Electrokinetic Phenomena	10-Feb-05	Delgado, Ángel	vol:77 iss:10
PAC-REP-04-03-03	NON-SPECIFIC SENSOR ARRAYS («ELECTRONIC TONGUE») FOR CHEMICAL ANALYSIS OF LIQUIDS	24-Mar-04	Vlasov, Yuri	vol:77 iss:11

Technical Reports and Recommendations: 2004-5

Manuscript ID	Title	Date Submitted	Submitting Author	Status
PAC-REP-04-07-02.R2	Atomic Force Microscopy and Direct Surface Force Measurements	6-Jun-05	Ralston, John	vol:77 iss:12
PAC-REP-04-06-08	Infrared and Raman Spectroscopy under Extreme Conditions of Pressure and Temperature	18-Jun-04	Heyns, Anton	Lost communication with author
PAC-REC-04-11-03	Nomenclature of Organic Chemistry (‘Blue Book’)	3-Nov-04	Powell, Warren	
PAC-REC-04-04-03	Nomenclature of Inorganic Chemistry (Revised Red Book)	21-Apr-04	Connelly, Neil	In print

Report 2004-5 of Division I, Physical and Biophysical Chemistry

FAX

To: Professeur Roberto Marquardt
From: Jeremy Frey

Fax no. 00861084970107

Tried to send to China
but it does not work
this is for ITCNS
Thanks

IUPAC Report from Div I to ITCNS
(Jeremy Frey)

The main issue that concerns Div I of importance to ITCNS is the next edition of the Green Book. There have been delays to the production of the final version, which I hope will have been resolved by the end of the Beijing meeting. Roberto Marquardt will be able to provide you with the most up to date information on the Green Book.

The majority of Div I projects are continuing satisfactorily. Several projects will now have databases as their outcomes and this may be an area that will impact on IUPAC more generally and need some coordination from ITCNS at some stage in the future.

In passing I should also note that I am also IUPAC's representative on SURAMCO (IUPAP equivalent of ITCNS) but I have to report that I have not had any contact with SURAMCO. My appointment was made via IUPAC so I have never had any contact or been informed of their meetings so I am unable to report any thing at this stage.

Jeremy Frey
University of Southampton

Report of the IUPAC Organic and Biomolecular Chemistry Division (III)

August 14th 2005

Minoru Isobe, President

I. Executive Summary and Highlights

The Mission of Division of Organic and Biomolecular Chemistry is to promote the goals of IUPAC in the field of organic and biomolecular chemistry in the broadest sense. To this end the Division consists of a Division Committee and six Subcommittees. Together these promote the formulation and execution of Projects on relevant chemical problems, the staging of chemical conferences on important areas of chemistry, the education and professional development of chemists worldwide, the advancement of chemical industry, and the application of chemistry to meet the world's needs. The Division is committed to utilizing the talents of chemists from around the world in these activities, and promoting diversity in our membership.

The Division covers such a broad area of multidisciplinary aspects, and stimulates fundamental and applied organic synthesis as top edge science. It includes asymmetric synthesis of Natural products, Process chemistry with Molecular catalysts, and the still explosively-expanding field of Organometallic chemistry. Chemical biology, or Post genomic chemistry, is a key science for the biomolecules in this century, and it is also close to Biotechnology. Physical organic chemistry has been a fundamental mechanistic science, and it is also important in spectroscopy and organic analysis. Photochemistry is of worldwide significance in the standardization for analytical chemistry as well. Green and sustainable chemistry is increasingly recognized as important for our environment and we have to protect scarce organic materials on a global scale. Division-III co-ordinates all of these subjects directly and as interdivisional activities, especially through the work of the following Subcommittees.

Subcommittee on Organic Synthesis (Chair: Frank McDonald, USA)
Subcommittee on Biomolecular Chemistry (Chair: Vadim Ivanov, Russia)
Subcommittee on Green Chemistry (Chair: Pietro Tundo, Italy)
Subcommittee on Photochemistry (Chair: Silvia Braslavsky, Germany)
Subcommittee on Structural and Mechanistic Chemistry (Chair: T. Marek Krygowski, Poland)
Subcommittee on Biotechnology (Chair: Romas Kazlauskas, USA)

The Subcommittees have been dealing with the IUPAC sponsored conferences in various locations around the world with great success. Some of them are recognized as major conference series with long advanced scheduling, and are integrated with schedules for related international conferences.

The following report is slightly different in style from standard IUPAC instructions, since the activities of the different subcommittees need to be integrated to make this report fit the six Goals in the current IUPAC Strategic Plan.

II. An overall report of Division activities 2004 – mid-2005

a) IUPAC will provide leadership as a worldwide scientific organization that objectively address global issues involving the chemical sciences. The Organic Synthesis Subcommittee has long held a key place in the worldwide leadership among synthetic chemistry communities: for example in asymmetric synthesis of natural products and in new reactions catalyzed by organometallic compounds. The Biomolecular Subcommittee is also recognized at a world leading level for promoting work on the elucidation of the molecular structures in trace amount and/or complexity and/or biochemical mechanisms. These have been identified through the divisional-supported series of conferences as Organic Synthesis (ICOS) and Natural Product Chemistry (ISCNP).

b) IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion. Photochemistry is a good example for such standardization as it has been widely applied to various kind of spectroscopy on the basis of physical chemistry such as NMR, Photoluminescence, and

Chemical Actinometry. It should be noted that our Photochemistry Subcommittee is in good collaboration with major photochemical societies in the world.

c) IUPAC will assist chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement in the quality of life. The Green Chemistry Subcommittee has contributed to this subject on a worldwide basis, starting from South East Asia, India, Arab region, Latin America, Russia, Africa in the strong connection with the economical growth and chemical industry activity and has fostered several projects in this field.

d) IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries. The Division-III Biomolecular Subcommittee has been developing its Biodiversity project, completed in the form of IUPAC recommendation (*Pure Appl. Chem. 74,* 697-702, **2002**). This project was discussed in Thailand, Brazil, China, and Turkey before the recommendation was finalized. A further workshop was held in New Delhi in 2004 during the 4th IUPAC Conference on Biodiversity to discuss the proposal for a Natural Product Center in Bangladesh.

e) IUPAC will utilize its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists and the public appreciation of chemistry. IUPAC prizes have been awarded to young chemists in the ICOS meeting as well as Poster Prize to 3 presentators. Many conferences have similar award system to give presentation awards to young chemists.

f) IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender, and age. The Division has been committed to these goals for some time, as witnessed by our current 31 members (11 TM, 6 AM, 12 NR, 2 PR), who are from 29 countries (Asia 8), (Europe 15), (North America 3), (South America 3), and (Africa 2). At present, just 4 are female but we aim to increase this representation. We are always keen to recruit younger chemists, while recognizing the impact that dedication to an IUPAC Committee can have on their career development. In addition our Subcommittees include 73 additional individuals, many of them younger chemists.

SUBCOMMITTEES:

Subcommittee on Organic Synthesis

Synthesis covers a central part of the organic chemistry spectrum and ethos. The mission of the Sub-committee on Organic Synthesis is to provide a focus for the dissemination of current knowledge and the development of future directions in all aspects of organic synthesis, including: 1) The development of new molecular transformations; 2) The development of new reagents; 3) The development of environmentally benign synthetic processes; 4) The synthesis of new types of organic structures; 5) The synthesis of target molecules for specific applications; 6) The total synthesis of natural products; 7) Combinatorial and high throughput techniques

The 15th IUPAC International Conference on Organic Synthesis (ICOS-15) was held in Nagoya, Japan in August 2004, and was very successful, attracting nearly 1000 participants. The IUPAC Prize was awarded to Prof. Hartwig, and the nomination process for the next Prize has just begun in June in collaboration with our co-sponsor, Theme. It will be awarded at ICOS-16, which will be held in Merida, Yucatan, Mexico June 11-15, 2006 by the organizer Professor Eusebio Juaristi. It is proposed that ICOS-17 should be held at Daejeon in Korea during Aug 17-23, 2008; ICOS-18 (2010) in Bergen, Norway; and ICOS-19 (2012) in Taiwan. A Heterocyclic Chemistry conference (FHC-5) was held in Florida, USA in March 2004, and its successor will be held in 2006. The most recent Organometallic Chemistry Conference (ICOMC-21) was held in Vancouver, Canada in July 2004. There are 2 more conferences planned in 2005: Heterocyclic Chemistry (ICHC) in Palermo, Italy in July-Aug, and Organometallic Chemistry (OMCOS-13) in Geneva in July.

Subcommittee on Biomolecular Chemistry

The Subcommittee seeks to deliver the long-range goals of IUPAC, particularly at the vital interfacial area of molecular science that lies between organic chemistry and biology. It will support the application of the powerful methods of chemistry to current and emerging problems in biology to achieve understanding and, where appropriate, modification of the systems of living organisms at the molecular level. To that end, the Sub-Committee will provide a focus for the dissemination of current knowledge and the development of future directions in the following fields: 1) Structure, function and applications of biomolecules and their analogues; 2) Molecular mechanisms of biological processes and their modulation; 3) Molecular engineering *via* chemo-enzymatic processes; 4) Analysis, manipulation and application of biomolecular information systems.

The 4th International Conference on Biodiversity and 24th meeting on Natural Products: Chemistry and Medical Applications were held in tandem in New Delhi, India in January 2004 under the able organization of Prof. V. S. Parmar with some 1000 participants. A Satellite symposium on Bioresources toward drug discovery and development was held in Mauritius in Feb. 2004 (Org. by Prof. Am. G. Fakim). The next joint symposia (5th and 25th respt.) will be held in Kyoto, Japan (D. Uemura) in July 2006; and then (6th and 26th) will be held in Australia (Mary Garson).

The 7th International Symposium on Biomolecular Chemistry (ISBOC-7) was held at the University of Sheffield, UK in July 2004, which was masterminded by Professor Michael Blackburn in collaboration with the Royal Society of Chemistry. In the Subcommittee meeting in Sheffield, the proposal (# 2004-013-1) submitted by Prof. Mosihuzzaman was recommended in modified form for the organization of a Symposium in Print. Progress reports of the projects on "Post-genomic chemistry" (#2001-005-1-300) and "Fighting microbial resistance through development of new antimicrobial agent, directed against new specific targets" (#2002-030-1-300) was reported by Prof. Koomen. The next ISBOC-8 is under active development for 2007.

Subcommittee on Photochemistry

Implementation of the overall goals and objectives of IUPAC in the multidisciplinary area of photochemistry and its links to the photosciences (e. g., materials sciences, photobiology, photolithography, photography) can be accomplished only with the inputs of a broad spectrum of experts in the field, including those with ancillary interests in areas covered by all Divisions within IUPAC. 1) Renewable energy sources; 2) Green chemistry; 3) Atmospheric photochemistry; 4) New analytical methods in the biosciences including trace analysis of proteins, nucleic acids, and small bioregulators, both *in vivo* and *in vitro*; 5) Industrial photochemistry; 6) Advanced spectroscopic methods in ultra-fast time and ultra-small space resolution; 7) Methods for identifying material fatigue and temporal changes.

The Subcommittee works in close contact with the three major Photochemical Societies of the world, i.e., the Inter-American Photochemical Society, IAPS, The European Photochemical Association, EPA, and the Japanese Photochemical Association.

Prof. Miguel Miranda organized a meeting of the Sub-Committee on Photochemistry, plus colleagues participating in or chairing projects, during the XX-IUPAC Sponsored symposium of Photochemistry in Granada, Spain in July 2004. The 21st Symposium is planned for Kyoto, Japan in April 2006 (Prof. Masahiro Irie).

The Project on Chemical Actinometry (#2002-008-1-300) has been published in *Pure Appl. Chem. 76*, 2105-2146 (**2004**) by H. J. Kuhn etc. Reference methods, standards and applications of photoluminescence Project (#2004-021-1-300) was carried out (by interdivisional collaboration with Divisions III, I and V) by Task group (Chair E. S. Roman and F. Brouwer). This is an updating of the previous 2 relevant documents *PAC, 60(7)*, 1107-1114 (1988), and *PAC, 62(8),* 1631-1648 (1990). The scope of this work not only covers the theoretical field in single molecule fluorescence, but also is applicable to material sciences and biology through fluorescence microscopy, etc.

Subcommittee on Structural and Mechanistic Chemistry

The Subcommittee should handle problems concerning the many aspects of structural and mechanistic organic chemistry. Specific examples include: 1) Environmentally friendly chemical processes and degradative pathways of organic contaminants; 2) Reactions in solution, gas phase, and solid state; 3) Solvents for organic reactions; 4) Acidity and basicity of organic compounds; 5) Supramolecular chemistry.

The 17th IUPAC Conference on Physical Organic Chemistry (ICPOC-17) was held in Shanghai, China in August 2004 (Prof. Guo Zhen Ji). The next ICPOC-18 is planned in Warsaw in Aug 2006 (Prof. Marek Krygowski); and ICPOC-19 will be in Santiago, Spain (Galicia) in 2008. The next group conference will be

held in Essen, Germany in 2007 (Roland Boese). CAIC-10 was held in Bussan, Korea in August 2004 (Prof. Dae Dong Sung).
The Subcommittee meeting in Shanghai approved the change in name of orrelation Chemistry to orrelation and Modeling in Chemistry This change aims at fostering research in all aspects of the modeling of the structure-property quantitative relationship (SPQR); thus, between structural variations and measurable properties as equilibrium constants, (enzyme catalyzed) reaction rates, etc.

Subcommittee on Green Chemistry

The aim of this Subcommittee is to develop actions devoted to the cause of green chemistry for its wider benefit to the future of chemistry and society as whole.

Its activities are introduced in *Chemistry International, Vo. 26, No. 2, March-April, 2004* by Pietro Tundo and Mohamed Tawfic Ahmed as follows. reen Chemistry is an emerging field concerned with the safe practice of chemistry a goal that people all over the world are interested in attaining. Green chemistry addresses some of our most precious values; human well-being, environmental sustainability, integrity, and safety, and the worldwide need for green chemistry practices should allow human development and property, along with environmental ethics. The IUPAC working party on Synthetic Pathways and Processes in Green Chemistry defined Green Chemistry (2000) as *The invention, design, and application of chemical products and processes to reduce or to eliminate the use and generation of hazardous substances.*

Projects of Green (Sustainable) Chemistry in the South East Asian (#2002-028-1-300), IUPAC coordinated web page (#2002-029-1-300), and the Arab (#2003-043-1-300) regions are still in progress; while Projects on Green Chemistry in Russia (#2003-026-1-300) and in Latin America (#2002-064-1-300) have been completed. There has been a proposal for the translation and dissemination of a monograph for secondary schools on lobal Climate Change by Tundo (#2005-015-1).

Subcommittee on Biotechnology

This is the youngest Sub-Committee of Division-III and under its Chairman (Prof. Romas Kazlauskas) is formulating its scope, remit and future activities. The International Biotechnology Symposium and Exhibition (IBS-12) was held in Oct. 2004 in Santiago, Chile (J. A. Asenjo). The program included 10 sections with newer areas of Molecular tools, Cellular tools, Genomic tools, applied genome research, Cultivation technology, downstream processing, Biocatalysis, Health care, Plant and food biotechnology, and Environmental Biotechnology. A proposal for an inaugural Meeting in W.Europe is being developed for 2007.

VII. Any other substantive information

The Budget of Division III for 2004-2005 has been allocated to the 6 Subcommittees in part, and the rest is available for projects. Further funding is available for good proposals. The generation of new projects remains the most urgent business of the Division.
Many potential proposals have been discussed among the subcommittee meetings to generate most important and timely projects.

VIII. Tabular material

List of publications

Current Projects

2000-012-1-300 - Single molecule spectroscopy*
2001-005-1-300 - Post-genomic chemistry*
2001-018-1-300 - Space- and time-resolved fluorescence spectroscopy and photochemistry
2001-020-1-300 - Glossary of terms and basic protocols used in photodynamic therapy
2001-036-1-300 - Glossary of terms in photocatalysis and radiation catalysis*
2002-024-1-300 - Glossary of terms used in photochemistry (3rd version)*
2002-028-1-300 - South East Asian, and neighbouring countries, Green Chemistry Network

2002-029-1-300 - A IUPAC coordinated web page on Green/Sustainable Chemistry
2002-030-1-300 - Fighting microbial resistance through development of new antimicrobial agents, directed against new specific targets
2003-043-1-300 - Green chemistry in the Arab region
2003-046-1-300 - Workshop for formulation of plans for the establishment of a "Center of Natural Products Research (CNPR)"
2004-021-1-300 - Reference methods, standards and applications of photoluminescence*
* Interdivisional project

OTHER INTERDIVISIONAL PROJECTS
2001-014-1-800- Fullerene nomenclature - part II
2001-031-1-800 - Alignment of nomenclature in areas of overlap between the preferred names for organic nomenclature and the revision of the nomenclature of inorganic chemistry
2001-043-1-800 - Preferred names in the nomenclature of organic compounds
2002-010-1-050 - Toward a core organic chemistry curriculum for Latin American universities
2003-006-1-100 - NMR chemical shifts: updated conventions

PROJECTS NEAR COMPLETION / IN PRESS
301/1/93 - Development of guidelines for the transmission of information on organic synthesis (Abbreviation guidelines and glossary of terms for protecting groups in synthesis)

RECENTLY COMPLETED
2003-026-1-300 - Green chemistry in Russia
2002-064-1-300 - Green Chemistry in Latin America
2002-008-1-300 - Chemical actinometry

Representation on other IUPAC Bodies

Committee on Chemical Education (CCE) M. Fatima G. F. da Silva.
Interdivisional Committee on Nomenclature, Terms, and Symbols (ITCNS) Gerrit Koomen.
Subcommittee on Materials Chemistry Shunichi Fukuzumi and Istvan Horvath.
Division VIII Nomenclature Warren Powell.

Recent Reports from ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION (III)
Chemical actinometry (IUPAC Technical Report)
Pure Appl. Chem. **76**(12), 2105-2146 (2004)
Phane nomenclature. Part II. Modification of the degree of hydrogenation and substitution derivatives of phane parent hydrides (IUPAC Recommendations 2002) (III)
Pure Appl. Chem. **74**(5), 809-834 (2002)
Molecular basis of biodiversity, conservation, and sustained innovative utilization
Pure Appl. Chem. **74**(4), 697-702 (2002)
Nomenclature for the C60-*I*h and C70-*D*5h(6) fullerenes (IUPAC Recommendations 2002) (III.1)
Pure Appl. Chem. **74**(4), 629-695 (2002)
Critical evaluation of proven chemical weapon destruction technologies
Pure Appl. Chem. **74**(2), 187-316 (2002)
Organic photochromism (IUPAC Technical Report) (III.3)
Pure Appl. Chem. **73**(4), 639-665 (2001)

Figures-of-merit for the technical development and application of advanced oxidation technologies for both electric- and solar-driven systems (IUPAC Technical Report) (III.3)
Pure Appl. Chem. **73**(4), 627-637 (2001)
Synthetic Pathways and Processes in Green Chemistry. Introductory Overview (III.2)
Pure Appl. Chem. **72**(7), 1207-1228 (2000)
That is the *Introductory Overview* to the *PAC* special topic issue on Green Chemistry.
Revised Section F: Natural products and related compounds (III.1)
Pure Appl. Chem. **71**(4), 587-643 (1999)
+ Errata, *Pure Appl. Chem.* **76**(6), 1283-1292 (2004)

Report of Organic and Biomolecular Chemistry Division

July 1, 2004 Sheffield; August 4, Nagoya

New term of IUPAC Division of Organic and Biomolecular Chemistry has started since January of this year. This Division in 2004-2005 is supported by the Division Committee and Subcommittees of the members as attached file, and further details are available at http://www.iupac.org/divisions/III/index.html. You can find the updated activity of this Division in this URL about items such as Recent Report (Note 1), Subcommittee (Note 2), Current Project (Note 3), Conferences (Note 4), etc. Material for inclusion can be sent to Fabienne Meyers: fabienne@iupac.org

Division's Aims

The Mission of the Division of Organic and Biomolecular Chemistry is to promote the goals of IUPAC in the field of organic and biomolecular chemistry in the broadest sense. To this end the Division consists of a Division Committee and six Subcommittees. Together these promote the formulation and execution of Projects on relevant chemical problems, the staging of chemical conferences on important areas of chemistry, the education and professional development of chemists worldwide, the advancement of chemical industry, and the application of chemistry to meet the world's needs. The Division is committed to utilizing the talents of chemists from around the world in these activities, and promoting diversity in our membership.

Division Rules (draft, Oct 2003) [attached file]

Subcommittees (*Note 2*)

Organic Synthesis
Structural and Mechanistic Chemistry
Photochemistry
Biomolecular Chemistry
Green Chemistry
Biotechnology

Projects (*Note 3*): Current projects supported by the Division are listed at **http://www.iupac.org/divisions/III/cp3.html** Our budget for 2004-2005 is allocated to the 6 Subcommittes in part, and the rest are available for projects. Further funding is available for good proposals. The generation of new projects remains the most urgent business of the Division.

Conferences (*Note 4*): We are the primary sponsors of a number of conferences for 2004-5, and these provide the opportunity for meetings of many of our Subcommittees. A one page description of the Division has been prepared and can be sent by email to any conference organizers who wish to distribute this at conferences, or include it in the abstract books.

Representation on other IUPAC Bodies

Committee on Chemical Education (CCE) M. Fatima d. G. F. da Silva.

Interdivisional Committee on Nomenclature, Terms, and Symbols (ITCNS) Gerrit Koomen.
Subcommittee on Materials Chemistry Shunichi Fukuzumi and Istvan Horvath.
Division VIII Nomenclature Warren Powell.

Provisional Division Rules and Subcommittee Mission Statements. These were adopted year 2003 and are posted on the Division website. Subcommittees may wish to consider if these accurately reflect their activities. (attached file).

Diversity: Former executives have done well in geographic diversity, with 29 countries represented on our Division Committee. However our inclusion of female members is low (6), and we hope this will improve in the future.

IUPAC former Division Vice-President David Black (new Secretary General of IUPAC), former Division President Torbjorn Norin (still on Interdivisional Subcommittee on Biological Chemistry), and Titular Members Norma Nudelman (now on CHEMRAWN Committee), Silvia Braslavsky (now National Representative from Germany and still Chair of the Photochemistry Subcommittee), Milton Hearn, and Govardhan Mehta.

Minoru Isobe
Nagoya University

Note 1

Recent Reports from ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION (III)

Phane nomenclature. Part II. Modification of the degree of hydrogenation and substitution derivatives of phane parent hydrides (IUPAC Recommendations 2002) (III)
Pure Appl. Chem. **74**(5), 809-834 (2002)

Molecular basis of biodiversity, conservation, and sustained innovative utilization
Pure Appl. Chem. **74**(4), 697-702 (2002)

Nomenclature for the C60-*Ih* and C70-*D*5h(6) fullerenes (IUPAC Recommendations 2002) (III.1)
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Figures-of-merit for the technical development and application of advanced oxidation technologies for both electric- and solar-driven systems (IUPAC Technical Report) (III.3)
Pure Appl. Chem. **73**(4), 627-637 (2001)

Synthetic Pathways and Processes in Green Chemistry. Introductory Overview (III.2)
Pure Appl. Chem. **72**(7), 1207-1228 (2000)
That is the *Introductory Overview* to the *PAC* special topic issue on Green Chemistry.

Note 2

The six Subcommittees are:

> Subcommittee on Organic Synthesis
> Subcommittee on Biomolecular Chemistry
> Subcommittee on Green Chemistry
> Subcommittee on Photochemistry
> Subcommittee on Structural and Mechanistic Chemistry
> Subcommittee on Biotechnology

Subcommittee on Organic Synthesis
Synthesis covers a central part of the organic chemistry spectrum and ethos. The mission of the Subcommittee on Organic Synthesis is to provide a focus for the dissemination of current knowledge and the development of future directions in all aspects of organic synthesis, including:

1. The development of new molecular transformations
2. The development of new reagents
3. The development of environmentally benign synthetic processes
4. The synthesis of new types of organic structures
5. The synthesis of target molecules for specific applications

6. The total synthesis of natural products
7. Combinatorial and high throughput techniques

Subcommittee on Biomolecular Chemistry
The Subcommittee will seek to deliver the long-range goals of IUPAC, particularly within the vital interfacial area of molecular science that lies between organic chemistry and biology. It will support the application of the powerful methods of chemistry to current and emerging problems in biology to achieve understanding and, where appropriate, modification of the systems of living organisms at the molecular level.

To that end, the Sub-Committee will provide a focus for the dissemination of current knowledge and the development of future directions in the following fields:

* Structure, function and applications of biomolecules and their analogues.
* Molecular mechanisms of biological processes and their modulation.
* Molecular engineering via chemo-enzymatic processes.
* Analysis, manipulation and application of biomolecular information systems.

Subcommittee on Green Chemistry
The aim of this Subcommittee is to develop actions devoted to the cause of green chemistry for its wider benefit to the future of chemistry and society as whole.

Subcommittee on Photochemistry
Implementation of the overall goals and objectives of IUPAC in the multidisciplinary area of photochemistry and its links to the photosciences (e. g., materials sciences, photobiology, photolithography, photography) can be accomplished only with the inputs of a broad spectrum of experts in the field, including those with ancillary interests in areas covered by all Divisions within IUPAC.

- renewable energy sources
- green chemistry
- atmospheric photochemistry
- new analytical methods in the biosciences including trace analysis of proteins, nucleic acids, and small bioregulators, both in vivo and in vitro
- industrial photochemistry
- advanced spectroscopic methods in ultra-fast time and ultra-small space resolution
- methods for identifying material fatigue and temporal changes

The Subcommittee will work in close contact with the three major Photochemical Societies of the world, i. e., the Inter-American Photochemical Society, IAPS, The European Photochemical Association , EPA, and the Japanese Photochemical Association.

Subcommittee on Structural & Mechanistic Chemistry
The Subcommittee should handle problems concerning the many aspects of structural and mechanistic organic chemistry. Specific examples include:

- Environmentally friendly chemical processes and degradative pathways of organic contaminants
- Reactions in solution, gas phase, and solid state
- Solvents for organic reactions
- Acidity and basicity of organic compounds
- Supramolecular chemistry

Subcommittee on Biotechnology
TBA

Until December 2001, the work was carried out through four commissions and subcommittees

Note 3

Organic and Biomolecular Chemistry Division (III) Current Projects

2000-012-1-300 - Single molecule spectroscopy*

2001-005-1-300 - Post-genomic chemistry*

2001-018-1-300 - Space- and time-resolved fluorescence spectroscopy and photochemistry

2001-020-1-300 - Glossary of terms and basic protocols used in photodynamic therapy

2001-036-1-300 - Glossary of terms in photocatalysis and radiation catalysis*

2002-008-1-300 - Chemical actinometry*

2002-024-1-300 - Glossary of terms used in photochemistry (3rd version)*

2002-028-1-300 - South East Asian, and neighbouring countries, Green Chemistry Network

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2002-030-1-300 - Fighting microbial resistance through development of new antimicrobial agents, directed against new specific targets

2002-064-1-300 - Green Chemistry in Latin America

2003-026-1-300 - Green chemistry in Russia

2003-043-1-300 - Green chemistry in the Arab region

2003-046-1-300 - Workshop for formulation of plans for the establishment of a "Center of Natural Products Research (CNPR)"

* Interdivisional project

OTHER INTERDIVISIONAL PROJECTS

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2001-031-1-800 - Alignment of nomenclature in areas of overlap between the preferred names for organic nomenclature and the revision of the nomenclature of inorganic chemistry

2001-043-1-800 - Preferred names in the nomenclature of organic compounds

2002-010-1-050 - Toward a core organic chemistry curriculum for Latin American universities

2003-006-1-100 - NMR chemical shifts: updated conventions

PROJECTS NEAR COMPLETION / IN PRESS

301/1/93 - Development of guidelines for the transmission of information on organic synthesis (Abbreviation guidelines and glossary of terms for protecting groups in synthesis)

Note 4 Coming Events and Sponsored Conferences 2004-2005

2004

Agriculture, 30 Nov - 3 Dec 2004 !! new dates!!
Analytical Chemistry (Euroanalysis XIII), 5-10 Sep 2004
Biodegradable Polymers and Plastics, 1-4 June 2004
Bio-interfaces, 23-26 May 2004
Biological Polyesters, 22-28 Aug 2004
Biomolecular Chemistry (ISBOC-7), 27 Jun - 1 Jul 2004
Biotechnology Symposium, 17-22 Oct 2004
Carbohydrates, 23-27 Jul 2004
Chemical Education, 3-8 Aug 2004
Chemical Sciences in Changing Times, 18-21 Jul 2004
Chemical Thermodynamics, 17-21 Aug 2004
Chemistry in Africa, 2-7 Aug 2004
Chemistry of Ge, Sn, and Pb, 27 June - 2 Jul 2004
CHEMRAWN XV - Chemistry for Water,* 21-23 June 2004
Coordination Chemistry (ICCC), 18-23 July 2004
DNA Supramolecular Assemblies, 5-6 May 2004
Fats, Oils and Oilseeds Analysis and Production,* 6-8 Dec 2004
Functional and Nano-Systems, 13-17 June 2004
Heteroatom Chemistry, 20-25 Aug 2004
Heterocyclic Chemistry, 12-15 Sep 2004
Macromolecules (MACRO 2004), 4-9 Jul 2004
Mycotoxins and Phycotoxins, 17-21 May 2004
Organic Synthesis (ICOS-15), 1-6 Aug 2004
Organometallic Chemistry, 25-30 Jul 2004
Phosphorus Chemistry, 4-9 Jul 2004
Photochemistry, 17-22 Jul 2004
Physical Organic Chemistry (ICPOC-17), 15-20 Aug 2004
Physical Chemistry of Bio-interfaces, 23-26 May 2004
pi-Electron Systems, 14-18 Jun 2004
Plasma Chemistry, 22-27 Jun 2004
Polymer Biomaterials, 11-15 Jul 2004
Polymers, 15-19 Aug 2004
Polymers and Organic Chemistry (POC '04), 18-23 Jul 2004
Soil Science, 20-23 Sep 2004
Solubility Phenomena, 25-29 Jul 2004
Trace Elements in Foods, 7-8 Oct 2004
Vanadium, Chemistry and Biological Chemistry, 3-5 Sep 2004

2005

Boron Chemistry, 11-15 Sep 2005
Carotenoids, 17-22 Jul 2005
Crop Protection Chemistry,* 14-17 Feb 2005
IUPAC 43rd General Assembly, 13-21 Aug 2005
IUPAC 40th Congress - *Innovation in Chemistry*, 14-19 Aug 2005
Heterocyclic Chemistry, 27 Feb - 2 Mar 2005
Organometallic Chemistry, 17-22 Jul 2005

Attachment 9
Re Item 10.4

IUPAC POLYMER DIVISION (IV)

Report to the ICTNS for 2003 - 2005

To reflect the continuing expansion of its work to include polymers as substances and materials as well as individual macromolecules, the Division has changed its name from Macromolecular Division to **Polymer Division**

Associate and Titular Members have defined, co-ordinating roles to play in the activities of the Division.

Two more areas of activity, namely, the **Structure and Properties of Commercial Polymers** and the **Modelling of Polymerisation Kinetics and Processes**, are now structured as **Sub-Committees**.

The **areas of activity** of the Division and the associated co-ordinators are:

Sub-Committee on the Structure and Properties of Commercial Polymers
(Co-ordinators R.S. Bailey (AM), S.C. Kim (TM))

Molecular Characterization of Polymers (Co-ordinator H. Pasch (AM))

Sub-Committee on the Modelling of Polymerisation Kinetics and Processes (Co-ordinator M. Buback (TM))

Sub-Committee on Macromolecular Terminology (Co-ordinators M. Hess (AM) (Chairman), R.G. Jones (TM) (Secretary))

Developing Polymer Materials Systems (Co-ordinators C. Ober (TM), J. Vohlídal (AM), W.J. Work (TM))

Education (Co-ordinators J.-Il Jin (TM), R.D. Sanderson (TM), J.-P. Vairon (AM))

Conference Sponsorship and Recruitment at Conferences
(Co-ordinators P. Kubisa (TM), S. Penczek (AM))

Electronic Publications and Communications
(Co-ordinators R.G. Jones (TM), W.J. Work (TM))

Division Strategy (Co-ordinators K. Horie (TM), J.-Il Jin (TM))

The Division pursues a policy of having all its reports and recommendations available on the **Division web site**.

The Division's work on the **Structure and Properties of Commercial Polymers** continues to make a significant input in this vital industrial and academic area. It represents an enormous effort and a sizeable industrial investment in terms of facilities and manpower. The work involves 76 active task group members from 17 countries, with 30 members from industry and 46 from academia and research institutes. The Division sees the work as a flagship activity. 7 papers have been published in the last two years (publications [23,24,27,29,33-35]). There are 2 continuing projects, 3 new projects, 7 projects in the final publication stage, 2 project submissions being reviewed and 5 projects under feasibility study.

Activities are now organised by the **Sub-Committee on the Structure and Properties Characterisation of Commercial Polymers** and Rob Bailey (Europe) and Sung Chul Kim (East Asia), the Co-Chairmen of the Sub-Committee, co-ordinate the projects. Since the GA in Ottawa, there have been 6 S-C meetings, 4 in Europe and 2 in East Asia.

A comprehensive summary of the Division's work on the structure and properties of commercial polymers since 1963 is now available on the Sub-Committee web site.

The projects under the **Molecular Characterisation of Polymers** involve about 36 task group members. The work is presently based on evaluating and developing size-exclusion chromatography methods and the Division is seeking to broaden the investigations to include other methods.

The co-ordination of projects in this area is now under Harald Pasch. During the last year, 1 project has been completed, resulting, so far, in 2 publications (publications [41,42]). There has also been 1 publication from an earlier project [40]. 2 new projects have been started, one of them interdivisional. There is also a terminology project associated with molecular characterization that is run by the Sub-Committee on Macromolecular Terminology and is joint with Division V. 3 new project proposals are presently under review.
The projects in the area of polymerisation are now run by the **Sub-Committee on the**

Modelling of Polymerisation Kinetics and Processes. The work is related to polymerisations of industrial relevance. The Chairman of the S-C and the person co-ordinating the projects is Michael Buback. The S-C has 28 members from 12 countries, with 2 members from industry. It has had 1 meeting since Ottawa.

There are 2 completed projects, 2 continuing projects, 2 new projects and 3 feasibility studies under consideration. In 2003-5, there have been 3 publications and 1 publication is in press [43-46]. Publications continue to receive very high numbers of citations. The S-C is also organising a conference in 2006 (see list of conferences, Section IV).

The **Sub-Committee on Macromolecular Terminology** has Michael Hess as Chairman and Dick Jones as Secretary. The Subcommittee has 29 members and about 25 additional, active task-group members. The S-C collaborates actively with Division VIII on macromolecular nomenclature projects, with the Chairman of the S-C being an AM of Division VIII.

2 projects have been completed since Ottawa, resulting in 2 publications [47,48]. The S-C has 13 current projects, with 7 nearing completion, and 4 new projects. Included in these are 7 joint projects, 1 with Division II, 1 with Division V, and 5 with Division VIII. There are also 8 feasibility studies, including a new initiative on bio-related projects. 1 meeting of the S-C (in Paris) has been held since Ottawa.

The area of activity **Developing Polymer Materials Systems** is co-ordinated by Chris Ober, Jiri Vohlidal and Bill Work. The intention is to keep the projects and activities of Division IV at the forefront of scientific and technological developments in polymer science and technology. Thus far, there have been two dedicated projects on conducting polymers under Jara Stejskal (Institute of Macromolecular Chemisty, Prague). The second project has just been completed and a Technical Report published in Pure and Applied Chemistry [49].

Notably, in the last year or so, efforts in developing polymer materials systems have led to new feasibility studies in biopolymers (characterization and terminology), field-responsive polymers (terminology), conducting polymers (characterization), and assembly and aggregation (terminology). The intention is that some of these feasibility studies will generate projects in other areas of Division IV's activities.

The Division continues to see **Education** (in Polymer Science), particularly of young people and for those from educationally hindered countries, as an important activity. About 15 active task-group members are involved and the work is co-ordinated by Jung-Il Jin, Ron Sanderson and Jean-Pierre Vairon, with contributions from Chris Ober.

During the biennium, the Division will have partially sponsored and supported 1 educational course (Prague) (leading to some of the publications [50-104]) and 1 workshop (Guimaraes, Portugal).

Increased co-operation with the CCE led to a significant participation of polymer scientists in the IUPAC Conference on Chemical Education in Istanbul in 2004. The next conference in the series will be held in Seoul in 2006 under the Chairmanship of Jung-Il Jin.

In conjunction with Professor Richard Stein (UMASS, Amherst) the Division is trying to establish a web site for polymer education.

The Division is grateful to the **Project Committee** for supporting its 2 applications for financial support for UNESCO/IUPAC conferences in South Africa (2004) and Mauritius (2005), related particularly to the IUPAC programme for developing countries. (See list of Sponsored Conferences in Section IV.) These conferences originated through Division IV's initiatives in education.

Support from the Project Committee was also received for a conference in St. Petersburg, involving participants from countries of the former Soviet Union.

Linked with its work in **Education**, the first awards from the interest on the endowment from the **Samsung General Chemicals Company of South Korea**, were made in 2004. An **IUPAC-Samsung Young-Scientist Award** was presented at the IUPAC World Polymer Congress in Paris and **Bursaries** were given to help 12 students attend the Congress. The first **IUPAC-Samsung Education Award** (2005) will be presented shortly.

A successful **Symposium on Polymer Education** was held as part of the 2004 IUPAC World Polymer Congress in Paris. This was a new venture that the Division hopes to continue at future WPCs.

At the IUPAC-sponsored Polymer Networks 2004 Meeting, in Bethesda, USA, the first **IUPAC Poster Prizes** were awarded for posters from young scientists.

As with Education, the Division continues to place particular emphasis on **Conference Sponsorship**. Largely through the efforts of the Co-ordinators for Conference Sponsorship, Przemyslaw Kubisa and Stan Penczek, and other Division Members, a total of **31 IUPAC-sponsored polymer conferences** have been and will be held in 2003-5, maintaining the high level of conference sponsorship from the previous biennium.

16 conference volumes of Macromolecular Symposia have been published in 2003-5. See publications [1-16]. In fact, more than half of the issues of Macromolecular Symposia are devoted to IUPAC-sponsored conferences, representing a significant income to IUPAC, some of which is now used to supplement the budget of Division IV.

The IUPAC World Polymer Congress of 2004, organised through the Division, was held in Paris. It is generally recognised that the biennial IUPAC World Polymer Congress, is the main event in the international polymer conference calendar. This year's Congress, with about 2500 participants, was the largest ever.

The future WPCs presently planned are 2006 Rio de Janeiro, 2008 Taipei and 2010 Glasgow.

Regarding **Recruitment at Conferences**, the Division Brochure is distributed at all IUPAC-sponsored conferences. In addition, the Powerpoint presentations issued by the Secretariat have been augmented to emphasise Macromolecular Division activities. Electronic versions of the brochure and the presentations are given to all conference organisers and IUPAC representatives.

The consideration of **Polymer World and Division Strategies**, started during the last biennium, has continued. As recognised in the change of name of the Division, polymer science and technology is no longer based primarily on the macromolecule but it is central to many modern functional and structural materials. The Division's aims and activities need to change continually and to grow in order to reflect the new emphasis and increasing diversity. The work is co-ordinated by Kazuyuki Horie and Jung-Il Jin.

5 publications [7,17-20] have resulted from the successful **Strategic Polymer Conference** in Kyoto in December 2002 on the **Mission and Challenges of Polymer Science and Technology**. A second strategic conference is planned for New York in 2007 under the Co-Chairmanship of Kalle Levon and Chris Ober.

Division IV has a **strategic project** on future developments in polymer science under the direction of Mitsuo Sawamoto. Work on the project helps to prepare, together with the Society of Polymer Science, Japan, a continually up-dated booklet giving details of all World Polymer Organisations and their activities.

During the 2004 World Polymer Congress, a **Symposium on International Collaboration in Polymer Science and Technology** was held for the first time as part of a WPC. The symposium involved representatives from the polymer organisations of many countries and world regions and subsumed the biennial Polymer Summit Meeting in its proceedings. The Division hopes to maintain this type of symposium at future WPCs.

The basic budget for the biennium has not been sufficient to fund all the division's project activities.

Division IV is grateful for the additional financial support it has received from the **Project Committee** and the **Division Reserve**. The division also has collaborative projects with Divisions V, VI, VIII and the CCE.

Future Plans and Structure

The Division intends to maintain its existing project areas, Structure-Property Characterization, Molecular Characterization, Polymerization Modelling, Terminology and Nomenclature, Developing Polymer Materials Systems and Education and also its efforts in Conference Sponsorship.

It will seek to expand its profiles in Molecular Characterization and Developing Polymer Materials Systems and maintain its high level of activity and throughput in all project areas and in Conference Sponsorship.

The Division will seek to play a strategic role in defining the important areas of world polymer research through its strategic study and conferences.

In order to give continuity to the Division's structure and range of activities, the elections to the Division Committee in 2005 have been to positions designated for particular responsibilities, essentially those listed at the beginning of this report.

Attachment 10
Re Item 10.5

Report of the IUPAC Analytical Chemistry Division (V)

August 2003 – August 2005

Kip Powell, President

I. Executive Summary

The Division has made significant moves to build partnerships with
chemists in "developing countries",
organizations that have field experience in developing countries (IAEA, UNIDO, IOCD),
other unions and expert bodies (IUPAP, BIPM, IUGS).

The Division has arranged a series of articles for *Chemistry International* on the topic of *"Emerging needs of developing countries".* This series should run for 8-10 issues and will carry contributions from several Divisions. A further series is envisaged.

The Division has started a significant number of inter-Divisional projects. These link us with Divisions I, III, IV, VI and VII, and with COCI.

To ensure attention to critical areas it has identified a limited number of "priorities" for the biennium. It has focused its energy on these.

To cultivate a spirit of "collective responsibility" it has formed seven Teams, each with responsibility for one priority area. All NR, AM and TM are assigned to one or two teams. The Team structure should facilitate continuity of effort into the next biennium.

Communication within the Division and with other officers of the union is maintained through the electronic newsletter *"Teamwork".*

The Division is working on the maintenance and updating of two key IUPAC publications, *The Compendium of Analytical Nomenclature* (Orange Book) and the *IUPAC Stability Constant Database* (SCDB).

To facilitate the development of new projects the Division involved external experts in a mini-symposium on "*Metrological traceability*" held at the IAEA in conjunction with its even-year meeting.

II. Report on Division activities in relation to IUPAC goals

2.1. *IUPAC will provide leadership as a worldwide scientific organisation that objectively addresses global issues involving the chemical sciences.*

The Division has 'Core activities' that are an on-going responsibility. But it also identifies a set of priorities that are based on perceived emerging needs of the scientific community. These 'Emerging issues' are more time-dependent and are likely to change to some degree from one biennium to the next:

***Core Activities**:*

Communication

Project initiation and management in the areas of:

Quality Assurance
Terminology – Orange Book: maintaining and updating
Critical evaluation of data

Emerging issues in analytical chemistry:

in bioanalytical chemistry
in process chemistry and nano-chemistry
in developing countries and scientific communities.

Teams of 4-6 members (TM + AM + NR) are formed for each priority area. Each Team has a collective responsibility and is encouraged to:

Determine the scope of its responsibility and activities;
Develop a strategy for effective communication between and by its members.
Identify activities that advance the goals of IUPAC in its designated area.
Achieve at least one significant output each year (*e.g*. letters to Editors; an IUPAC or ACD presentation at a Conference; an article for *CI*; a Project Proposal; etc.)
Accept responsibility for leading Division activities in its designated area
Facilitate a 'roll-over' of its activities at the end of the current biennium.

Communication.
The Division maintains communication with all its members, and officers of other Divisions and Operational committees, through its newsletter *Teamwork*.

The Division interacts with all Task Groups on a half-yearly basis (to be changed to eight-monthly) via a Project reporting system. The reports are read by all Division members and are reviewed at Division meetings. They provide an 'early warning system' for any projects that are struggling, alert the Division to the need for reviewers and allow re-assessment of Dissemination plans as the projects near completion. As from November 2004 these reports are appended to the respective Project pages on the IUPAC website, so that Project progress is in the public domain.

Global issues.
One global issue being addressed is the measurement of pH, through the project: *Comparable pH measurements by metrological traceability. Part I: Water quality monitoring and assessment; Part II: Clinical and biochemical matrices.* This project sees a continuation of work by the "pH task group" [Measurement of pH. Definition, Standards and Procedures] and it has the financial and professional backing of three Divisions and COCI.

Another global issue addressed is the concept of *'fair trade'*. Fair Trade can only arise between nations when all have adequate and *quality-assured laboratories* and their methodology meets the current requirements for *metrological traceability*. These issues are particularly relevant to the less developed nations. These concepts were the basis of:

(a) A successful joint project proposal with IOCD which includes several Division V members, titled: "*Standardisation of analytical approaches and analytical capacity building in Africa*". This project involves a melding of IUPAC technical expertise with IOCD appreciation of geopolitical issues in developing countries.

(b) Division V support for the WPQA in preparation of an ICSU proposal on "*Measurement traceability – a fair basis for trade'*. This application for funds was not successful but the process of preparing the proposal generated very positive interactions with project partners UNIDO and IUPAP (including their participation in a WPQA/Division V workshop).

Symposia and Workshops.
The Division attempts to capture external expertise to introduce and scope emerging issues or opportunities in analytical chemistry. This is assisted through mini-symposia held in conjunction with the Division even-year meeting and the GA.

From the mini-symposium on "***New Challenges for Analytical Chemists in Genomics, Proteomics, and Genetically Modified Organisms***" held during the Ottawa GA, two new projects were identified. One has been funded in this biennium ("*Standard definition of terms related to mass spectrometry*") while the other on "*Terminology related to analytical chemistry of metal forms in biological systems: metallomics*" has been thoroughly scoped and a Task Group identified.

At the even-year meeting in Vienna 2004 a mini-symposium on "*Metrological traceability*" was held jointly with IAEA staff and the WPQA. It attracted speakers from IUPAP, UNIDO, BIPM, IAEA and WPQA. The meeting identified several areas in which IUPAC expertise might be applied. We now try to identify possible 'concrete' outcomes from that meeting - IUPAC projects that could be crafted around the ideas and concerns that were shared. IUPAC will benefit through any projects that link it with agencies that are working much closer to the geopolitical coal-face.

2.2. IUPAC will facilitate advancement of research in the chemical sciences through the tools that it provides for international standardisation and scientific discussion

Division V actively pursues these goals through its program of critical evaluations of data, the establishment of guidelines for Quality Assurance in chemical methods and associated sampling, and by the updating of analytical nomenclature and making it readily available via the web:

(a) ***The Orange Book***. This is now on-line at (http://www.iupac.org/publications/analytical_compendium/)

The route for updating terminology in the OB is via formal publication in *PAC*. Examples of issues being currently addressed through projects are: *Glossary of Terms related to Solubility; Revision of terminology in separation science; Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanlytical chemistry; Internationally agreed terminology for observations in scientific communications; Standard definitions of terms relating to mass spectrometry.*

The text will be progressively converted to ICTNS-accepted format; it will also be aligned with the Gold book version, so that there is only one version of terminology within the IUPAC database.

(b) ***The IUPAC Stability Constants Database*** (SCDB) is the most comprehensive compilation of stability constants available, covering the years 1877 to 2002. It is the primary source of data for the Critical evaluations of Stability Constants that are published on a regular basis by Division V. It is a major research tool for those involved in equilibrium modelling of environmental, biological and industrial systems.

Division V has in place a Project to continue the evaluation, collection and entry of data through to 2008. To minimise risk the data collection team has been expanded from one site to now involve experts in four countries.

The future of SCDB was the subject of a Division V presentation to the Bureau meeting in 2004. All aspects of the management of the database – program development, data conflation, advertising, marketing – have for the last 16 years been undertaken on behalf of IUPAC by the developers of the current database, Academic Software. This company has now signalled that it wishes to transfer the responsibility for management and maintenance of SCDB to IUPAC within about 3 years.

Division V has formed a consultative team (Folke Ingman, David Moore and Kip Powell) to work with Academic Software and the Executive to effect a successful transition to management by IUPAC or an alternative external systems manager. The Bureau meeting identified the future management of commercial databases as a generic issue that now needs to be addressed by IUPAC. It is possible that appropriate secretariat resources may need to be assigned in future.

(c) ***The Working Party on Quality Assurance*** continues to produce publications that are of value to chemists in analytical laboratories; e.g. *Revision of the IUPAC/ISO/AOAC protocol for proficiency testing; Harmonised guidelines for single-laboratory validation of methods of analysis; and Terminology for soil sampling*. The WPQA will make a major presentation at the GA on *"Metrological Traceability of Results in Chemical Measurement."*

(d) ***The Solubility and Solution Equilibrium Data sub-committee (SSED)*** has a very active program of projects that embrace the critical evaluation of solubility data related to (a) mobility of metals in the environment, (b) to industrial processes, (c) human health. The outputs appear as papers in the Journal of Physical and Chemical Reference Data or as book volumes and are thence transferred to the NIST-IUPAC Solubility Database: http://srdata.nist.gov/solubility/. A significant new project is a 25-Chapter book volume on "*Solubility for Industry*". Another project is concerned with *Chemical speciation of environmentally significant heavy metals with inorganic ligands.*

2.3. IUPAC will assist chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement of the quality of life.

Chemistry-related industry is served by the active program of critical evaluations of solubility data and of solution equilibrium data, and by the continuance of data evaluation and compilation for the IUPAC Stability Constant Database. The current projects on pH

(*Comparable pH measurements by metrological traceability.)* and metrological traceability *(Metrological Traceability of Results in Chemical Measurement*) are highly relevant to industry. The SSED were joint organisers of the 11th International Symposium on solubility phenomena (Aviero, 2004) at which there was significant emphasis on industrial issues and involvement of industrial chemists (*PAC*, 77(3), 2005). A significant new project is a 25-Chapter book volume on "Solubility for Industry".

2.4. IUPAC will foster communication among individual chemists and scientific organisations, with special emphasis on the needs of chemists in developing nations.

Analytical Chemistry in Developing countries

The Division seeks to expand activities in this area. "Emerging needs in developing countries" is one of its priority areas and is the responsibility of one Team. The Division is fortunate in having several members with established professional links with the African continent (Jan-Åke Jönsson, Walter Lund and Roger Smith). Nelson Torto (Botswana) has joined the ACD as a Provisional Member representing the IUPAC Associate Organisation, SEANAC. The Division is significantly involved in the project with IOCD: "*Standardisation of analytical approaches and analytical capacity building in Africa*".

One potential difficulty in establishing links with developing countries is that few are members of IUPAC. Is there any effective way that IUPAC can generate an outreach though chemical societies in counties which are currently not NAO?

To increase awareness of the needs of developing countries the Division has arranged a series of 8-10 articles for *Chemistry International.* These articles on *Emergingissues in developing countries* commenced in the March 2005 issue. Division V is well-supported by other Divisions in this venture.

Building bridges with other organisations.

The SSED works actively with NIST in the preparation of critical evaluations for publication in the NIST-IUPAC Solubility Data Series. The joint Division V - WPQA meeting in Vienna showed that many new dynamics can be brought to our activities by discussion and collaboration with other organizations, in this case IUPAP, IAEA, UNIDO.

Through the WPQA the Division is represented on the Coordinating Committee on Chemistry and Materials, ISO-Committee on Reference Materials, the International Committee on Weights and Measures, the Consultative Committee for Amount of Substance (BIPM), EURACHEM and CITAC.

Better Communication.

Dissemination of project outcomes is a crucial issue for improving the impact of our work in the chemistry community. This is overseen by the "Communications" team. The ACD website has been made more intuitive. Working with Dr. Meyers we are attempting to make it better attuned to the needs of those who are not familiar with the IUPAC system and processes. Improved lines of communication between TG chairs and the Division have been facilitated by the establishment of a 6-monthly Project reporting system in which the TGC responds to questions re progress, milestones, difficulties, and opportunities for further work etc. These progress reports are now filed on the web on the respective project pages.

The Division has been pro-active in recommendations for improved IUPAC representation at conferences. It considers that there is scope for enhanced involvement

of IUPAC representatives at IUPAC-sponsored conferences. This could be aided if conference organisers were required to discuss the nomination of an IUPAC representative with the relevant Division ahead of submitting the AIS. It is all too easy for Conference programs to be 'finalised' ahead of representative appointment, or without reference to IUPAC requirements.

2.5. IUPAC will utilise its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.

The Division was represented in the Task Group for the project: *Chemistry's contributions to humanity.* It actively participates in the General Assembly Young Observers scheme. The question of career development for young chemists (in developing countries) will be raised in one of the proposed articles for *CI.*

2.6. IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender and age.

Division V has in place a strategy, which is communicated to the Nominations' Committee, to ensure the widest possible geographic representation. The Division actively sought participation of Nelson Torto as a Provisional Member representing the ANO, SEANAC. Within its own structures, the Division works to ensure **active** involvement of all AM, TM and NR.

III. Challenges and Solutions

The principal challenges to the ACD are typical of many IUPAC Divisions:
The breadth of its portfolio.
The generation of members' collective responsibility for
the goals of the Division
the needs of countries not represented
the long-range goals of IUPAC
Maintaining momentum through the biennium and with the change of biennia.

Strategy adopted by the ACD to address these challenges:
Identification of a manageable number of priorities for the biennium (see Section 3.1).
Formation of Teams, each with collective responsibility for one priority area.
Effort focused on the needs of developing countries and on links with other agencies (Section 3.4).
Use of mini-symposia to bring in external expertise.
Maintaining active communication between members, e.g. through the newsletter, *Teamwork*.

Roger is updating this section

4. Publications since August 2003:

CURRENT PROJECTS

* Interdivisional project

1999-044-2-500 - Terminology for the description of peak asymmetry in chromatography
1999-050-1-500 - Chemical speciation of environmentally significant heavy metals and inorganic ligands
2000-003-1-500 - Ionic strength corrections for stability constants
2000-004-2-500 - IUPAC stability constants database - completion of data collection up to 2000+
2001-041-2-500 - Recommendation on the use of countercurrent chromatography in analytical chemistry
2001-063-1-500 - Revision of terminology of separation science
2001-072-1-500 - Low activation materials for fusion technology: State and prospects
2001-073-1-500 - Determination of alpha-emitting radionuclides in diet: Review and evaluation of analytical methods for artificial and natural alpha-emitting nuclides in food and human tissue
2002-002-2-500 - Recent advances in electroanalytical techniques: characterization, classification and terminology
2002-003-2-500 - Performance evaluation criteria for preparation and measurement of macro and microfabricated ion-selective electrodes
2002-009-2-500 - Optical spectrochemical analysis using waveguides and optical fibers; Series on Nomenclature, Symbols, and Units in Spectrochemical Analysis
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
2003-011-3-600 - A critical compendium of pesticide physical chemistry data*
2003-015-2-500 - Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry
2003-037-1-500 - Optical biosensors and bioprobes; Series on Nomenclature, Symbols, and Units in Spectrochemical Analysis
2003-056-2-500 - Standard definitions of terms relating to mass spectrometry*
2003-060-2-400 - Terminology on separation of macromolecules*
2004-017-1-500 - Standardization of analytical approaches and analytical capacity-building in Africa*
2004-021-1-300 - Reference methods, standards and applications of photoluminesence*
2004-023-1-70 - Internationally agreed terminology for observations in scientific communications*

INTERDIVISIONAL WORKING PARTY ON HARMONIZATION OF QUALITY ASSURANCE

2000-033-1-500 - Assessment of uncertainty associated with soil sampling in agricultural, semi-natural, urban and contaminated environments (SOILSAMP)
2001-010-3-500 - Metrological traceability of measurement results in chemistry
2003-004-1-500 - Interdisciplinary harmonised approach to metrological traceability of chemical measurement results

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

2002-025-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Inorganic actinide compounds
2002-031-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates
2002-032-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates
2002-033-1-500 - Solubility data related to oceanic salt systems. Part I - Binary systems containing sodium, potassium, and ammonium sulfate
2002-034-1-500 - Solubility data related to oceanic salt systems. Part II - magnesium chloride-water and calcium chloride-water and their mixtures
2002-035-1-500 - Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis
2002-036-1-500 - Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates

2002-037-1-500 - Solubility data of compounds relevant to human health. Solubility of haloganated aromatic hydrocarbons
2002-038-1-500 - Solubility data of compounds relevant to human health. Antibiotics: peptide antibiotics and macrocyclic lactone antibiotics
2002-042-1-500 - Solubility data related to industrial processes. Lead sulfate
2002-043-1-500 - Solubility data related to industrial processes. Carbon dioxide and the lower alkanes at pressures above 2 bar: methane to butane
2002-044-1-500 - Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions
2002-045-1-500 - Solubility data related to industrial processes. Solids and liquids in supercritical carbon dioxide
2002-050-1-500 - Solubility data related to industrial processes. Acetonitrile: ternary and other multicomponent systems
2003-018-1-500 - Mutual solubility of hydrocarbons and water (update of SDS Vol 37 & 38)

PROJECTS NEAR COMPLETION / IN PRESS

1999-050-1-500 - Chemical speciation of environmentally significant heavy metals and inorganic ligands. Part I Mercury.
2001-052-1-500 - Solubility of volatile and gaseous fluorides in all solvents
2001-085-1-500 - IA and IIA azoles, cyanates, cyanides and thiocyanates
2003-018-1-500 - Mutual solubility of hydrocarbons and water (Part 1)

UNDER REVIEW BY ICTNS OR AUTHORS

550/64/97 - Non-selective sensors arrays ("Electronic Nose", "Electronic Tongue") chemical analysis: classification and characterization
2000-033-1-500 Terminology in soil sampling (V)
http://www.iupac.org/reports/provisional/abstract03/fajgelj_301103.html
2001-055-1-500 - Critical evaluation of stability constants of metal complexes of complexones for biomedical and environmental applications
2001-075-1-500 - Compilation of k0 and related data for NAA in the form of electronic database
2001-038-2-500 - Recommendations for NMR measurements of high pK values and equilibrium constants in strongly basic solutions
2001-009-1-500 - Revision in the international harmonised protocol for the proficiency testing of (chemical) analytical laboratories

PUBLISHED REPORTS (2003 - 2004)

Alkali and Alkaline Earth Metal Pseudohalides *J. Phys. Chem. Ref. Data*, **2004**(1), *33,1-176.*
Ionic strength corrections for stability constants http://www.iupac.org/projects/2000/2000-003-1-500.html
Chemical speciation of Hg(II) with environmental inorganic ligands. *Australian J.Chem.,***57**, 1-8 (2004)
Guidelines for calibration in analytical chemistry. Part 2: Multicomponent calibration (IUPAC Technical Report)
Pure Appl. Chem. **76**(6), 1215-1225 (2004)
id464146 Critical evaluation of the state of the art of the analysis of light elements in thin films demonstrated using the examples of SiO_xN_y and AlO_xN_y films (IUPAC Technical Report)
Pure Appl. Chem. **76**(6), 1161-1213 (2004)
Piezoelectric chemical sensors (IUPAC Technical Report)
Pure Appl. Chem. **76**(6), 1139-1160 (2004)
Electrochemical detection in liquid flow analytical techniques: Characterization and classification (IUPAC Technical Report)
Pure Appl. Chem. **76**(6), 1119-1138 (2004)

Terminology for analytical capillary electromigration techniques (IUPAC Recommendations 2003)
Pure Appl. Chem. **76**(2), 443-451 (2004)
Determination of trace elements bound to soil and sediment fractions (IUPAC Technical Report)
Pure Appl. Chem. **76**(2), 415-442 (2004)
Critical assessment: Use of supersonic jet spectrometry for complex mixture analysis (IUPAC Technical Report)
Pure Appl. Chem. **75**(7), 975-998 (2003)
Critical review of analytical applications of Mössbauer spectroscopy illustrated by mineralogical and geological examples (IUPAC Technical Report)
Pure Appl. Chem. **75**(6), 801-858 (2003)
Critical evaluation of stability constants for alpha-hydroxycarboxylic acid complexes with protons and metal ions and the accompanying enthalpy changes. Part II. Aliphatic 2-hydroxycarboxylic acids (IUPAC Technical Report) (V.6)
Pure Appl. Chem. **75**(4), 495-540 (2003)
Critical evaluation of the chemical properties of the transactinide elements (IUPAC Technical Report) (V.7)
Pure Appl. Chem. **75**(1), 103-108 (2003)
Critical evaluation of stability constants and thermodynamic functions of metal complexes of crown ethers (IUPAC Technical Report) (V.6)
Pure Appl. Chem. **75**(1), 71-102 (2003)

Division representation at Conferences

Analytical Forum 2004, July 2004, Warsaw, Poland.

11th International Symposium on Solubility Phenomena, Aviero, Portugal; July 2004.

8th International Conference on Nuclear Analytical Methods in the Life Sciences - NAMLS8. Rio de Janeiro, Brazil; April 2005

Analytical Chemistry and Chemical Analysis, (AC&CA-05). Kiev, Ukraine; September 2005.

IUPAC, ITCNS
Division of Chemistry and the Environment (DCE) REPORT
August 2005

1. General

1.1 DCE Objectives and Strategy

The Division of Chemistry and the Environment (DCE) aims to provide timely authoritative reviews on the behavior of chemical compounds in food and the environment compartment: air, soil and water. The DCE undertakes both fundamental and applied evaluations, aiming to contribute to solving environmental problems and enhancing the quality of food on a global scale. Projects are customer oriented dealing with current problems of the environmental chemistry and food safety and communicating state of the art assessments through publications, workshops and regional and international conferences.

Cooperation with other International Organizations

The Division aims for IUPAC Interdivisional Cooperation and with other scientific bodies, international organizations including: ICSU/SCOPE, IOCD, WHO, FAO, the EU Commission OECD (Green Chemistry), IFCS and the industry via ICCA. The aim is for a case-by-case interaction, expanded and intensified as needed.

1.2 DCE Organization and Menbership

The Division Committee is currently comprised of 10 TM's, 7 AM's, and 6 NR's, as well as a range of interested scientists without official titles.. The work of the Division Committee is channelled through four sub-committees, namely:

Food Chemistry (Chair: Dr. Patrick Dysseler)
Biophysico-Chemical Processes in Environmental Systems (Chair: Prof. Nicola Senesi)
Chemistry of Environmental Compartments (Chair: Dr. Yehuda Shevah)
Crop Protection Chemistry (Dr. Ken Racke)

2. Ongoing Programme and Achievements

In the reporting period 24 projects were handled b the Division, of which eight were completed and 16 projects are ongoing. Of the ongoing projects, 3 are related to Biophysico-Chemical Processes. Five are related to Crop Protection Chemistry, seven to Chemistry of Environmental Compartments and two are related to Food Chemistry. Ten different papers were also published in 2004/5. Short description and status of the various project is given in the following.

2.1 Global Issues

Impact of transgenic crops on the use of agrochemicals and the environment (2001-24-2-600). This project was approved in January 2003 (leaders Gijs Kleter and Harry Kuiper). The aims are to portray IUPAC views on the environmental consequences of the transgenic crops, providing sound scientific, regulatory, political and public perception issues surrounding the controversial use of genetically modified crops.

Pest management for small-area crops: a cooperative global approach (2001-039-1-600)

Remediation Technologies for Removal of Arsenic from Water and Wastewater (2003-017-2-600). This project was approved in 2004 (leaders H. Garelick and Y. Shevah). The impetus for this project, in collaboration with WHO and other IUPAC initiatives, is on the toxicity of water supplies through natural arsenic contamination affecting the health of millions of residents. The project address the industrial and home made technologies and evaluate the suitability, effectiveness and health safety of current technologies used for routine treatment of large water works and water points for isolated homestead.

Air pollution models in environmental management and assessment (2003-058-1-600). The aim of the project is to provide researchers and environmental managers some guidance in selecting the right models

for a given purpose and ensuring that the models work in a proper way using appropriate input data. The project has been accepted for publication as a book by Kluwer Press. Author/Editors: Ole Hertel, Jørgen Brandt and Jes Fenger

Comparable pH measurements by metrological traceability (2004-05-1-600) Interdivisional project.

Development of simplified methods and tools for ecological risk assessment of pesticides (2004-011-1-600) A joint efforts of Government, industry, academic modellers and risk assessment experts.

2.2 Tools and Standardization.

Glossary of Atmospheric Chemistry (2003-030-1-600). *A.* Glossary of atmospheric chemistry, aiming to update IUPAC recommended definitions, is coordinated by T. Cvitas, classified into: 1. physical quantities and units, 2.measurements, analytical methods and abatement strategies, 3. chemical and physical constituents of the processes in the atmosphere, 4. theoretical aspects and 5. instrumentation in atmospheric chemistry. The work is progressing. Both printed and internet-based versions are envisioned.

Glossary of Pesticide Chemistry (2004-002-1-600). The project aims to provide authoritative updates of existing IUPAC recommended definitions. Collaboration with WHO-IPCS and OECD is being pursued to enable the broadest possible acceptance of the revised IUPAC recommendations. Both printed and internet-based versions are envisioned.

Terminology and Measurement Techniques of Starch Components (2004-022-3-400). This project will provide internationally needed guidance on the terminology for this complex carbohydrate class. Starches present a number of difficult issues relating to both terminology and methods for determination which are of importance to nutrition, food quality and international trade.

A critical compendium of pesticide physical chemical data (2003-011-1-600). An Interdivisional project coordinated by Wauchope.

Validation of ICP method for trace elements in fats (2002-013-1-600). A joint effort of IUPAC, AOCS, AOAC, EU Ref. Lab and others, coordinated by Cantrill.

Use of reference soils for testing fate & effects of chemicals (2001-026-1-600). The first draft is due beginning of next year and a working group meeting, end of 2005.

Global availability of information on pesticides (2001-022-1-600). A joint effort of IUPAC, FAO/IAEA and others, coordinated by Racke.

2.3 Chemistry Needs in Developing Countries.

Regional Workshops on Fats, Oils, Oilseeds Analysis and Production (2002-011-2-600). The first such IUPAC workshop on this topic occurred in Brazil during 2000 (1999-042-1-600). The second workshop, in this series, was held in Tunisia during December 2004

Regional Pesticide Chemistry Workshops (2003-013-1-600). During the past 15 years DCE has sponsored a series of regional workshops focused on broadening the adoption of harmonized, international approaches to pesticide research and regulation in developing countries. Following sessions in China, Thailand, Taiwan, Brazil and Korea, the *Workshop on Crop Protection Chemistry in Latin America* was held in San Jose during February 2005.

Development of Simplified Methods for Ecological Risk Assessment of Pesticides (2004-011-1-600). This project addresses the lack of capacity and risk assessment ability in many of the developing countries. A project team consisting of leading government, industry, and academic modellers and risk assessment experts has been assembled to review the situation and propose practical solutions.

Standardization of Analytical Approaches and Analytical Capacity-Building in Africa (2004-017-1-500). This is a cooperative project with the IUPAC Analytical Chemistry Division, the International Organization for Chemical Sciences in Development (IOCD), and the Association of Official Analytical Chemists International (AOAC). Uganda and Kenya are the initial focus, with Nigeria, South Africa, and Mozambique of future interest in conjunction with an ongoing World Bank project. The project aims to build regional analytical laboratory capabilities in relation to monitoring and enforcement of international trade standards. Key activities will involve lectureships, local workshops, visiting scientist apprenticeships, and laboratory equipment procurement initiatives.

2.4 Book Series

Wiley-IUPAC book series *"Analytical and Physical- Chemistry of Environmental Systems"* Professor Nicola Sensi provides the impetus at the Divisional level for the continuing publication of this series of multi-chapter critical-reviews (Series Editors, J. Buffle and H. Van Leeuwen). No. 9 in the series "*Physicochemical Kinetics and Transport at Chemical-Biological Membranes*" was published in 2004. Two current projects are producing volumes No. 10 and 11: "*Biophysico-Chemistry of Fractal Structures and Processes in Environmental Systems*" (2003-014-2-600) and "*Environmental Colloids: Behaviour, Structure & Characterisation*" (2004-015-1-600). A related project is producing another book to be published by Wiley but not in the above series: "Biophysico-chemical process of heavy metals and metalloids in soil environments" (2004-003-2-600).

2.5 Symposiums

XI International IUPAC Symposium on Mycotoxins and Phycotoxins, Maryland, USA, May 2004. This symposium, strongly supported by IUPAC and DCE, was the latest in a long-standing series on the chemistry aspects of biotoxins. The next symposium is planned for Istanbul, Turkey in 2007. This symposium has become the forum for exchange of research results and methodologies related to these important naturally occurring toxins.

International Workshop "Fats, Oils and Oilseeds Analysis and Production" Tunis, Tunisia, December 2004 (2002-011-2-600). Organized by IUPAC and AOCS in cooperation with the Tunisian Office National de l'Huile (ONH), the American Soybean Association (ASA), and the International Olive Oil Council (IOOC). This workshop continued a series supported by IUPAC, the last in Brazil in 2000. The analytical sessions provided support for the oil refining/oil processing sessions, with an emphasis on the needs of the host and other developing countries.

International Workshop "Crop protection chemistry in Latin America", San Jose, Costa Rica, February 2005 (2003-013-1-600) Organized by IUPAC in cooperation with the Costa Rica Ministry of Agriculture, the University of Costa Rica, and the agrochemical industry association Crop Life Latin America. This workshop continued a series supported by IUPAC-DCE, the last in Korea in 2003. Major topics: pesticide environmental fate and impacts, analysis and monitoring of residues, risk assessment, and regulation.

"Environmental Chemistry & Green Chemistry" - Symposium at 40th IUPAC Chemistry Congress, Beijing, August 2005. *A special session* ***is organized by DCE*** along with Professor Xiaoba Xu (China).

3. PUBLICATIONS (January-2004 to June-2005)

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Carazo, E.; Racke, K.D. (eds.) *Proceedings of the IUPAC-UCR-MAG Internat Workshop on Crop Protection Chemistry in Latin America.* University of Costa Rica, San Jose, (**2005**) 217 pages.

Hamilton, D.J.; Ambrus, A.; Dieterle, R.; Felsot, A.; Harris, C.; Petersen, P.; Racke, K.; Wong, S., Gonzalez, R.; Tanaka, K. ; Earl, M.; Roberts, G.; Bhula, R. "Pesticide Residues in Food: Acute Dietary Exposure." *Pest Manag. Sci.* (**2004**), 60:311-339.

Kleter, G.A., R. Bhula, K. Bodnaruk, E. Carazo, A.S. Felsot, C.A. Harris, A. Katayama, H.A. Kuiper, K. Racke, B. Rubin, Y. Shevah, G.R. Stephenson, K. Tanaka, J. Unsworth, S.S. Wong. The effect of the cultivation of genetically modified crops on the use of pesticides and the impact thereof on the environment **(2005).** A paper presented at the Costa Rica workshop, February 2005.

Koester, W.; Van Leeuwen, H. (eds.) *Physicochemical Kinetics and Transport at Chemical-Biological Membranes*, Series on Analytical and Physical Chemistry of Environmental Systems, Vol. 9, John Wiley & Sons, New York (**2004**) 576 pages

Racke, K.D. "Pesticide Science - Harmonization of Data Requirements and Evaluation. Report on Workshop " *Chem. Int.* (**2004**) 26:18-20.

Shevah Yehuda. Wastewater Treatment and Reuse for Irrigation. In Encyclopedia of Life Support Systems (EOLSS), Developed under the auspices of the UNESCO, Eolss Publishers, Oxford, UK, **(2004),** [http://www.eolss.net].

Slanina, S.; Zhang, Y. "Aerosols: Connection between Regional Climate Change and Air Quality." *Pure Appl. Chem.* (**2004**) 76:1241-1253.

Zhang, Y.; Zhu, X.; Slanina, S.; Shao, M.; Zeng, L.; Hu, M.; Bergin, M.; Salmon, L. "Aerosol Pollution in Some Chinese Cities." *Pure Appl. Chem.* (**2004**) 76:1227-1239.

Attachment 12
Re Item 10.7

Biannual report to the ITCNS by Urban Forsum (Division VII) 2005-07-22 (appended are: draft EN1614 document and Div. VII meeting protocol Leiden, the Netherlands March 2005)

Meetings with focus on terminology and nomenclature conducted during the time covered by the report. (minutes are available at the IUPAC web site)

C-NPU committee (subcommittee, IUPAC)
Lund Sweden 2003-10-25 - 27
Project, Global use of the C-NPU concept system for properties in toxicology:
Ottawa Canada 2003-08-10 - 12
Meeting with the MEQUALAN project
(U. Forsum on behalf ot hte C-NPU)
Budapest Hungary 2003-11-07 – 08
C-NPU committee (subcommittee, IUPAC)
Sousse Tunisia 2004-05-14 – 17
C-NPU committee (subcommittee, IUPAC)
Leiden the Netherlands 2005-03-06 -08.
Subcommittee on Medicinal Chemistry and Drug Development
Copenhagen, Denmark 2004-08-14
Subcommittee on Medicinal Chemistry and Drug Development
Anaheim, CA, USA 2004-03-27
Subcommittee on Medicinal Chemistry and Drug Development
London, UK 2003-12-12

C-NPU generic database
The C-NPU generic database is, as of 2002-04-25, 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. A major up-grade was done November 2004 and new properties in clinical chemistry, transfusion medicine and clinical molecular biology were added.
The costs for running the server, updating the server and updating and maintaining the content is still shared between funds available from the University of Linköping, EQUALIS AB and the National Board of Health, Denmark. A more permanent, truly international solution must be sought.

Metrology, concepts and international standards
The European prestandard ENV 1614 that defines the concept system used by the C-NPU is up for acceptance as a standard. Parallel work on a new edition of the VIM (now anticipated to be finished during 2005) will influence the definitions of some concepts in the ENV 1614. The C-NPU has in conjunction with WG2 of the CEN TC 251 decided to revise the ENV 1614. A revised draft EN 1614 has been prepared by Urban Forsum and Daniel Karlsson and is currently circulated (CEN, ISO) (the draft appended to the report).

The modifier “arbitrary” is used in the C-NPU coding scheme for properties The standing of this modifier is unclear and the C-NPU is still actively seeking a metrologically sound solution.
The C-NPU has decided to add NPU codes for mass-based kinds-of-quantities to the coding scheme. Accomplished early 2004.

Ongoing and finalized projects during fall 2003-summer 2005
1. Properties and units for function examinations (IUPAC: 2001-067-1-700). Still not finalized.
2. Properties and units in Medical Molecular Biology (IUPAC: 2001-068-1-700) Finalized 2004, published in Pure and Applied Chemistry (introductory text) and (list of properties and code values) on the net (the C-NPU server) 2004.
3. Properties and units for urinary calculi (IUPAC: 2001-070-1-700) Still not finalized.
4. Concepts and structure for requests in clinical laboratories (IUPAC: 2001-058-1-700) finalized 2005.
5. Global use of the C-NPU concept system for properties in toxicology (IUPAC: 2001-066-1-700) under review and revision for publication in Pure and Applied Chemistry.
6. Internationally agreed terminology for observations in scientific communication. (IUPAC 2004-023-1-700) Started 2005-01-01.
7. Translation of C-NPU database elements and properties into French and German. To continue through 2005.
8. Paper on IFCC WG-HbA1c name and units submitted to the IFCC executive board for possible publication as an IFCC recommendation (G. Nordin and D. Kenny). Ongoing discussion on the impact of systematic nomenclature on the naming of this particular important property has evolved and is expected to continue during 2005 before finalized.

LOINC co-operation?
Urban Forsum Daniel Karlsson Clem McDonald, Stan Huff and Gill Hill met November 2004 in Indianapolis, USA .
Purpose of the meeting was to suggest ways of interaction between the C-NPU and LOINC in meeting communication and laboratory needs for systematic and metrological correct nomenclature in describing and communicating properties in laboratory medicine.
The mapping of the C-NPU and the LOINC databases item per item was brought up as feasible and as a necessary task. The C-NPU and LOINC representations of properties are different but not without common ground. The C-NPU uses a multi axial approach while the LOINC database is a flat table of fields with specified contents. It was agreed that the C-NPU generic database should be compared for similarity with the LOINC database using the RELMA software tool developed by Regenstrief Institute developers. The outcome was expected to be a list of properties that are represented in the C-NPU and LOINC databases in a mutual exact 1 to 1 relationship. A list where this 1 to 1 relationship does not exist will thus also be produced and was expected to be much larger. The 1 to 1 matches are candidates for adoption of the C-NPU properties for publication in the LOINC database while the other properties needs careful reasoning, property by property, by domain experts and informatics specialist. The task is in all probability huge and personnel recourses and financing was discussed.
<u>Implications for C-NPU and the IFCC and IUPAC.</u>
The generic C-NPU database must be a metrological project in the domain of laboratory medicine that is driven by the experts (i.e. IFCC and IUPAC). How to publish the properties in real informatics milieus is a different story that in part depends on cultural and business

driven differences on how health care is provided. The LOINC project is perhaps the most successful project for coding laboratory examinations in IT milieus.
The C-NPU should join forces with LOINC (and possibly other national or regional coding efforts) to foster prudent use of systematic terminology for properties. Other parts of LIS information contents (such as list of properties, narratives, administrative information objects for expressing requests that depends on local convenience considerations or local preferences in billing), is not a main concern of the C-NPU.

Future projects

The C-NPU is currently working on the following projects to become work items:
Properties and units in proteomics of medical interest (working title).
Maintenance and development of the C-NPU generic database.
Revision of the "Silver book". No progress can be reported because a working group leader has been hard to find, the item has high priority and is not abandoned.
Possible further projects include properties and units in pharmacogenetics, nuclear medicine, forensic medicine, mycology, parasitology and flow cytometry, pre-analytical solutions for sampling systems.

Reports

1.
Properties and units in the clinical laboratory sciences. Part XVIII. Properties and units in clinical molecular biology (IUPAC Technical Report)
Pure Appl. Chem. **76**(9), 1799-1807 (2004)
2.
Diagnostic relevance of the lymphocyte transformation test for sensitization to beryllium and other metals (IUPAC Technical Report)
Pure Appl. Chem. **76**(6), 1269-1281 (2004)
3.
Mechanisms of immunosensitization to metals (IUPAC Technical Report)
Pure Appl. Chem. **76**(6), 1255-1268 (2004
4.
R. Dybkaer, Units for quantities of dimension one, Metrologia 41 (2004) 69–73
5.
R. Dybkaer, An ontology on property for physical, chemical and biological systems" December 2004 (APMIS, Supplement 117, vol 112 2004, Munksgaard Blackwell)
6.
Forsum U, Karlsson D, Terminology, categories and representation of examinations in laboratory medicine. Clin. Chem. Lab. Med. 2005;43.344-345.
7
Forsum U, Hallander HO, Kallner A, Karlsson D, Impact of qualitative analysis in laboratory medicine. TrAC-Trends in Analytical Chemistry, 2005, 24: 546 -555.
8.
Nordberg M, Duffus JH and Templeton DM (2004) Glossary of Terms used in Toxicokinetics (IUPAC) Recommendations 2003, Pure Appl. Chem., Vol. 76, No. 5, pp. 1033-1082

Comité Européen de Normalisation
Technical Committee 251 - Medical Informatics

Project Team 002 (Laboratory)

Draft European Prestandard – FFV

Health care informatics
Structure for representation of dedicated kinds of property in laboratory medicine

Draft, C-NPU working group UF, DK, 2005-04-07

Status of the attached document:

DRAFT
prENV xxxxx-x

EUROPEAN PRESTANDARD

PRÉNORME EUROPÉENNE

EUROPÄISCHE VORNORM

Month 2005

UDC 000.0:000.00:000.000

Descriptors

English version

Health care informatics
Structure for representation of dedicated kinds of property in laboratory medicine

[French title] [German title]

[Text of
PNE Rules:1991
Annex D.3.2.4]

[Dummy title page - definitive version to be supplied by CEN-CS]

CEN

European Committee for Standardization
Comité Européen de Normalisation
Europäisches Komitee für Normung

Central Secretariat: rue de Stassart 36, B-1050 Brussels

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Contents list

Annexes

Foreword

This European Prestandard has been prepared by CEN/ TC 251 "Medical Informatics".

Introduction

This European Prestandard provides a model for the representation of ***dedicated kinds of property***[1] in Laboratory Medicine.

The need for this work stems from the increasing use of computerized clinical laboratory information systems, and the increasing need for reliable communication between laboratory information systems and between laboratory and other health care information systems (HCIS).

Potential users of this European Standard are:

- International and national organizations responsible for development, maintenance or registration of nomenclatures, classifications and coding systems;
- Designers and developers of HCIS, e.g. laboratory information systems (LIS);
- Persons responsible for acquisition of HCIS and checking compliance with standards;
- Designers and developers of computerized diagnostic devices and data acquisition systems;
- Developers of communication standards.

The degree to which a message (such as a clinical laboratory report) needs to be expressed in a formal, systematic language depends on the geographical, linguistic, social or professional distance between the communicating parties. The greater the distance, the greater the risk of misunderstanding.

Within any one clinical laboratory, local jargon terms may be used which are usually well understood between colleagues (Local Dialect A in Figure 1), but which would not be sufficiently widely known for communication with the outside world. Likewise, a laboratory and its local community of users, such as hospital or community physicians, may use a "local dialect" of the language of clinical laboratories which

[1] This concept has in some contexts previously without distinction between type and instance levels been called “property”

is well understood by all concerned; but if communication possibilities are wider, even transnational, risks of serious misunderstanding arise.

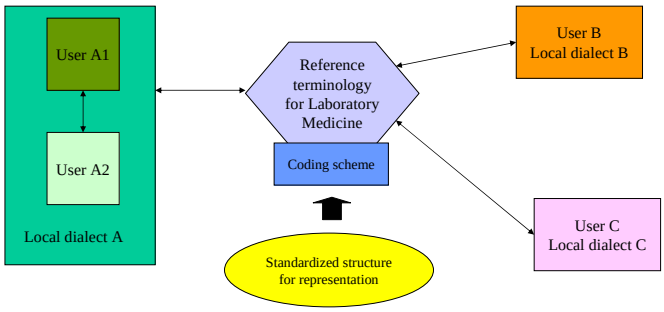


Figure 1 — Reference terminology as the bridge between local dialects

Risks of misunderstanding also increase when the "professional distance" between communicating parties increases, e.g. laboratory to health administrator rather than laboratory to clinician.

Two approaches to reducing this risk are:

1. To standardize the technical language used by clinical laboratory workers, users of the service, and other interested parties throughout the whole area in which communications may take place by eliminating all "local dialects".

This is obviously impracticable. Laboratory workers and clinicians would object to any such attempt from medical informatics. In the long run, agreement between professional bodies, with the cooperation of educational institutions, may lead to a greater degree of uniformity in the language of clinical laboratories, but this will not happen quickly and cannot be forced.

2. To create a coding scheme and a reference terminology for laboratory medicine which can be used as the basis for coding the dedicated kind-of-property part of a clinical laboratory messages for transmission between different locations and which contains sufficient information to allow the message to be translated from and to the required "local dialect" at each end. The coding scheme should be based on a standardized representation structure.

This is the more practical approach.

Title

Health care informatics.
Structure for representation of dedicated kinds of property in laboratory medicine.

1. Scope

1.1 Purpose

This Prestandard provides a structure aiding the representation, e.g. systematic terms or coding systems, of dedicated kinds of property, including dedicated kinds of quantity, in laboratory medicine. The structure for representation is intended to facilitate the unambiguous communication of messages containing information about properties.

1.2 Field of application

This standard is applicable to all branches of laboratory medicine and other bodies offering laboratory analytic services. Examinations performed in the physician's office, at the bedside, or in the home are considered to be part of the laboratory medicine domain and thus this standard applies.

1.3 Uses

This structure for representation constitutes the essential basis for development of nomenclatures and coding systems intended for use in unambiguous and fully informative communication about properties which fall within the field of application. Every such communication, including requests to and reports from clinical laboratories, and information retrieval for management reporting, research and reimbursement, will require additional information which are outside the scope of this standard.

1.4 Limitations

It should be emphasized that it is not the purpose of this standard to standardize the language used by health care practitioners in requesting or reporting clinical laboratory data. It may, however, be used as a guide by those who wish to adopt systematic terms for routine requesting and reporting of laboratory data.

The syntax used for representing dedicated kinds-of-property is outside the scope of this standard, as are syntactic rules for the construction of codes in coding schemes.

The purpose is not to standardize the presentation of properties or kinds-of-property in user interfaces of computer systems nor the presentation in printed documents.

2. Normative references

This European standard incorporates by dated or undated reference provisions from other publications. These normative references are cited at the appropriate places in the text and the publications are listed hereafter. For dated references, subsequent amendments to, or revisions of, any of these publications apply to this European standard only when incorporated in it by amendment or revision. For undated references the latest edition of the publication referred to applies.

BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, OIML.
International vocabulary of basic and general terms in metrology / Vocabulaire international des termes fondamentaux et généraux de métrologie. 2nd ed. Geneva: ISO, 1993
NOTE: This document is referred to by the abbreviation VIM
NOTE: Currently undergoing major revision

ISO 31 ISO STANDARDS HANDBOOK, Quantities and units – Parts 0 – 13
NOTE: Currently undergoing revision

ISO 10241 International terminology standards – Preparation and layout

IUPAC-CCC; IFCC, 1967.
Dybkaer R, Jørgensen K. Quantities and units in clinical chemistry. Recommendation 1966. Copenhagen: Munksgaard; 1967.

Dybkaer04 Dybkaer R. An Ontology on Property for physical, chemical, and biological systems. APMIS. 2004; 112(Suppl. no. 117).

3. Definitions

For the purpose of this standard, the following definitions apply and serve to facilitate the understanding of this document:

3.1
system
part or phenomenon of the perceivable or conceivable world consisting of a demarcated arrangement of a set of elements and a set of relationships or processes between these elements [Dybkaer04]

EXAMPLES – A given human being; a given portion of urine; the blood of a given person.

NOTE – A system is, with the exception of the universe, a part of at least one more comprehensive supersystem and can itself contain one or several subsystems, also called **components** (3.2).

3.2
component
part of a **system** (3.1) [Dybkaer04].

EXAMPLES – Body of a given human being; glucose in a given portion of urine; the process of coagulation of the blood of a given person.

NOTE – Systems are open, i.e. transport occurs across their borders, both as input and output. Such transported entities conveniently may be regarded as components of the system.

3.3
property
inherent state- or process-descriptive feature of a **system** (3.1) including any pertinent **components** (3.2) [Dybkaer04]

EXAMPLE – Mass of the body of a given person at a given point in time; amount-of-substance concentration of glucose in a portion of urine at a given point in time.

3.4
quantity
attribute of a phenomenon, body or substance that may be distinguished qualitatively and determined quantitatively [VIM].

Comment: VIM is currently under revision, the draft definition of quantity is as of April 2004 “property of a phenomenon, body, or substance, to which a magnitude can be assigned”.

EXAMPLE – Mass of a given object at a given point in time.

NOTE – **Quantity** is as specific in relation to **property** (3.3).

NOTE – The adjectives "measurable" and "physical" are used in VIM and in ISO 31, respectively, when required to point out that the word "quantity" is used in its metrological sense. In general, these adjectives can be omitted.

3.5
kind-of-property
common defining aspect of mutually comparable **properties** (3.3) [Dybkaer04]

EXAMPLES – Colour; mass; amount-of-substance concentration

NOTE – The hyphens are used to clarify that the modifier should be seen as a connected whole.

3.6
dedicated kind-of-property
kind-of-property (3.5) with given sort of **system** (3.1) and any pertinent sorts of **component** (3.2) [Dybkaer04]

EXAMPLES – Mass of the body of a non-specified human being; amount-of-substance concentration of glucose in urine.

4. Requirements

4.1 Representation

The following elements shall be used for the representation of **dedicated kinds-of-property** (3.6) in laboratory medicine:

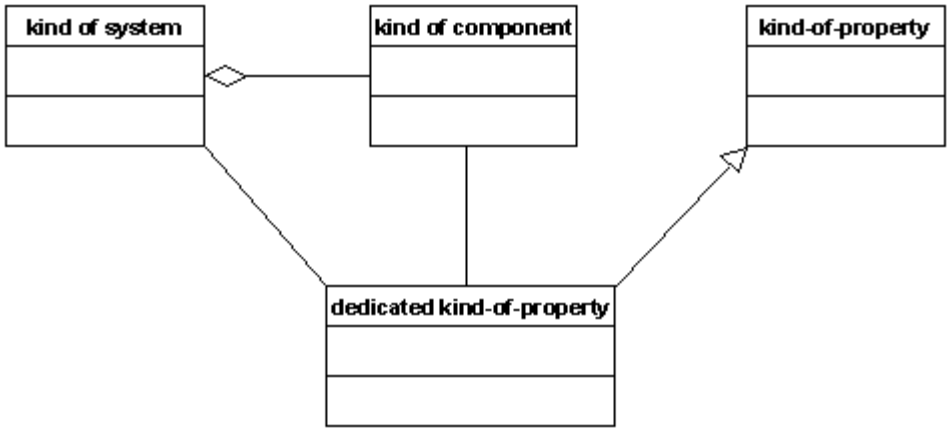
kind of **system** (3.1)
kind of **component** (3.2)
kind-of-property (3.5)

Representations of additional entities shall be appended to any or all of the elements when this is necessary to further specify the **dedicated kind-of-property** (3.6) to the degree required for a given purpose. Specifications to system and component may be super- or subsystem, or subcomponent. Specifications to kind-of-property may be metrological information concerning the examination. Specifications may also apply to the dedicated kind-of-property as a whole; to all elements of dedicated kind-of-property.

EXAMPLES – Specification to the system *plasma*, may be the supersystem *venous blood*; to the component *chromium*, the specification *Stock notation IV*; to the kind-of-property *mass concentration*, the specification may be the measuring *scale*. Procedure specifications often apply to the whole dedicated kind-of-property.

NOTE – Components may be complex, i.e. consist of aggregates of other components, e.g. in the case of sums or ratios.

4.2 UML diagram



UML representation of dedicated kind-of-property

Annex A (informative)
Representation of dedicated kinds-of-property

In reports for medical diagnosis and treatment it is necessary to ensure connectivity between laboratory production databases, medical health records and request and report systems. A prerequisite to enable this connectivity is the ability to represent examined properties in a systematic standardized way. This standard aims to provide such a systematic standardized way of representing the part of laboratory messages pertaining to the kind-of-property examined.

To illustrate how a property can be represented in a laboratory message, the following diagram is given. The example chosen is the amount-of-substance concentration of glucose in plasma from venous blood of a fasting patient examined in a sample from the patient at a given point in time. The laboratory message representing the examined property contains, among other things, the spatiotemporal specification, i.e. the subject of care and the time of examination, and the dedicated kind-of-property examined. In a practical context more complex message formats are of course needed. The message refers to a representation of a dedicated kind-of-property, usually using a code value obtained from a laboratory reference terminology, which in turn uses a representation structure according to this standard [2].

The representation of the dedicated kind-of-property consists of representations for the kind of system, the kind of component, and the kind-of-property. In the example, the kind of system **plasma** is specified by stating that the **plasma** is taken from **venous blood** from a **fasting patient**, where **venous blood** and **fasting patient** are specifications to the kind of system **plasma**. In terms of Aristotelian definition, the system is the genus and the specifications are the differentiae. The kind of component and the kind-of-property as well as the dedicated kind-of-property can be specified similarly.

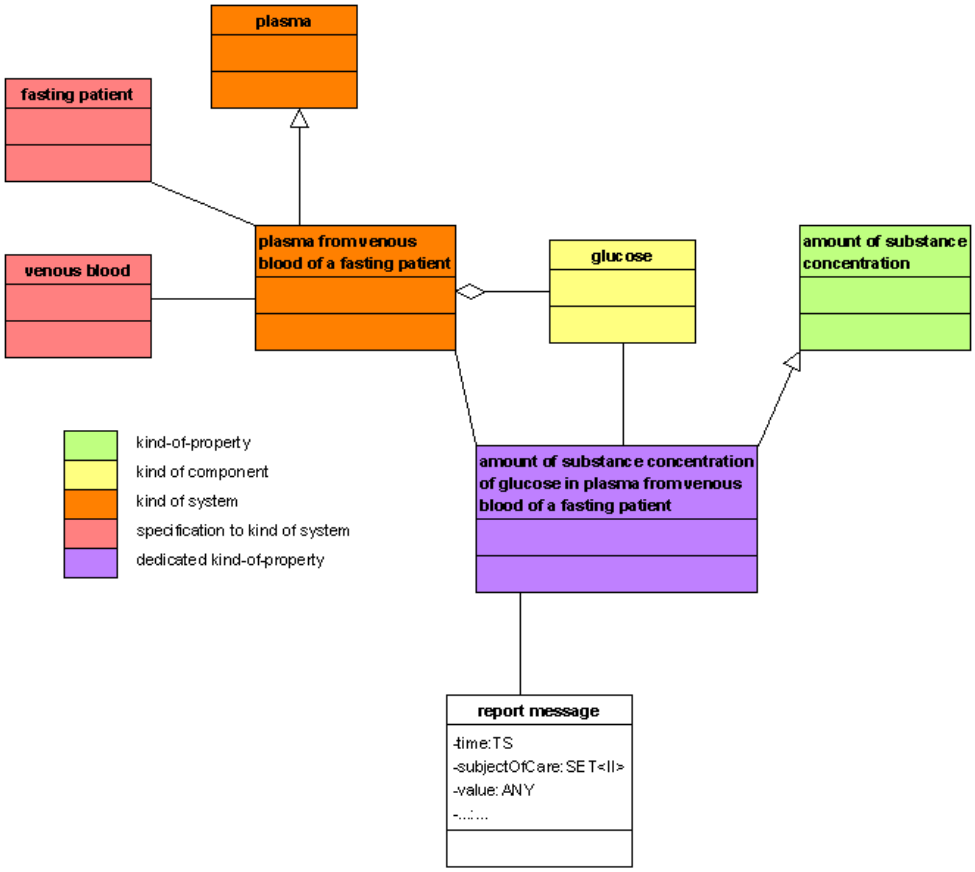


Figure – Example of representation of a dedicated kind-of-property

Two important distinctions when reasoning about properties are the instance—kind distinction and the semiotic level distinction. Consider the following example: There are two properties examined, the amount of substance concentration of glucose in plasma from venous blood of two distinct fasting patients at two different points in time. These two properties are two instances of one kind. Considering that these two properties have been examined in the real world in some real patients, these two properties can exist on a conceptual level in the mind of observers of the examination and on a representational level, e.g. in report messages or in laboratory information system (LIS) databases. The scope of this standard is solely the representation of kinds, specifically of dedicated kinds-of-property. The standard does not aim to standardize representation of instances.

Property		
	Instance	Kind (dedicated)
Representation	E.g. LIS database record or laboratory message	Systematic term for dedicated kind-of-property (e.g. according to C-NPU [2] or LOINC [3])
Concepts	Individual concept	General concept
Reality	Object	Universal [4]

References

1. Dybkaer R. An Ontology on Property for physical, chemical, and biological systems. APMIS. 2004; 112(Suppl. no. 117).
2. C-NPU. Subcommittee on Nomenclature, Properties, and Units in Laboratory Medicine. Available from: URL: http://www.iupac.org/divisions/VII/VII.C.1/
3. LOINC®. Logical Observation Identifiers Names and Codes. Available from: URL: http://www.regenstrief.org/loinc
4. Johansson I. Determinables as Universals. The Monist. 2000; 83(1): 101-21.

Annex B (informative)
C-NPU

IFCC / Committee on Nomenclature, Properties and Units
IUPAC / Subcommittee on Nomenclature, Properties and Units

Properties and Units in the Clinical Laboratory Sciences

A structure for reporting of results in clinical chemistry was given in detail by IFCC and IUPAC in "Recommendation 1966" [1]. The recommendation has been the basis for much of the work in representation of kinds of property in laboratory medicine [2]. Over the years, the model of representation of “Recommendation 1966” has been developed to encompass all examinations in laboratory medicine. The more general concept of property (in relation to quantity) was introduced and a thourugh terminological analysis has been performed.

In printed text, the systematic term for a dedicated kind-of-property shall have the format:

System(specification)—Component(specification); Kind-of-property(specification)

The element "(specification)" shall be empty when no specification is required. The em dash following the name of the system and the semicolon following the name of the component are part of this syntax and these characters shall not be used within terms for kind of system, kind of component nor kind-of-property.

To use the C-NPU coding scheme for representation of properties, the examination must be specified in space and time, i.e. a patient id and date and time must be given.

The C-NPU publishes lists of codes for dedicated kinds-of-property at http://dior.imt.liu.se/cnpu.

References

1. Dybkaer R, Jørgensen K. Quantities and Units in Clinical Chemistry. Recommendation 1966. Chopenhagen: Munksgaard; 1967.
2. Rigg JC, Brown SS, Dybkaer R, Olesen H, editors. Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences. Recommendations 1995. Oxford: Blackwell Science Ltd;1995.

Annex C (informative)

LOINC

LOINC Committee, The Regenstrief Institute, Indianapolis, Indiana, USA

Logical Observation Identifier Names and Codes

The LOINC database provides a set of universal names and ID codes for identifying laboratory and clinical test results. Currently, many US laboratories are using ASTM 1238 or its sister standard HL7, (Health Level Seven, http://www.hl7.org), to send laboratory results electronically from producer laboratories to clinical care systems in hospitals. A HL7 message carries one record for each separate test observation. Within this record is one field that identifies the test, and another that reports its value. In HL7 nomenclature, the field that carries the observation identifier is called OBX-3, and the field that carries the observation value is called OBX-5.

The LOINC database provides universal identifiers for observations in HL7 messages. The scope of the LOINC includes the codes that identify the test observation per se, not the codes that might be reported in the values of some test observations. If observations are seen as a question and the observation values as answers, LOINC provides codes for the questions. Other code systems provide codes for the answers.

LOINC names are defined in terms of six major, and up to four minor, axes. The formal LOINC name must include entries for the first six major axes. The method axis is included only when the method distinction makes an important difference to the clinical interpretation of the result.

Syntax of LOINC names:

> <Analyte/component>:<kind of property of observation or measurement>:<time aspect>:<system (sample)>:<scale>:<method>

The minor axes include challenge information, adjustments, supersystem and time operators. The challenge axis is the most complex and includes amount, route, and timing.

The LOINC code used to report a single observation can also be used to order that observation. The LOINC database includes codes for some test packages (panels) but only the most common and standardized ones. Each record carries the formal six-part LOINC name; the LOINC code, a number with a check digit, the observation class, related names, and other attributes. For most classes of laboratory observations, the database also includes a "short" report name that is <30 characters.

The LOINC database is published at http://www.regenstrief.org/

Referencies

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2. McDonald, C. J., Huff, S. M., Suico, J. G., Hill, G., Leavelle, D., Aller, R., Forrey, A., Mercer, K., DeMoor, G., Hook, J., Williams, W., Case, J., & Maloney, P. (2003). LOINC, a universal standard for identifying laboratory observations: a 5-year update. Clin Chem, 49(4), 624-633.

DIVISION VII

Chemistry and Human Health

Minutes Division Committee Meeting

Leiden, March 4-6th 2005

Location and Schedule: Oud-Poelgeest Estate, Leiden-Oegstgeest, NL

Saturday, March 5th, 2005; 9:00 - 19:30

Division Committee:

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Associate Members:

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Thomas Perun Tjperun@aol.com (chair: Subcommittee on Membership and Elections)

cc.

National Representatives:

Dr. Pierre-Etienne Bost (2002-2005 France) E-MAIL: pebost@pasteur.fr

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Prof. Nikolay E. Nifantiev (2002-2005 Russia) E-MAIL: nen@ioc.ac.ru

Prof. Masayuki Totani (2002-2005 Japan) E-MAIL: mtotani@swu.ac.jp

Observers

Francoise Pontet francoise.pontet@wanadoo.fr (invited by U. Forsum)

Excused/Not Participating

John Duffus

Pedro Soares

NRs

1. Opening, Welcome

Paul Erhardt (PE) welcomed the Division Committee members and the project leader Dr. Francoise Pontet from Paris/France, and thanked Prof. Henk Timmerman who served as the meeting's host at Leiden, NL.

2. Approval of the Agenda and Minutes from the previous Division Committee Meeting, Boston, June 11-13th – 2004, Wellesley College Club

The minutes, already made available on the internet (www.IUPAC.org), were formally approved.

3. Division VII Presidents Report

PE discussed the results of the Division Presidents and Bureau Meetings that were recently held in Bled, Slovenia. He described the group of Division Presidents to be extremely collegial and eager to co-operate as appropriate amongst their own Division's activities and projects. They reached agreement with regard to several items scheduled for the Bureau meeting's agenda. PE was also impressed by the flexible and constructive way the Bureau operated within the framework of IUPAC's constitution.

The Division should not be hesitant to get involved with political-related topics. If our technical specialty has something to contribute or inform others about in such an area, we should do so in a neutral or unbiased manner. He noted that this operational philosophy impacts directly upon the discussions and reservations that the DC previously had, related to submission of a project proposal that deals with issues on patenting chemical-related intellectual property and its interface with the harmonization of global trade agreements. As a consequence PE will now move forward with this particular submission without any additional delay (see 7.12).

Independent fund raising is strongly encouraged and there are already several cases that serve as precedent. Likewise there is some flexibility about how royalties from book and monograph publications might be directed back to the Division associated with the project. However, this could occur only after the IUPAC had recouped all of its expenses for the project and publication costs.

It is strongly requested to add more outside reviewers in order to expedite the initial submission approval process and to expand the range of experts that might become involved in the project at a later stage.

The 25 % restriction for operational expenses within the DC budget was criticized by the Divisions and agreement was reached that 30 % would be considered acceptable. In addition, an even larger percentage may be deployed toward administrative costs by simply communicating the need for this directly to the secretariat in advance.

PE also pointed out that there is a special mechanism for interdivisional projects to obtain additional funding from reserves.

The Division president reported briefly about the Project Evaluation Committee, which will attempt to assess the impact of each project, once completed. He reminded the DC and SC to bring issues of impact, other than just citations indices, to attention.

4. Prof. Brian Henry's Visit of the DC

Prof. Henry, who visited the DC meeting at Boston, was quoted as saying that his visits to the various Division Committees in general had been very beneficial in improving communications. He further commented favourably on Division VII, indicating our handling of the Project System had been well adopted, especially as a vehicle to bring in new colleagues and experts.

5. Reports from Subcommittees

5.1 Subcommittee on Medicinal Chemistry and Drug Discovery (RG)

Draft minutes from the Subcommittee for Medicinal Chemistry and Drug Development (SCMCDD), meeting in Copenhagen, August-2004, were circulated within the SC and will be made available soon. The meeting was held prior to the EFMC meeting and had an attendance of 10.
In February 2005 the group met in Rio de Janeiro, in conjunction with the XI SSMC (Summer School Course on Medicinal Chemistry), which was organized by the Universidad Federal do Rio de Janeiro (Prof. E.J. Barreiro). 7 members of the subcommittee lectured on "Highlights in Medicinal Chemistry". RG reported that Dr. Bogsch, the CEO of the pharmaceutical company Richter/Hungary, will sponsor an "IUPAC- Richter-Prize in Medicinal Chemistry", and that he and Janos Fischer are currently drafting the details. This development and the generous contribution from Richter Company was very much welcomed by the DC and it was recommended to make this attractive award distinguishable from other prizes, e.g. by building a symposium around the prize-winner lecture and to use the opportunity to strengthen relationships to ACS, EFMC and AFMC.

A proposal was discussed to introduce an honorary title (e.g. "distinguished or emeritus fellow") for previous members with outstanding service to IUPAC. The DC president will bring this suggestion up at the next Presidents` and Bureau meetings. He asked the SC chairs to provide names of potential nominees for such a title from each of their areas

5.2 Subcommittee on NPU (UF)

The SC met in Tunis and Indianapolis. Close co-operation with IFCC continues in the search for financing the generic database in order to maintain and update the 20,000 terms. UF worked during his sabbatical leave at Indianapolis on the conceptual description and alignment of the LOINC and C-NPU databases. The positions of the two concepts were exchanged and co-operation is moving forward to overcome the difference of representation of properties in laboratories.
New projects under consideration address concepts of properties and quantities, as well as revision of the Silver Book which is now 10 years old and needs an update in syntax and semantics. S. Anderson (DK) has been contacted for this project. New members for the SC have been recruited at the IFCC meeting and these were welcomed by the DC. UF will convey the necessary details to the Secretariat.

René Dybkaer, who turned 80 recently and is still very active, received a PhD from the University of Copenhagen in 2004 for his outstanding thesis: "*Ontology of properties for physical, chemical and biological systems"*. The work has been published by Blackwell, Munksgaard, APMIS, Suppl. 117, Vol 112, 2004. Availability on the IUPAC website will be pursued.
The Subcommittee is considering two new projects entitled: the "concepts of traceability and calibration", and "NPU in environmental chemistry". AK suggested writing a short position paper for CI and to discuss interdivisional co-operation at the next GA. The NPU project on Toxicology might serve as an example for successful partnership across disciplines.
A SC-NPU-meeting was held following the DC-meeting at Leiden the next day; participants were Urban Forsum (Sweden), Francoise Pontet (France), Gunnar Nordin (Sweden), Wolf Kuelpmann (Germany), Ivan Bruunshuus (Denmark), Arne Kverneland (Denmark), Daniel Karlsson (Sweden), and René Dybkaer (Denmark).

5.3 Subcommittee on Toxicology and Risk Assessment (based upon written report forwarded by JD)

The Subcommittee on Toxicology has not met since the last meeting of the Divisional Committee. However, it is intended that the officers of the Subcommittee will meet in May, 2005.
At the last IUTOX Congress in Tampere, Finland, JD gave an invited lecture on the activities of IUPAC in facilitating education in toxicology. The IUPAC Toxicology Modules, the development of glossaries, and the related textbook "Fundamental Toxicology for Chemists' were put in context and their origins in the IUPAC system were described. A paper based on this lecture has been accepted for publication in the ICTX special issue of Toxicology and Applied Pharmacology. As a consequence of the lecture, JHD has been asked to contribute a similar presentation to a proposed education session at the SOT Congress in San Diego. Any suggestions of related IUPAC activities with internet components which might be referred to would be welcomed.
A version of the glossary, prepared by JHD, has been incorporated into the forthcoming 'Encyclopaedia of Toxicology', 2nd edition, with full acknowledgment of its IUPAC origins. The encyclopaedia will also include an entry on the role of IUPAC in toxicology written by JHD.
Monica Nordberg is a task group member of the Revision of the IUPAC Compendium of Chemical Terminology (the gold book) and started correspondence with Gerry Stephenson on his first draft of an IUPAC Pesticide Glossary.
New fields to generate new projects might be human health aspects related to nano-technology (nanoparticles) and a glossary of terms in metabolomics.

6. Review of Activities

PE reminded the DC and SC chairs that all completed project manuscripts should be sent to the DC President, the SC chairs and the secretary (cc) prior to publication. To reduce the workload of the DC president and in order to progress faster with publications, he delegated the editorial responsibility to the SC chairs, except for those cases, where the SC-chairmen are themselves the project leaders. PE will inquire at the secretariat if this delegation can be officially accommodated within the IUPAC rules, or if it will just be so practiced within our Division.

6.1 Completed Projects

Completed projects 2003-2004

6.1.1 2001-048-2-700 - Research and training in medicinal chemistry in India, Pakistan and Sri Lanka (MC). The report has been finalized and a recommended IUPAC curriculum will be included. The msc is ready for submission to PAC. The project will be extended and continued (see 6.2.5).

6.1.2 2000-034-2-700 - Glossary for Toxicokinetics for chemists (M. Nordberg).The project has been completed. The glossary has approximately 300 entries and was printed in PAC, May issue. Nordberg M, Duffus JH and Templeton DM (2004) *Glossary of Terms used in Toxicokinetics (IUPAC Recommendations 2003,* Pure Appl. Chem., Vol. 76, No. 5, pp. 1033-1082.
Other publications related to this project are: Nordberg M. (2002) *Glossary of Toxicokinetics of Chemicals.* Chemistry International 24, no. 3, 15 and Nordberg Monica (2004) *Glossary of Terms used in Toxicokinetics (IUPAC Recommendations 2003),* Chemistry International Vol 26, no. 5, 21

6.2. Current Projects

6.2.1 1999-047-1-700 - Immunochemistry of metal sensitization

(DT)Two manuscripts appeared in PAC in 2004: Templeton, D.M., *Mechanisms of immunosensitization to Metals*, Pure Appl. Chem. **76**, 1255-1268 (2004). Klein, R., Schwenk, M., Heinrich-Ramm, R. & Templeton, D.M., *Diagnostic Relevance of the Lymphocyte Transformation Test for Sensitization to Beryllium and other Metals*, Pure Appl. Chem. **76**, 1269-1281 (2004).
A draft of a third paper on cytokine profiling is nearing completion. The authors will be meeting in Tübingen/Germany in May to finalize this paper. At that time they will also discuss whether this completes the project or what additional work is needed. In the original proposal they stated that "The results would be published in two manuscripts, one dealing with structural aspects and one on standardized immunological test methods for sensitization to specific metals." This field is changing quickly and it seemed logical to split the second paper into two or perhaps three parts.

6.2.2 2000-009-1-700 - Metabolism terms

(PE) The glossary is nearly completed and was discussed at the SCMCDD meeting in Rio last month. It will soon be passed on to external review. A poster describing the activities related to metabolism was presented by PE at the last ISSX meeting, September 2004, in Canada (see also 6.2.3)

6.2.3 2000-010-1-700 - Human drug metabolism database

(PE). The project has received great interest and praise at the ISSX meeting, but is still delayed due to lack of financing. PE will now approach the private sector; negotiations with a publisher from Spain have just started. PE noted that free public availability will remain a condition of any collaboration

6.2.4 2000-014-1-700 - Recommendations for the use of nanotechnology in clinical laboratories

(Peter Wilding, AK). The project is nearly finished, final comments together with approval were handed back by PE. One article has already been published in J Clin Chem.

6.2.5 2001-048-2-700 - Research and training in medicinal chemistry in India, Pakistan and Sri Lanka

(MC) A follow-up of the project will be to run workshops according to the recommended curriculum. MC together with the Indian IPP will organize a series of one-week training courses with distinguished lecturers in India.

6.2.6 2001-049-2-700 - Glossary of terms used in process chemistry/manufacturing of active pharmaceutical ingredients and pharmaceutics

(MC and E. Breuer) This project encompasses two different glossaries. Both will be incorporated in the Compendium. MC's glossary of Terms used in process chemistry with 190 terms has nearly been completed and has been circulated for external review. The other glossary, from E. Breuer is of Terms in Pharmaceutical Technology. This has been reviewed by external reviewers and comments have been incorporated.

6.2.7 2001-050-2-700 - Chemical, pharmacological aspects of natural products with medicinal and nutritive value

(MC). The survey has been completed and the final document is currently under review by PE. PE intends to provide recommendations to restructure the paper.

6.2.8 2001-053-2-700 - Fundamental toxicology for chemists

(JD) The editing of the texts for the second edition of 'Fundamental Toxicology for Chemists' is proceeding to completion. Howard Worth and JD hope to deliver the complete edited version to the Royal Society of Chemistry within the next few weeks. All existing chapters have been revised and a number of new chapters were prepared, including chapters on pharmaceutical toxicology, toxicology in the clinical laboratory, and pathways and behaviour of chemicals in the environment.

6.2.9 2001-058-1-700 - Concepts and structure for requests in clinical laboratories

The project is moving ahead and will be completed during the SC meeting. A publication will be produced next month.

6.2.10 2001-066-1-700 - Global use of the C-NPU concept system for properties in toxicology

(Wolf Külpmann)The final paper resulting from this project was submitted to PAC on October 26, 2004. Jack Lorimer, UF, PE and JD have been corresponding about it and there is now a final list of suggestions from Jack (January 22, 2005) as to how it should be prepared in a form suitable for publication in PAC. The project will be finalized before summer.

6.2.11 2001-067-1-700 - Properties and units for function examinations

(A.Jabor). AJ has retired and therefore the project is not finished but it is anticipated that work will restart 2005 and be finalized once a replacement for AJ has been identified

6.2.12 2001-070-1-700 - Properties and units for urinary calculi

(A.Jabor). The project is not finished but it is anticipated that this work will also restart in 2005. The two projects by A. Jabor are considered very important and are already in an advanced stage. The continuation will be discussed at the forthcoming SC meeting and a replacement for A Jabor will be sought.

6.2.13 2002-001-1-700 - Compendium of terms associated with drug discovery and development

(RG). There is good progress and 6 glossaries will be included. A single editorial format is being developed. Details will be discussed with the publisher (Wiley) at the ACS in San Diego. It was noted by TP, referring to the recent book of Prof. Wermuth, that the publisher Wiley should be informed that advertisement of books could still be improved by the publisher. PE indicated that he would convey this situation during the Wiley meeting.

6.2.14 2002-051-1-700 - Analogue-based drug discovery

(J.Fischer). The project has made excellent progress, with 20 msc already received. The new deadline is March, 2005, for receipt of the last 6 pending manuscripts and the end of April for submission to the publisher (Wiley). The book will have about 300 pages.

6.2.15 2003-001-2-700 - Explanatory dictionary of concepts in toxicokinetics

(Monica Nordberg) The project has just started.
The only publication so far is: Nordberg M. (2004) *Explanatory Dictionary of Concepts in Toxicokinetics*, Chemistry International Vol **26**, no. 4, 23-24.

6.2.16 2003-028-1-700 - Glossary for chemists of terms used in toxicology - revision and updating

The original glossary has been merged with the new Glossary of Terms Used in Toxicokinetics which was published in PAC last year. The combined glossary has been circulated to a number of possible reviewers including representatives of IUTOX and EUROTOX but little comment has been received. It appears that the definitions in the glossary are acceptable but further comment will be sought.

6.2.17 2003-044-1-700 - Glossary of terms used in combinatorial chemistry

Derek Maclean had difficulties in finding external contributors but continues with the work. He became a member of the editorial board of the J.Combinatorial Chemistry and was involved in writing (style guide) the instruction for authors.

6.2.18 2003-059-1-700 - Quantifying the effects of compound combinations

Dr. Joseph Lehar from Computational Biology in Boston/US continues with the project, previously initiated by Prof. Poech from Austria. JL will contact potential subcommittee members over the next two months and plans some form of gathering for the summer to agree upon the contents of the report. He estimates a period of 4-5 months to write up the IUPAC recommendation on quantifying the effects of compound combinations. JL shall be encouraged to provide a short summary of the project for Chemistry International (CI).

6.2.19 2004-019-3-700 - Glossary of terms used in biomolecular screening

(J Proudfoot) The project started last year and 175 terms were collected by the team which met in Orlando. Larry Walter the editor of J. Biomolec. Screening has joined the working group and an article has appeared in the newsletter of the Society of Biomol. Screening, from which several members participate: (www.sbsonline.org). Target for completion is summer 2005.

6.2.20 2004-023-1-700 - Internationally agreed terminology for observations in scientific communication*

Dr. Pontet`s project has been initiated at the SC-NPU meeting in Leiden 03-06-05. The project addresses nominal results, terms that are not described by numerical quality as in classical metrology.

6.2.21 2004-025-1-700 - Compendium of targets of the top 100 commercially important drugs

(John Proudfoot) This project originated from a report stating that only a limited number of targets exist for the top 100 commercially important drugs. The project has started last year and 3 main target groups have been identified and drafted: nuclear receptors, antibacterial and protein targets. It was recommended to include an editorial comment on commercial versus essential drugs and make a comparison with the WHO listed 100 essential drugs.

6.2.22 2004-028-1-700 - Practical studies for Medicinal Chemistry - An integrating approach for developing countries

(MC and A Monge) The project will produce educational material for IUPAC Courses in the field of Medicinal Chemistry in the form of a book on practical aspects, involving small scale experiments. Antonio welcomes contributions in the form of experiments/descriptions. HT will contact AM and provide input. The results of the project will be made available also on the internet and it was recommended to produce an English version. MC will contact and inform CCE.

6.3 Interdivisional Activities

6.3.1 2001-005-1-300 - Post-genomic chemistry is to be dropped from our listing.

6.3.2 2001-020-1-300 - Glossary of terms and basic protocols used in photodynamic therapy. (Prof. Davies, UK) No update on the latter project has been received for some time and the status remains unclear.

The Division has offered co-operation in the review process of recently initiated projects:
Development of simplified methods and tools for ecological risk assessment of pesticides
(Ronald Parker) and
Glossary of terms related to pesticides
(Gerald R. Stephenson) Monica Nordberg has become involved.

6.4 **Project Applications under review (March 2005)**

6.4.1 2004-45-1 Educational material for education in Toxicology (W. Temple)

This project pertains to educating children about toxicology, i.e. the hazards and safe use of pesticides. After mixed responses the review by CCE has been positive and a contribution has been offered. The DC accepted the project and PE will inform the secretariat that the project shall be funded.

6.4.2 2004-20-1 Molecular gastronomy (H.This)

Several positive reviews for this project application have been received. Addition of a team member who is an actual food specialist (e.g. nutritionist) was also recommended but not accepted by the project leader. The project, as it is, has again received approval of the DC and AK was asked to communicate this favourable decision to Prof. This and ask him to start the project.
Post-meeting note: Since the budget for this project is rather high, AK has also been asked to see if the budget can be reduced to $ 5 K and, if not, then to directly convey to the Project Team that they need to provide further justification for their costs.

6.4.3 2001-69-1 CNPU concepts and traceability (G. Nordin)

This joint project (IFCC and IUPAC) will make use of co-operation with Prof. de Bievre, BIPM, IFCC, EU and WHO to proceed with this important aspect in the clinical laboratory. Rene Dybkaer joined the working party.

6.4.4 2004-022-1 “Starch project” (Fitzgerald)

1500, - USD were offered from the Division budget for this interdivisional project.

6.4.5 2004-43-1 Terminology of biomedical polymers(Vert)

Interdivisional financial contribution from DC VII was declined, because there was no interest in participation of any type.

7. Discussion of future plans

7.1 New projects

7.1.1 ”Bioinformatics”: Prototype Analysis of Molecular Biomarkers of diseases (M. Liebman): The already approved project had not been submitted yet. Again approved by the Division pending submission including bridging with SC on NPU and IFCC and inclusion of terms of evidence based medicine and quality control. AK will provide the name of a Hungarian colleague.

7.1.2 Prototype Analysis of Glossary Terms to establish Biological Context by Text Data-mining (M. Liebman): Already approved by the Division for submission. ML outlined his ideas on data mining in the field of cancer research and estrogenic compounds by use of information technology. ML explained that the application was delayed because of software problems, which have been solved only recently. He promised that the project application will be forwarded within the next weeks for external review.

7.1.3 IUPAC Survey and Discussion Group on Present Trends in Patenting Drug-Related Technologies (P. Ehrhardt & P. Lindberg): Approved theme, and having cleared the question of political impact, PE will submit the project application very soon.

7.1.4 Nutraceuticals derived from plant sources of South America (Antonio Monge)

There is still strong interest to develop this project and analysis of health importance and economic changes recommended. A team from Latin America has been put together and a draft has been received by RG, who will assist in preparing the proper submission.

7.1.5 Nutraceuticals derived from marine sources (NF)

ML provided contact information, but no response from Prof. Nifantiev was received, RG will contact Prof. Nifantiev again.

Related to the two former projects, the term "Nutraceutical" was critically discussed and it was recommended to avoid this expression, which has been developed solely for commercial reasons and bears no scientific value.

7.1.6 Prediction of storage stability of drugs and compound libraries. (MC and Richard Wife from Biospex)

MC was encouraged to follow this proposal up and mentor Dr. Wife into a submitting the project. The data are already available and a contribution of 1000, - USD from the Division budget was offered.

7.1.7 Introduction of the NPU-database into the Russian system.

The DC has not received a response from Prof. Nifantiev, and inquiries made by AK during his recent visits to Moscow failed to find any organizations who might be interested to use the NPU codes. All efforts have not yielded real interest from the Russian participants. It is anticipated, that with the increasing use if IT in Russia in clinical laboratories, the need of a database will soon be recognised. Russia does not have Russian equivalents for the majority of biology terms and thus "English originals" are in use just with spelling in Russian letters. Nevertheless, the SC will continue to search how to introduce NPU codes into Russian practice. In the meanwhile, the system might be introduced to Estonia with good chances; negotiations with the Estonian Society of Clin Chem have begun.

7.1.8 Revision of the Silver Book (Chris Rigg)

The silver book needs revision and updating, however neither C. Rigg nor R Dybkaer will take up the task. The issue will be discussed at the forthcoming SC meeting and the search for a project leader continues.

7.1.9 Extension of the SCNPU-system to Imaging (UF)

The field needs a unifying concept and a systematic structure. Contacts with producers of imaging equipment (Siemens, Philips, and GE) might be a way to explore the possibility to develop a system for reporting information according to the NPU system.

7.1.10 Problems of metrology dealing with uncertainty.

Co-operation with DC V will continue, but no own project will be formulated. AK has written a compendium of uncertainty for Lab. Med. This will be made available upon request.

7.1.11 Educational Material / ToxLearn (J Duffus)

The topic will be discussed at the next SOT meeting.

7.1.12 Joint project clinical and medicinal chemistry (JF)

JF outlined a proposal for a bridging project between clinical and medicinal chemistry on validated targets of isolated drugs and analogues. He was asked by the DC to prepare a sketch for the Beijing meeting.

7.1.13 Kids in science (MC, Jack Wife).

MC presented a correspondence with Dr. Wife, who seems willing to start a project on kids in science. The DC considered the theme interesting but more appropriate to be transferred to the responsibility of CCE. MC was asked to establish the contact between Dr. Wife and CCE.

7.1.14 Properties and Units in CD markers (UF)

This might become a new project; a possible project leader has already been identified.

7.2 Conferences

PE asked the SC chairmen to submit a list of conferences in their field that they would like to be aligned with IUPAC sponsorship either in a new manner or as a new relationship. He wants to explore the possibility of an IUPAC (blanket) sponsorship for these conferences by reducing the terms of sponsorship and further opening the possibility for poster prizes.

7.2.1 IUPAC conference, 2005 in Beijing (12-14.August 2005). See item # 12.

7.2.2 ACS, San Diego. PE will present a Division-Poster at the forthcoming ACS conference describing the work of Division VII. Also see item # 7.3

7.3 Preparation of Division VII PR Materials

A poster for use at various meetings has been prepared by PE (see item 7.2.2)

MC volunteered to write a Division VII brochure. He will provide the draft to PE within a week.

The issue of a Division newsletter will be further discussed in Beijing.

7.4 Division VII Fund Raising Plan

PE has drafted and circulated a plan of how the Division might go about fund raising.

1. Subcommittee member/team proposes a fund-raising effort on behalf of his/her/their subcommittee activities and/or project(s).

2. Subcommittee Chairperson submits summary to the Division about how funds are to be sought and specifies how the money will be spent in a non-profit manner to enhance the Subcommittee's activities and/or to further support its ongoing projects.

3. Division provides approval for Subcommittee to initiate fund-raising effort and forwards the summary to the Secretariat.

4. Incoming money is deposited directly into general IUPAC account(s) via Secretariat.

5. Secretariat sets-up a “Fund” Project using its Project System mechanism specifying the Subcommittee Chairperson as the Project Leader who can then spend the money via the same expense submission process used for any other projects. No “cuts” will be excised by either the Secretariat or the Division, i.e. 100 % of the funds that are raised will be returned to the Subcommittee.

The same process may be undertaken on behalf of the Division wherein the President then becomes designated as the “Fund” Project Leader.

Depending upon various goals of the fund-raising effort, other spending scenarios may be able to be set-up by the Secretariat as well. For example, a self-sustaining sum of ca. $ 5 K per year could be established by “banking” ca. $ 100 K of raised funds into an IUPAC account so as to produce such a level of annual interest income in a perpetual fashion. The latter, in turn, might then be used to support some initiative that the Subcommittee or Division wants to run in an ongoing manner for several years, such as a continuing IUPAC poster award at some regular conference that is specifically relevant to the Subcommittee’s or the Division’s technical area.

7.5 Division VII Project Update Form

The DC President would like to see the Division adopt a more formal tracking system for our projects in a format that would go out to all of the Project Leaders on a regularly scheduled basis, e.g. just prior to our DC meetings or at least an annual basis. Division V already uses such a tool and they have found it to be extremely useful. A draft was circulated by PE. It was decided to adopt this tool on a trial basis and to use the form for tracking projects and reporting at the next DC meeting (Beijing). We will then discuss what the experience has been, before a final decision is made.

Each Subcommittee chairperson should ensure that the following form is delivered to each of the project leaders in their respective areas. The form shall contain the following information in this same language and sequence:

1. IUPAC Project # and Title:
2. Project Leader:
3. E-Mail, Telephone # and FAX #:
4. Project Start Date:
   Amount Budgeted:
   Recorded Completion Date:
5. Estimate Completion Percentage:
   Amount Spent:
   Anticipated Completion Date:
   What Will Be Delivered First:
6. List of changes in the Project Team’s membership (provide complete contact information for any new members):

8. Cooperation within IUPAC

ICTNS: Clarification of glossary entries with John Lorimer is continuing.

CCE: MC will continue in representing Division VII.

COCI: Tom Perun was nominated to represent Division VII.

PAC: As DC President, PE is a member of the editorial board. As mentioned earlier in the Minutes, PE proposed to have three technical editors for PAC and will proceed with this proposal as appropriate via the secretariat.

CI: Newsletter Project. Antonio Monge will on behalf of Div.VII work with Div V to deliver an article for their series entitled: "Emerging needs in developing countries-challenges for IUPAC"

9. Cooperation with other Organizations

US-NC: PE participated in a meeting and discussed experiences in fund raising.

ICSU: AK attended the annual meeting. The drug metabolism database will remain an initiative and AK will write a letter to endorse the latest draft.

NIH: Co-operation with Phil Wexler's"World Library on Toxicology" and the"Tox-Learn" concept is continuing. Work is progressing on the development of introductory material on toxicology, presently called TOXLEARN, for the forthcoming US National Library of Medicine Toxicology Portal. John Duffus provided the glossary and will be involved in the review of the ToxLearn format.

WHO: A formal request for a report of activities of DC VII was received and PE will forward the information by sending them our most recent annual report. AK will inform him about the contact.

WHO/IPCS: BH contacted Dr. Besbellin (IPCS, WHO Geneva) and was assured that the joint project on Educational Material (W. Temple) is still supported by WHO.

IFCC: Projects are continuing and vested interests relate to traceability and uncertainty. UF will represent IUPAC.

SOT: JD attended the SOT Congress in Baltimore. JD and ML have been invited to give a lecture at the next SOT conference.

SBS: Contact with SBS was established by PE and will be continued by John Proudfoot relative to his project and PE.

IUPHAR: PE remains in contact via his joint project on a drug metabolism database, and HT plans to make additional contacts.

ACS, EFMC, AFMC: PE intends to be more proactive towards collaborating with these organizations on behalf of Div. VII.

10. Personalia, Report from the Election Committee (TP)

Tom Perun, chairmen of the Nominating Committee, attended the DC meeting. TP conveyed the final membership of his nominating committee as approved by the secretariat: TP (chair), Rita Cornelis (Belgium), Monica Nordberg (Sweden), Giorgio Tarzia (Italy), Hugo Kubinyi (Germany). TP distributed names of 7 candidates that have been approached and are willing to serve on the DC. The SCCC will discuss and provide another nomination and will inform TP and the Election Committee within a week. Four positions on the DC are to be filled plus the position of vice president and secretary of the DC, due to end of term. The question of Pedro Soares de Araujo continuing on the DC will need to be resolved.

The ballot for election of the TMs will be handled by the secretariat. PE asked that each of the Division's three technical subcommittee chairpersons propose five (5) additional names from their SC and/or people on their various projects, who under the new balloting system, would then become added to the traditional group that comprises the Division's electorate.
BH offered to vacate his position as secretary of the Division and MC expressed his interest in assuming this position. The motion to have MC become the new secretary was discussed and then acknowledged by PE. An official election of the Division Secretary will be made by the DC at the GA in Beijing.
Likewise, the possibility for someone to assume the Vice President was discussed. Formalized election of a VP will also take place in Beijing.
The list of nominated national representatives (NR) from the NAOs will also be forwarded by TP to the DC and their formal election to the DC will be conducted in Beijing.

11. Finances

The DC has spent about 70 % of the budget and if, after also covering this last round of administrative costs, the remaining funds do not cover the pending project submissions, PE will ask for additional funds from the secretariat reserve.

12. Any other business

Next DC meeting

The next DC meeting will be held at the IUPAC General Assembly, 2005 in Beijing (12-14. August 2005). The schedule for DC members should be to arrive no later than Friday, because our DC meetings are scheduled for Saturday and Sunday (specific times and location will be provided later). Joint meetings with DC III and VI shall be requested to discuss interdivisional co-operation on NPU in environmental analysis.
The TMs were reminded to follow strictly the information requested in the brochure (available from IUPAC website) and timely application of visa.

PE will request travel reimbursement for the subcommittee and nomiating committee chairmen (RG and TP) to participate in the DC/GA meeting at Beijing. PE also intends to extend an invitation to our Chinese hosts, to attend the DC meeting. PE encouraged the SC chairs to do the same for any meeting they intend to hold while at the GA. For the latter, chairpersons were reminded to contact the Secretariat immediately for assistance with scheduling of non-conflicting times and for the availability of rooms.

IUPAC DIVISION (VIII) OF CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION

Report to ICTNS, August 2005

I *Current projects*

I.1 IUPAC International Chemical Identifier (InChI).

A further test version of the software was distributed in July 2004, and comments were accommodated in a final test version issued in February 2005. To allow trademark copyright and licensing issues to be resolved, the name of the Identifier was changed to International Chemical Identifier (InChI) [formerly IUPAC-NIST Chemical Identifier (INChI)]. Version 1 was finally released in April 2005: see www.iupac.org/inchi and an announcement in *Chemistry World*:

"International chemical identifier goes online", *Chem. World*, 2005, **6**, 7: http://www.rsc.org/chemistryworld/Issues/2005/June/this_month/International_chemical_identifier.asp

The Identifier has been incorporated into Chemical Markup Language and its potential is being explored by various groups; see for example:

P. Murray-Rust, H. S. Rzepa and Y. Zhang, "Googling for INChIs; A remarkable method of chemical searching": http://lists.w3.org/Archives/Public/public-swls-ws/2004Oct/att-0019/index.html

S.J. Coles, N.E. Day, P. Murray-Rust, H.S. Rzepa and Y. Zhang, "Enhancement of the chemical semantic web through the use of InChI identifiers," *Org. Biomol. Chem*., 2005, **3**(10), 1832-1834: http://pubs.rsc.org/ej/OB/2005/b502828k.pdf

M.D. Prasanna, J. Vondrasek, A. Wlodawer and T.N. Bhat, "Application of InChI to Curate, Index, and Query 3-D Structures," *Proteins: Structure, Function, and Bioinformatics*, 2005, **60**, 1-4

One of the graduate students in Murray-Rust's group has prepared a very useful InChI information source:

http://wwmm.ch.cam.ac.uk/inchifaq/

InChI is currently being incorporated into a variety of public and commercial chemistry databases:

NIST - 150,000 structures

NIH/NCBI/PubChem project - 800,000+ structures

ISI - 2+ million structures

NCI Database - 23 million+ structures

EPA-DSSToX Database - 1450 structures

KEGG database - 9584 structures

UCSF ZINC - 3.3 million structures

Chemical Entities of Biological Interest (ChEBI) database of the European Bioinformatics Institute – 5000 structures

BRENDA database (University of Cologne) – 36,000 structures

Other InChI developments include:

Integration by ACD/Labs into their chemical structure drawing program, ChemSketch.

Discussions on adoption by the new *Nature Chemical Biology*

Discussions on use in the new *Beilstein Journal of Organic Chemistry*.

A Supplementary Project is now in progress with the following objectives:

to promote the use of the Identifier throughout the chemical information community

to extend its applicability to include polymeric structures

to explore the need for other extensions, including the ability to handle Markush structures, and to include information on other attributes such as phases and excited states

A meeting in Prague in June 2005 has established requirements for extension to polymers.

To enable development of InChI facilities and applications in an Open Source context, a project to encompass this work has been registered with SourceForge.net (see http://sourceforge.net/projects/inchi).

I.2 Organic Preferred IUPAC Names (PINs)

Work on the new Nomenclature of Organic Chemistry (IUPAC Blue Book), including recommendations for identifying IUPAC-preferred names, is approaching completion. Final revision of the book (more than 1300 pages) is in progress following ICTNS and public review, and publication is expected in 2006.

I.3 Revision of "Nomenclature of Inorganic Chemistry"

The revised IUPAC Red Book is scheduled for publication in August 2005.

I.4 Rotaxanes

Recommendations for naming rotaxanes are almost ready to be issued for expert review.

I.5 Fullerene nomenclature Part II

This extension of the published Part I recommendations to larger and more complicated molecules, with emphasis on numbering systems, was published in *Pure Appl. Chem*:

http://www.iupac.org/publications/pac/2005/7705/7705x0843.html

I.6 Extension of rules for stereodescriptors to include coordination numbers 7-12

The first meeting of the project group took place in March 2005, in London.

I.7 Nomenclature of cyclic peptides

The document is undergoing revision following ICTNS and public review.

I.8 Graphical representation standards for chemical structures

The first component of this project, consisting of guidelines for two-dimensional representation of configuration, is being revised following ICTNS and public review. Draft guidelines for many other aspects of graphical representation were discussed at a Task Group meeting in Beijing immediately preceding this General Assembly.

Macromolecular Nomenclature Projects

The following projects are managed in full cooperation with Division IV's Subcommittee on Macromolecular Terminology:

I.9 Terminology and nomenclature of macromolecules with cyclic structures

This project has been extended to cover polycyclic and spirocyclic macromolecules, and the new draft is expected to be ready for expert review after the Beijing meeting.

I.10 Terminology and structure-based nomenclature of dendritic and hyperbranched polymers

This is almost ready for expert review.

I.11 Nomenclature for chemically modified polymers

The nature of this project has been reconsidered, and the project group reconstituted. It has a new title: 'Source-based Nomenclature for Modified Polymer Molecules'

I.12 Source-based nomenclature of single-strand organic polymers

This is a new project; it is now proposed to change the title to the more explicit "Source-based Nomenclature of Organic Homopolymers and Copolymers".

I.13 Nomenclature of macromolecular rotaxanes

This project is on hold pending completion of the non-polymeric rotaxane document (item II.3.4).

II Joint IUPAC-IUBMB Commission on Biochemical Nomenclature (JCBN)

Joint activities of the two Unions are channelled through this Joint Commission. Its main activities are:

II.1 Maintenance and updating of the Enzyme List

This is a very substantial and continuous operation drawing on advice from IUPAC participants on chemical names for substrates, reagents and products.

II.2 Maintenance and development of specialised naming systems for natural products

Classes of natural product of interest to biochemists, especially steroids, amino acids and peptides, carbohydrates, lipids and nucleic acids require local specialised systems for naming. A project to review and update carbohydrate nomenclature is being developed.

II.3 Advice for biochemists on names for specific compounds of biochemical importance

II.3.1 Synonyms databases.

Synonyms databases for compounds in common biochemical use are being assembled by various groups, and JCBN members are involved with this work. Examples are the ChEBI database at the European Bioinformatics Institute and the Biochemical Names Database at the University of Missouri.

II.3.2 Phosphorus compounds

Recommendations on the naming of phosphorus compounds of biochemical importance are being revised.

II.3.3 Small molecules glossary

There are plans to compile advice for biochemists for naming a selection of small molecules of biochemical importance not covered elsewhere

III Project Development

As noted previously, Division VIII has not received any unsolicited project proposals from the community. The responsibility for developing proposals rests with the Division Committee. The Division therefore carries out scoping exercises from time to time, to establish needs and feasibility. In the most recent such exercise, a group of Division Committee members and other potentially interested people met on September 29th 2004 in Budapest to consider approaches to development of Preferred IUPAC Names for inorganic compounds, bearing in mind the almost-completed similar exercise on organic compounds The consensus was that a Task Group should be assembled and a proposal developed; however it has so far proved difficult to identify people willing to commit the considerable amount of time and effort necessary for this work to proceed..

IV Division VIII Publications

Since January 2004, the following publications have appeared:

IV.1 Corrections to Revised Nomenclature of Organic Chemistry Section F: Natural Products, *Pure Appl. Chem.,* 2004, **76**, 1283-1292:

http://www.iupac.org/publications/pac/2004/7606/7606x1283.html

A number of errors and inconsistencies in the original Revised Section F had been pointed out in the course of translation, and this substantial Corrections and Modifications document was developed and published both in print and on the web. The changes were incorporated into the web version of Revised Section F, with links to the original text.

IV.2 Numbering of Fullerenes, *Pure Appl. Chem*, 2005, **77**, 801-923:

http://www.iupac.org/publications/pac/2005/7705/7705x0843.html

IV.3 "International chemical identifier goes online", *Chem. World*, 2005, **6**, 7:

http://www.rsc.org/chemistryworld/Issues/2005/June/this_month/International_chemical_identifier.asp

Alan McNaught
21 July 2005

Attachment 14
Re Items 10.8 and 15.6

Comments of Prof Jan-Gerritt Koomen on
Jonathan Brecher
Provisional Recommendation on
Graphical Representation of Stereochemical Configuration

I compliment the task group with all the work they carried out. The proposal is clearly written and seems to cover all existing possibilities. In general however, in several situations the amount of different "acceptable" representations is rather large (sometimes six or more). In my opinion, IUPAC should try to reduce this within a couple of years to one "preferred" representation, to be used worldwide. I wonder whether plans have been developed to achieve this.

Detailed comments:
page 8. line 23-28. It seems illogical that in the solid wedged bond the wide end is nearer to the viewer and in the hashed wedged bond the wide end is further away from the viewer. On the other hand this is so widely accepted that it will be difficult to change the direction of the hashed wedged bond, which is now qualified as "acceptable" (line 46)
page14, 16, 18, 19. Too many 'wrong" structures which probably nobody ever used.
page 21. line 15-22 refer to ST-0.5 page 10, identical structures.
page 22. line 23-29 is it better to use an identical sign instead of = ? (also on pages 23 and 24)
page 29.line32-44, To recah uniformity, my suggestion is: first structure "preferred", stuctures on page 30 "not acceptable"
page 31 line 8-13. substituents disappearing or hydrogen?
page 32. line 12-33. One "preferred" structure, others "not acceptable' would be better.
page 34. line 28-44. ST-1.9. Only the first structures are acceptable and should be used. If the last ones are "acceptable" one should describe that the ring oxygen is away from the viewer. Better forget them.
page 36. line 18-24. last structure non-sense.
page 54 line 39-45. Last structure "wrong"
page 55 line 31-38. same problem as with Hayworth projections. Ring oxygen should be away from the viewer. "Not acceptable".
page 61 line 14-23. First structure OK. Others "not acceptable"

BIPM REPORT TO THE IUPAC GENERAL ASSEMBLY 2005

BIPM has pleasure in submitting a short report of its activities in 2004 and 2005.

1. The Metre Convention.

During the last two years, the number of Member States of the Metre Convention remained at 51 whilst the number of Associates of the General Conference on Weights and Measures has risen to 18.

2. The CIPM MRA.

In 1999, the International Committee for Weights and Measures (CIPM) drew up a Mutual Recognition Arrangement between signatory National Metrology Institutes (NMIs). This was aimed at establishing a scientific framework within which NMIs could demonstrate their technical capabilities through a combination of:

comparisons and peer-reviewed statements of their calibration and measurement capabilities (CMCs) ; and

quality systems which conformed with ISO/IEC 17025 or other appropriate international standards such as ISO Guide 34 for the production of certified reference materials.

The Key Comparison Data Base (KCDB) on the BIPM's web site (www.bipm.org) hosts data from the comparison reports and provides a searchable data base of the peer reviewed CMCs. This is the first ever authoritative data base which provides evidence of peer-reviewed traceability to the International System of Units (SI). It covers measurement capbilities in the physical and chemical areas and is being promoted strongly to regulators and others as a means to reduce technical barriers to trade which may result from the lack of acceptability of measurements between countries.

NMIs from forty-five Member States of the Metre Convention and from 17 Associates have now (11July 2005) signed the CIPM MRA, so bringing the number of institutes and designated organisations committed to the CIPM MRA to nearly 160. There are currently over 17 000 CMCs and 612 comparisons in the KCDB.

2. BIPM and Laboratory Medicine

We are especially pleased by recent progress in laboratory medicine under the Joint Committee for Traceability in Laboratory Medicine, the JCTLM. This programme is now well on the way to the creation of a widely acknowledged and internationally accepted framework for the recognition of reference materials "of a higher order" as required by the In Vitro Diagnostic community. It will also help to identifying best practice for the validation of measurement methods used in competent laboratories. In addition to the co-operation with our formal JCTLM partners, the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC) and the

International Laboratory Accreditation Cooperation (ILAC), we are working with the World Health Organisation, especially in the area of biological units and traceability. JCTLM's working group 1 is well advanced with lists of "standards of a higher order" which will be entered onto the BIPM's JCTLM database later this year or in early 2006. Some 300 reference materials and about 75 reference methods have been nominated for review. Working Group 2 is concerned with lists of laboratories which are recognised as having the appropriate competences in diagnostic and laboratory medicine. It is currently deciding on the criteria against which these laboratories will be judged.

3. Collaboration with other international organisations.

BIPM is now an observer on the **CODEX Alimentarius**, thereby providing a connection for us to world-wide activities in food. Already a number of comparisons and pilot studies, led by the BIPM and ithe CIPM's Consultative Committee for Metrology in Chemistry (CCQM), are dealing with food - relevant subjects and we expect this activity to increase in the future as we have a better view of priorities in this sector.

We have been working with the **World Meteorological Organisation** for some time and are pleased to see that they would like to become a signatory to the CIPM MRA and to bring some of their global atmospheric watch laboratories into the MRA with CMCs in relevant areas.

On behalf of Member States we have been working more closely with **ISO**, especially in the CASCO and REMCO committees.

4 BIPM's Quality System

Within the BIPM we have seen the successful, implementation of our own self-declared/peer reviewed quality system. Progressively, other aspects of BIPM's work will be brought within either our ISO/IEC17025 system or a system based on ISO 9001. Whilst we do not publish "CMCs" in the KCDB, the BIPM web site contains details of the uncertainties normally associated with the BIPM's calibration services.

5. Science at the BIPM

5.1 Chemistry

The Chemistry section has laboratory programmes and coordinates international comparisons in the fields of gas analysis (air quality standards) and organic analysis (primary calibrators for laboratory medicine). The section provides the secretariat for the Joint Committee for Traceability in Laboratory Medicine (JCTLM), and coordinates the JCTLM database of higher order certified reference materials and reference measurement procedures.

The BIPM is coordinating the ozone reference standard comparison (CCQM-

P28), and measurements for the comparison were completed in March 2005. This comparison has allowed the degree of equivalence of 23 reference standards to be determined in relation to the BIPM maintained standards, and will be followed by an on-going key comparison (BIPM-QM-K.1). A collaboration with the BAM on the statistical treatment of ozone comparison data has continued, and a software programme (OzonE) developed for the treatment of data. The study of systematic biases and measurement uncertainty in SRPs has been completed, and a new uncertainty budget for the instrument will be published in collaboration with the NIST. A feasibility study has demonstrated the advantage of introducing a laser-based light source into the SRP, and a programme to develop a candidate primary ozone photometer based on a laser light source has been initiated. A gas-phase titration (GPT) facility for ozone concentration measurements has been modified and its performance and measurement uncertainty improved. The system was used in the CCQM-P28 study, producing a result consistent with that of an independently developed GPT facility, but biased with respect to the ozone photometer measurements. The source of this bias will be investigated in the future programme.

The BIPM's primary gas standard facility for the dynamic preparation of nitrogen dioxide gas standards in the range (0.5-10) μmol/mol has been automated and software control developed. A multiple gas mixture sampling module for this facility is currently under construction which will allow static gravimetric NO_2 gas reference mixtures (prepared in cylinders) to be compared with the facility's dynamically generated reference mixtures.

A feasibility study on high accuracy comparisons of nitrogen monoxide gas standards has been completed, and presented to the CCQM's Gas Analysis Working Group. A BIPM coordinated comparison (CCQM-P73) of NO gas standards from 12 NMIs is planned to start at the end of the year.

The BIPM is coordinating subsequent rounds of the CCQM-P20 series of organic substance purity analysis comparisons, with two comparisons approved by the CCQM: CCQM-P20.e for theophylline; and CCQM-P20.f for digoxin. The substances to be studied have been prioritized taking into account the current programmes of the CCQM and the JCTLM and the ongoing requirements of laboratory medicine. Investigations into the extension of the comparison series to include clinically-important steroid hormones such as progesterone, β-estradiol and testosterone are also being undertaken. Two scientists and a technician have been recruited to the section, and laboratory facilities to support ongoing activities in this area have been established including capabilities for analysis by liquid chromatography with mass spectrometry (LC/MS), gas chromatography with mass spectrometry (GC/MS), gas chromatography with a flame ionization detector (GC/FID) and differential scanning calorimetry (DSC), supplemented by Karl Fischer titration and thermogravimetric analysis.

Collaborations to develop methods for purity determination for therapeutic drug monitoring and steroid hormones have been established with the LGC and the NMIJ,

respectively. Theophylline and digoxin materials have been prepared by the LGC and will be transferred to the BIPM. The NMIJ has obtained 200g batches of testosterone, progesterone and β-estradiol materials. Initial analyses of the materials have been performed at the NMIJ, and will continue at the BIPM.

5.2 Materials metrology

In October 2004, the CIPM considered a proposal from the materials community for an activity, within the Metre Convention, on traceability and uncertainty in materials metrology. This is currently the subject of a working group led by Dr Seton Bennett of the UK's National Physical Laboratory and which will report to the CIPM in October 2005. Meetings of Dr Bennett's group will look at how a more rigorous approach to SI traceability may be of benefit to the materials community and will outline possible workplans in a number of areas. CIPM will decide on whether to adopt an activity in materials metrology and how it would be handled administratively.

5.3 Publications

Work continues on the 8th SI brochure, on supplements to the Guide to uncertainty in Measurement (GUM) and the next edition of the international vocabulary of metrology (VIM), all of which will have particular attention paid to the needs of the chemical community. We hope to see publication of all three documents during 2005 and early 2006.

5.4 The SI

In recent years there has been increasing discussion on the possibility of redefining a number of base units of the SI. Encouraged by results from a number of NMIs working on the so called " Watt Balance" experiments which relate the international prototype kilogram to the electrical units, there is the real possibility of a redefinition of the kilogram based on a fixed value of the Plank Constant or the Avogadro Constant. In addition, should the kilogram be redefined, there are implications for the ampere and, perhaps somewhat more distantly, the mole. Similar moves are afoot to consider a redefinition of the kelvin based on new and better knowledge of the Boltzmann Constant. This may also have implications for the candela.

All these new concepts will be reported to the 2007 General Conference on Weights and Measures with the possibility of new definitions being confirmed by the CGPM in 2011. We are now entering an intensive period of consultation with bodies, including IUPAC, and other user communities which may be affected by these changes.

6. Collaboration with the International Laboratory Accreditation Cooperation, ILAC

BIPM's collaboration with the accreditation community continues to develop and ILAC supports BIPM's overall responsibility for the world measurement system - essentially a combination of:

equivalent national standards, demonstrably traceable to the SI through their realization and maintenance at the NMI level and validated through the CIPM MRA; and

effective national traceability and measurement systems in which measurements are traceable to these national standards, at whatever level of accuracy is appropriate to the user. This traceability is generally achieved through a network of technically competent calibration and testing laboratories accredited to ISO/IEC 17025 or other appropriate written standard by a National Accreditation Body (NAB) which is a signatory to the ILAC Mutual Recognition Arrangement.

The CIPM MRA and the ILAC Arrangement are clearly complementary and mutually supportive and their unique combination helps to provide confidence in the equivalence of SI traceable measurements worldwide. This infrastructure is increasingly recognized as providing the technical basis for consistency of measurements and their acceptance in international trade and its use can help reduce or eliminate Technical Barriers to Trade

BIPM and ILAC are working on a joint statement which will outline the roles and responsibilities of the metrology and accreditation bodies. The aim is to have an agreed document for the meeting of NMI Directors to be held in September 2005 at the BIPM and the ILAC General Assembly in October 2005. After that, the joint statement will be promoted vigorously to both communities as well as standardisation bodies, regulators and governments.

Andrew Wallard,
Director, Bureau International des Poids et Mesures, Sévres
27 July 2005

Attachment 16

Re Item 11.3

2005 Report to ITCNS by the IUPAC Joint Commission on Biochemical Nomenclature

August 2003 July 2005

The IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) works in collaboration with the Nomenclature committee of IUBMB (NC-IUBMB). Annual meetings were held in London (May 1-2, 2004) and Columbia, USA (April 30-May 1, 2005).

Membership
Titular members of JCBN are Dr G.P. Moss (UK) and Dr S. Boyce (Ireland, Secretary). Joint members of JCBN and NC-IUBMB (sponsored by IUBMB) are Prof. R. Cammack (UK, present Chairman); Prof. D. Horton (USA) and Prof. K.F. Tipton (Ireland). Other members of NC-IUBMB are Prof. H. Berman (USA), Prof. C.R. Cantor (USA), Prof. M. Kanehisa (Japan), Prof. J.F.G. Vliegenthart (Netherlands) and Prof. Dr. D. Schomburg (Germany). Associate members for JCBN are Dr M.A. Chester (Sweden) and Dr A. Cornish-Bowden (France); for NC-IUBMB are Dr R. Apweiler (UK), Dr H.B.F. Dixon (UK), Dr T. Kazic (USA), Dr A.D. McNaught (UK).
At the 2005 annual meeting, Prof Dietmar Schomburg was nominated as chairman, with effect from 1 January 2006.

The *Nomenclature website* (Moss)
This contains full nomenclature recommendations by the biochemical nomenclature committees, at http://www.chem.qmw.ac.uk/iubmb/. The site has been accessed from 196 countries since 1996, with the number of hits increasing annually.

The *Enzyme List* (Tipton, Boyce)
This is the major activity of the committees. It currently lists 3874 different enzyme-catalysed reactions and is being actively maintained. There is an emphasis on interoperability with other databases, and a great deal of effort has gone into cleanup of information deposited over the past 40 years, to ensure consistency of nomenclature.
Many enzymes in the list on the nomenclature website are now linked to metabolic pathways and mechanism diagrams, provided by H.B.F. Dixon and G.P. Moss.
Methods for automatic assignment of EC numbers for newly discovered enzymes are being developed by the group of M. Kanehisa. The algorithms are based on substructure matching of the molecular structures of substrates and products.

The EC list is the benchmark for classification of enzymes and is used in a wide array of bioinformatics databases, including ontologies and those providing gene annotation and metabolic pathway information. Increasingly the EC class of an enzyme is used as an identifier for regulatory purposes and in patents.
The list is being expanded as new enzymes are isolated and described in the literature. The creation of new enzyme names, numbers and classes is carried out in a continuous process of public consultation.
Methods for automatic assignment of EC numbers for newly discovered enzymes are being developed by the group of M. Kanehisa. The algorithms are based on substructure matching of the molecular structures of substrates and products.

Bioinformatics
The following primary bioinformatics databases are represented by members of the committee.

INTENZ, (http://www.ebi.ac.uk/intenz/); maintained by R. Apweiler. This database is also linked to ChEBI (Chemical Entities of Biological Interest), a dictionary of small molecular entities.

BRENDA, the Comprehensive Enzyme Information System (http://www.brenda.uni-koeln.de), maintained by the group of D. Schomburg

KEGG: the Kyoto Encyclopedia of Genes and Genomes (http://www.genome.jp/kegg/), maintained by the group of M. Kanehisa

PDB: the Protein databank maintained by the group of H. Berman.

Other activities
The committees have also participated in the following nomenclature activities

Standards for reporting Enzyme Data (Tipton, Schomburg, Cornish-Bowden).
The STRENDA commission (http://www.strenda.org), with support from the Beilstein Institute, has published recommendations for standard information to be provided when publishing enzyme activity data.

Symbolism for carbohydrates (Horton, Vliegenthart)
Symbols for the more commonly-occurring monosaccharides are used in a number of different applications, for example labelling of mass spectra. The committee is working with two organizations who use different systems, namely the Oxford Glycobiology Institute (UK) and the Consortium for Functional Glycomics (USA). At present the differences between the two systems have not been resolved.

Lipid classification (Cammack)
The Lipid metabolites and pathways strategy classification of lipids has been published (Fahy et al., 2005, *J. Lipid Res.* **46**, 839-862). This classification has also been adopted by the KEGG database. It divides lipids into eight categories: fatty acyl compounds, glycerolipids, glycerophospholipids, sphingolipids, sterol lipids, prenol lipids, saccharolipids, and polyketides. Nomenclature of the lipids is based on, and extends, the published JCBN recommendations.

THE INTERNATIONAL UNION OF PHARMACOLOGY COMMITTEE ON RECEPTOR NOMENCLATURE AND DRUG CLASSIFICATION, 2004-2006

Role, procedures and goals. Report IUPAC.

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The International Union of Pharmacology Committee on Receptor Nomenclature and Drug Classification (NC-IUPHAR, Table 1) has the mission of:

1. issuing guidelines for receptor and ion channel classification,

2. classifying the major receptor and ion channel systems,

3. facilitating the interface between the discovery of new sequences from the Human Genome Project and the designation of the derived proteins as functional receptors and ion channels.

4. setting up a website with access to data on all known receptor systems, freely available to all scientists. This site is the starting point for this endeavour.

Pharmacology is at a crucial point, because for the first time we have access to sequences for almost all of the receptors in the human genome. This is a unique opportunity to make a rare definitive scientific statement because the task of annotating sequence for function is a task for pharmacologists, in conjunction with our other scientific partners. Receptors are the site of action for many of the currently available drugs and the absolute definition of the majority of the receptors in genome is eagerly awaited. The IUPHAR receptor lists for G-protein-coupled receptors, and for voltage-gated ion channels (which are listed in the database) are steps forward, and will be rapidly followed by the list for nuclear receptors, and for ligand-gated ion channels. The database will list the main pharmacology associated with these proteins, as proposed by our subcommittees.

NC-IUPHAR has established close links with the Human Genome Organisation (HUGO), which attributes gene names; the International Union of Pure and Applied Chemistry (IUPAC), to standardise correct use of drug names; and the International Union of Biochemistry and Molecular Biology (IUBMB) to collaborate on receptor-related enzyme nomenclature.

CURRENT STRATEGY

NC-IUPHAR now comprises >50 subcommittees on receptor and ion channel nomenclature and each subcommittee comprises between 6–20 international experts. The plethora of new targets means that now we may invite single scientists to contribute to receptors for which there is sufficient evidence to indicate a genuine receptor, but where the classification of this receptor is not controversial. As controversy may be inherent to pharmacology, we have also set up a bulletin board (iupharbb.org) allowing pharmacologists to express their opinions. Important new initiatives are addressed by working groups, which explore and develop possible future directions for the committee, and for receptor pharmacology. An example of this is the issue of receptor dimers, which may markedly change the pharmacology of a given site – but how real are the changes? What criteria must be fulfilled to show that the changes exist? The subgroup (chair – J-P Pin) has an important question to answer.

A high priority for NC-IUPHAR has been the complex issue of nomenclature for the plethora of multi-subunit receptors and ion channels. The compendium, edited by Bill

Catterall, George Chandy and George Gutman, addressed the challenges for the nomenclature of the voltage-gated ion channels and breaks new ground in resolving old difficulties. The NC-IUPHAR subcommittees have proposed nomenclature for the major ion channel families which is, for the most part, consistent with the recommendations for receptor nomenclature. Unlike previous compendia, the ion channel compendium also covers data for proteins that are only functional when expressed with other subunits.

The list of non-sensory 7-transmembrane receptors (7-TMRs) in the human genome, divided into their main structural classes, designated by Steve Foord, is a major step forward in this area, as we consider that there will be few other structurally-related receptors left to discover. Gordon Shepherd is maintaining a database of all the sensory 7-TMRs. An evolving pharmacology committee has been formed, chaired by Anthony Davenport, to ascribe changes in the status of 7-TM receptors (orphan receptors)
However, NC-IUPHAR has limited funds, and is made up of busy scientists who give up their free time to perform their work in the committee. This means that resources are limited and we have had to prioritise our activities. We have not yet achieved a classification of receptors linked to tyrosine kinase (TKRs), and this can only be started after 2006. Receptors linked to ion channels are extremely complex to classify and Richard Olsen, the group leader for this task, is studying the possibilities in this area, where our previous classifications have been based on the established nomenclature of subunits, used in the field.

ORIGINS OF NC-IUPHAR

The mission for NC-IUPHAR was initiated in 1987 at the Xth International Congress of Pharmacology, with Sir Colin Dollery playing a role in the initiation. In 1989, the Executive Committee of IUPHAR named Paul Vanhoutte (France) as chairman of a revised and enlarged committee. This committee energetically expanded its activities and the number of subcommittees (to 33), eventually producing the first official compendium on the occasion of the XIIIth International Congress of Pharmacology at Munich in 1998. Paul Vanhoutte was elected president of IUPHAR in 2002, and Robert Ruffolo (USA) was Chairman of NC-IUPHAR from 1998-2002 with Michael Spedding as Secretary, who became chairman from 2002.

MEMBERSHIP

The current membership of NC-IUPHAR is listed in Table 1. The Committee comprises **17** researchers who have established reputations in the field of research on receptors and ion channels, in a range of disciplines from molecular biology, signal transduction, electrophysiology, structure–activity relationships, to drug discovery and development. Each member is a liaison officer with a group of activities. NC-IUPHAR meets every six months. At each meeting there is a particular theme (ion channel classification, receptor databases etc.) and a review of the progress of the various subcommittees. Individual members of NC-IUPHAR liaise with the subcommittees, communicating general recommendations from the committee and reporting back on proposed changes in nomenclature, or on the discovery of new receptors.

SUBCOMMITTEES

Subcommittees are established to provide receptor classification for a particular family of receptor and attempt to bring consensus amongst the experts in the field. Subcommittee chairs are asked to propose a list of experts, embracing a wide range of different disciplines. The composition of the subcommittee, both initially and for any changes in membership, must be ratified by NC-IUPHAR, to ensure adequate representation of the field. The chairman of each subcommittee plays a critical role co-ordinating the actions of the subcommittee, organising meetings and finalising documents. The subcommittee meets to establish consensus on classification, and to ensure that the NC-IUPHAR guidelines are complied with.

PUBLICATIONS

The recommendations of the various subcommittees are published as definitive articles in *Pharmacological Reviews*, after ratification by NC-IUPHAR, and revisions appear in the compendia. Occasionally, editorials in other specialist journals are published to ensure widespread dissemination of the propositions.

In the past, NC-IUPHAR has also convened the editors of the major pharmacology journals in order to communicate its recommendations and assess the feedback from the various NC-IUPHAR user-groups.

THE IUPHAR RECEPTOR DATABASE

In addition to the publication of the new classifications for ion channels, NC-IUPHAR is launching the present IUPHAR Receptor Database (www.iuphar.org) in 3. Although at present in draft, preliminary form, this fully relational database will eventually contain the data published in the two previous receptor compendia, as well as essential links to accompanying information, such as sequences, chemical formulae and references, which are not easily presented in paper format. The database will be regularly updated and the data from the ion channel compendium will be incorporated in the second phase of development. The IUPHAR Receptor Database has been developed initially from funds from an educational grant from Incyte Genomics, and subsequently from ICSU. The database was housed at the European Bioinformatics Institute, where it was developed through an academic collaboration with SWISS-PROT. The database is now independently maintained at the University of Edinburgh (Pr A. Harmar; curator, E. Rosser).
A key issue for us (and potentially IUPAC) is the ability to show (in the database, available freely to all scientists) the chemical names of all ligands interacting selectively with the receptors of interest and potentially their structures. NC-IUPHAR is considering interacting with Pubchem in this regard.

The development of the database has been supported by a major educational grant from Incyte Genomics, and from ICSU for which NC-IUPHAR is very grateful.

FUTURE INITIATIVES

NC-IUPHAR is addressing novel ways of addressing which receptor sequences from genomic databases represent crucial information for the design of new drugs, and also for the recognition of hitherto unsuspected endogenous ligands.

The scope of NC-IUPHAR has grown immensely during the last few years, and the work required to co-ordinate the large number of subcommittees has rapidly expanded. This has resulted in a change in the organisation of NC-IUPHAR, whereby members are charged with certain responsibilities for groups of receptor subcommittees (group leaders). Corresponding Members now have major roles to play in several areas, as well as reviewing documents.

The rapid extension of crystal structures is changing drug discovery and the characterisation of the sites for drugs. Molecular modelling is becoming more predictive and NC-IUPHAR will establish a working group on this topic. NC-IUPHAR now has a

unique opportunity to be proactive, because we have available to us, via committee members, a curated list of all the GPCRs, ion channels and nuclear receptors in the human genome. *This is a unique tool for pharmacologists (indeed for all scientists involved in receptor research) and we believe it should fundamentally change the way in which we work.*

Table 1. **NC-IUPHAR Membership, 2004–2006**.

	Specific responsibility
Chairman **Michael Spedding** Institut de Recherches Internationales Servier (IdRS) 11 Rue des Moulineaux, Suresnes, France	
Vice chairman **Franz Hofmann** Institut für Pharmakologie und Toxicologie Technische Universität München Biedersteiner Strasse, 29 80802 München Germany	
Vice chairman **Eliot H. Ohlstein** Beecham Pharmaceuticals Cardiovascular Urogenital Drug Discovery 709 Swedeland Road King of Prussia PA 19406-0939 U.S.A.	**Group Leader GPCR class 1** SmithKline
Editor	
Members **Tom I. Bonner** Laboratory on Genetics National Institute of Mental Health Building 36 Room 3D-06 Bethesda MD 20892-4094 USA	**Cochair technical committee**
William A. Catterall Department of Pharmacology University of Washington School of Medicine Box 357280 Seattle WA 98195-7280 USA	**Group Leader VGICs**
Colin T. Dollery Glaxo SmithKline New Frontiers Science Park (South) Third Avenue Harlow CM19 5AW UK	**Chairman Database Committee**
Steven M. Foord GlaxoSmithKline Medicines Research Centre	**Receptor Curator**

Gunnels Wood Road
Stevenage
SG1 2NY
UK

Anthony J. Harmar **Group Leader GPCR class 2 – Chairman Receptor Database**
Division of Neuroscience
School of Biomedical & Clinical Laboratory Sciences
University of Edinburgh
1 George Square
Edinburgh EH8 9JZ
U.K.

Vincent Laudet **Group Leader Nuclear Receptors**
Laboratoire de Biologie Moléculaire et Cellulaire
CNRS UMR 6556
Ecole Normale Supérieure de Lyon
46 allée d'Italie
69364 Lyon
France

Richard Neubig **Cochair technical committee, Group Leader GPCR class 1**
Department of Pharmacology
University of Michigan
1301 Medical Science Research
Building III
Ann Arbor, Michigan 48109-0632
USA

Richard W. Olsen **Group Leader RGICs**
Dept. of Molecular & Medical Pharmacology
UCLA School of Medicine
Center for the Health Sciences 23-120
650 Young Drive South
Los Angeles, CA 90095-1735
USA

Dr. Jean-Philippe Pin **Group Leader GPCR class 3**
CNRS UPR 9023
C.C.I.P.E.
141 rue de la Cardonille
34094 Montpellier
France

David Searls **Technical Advisor, Receptor database**
GlaxoSmithKline
709 Swedeland Road
King of Prussia PA 19406-0939
USA

Ex Officio Members

President, IUPHAR
Paul M. Vanhoutte

Secretary General, IUPHAR
Sue Piper Duckles

Treasurer, IUPHAR
Salomon Z. Langer

Past Chairman, NC-IUPHAR
Robert R. Ruffolo

2005 REPORT TO ICTNS BY IUPAP

Attachment 18
Re Item 11.6

2005 REPORT TO ICTNS[1] BY THE REPRESENTATIVE OF THE INTERNATIONAL UNION OF PURE & APPLIED PHYSICS (IUPAP)

IUPAP and the ICTNS

Concerning questions of terminology, nomenclature and symbols and the work of the ICTNS, it is the IUPAP Commission C2 SUNAMCO which acts as a link with pure and applied physicists in IUPAP and elsewhere.

The IUPAP Commission C2: Symbols, Units, Nomenclature, Atomic Masses & Fundamental Constants (SUNAMCO) [http://www.iupap.org/commissions/c2-mandate.html] has namely amongst its mandates 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.

IUPAP SUNAMCO Report to ICTNS

In reporting to the ICTNS, the following items are of particular interest to SUNAMCO with reference to the proposed agenda of the ICTNS Beijing meeting, August 2005:

[1] IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

2005 REPORT TO ICTNS BY IUPAP

ICTNS § 9. Report of June meeting of BIPM/CCU, §9.1 Redefinition of the kilogram

IUPAP is at present in the process of formulating its own recommendation about the possible redefinition of the kilogram. After a lively discussion within SUNAMCO, a draft recommendation was earlier this year forwarded to IUPAP Council where the intention is to circulate the draft amongst the other IUPAP Commissions prior to direct submission of the recommendation to the CGPM later this year. The IUPAP draft recommendation was presented amongst others at the June meeting of the CCU. Individual SUNAMCO members have also participated in related discussions of this issue in a number of fora, including within the Metre Convention, for instance, the Consultative Committees for Mass (CCM) for Electricity & Magnetism (CCEM) as well as CODATA.

ICTNS §9. PROPOSAL CONCERNING USE OF THE DALTON

In earlier discussions about the dalton at last ICTNS meeting, the IUPAP SUNAMCO Chairman (Dr Sharma) had noted that an earlier recommendation in this field, concerning the adoption[2] of the exact number 12 as the relative nuclidic mass of the carbon isotope of mass number 12, had been made jointly with IUPAC, and it would perhaps be fitting to co-ordinate similarly the current proposal about the dalton.

In the meantime, IUPAP SUNAMCO C2 has made a recommendation and a resolution has been passed by IUPAP council regarding the interim approval to use both the dalton and the unified atomic mass unit for a period of time, as follows:

IUPAP C2 SUNAMCO Resolution 15/Oct/2003

Introduction:
A suggestion has been made in the CCU (communicated to C2 through Brian Petley), that the time has come to replace the name and symbol of the unified atomic mass unit, *u*, with dalton, *Da*. The grounds are that the current name is a mouthful and the need to emphasize the concept of "unified" is long gone. The dalton is widely used in chemical mass spectrometry community (e.g. bio-chemistry). Its use will also bring the polymer chemists into the SI community. There is possible confusion with the astronomical unit *ua*, and people want to use *u* or *U* to denote the unit one. There was considerable comment on this matter from many of the SUNAMCO members. In the short term the proposed change simply endorses the present reality that both the atomic mass unit and Dalton are in use.

Recommendation:
IUPAP should endorse the use of both names, dalton (*Da*) and unified atomic mass unit (*u*) for the atomic mass unit and strongly recommends waiting for an extended period to see which physicists and others prefer to use before making any further decisions.

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[2] 10th General Assembly of the I.U.P.A.P. in 1960

2005 REPORT TO ICTNS BY IUPAP

ICTNS §12. Update on status of 'color' books

The IUPAP 'Red' book SUNAMCO 87-1 "Symbols, Units, Nomenclature and Fundamental Constants in Physics, is by all accounts still popular 18 years after publication of the latest edition. A revision, perhaps with an electronic publication, is needed however.

A number of other organisations such as IUPAC are also quite active in producing a number of guidance documents and books, such as the latter's 'green ' and 'orange' books. Some of these, for instance the 'orange' book[3] "Compendium on Analytical Nomenclature" have certain sections which directly overlap the contents of the IUPAP 'Red' book, such as accounts of the SI and tables of values of the fundamental constants and are already published on the Internet.

It is natural therefore that some amount of coordination would be in order is SUNAMCO is to go ahead with a new edition of the red book. SUNAMCO has already suggested and has had a positive response from IUPAC (both ICTNS and the Analytical Chemistry Division – see ICTNS §13 below).

SUNAMCO members expressed the wish to publish a revised red book, identifying clearly the physics part as distinct from chemistry and other engineering disciplines. While electronic versions are desirable, it was felt there was still a need for paper versions and the for translations.

ICTNS §13 Membership

Under this agenda point, I would like to mention some of the contacts between IUPAC and IUPAP SUNAMCO which have occurred during the period of this report. Amongst others, SUNAMCO was kindly invited by IUPAC Analytical Chemistry Division[4] to its meeting (040217, IAEA, Vienna) to discuss increased collaboration. Items discussed included:

- cooperation about terminology (initial contacts have been made with David Moore (Los Alamos) who is active in producing the latest Orange book – see ICTNS §12.2)
- a possible joint project about Metrological Traceability. A proposal to ICSU entitled "Measurement Traceability – A Fair Basis For Trade" lead by IUPAC, together with IUPAP and UNIDO did not unfortunately get a positive response.
- presentation of a talk at a Minisymposium "Emerging issues in Metrology in Chemistry"[5].

Due to funding restrictions, I am unfortunately unable to attend the Beijing meeting.

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[3] http://www.iupac.org/publications/analytical_compendium/

[4] http://www.iupac.org/divisions/V/index.html

[5] http://www.iupac.org/divisions/V/news/040217/index.html; Pendrill L R 2005 "Meeting future needs for Metrological Traceability – A physicist's view", *Accred. Qual. Assur.*, **10**, no 3, 133 - 9

2005 REPORT TO ICTNS BY IUPAP

I hope your meeting will be successful.

Sincerely

Dr Leslie R Pendrill

IUPAP C2 SUNAMCO Secretary

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REDEFINITION OF THE KILOGRAM AND OTHER SI BASE UNITS

1. ACCOMPANYING DOCUMENTS, OR THOSE DISTRIBUTED PREVIOUSLY

1. Mills et al. Redefinition of the kilogram: a decision whose time has come. *Metrologia* **42**, 71-80 (2005) – distributed previously.
2. Mills. On defining base units in terms of fundamental constants. *Mol. Phys.* (2005) (in press) – attached.
3. Mohr and Taylor. On defining the mole so as to fix the value of the Avogadro constant *N*A when the kilogram is defined so as to fix the value of the Planck constant *h*. CCU/05-29 (2005) – attached.

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2. COVER LETTER FROM IAN MILLS

Date: Tue, 12 Jul 2005 15:42:52 +0100
From: Ian Mills <i.m.mills@reading.ac.uk>
Subject: Redefining some base units of the SI
To: "Lorimer, Jack" <lorimer@uwo.ca>, weirr@rmc.ca, a.r.west@sheffield.ac.uk, k.powell@chem.canterbury.ac.nz, cvitas@joker.irb.hr, Jeremy Frey <j.g.frey@soton.ac.uk>, mweiser@ucalgary.ca, berglund@irmm.jrc.be, martin@quack.ch, peter.atkins@lincoln.ox.ac.uk, "John W. Jost" <secretariat@iupac.org>
CC: Andrew Wallard <awallard@bipm.org>, Barry Taylor <barry.taylor@nist.gov>, Peter Mohr <peter.mohr@nist.gov>, Terry Quinn <terry.quinn@physics.org>, Claudine Thomas <cthomas@bipm.org>, Bob Kaarls <rkaarls@euronet.nl>

Dear Colleagues,

I attach a letter concerning proposals that the CCU are making concerning redefining four base units of the International System of Units (the SI). I also attach four further files which relate to aspects of these proposals. Your comments are invited. We would be particularly happy to receive comments on the proposal concerning the mole. If these proposals were to be discussed at the IUPAC general assembly in August, I would be happy to receive comments early in September, so that I could pass then on to the CIPM at their meeting in October.
Yours sincerely, Ian Mills

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3. SUMMARY LETTER FROM IAN MILLS

From: Ian M Mills, FRS
President of the Consultative Committee for Units

Telephone: +44-(0)118 378 8456
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email: i.m.mills@rdg.ac.uk

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Professor R D Weir, Kingston, Ontario	weirr@rmc.ca
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Professor H K Powell, Canterbury, NZ	k.powell@chem.canterbury.ac.nz
Professor Tom Cvitaš, Zagreb	cvitas@joker.irb.hr
Dr Jeremy Frey, Southampton	j.g.frey@soton.ac.uk
Professor M Wieser, Calgary	mweiser@ucalgary.ca
Dr Michael Berglund, Geel, Belgium	berglund@irmm.irmm.jrc.be
Professor Martin Quack, Zurich	martin@quack.ch
Professor P W Atkins, Oxford	peter.atkins@lincoln.ox.ac.uk
Dr J W Jost, IUPAC Secretariat	secretariat@iupac.org

12 July, 2005

Dear Colleagues,

I am writing to tell you about proposals for redefining some of the base units of the International System of Units (the SI) that were discussed at a meeting of the Consultative Committee for Units (CCU) held at the BIPM 10 days ago. We seek your comments on these proposals. You could reply directly to me (i.m.mills@reading.ac.uk), with a copy to Claudine Thomas at the BIPM, the Executive Secretary of the CCU (cthomas@bipm.org).

Briefly, it is proposed that the kilogram, the ampere, the kelvin, and possibly the mole might all be given new definitions, simultaneously, for the reasons and in the manner that is described below. Changes to the definitions of base units of the SI can only be made by the Conférence Général des Poids et Mesures (CGPM), which meets every four years. It will meet next in October 2007, and then again in October 2011. If all the necessary preliminary conditions were met, and all were agreed, the suggested changes might be implemented at the meeting in 2011. (An earlier proposal that these changes might be achieved at the preceding CGPM meeting in 2007 is now considered to be unlikely.) The changes would be made in such a manner as to preserve continuity, so that the value of the units would not be seen to change, but the effect would be to reduce the uncertainty of measurement of many fundamental constants, and to simplify the SI and make it more robust.

Because one of the proposals concerns redefining the mole, it is particularly important that this should be widely discussed by the chemical community, and it is for this reason that I am sending this letter to many who are involved in the relevant Commissions of IUPAC.

Although the possibility of redefining the kilogram has been discussed for more than ten years, new arguments for the change were presented and reviewed in a paper by myself and four others

published in *Metrologia* earlier this year (Mills, Mohr, Quinn, Taylor and Williams, *Metrologia* 2005, **42**, 71-80). I attach a copy of this paper. Some of the background is also presented in a paper I have written that is currently in press for *Molecular Physics*, of which I also attach a copy (Mills, *Mol. Phys.*, in press July 2005; the attached manuscript is a copy of the proofs and does not include some proof corrections).

The CCU is recommending to the CIPM (Comité International des Poids et Mesures) that the kilogram should be redefined to fix the value of the Planck constant h; the ampere should be redefined to fix the value of the elementary charge e; and the kelvin should be redefined to fix the value of the Boltzmann constant k. The advantages of these changes are discussed briefly below. If these changes were implemented, it would also then be possible to redefine the mole to fix the value of N_A, and the advantage of this final possibility is presented in the third of the attachments to this letter, which is a paper by Mohr and Taylor, CCU/05-29, titled "On defining the mole so as to fix the value of the Avogadro constant …". This final possibility will be of particular concern to chemists, and is the immediate reason why I am sending this letter, and inviting your comments.

The fourth of the attachments to this letter is a copy of the recommendation 2005-U1 from the CCU to the CIPM, which will be discussed at their meeting to be held this coming October. If the proposal to redefine the mole, in particular, were to be discussed at the IUPAC General Assembly in August, and comments were to be returned to me early in September, I would be able to present these views to the CIPM at their meeting in October.

To redefine the kilogram: This proposal is presented in detail in the paper by Mills et al. which is attached. The present definition, which dates from 1889, is in terms of the mass of the International Prototype of the kilogram kept at the BIPM, and it has the effect of fixing the mass of this artefact to be one kilogram exactly. The proposal is to change to a new definition *either* in terms of the mass of the carbon-12 atom, which would fix the value of N_A, *or* in terms of the Planck constant, which would fix the value of h. Although a new definition to fix N_A is simpler to comprehend, a definition to fix the value of h is preferable from the point of view of fundamental physics, and is the choice preferred by the CCU. Either alternative would lead to a significant reduction in the uncertainty in many of the fundamental constants, and would be a definition related to an invariant of nature, in place of an artefact standard whose mass is believed to be drifting relative to a true invariant. Appropriate words for a new definition are presented in the attached paper.

To redefine the ampere: The present definition of the ampere has the effect of fixing the value of the magnetic constant, also called the permeability of free space, μ_0. The elementary charge e has then to be determined by experiment. The proposal is to adopt a new definition that fixes e, so that μ_0 (and hence also ϵ_0) would then have to be determined by experiment. A definition to achieve this might read: "The ampere is that electric current which corresponds to a flow of $1/(1.602\ 176\ ...\ \times 10^{-19})$ elementary charges per second". The advantage of this change is that it would lead to a further reduction in the uncertainty of many fundamental constants, and when combined with the redefinition of the kilogram to fix h it would lead to exactly defined values for h, e, and both the Josephson constant $K_J = 2e/h$, and the von Klitzing constant $R_K = h/e^2$. This would simplify and make more precise all electrical measurements that are now made using the

Josephson and quantum hall effects. Although the electric and magnetic constants ϵ_0 and μ_0 would no longer be known exactly by definition, the uncertainty in their values would be less than 2 parts in 10^9, based on the latest 2002 values of the fundamental constants.

To redefine the kelvin: The present definition of the kelvin has the effect of fixing the triple point of water to be 273.16 K. It can at present be realised with an uncertainty of about 2 mK, but there is a problem in obtaining sufficiently pure water of the appropriate isotopic composition for use in a triple point cell. The Boltzmann constant k has then to be determined by experiment, and it is at present known to about 2 parts in 10^{-6}. The proposal is to redefine the kelvin to fix the value of the Boltzmann constant k, so that the triple point of water would then have to be determined by experiment, and would be known with a similar uncertainty of about 2 parts in 10^{-6}. A definition to achieve this might read simply "The kelvin is that temperature which leads to a value for the Boltzmann constant of 1.380 ... $\times 10^{-23}$ joules per kelvin". Temperature measurements based on this definition would be realised with an uncertainty similar to that achieved under the present definition, but it would have the advantage of being a definition referenced to a fundamental constant rather than a property of water. It would lead to a much reduced uncertainty in the values of the molar gas constant $R = N_A k$ and the Faraday constant $F = N_A e$ (when combined with the redefined ampere).

To redefine the mole: This proposal, which can only be implemented if the kilogram is first redefined to fix h, is explained in the attached paper by Mohr and Taylor. The proposal is essentially to redefine the mole as being that amount of substance that contains exactly 6.022 ... $\times 10^{23}$ elementary entities, thus fixing the value of the Avogadro constant N_A to be exactly 6.022 ... $\times 10^{23}$ mol^{-1} by definition. The present definition of the mole is such as to fix the molar mass of carbon-12, $M(^{12}\mathrm{C})$, to be exactly 12 g/mol by definition, so that the Avogadro constant has then to be determined by experiment. The proposal of Mohr and Taylor would give the Avogadro constant an exact value by definition, at the expense of making the molar mass of carbon-12 a quantity to be determined by experiment.

The value of N_A it is at present known with an uncertainty of about 2 parts in 10^7, but if the kilogram were to be redefined to fix h this would be reduced to about 7 parts in 10^9. If the mole were then to be redefined in the manner proposed, the value of N_A would be known exactly, but the value of $M(^{12}\mathrm{C})$ would itself have an uncertainty of a few parts in 10^9. The actual value of $M(^{12}\mathrm{C})$ would still be (almost exactly) equal to 12 g/mol, but it would not have this value by definition. The advantages of redefining the mole in this way are presented in Mohr and Taylor's paper. Note that if the mole were redefined this way, in addition to the other three redefinitions described above, the Avogadro constant N_A, the molar gas constant R, and the Faraday constant F, would all have exactly defined values, and arguably this definition of the mole would be easier to understand. The disadvantage would be that the molar mass of an atom or molecule would no longer be given by definition as equal to its atomic or molecular weight multiplied by the unit g/mol, although the deviation from this relation would be very small.

I hope that this proposal might be widely discussed by the community of chemists, and I look forward to hearing your views.

Yours sincerely,

Ian Mills

cc. Andrew Wallard, Barry Taylor, Peter Mohr, Terry Quinn, Claudine Thomas, Bob Kaarls

4. RESOLUTION TO CIPM

Final Version, with small mods to 1st "requests", 4 July 2005 rec-U1-final-version.doc

Recommendation U1 (2005)

On possible changes to the definitions of the kilogram, the ampere, the kelvin and the mole

The CCU,

considering

the responsibilities of the CCU, namely:
those given to it at its creation in 1964 by the CIPM concerning the development of the SI,
its responsibility for the drawing up of successive editions of the SI brochure,
the further responsibility of giving advice to the CIPM on matters related to units of measurement;

the importance of taking a broad and profound view of the SI to ensure that it meets the needs of all users while at the same time ensuring that it reflects advances in science and in the understanding of the structure of physics;

the great improvements that have taken place in the accuracy of our knowledge of the values of most of the fundamental constants of physics since the last change in the definition of a base unit in 1983, which fixed the value of the speed of light in vacuum;

the impact on metrology of the application of the Josephson and quantum-Hall effects;

the consensus that now exists on the desirability of finding ways of defining all of the base units of the SI in terms of fundamental physical constants so that they are universal, permanent and invariant in time;

Resolution 7 of the 21st CGPM, 1999, concerning a future definition of the kilogram;

the recent (2005) recommendations from the CCM, the CCEM, and the CCT to the CIPM concerning possible redefinitions of the kilogram to fix, for example, the Planck constant, the ampere to fix the elementary charge and the kelvin to fix the Boltzmann constant, and also from the CCQM in relation to the interests of the chemical community;

the recent recommendation to the CCU from the CODATA Task Group on Fundamental Constants supporting the redefinitions above, and also on redefining at the same time the mole in terms of a fixed value of the Avogadro constant;

the broad view that has emerged from discussions at these meetings of Consultative Committees and the CODATA Task Group, that if changes do take place in the definitions of the kilogram, the ampere and the kelvin, they should all take place at the same time;

that further experimental results are essential, as noted by the Consultative Committees in their Recommendations cited above, before redefinition of the base units could be implemented;

that before such important changes are made to the definitions of base units of the SI, wide publicity must be given to the draft proposals so that the opinion of the broad scientific and other user communities, not directly touched by the Consultative Committee structure of the Metre Convention, can be obtained and taken into account;

requests that

the CIPM approve in principle the preparation of new definitions and *mise-en-pratiques* for the kilogram in terms of a fixed value of the Planck constant, the ampere in terms of a fixed value of the elementary charge, and the kelvin in terms of a fixed value of the Boltzmann constant, so that if the results of experimental measurements are indeed acceptable, all having beren agreed with the various consultative committees and other relevant bodies, the CIPM can prepare proposals to be put to Member Governments of the Metre Convention in time for possible adoption by the 24th CGPM in 2011;

the CIPM give consideration to the possibility of redefining, at the same time, the mole in terms of a fixed value of the Avogadro constant;

the CIPM prepare a Resolution that may be put to the 23rd CGPM in 2007 to alert member states to these activities;

the CIPM further encourage NMIs to pursue national funding to support continued relevant research in order to facilitate the changes suggested above and improve our knowledge of the relevant fundamental constants, with a view to further improvement in the International System of Units.

Molecular Physics, Vol. 103, Nos. 21–23, 10 November–10 December 2005, 2989–2999

Taylor & Francis
Taylor & Francis Group

On defining base units in terms of fundamental constants

I. M. MILLS*
Department of Chemistry, University of Reading, Reading, RG6 6AD, UK

(*Received 1 April 2005; in final form 18 May 2005*)

The definitions of the base units of the international system of units have been revised many times since the idea of such an international system was first conceived at the time of the French revolution. The objective today is to define all our units in terms of 'invariants of nature', i.e. by referencing our units to the fundamental constants of physics, or the properties of atoms, rather than the characteristics of our planet or of artefacts. This situation is reviewed, particularly in regard to finding a new definition of the kilogram to replace its present definition in terms of a prototype material artefact.

1. Introduction and history

Our present system of units for all the quantitative sciences, the International System of Units (abbreviated as the SI, from the French Système International d'Unités), has its origin at the time of the French revolution, when in 1791 Louis XVI set up a commission to recommend a system of weights and measures for world wide use. Although Louis XVI lost his head to the guillotine, the commission and its grand objectives were never abandoned: indeed they were adopted by the revolutionaries, and then later by Napoleon Bonapart. The members of the commission included some of the best French scientists and mathematicians of the time, such as Antoine Lavoisier, an outstanding chemist, Adrien-Marie Legendre and Pierre-Simon Laplace – the leading mathematicians in the country at that time, and Jean-Dominique de Cassini – a distinguished astronomer. They had the grand ambition to establish a new decimal metric system in which the definitions for the base units of length and mass would be based on a natural and universally available model that would be freely and equally available to all the peoples of the world at any time. They also included plans for a new Republican calendar with decimal division of the day and the hour, as well as a new decimal coinage. However, the decimal division of time never became established, and the division into days, hours, minutes, and seconds that had developed from Babylonian times was, in practice, incorporated into the new decimal metric system.

For the definition of the metre they chose one ten millionth of the distance from the pole to the equator (measured on a meridian through Paris, should there be any doubt!), and for the kilogram they chose the mass of a cubic decimetre of pure water at its temperature of maximum density, about 4°C (so that the definition of the kilogram depended on the definition of the metre). For the second they retained, in effect, the existing definition as (1/86 400) of the mean solar day.

They did consider an alternative definition of the metre as the length of a pendulum with a two-second period, for it was known that for small amplitude oscillations the period of a pendulum depends on its length but is independent of the amplitude of motion. However, it does also depend on the local gravitational acceleration, which varies from place to place, and perhaps for this reason they preferred the definition in terms of a quadrant of the earth.† They then instructed two of their members, Jean-Baptist-Joseph Delambre and Pierre-Francois-André Méchain, to go out and realize this definition,‡ and return with a metre stick according to the definition. It took them seven years, and they had to survive many adventures due to the

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†For small amplitude oscillations the period τ of a pendulum is given by the formula $\tau = 2\pi\,(l/g)^{1/2}$, where l is the length of the pendulum and g is the local gravitational acceleration. Using SI units, this gives $\tau/\mathrm{s} = 2\pi(l/\mathrm{m})^{1/2}\,(g/\mathrm{m\,s^{-2}})^{-1/2}$, where (l/m) is the length of the pendulum expressed in metres and $(g/\mathrm{m\,s^{-2}})$ is the gravitational acceleration expressed in metres per second squared. Since π^2 is approximately equal to the gravitational acceleration in metres per second squared, a pendulum of length one metre has approximately a two second period. It would have exactly a 2 s period if $g/(\mathrm{m\,s^{-2}})$ were exactly equal to π^2.

‡To realize a definition is to make use of it to make a measurement.

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revolutionary wars. They surveyed over the ground by triangulation, climbing church towers and measuring the angles to neighbouring towers, to determine the distance from Dunkirk to Barcelona, these two cities being chosen because they lie on the same north–south meridian. Then they scaled that distance up to the distance from the pole to the equator by using astronomical observations. Their story has been beautifully told in the recent book by Ken Alder [1]. In 1799 they returned to Paris with what they said was a metre stick 'according to the definition', and from this was constructed what came to be known as the 'platinum metre of the archives'. A platinum kilogram was also constructed according to the definition of the kilogram, and these two standard artefacts were placed in the archives of France.

However, none of these definitions proved entirely satisfactory. The measurement from the pole to the equator was never made a second time in the years that followed. A cubic decimetre of pure water at its maximum density cannot be easily reproduced with accuracy; and towards the end of the 19th century it was already known that the rotation of the earth was slowing down due to tidal friction, thus compromising the definition of the second. The leading physicists of the time were well aware of the importance to the world of having reliable standards that could be used to define the base units, but the solution was not easy to find. James Clerk Maxwell, in his Presidential address to the British Association of Science in 1870 (when he was just 39 years old, but already recognized as the leading physicist in Britain), said:

> 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.

This showed remarkable foresight, since at the time that he made those remarks neither the mass nor the dimensions of a molecule, nor the frequency of any oscillation within any molecule, were known to more than a rough approximation. But his wisdom is recognized today, as we strive to achieve exactly the kind of reference standards that Maxwell envisaged to define the base units.

Several qualities may be seen as desirable in choosing definitions for the base units of our system, and these are often difficult to meet and often conflict with each other. With the wisdom of hindsight we may summarize them as in table 1.

In the light of these requirements it is instructive to look at our experience with the base units of the metric system (now called the SI) since their first establishment at the time of the French revolution.

The Bureau International des Poids et Mesures (the BIPM, in English: the International Bureau of Weights and Measures) was created in 1875 by the Convention of the Metre, signed at the time by seventeen nations. It is situated at Sèvres, in the Pavillon de Breteuil overlooking the Seine, just over the Pont de Sèvres to the south west of Paris. The Pavillon was generously presented by the French Government as international land (akin to an embassy) for this purpose. Effort was then devoted to constructing international prototypes for the metre and the kilogram to replace the original

Table 1. Desirable qualities for the definition of a base unit.

1. We should choose reference standards that we have good reason to believe are stable and unvarying under translation in time and space on an astronomical scale, i.e. standards that are related to 'invariants of nature'.
2. We must be able to realize each of our definitions with a reproducibility and precision that is as good as that of the best measurements of the quantity concerned at the time. As science advances and we discover how to make measurements with ever greater precision this suggests that we shall have to keep revising our definitions as the years go by to match our ever increasing skills.
3. We should strive to choose definitions that are simple. Not only should the concepts concerned be easy to comprehend but the necessary apparatus to realise the definition should be easy to construct and should preferably not be expensive.
4. We should choose definitions that are freely available to anyone anywhere at anytime.

definitions of 1799, which were seen to be unsatisfactory. The first Conference Géneral des Poids et Mesures (CGPM) was held in 1889, at which the International Prototypes of the metre and the kilogram were sanctioned. These were kept at the BIPM, along with four official copies of the kilogram, but further copies were made that could be compared with the originals and then distributed to the various countries that had signed the metre convention. The international prototype metre and kilogram, and the copies, were constructed from an alloy of platinum-iridium,† and have been kept in a safe at the BIPM ever since. More than fifty copies were made of each. Clearly the prototypes allowed the units to be realized and compared with the copies much more easily and with far greater precision than was true for the 1799 definitions. The revised definitions in terms of the International Prototypes were thus significant improvements. However although they satisfied conditions 2 and 3 in table 1, they clearly fail on conditions 1 and 4, since they are not referenced to 'an invariant of nature', and they are only available at the BIPM. Most workers had to be content with one of the secondary standards distributed to the National Metrology Institutes (NMIs) of the signatory countries.

In fact the definition of the metre has been revised three times since it was first established at the time of the French Revolution, as summarized in table 2. The 1889 definition of the metre was replaced in 1960 because the use of an interferometer with an atomic spectral line as a source allowed reproducible measurements of length to be made, by counting fringes, with far greater accuracy than the scratches could be located at each end of the International Prototype – between which the metre was at that time defined. Since then the development of optical lasers has allowed even more precise measurements than can be made with the krypton spectral line, and the possibility of precise frequency counting up into the visible led to the 1983 definition of the metre which stands today. This definition, which fixes the speed of light in a vacuum to be 299 792 458 m/s exactly, is realized by determining the frequency and hence the wavelength of any one of many optical laser lines, and then making length measurements using an interferometer with the laser line as a source. Using this definition, distances of the order of a metre can now be measured with a relative standard uncertainty of about 1 part in 10^{11} [2].

Table 2. Successive definitions of the metre over the past 200 years.

1799:	The metre is one ten millionth of the distance from the pole to the equator measured on the meridian through Paris.
1889:	The metre is the length of the International Prototype of the metre, made from platinum iridium and kept at the BIPM at Sèvres (1st CGPM, 1889).
1960:	The metre is the length equal to 1650 763.73 wavelengths of the radiation corresponding to the transition between the $2p_{10}$ and $5d_5$ levels of the atom of krypton 86 (11th CGPM, 1960, Resolution 6).
1983:	The metre is the length of path travelled by light in vacuum during a time interval of 1/299 792 458 of a second (17th CGPM, 1983, Resolution 1).

Three things are notable about these successive revisions of the definition. The first is that they were driven by advances in science and technology. We must always define our units with a precision to match the accuracy with which we can make the measurements. The second is that each new definition was chosen to be equivalent to the preceding definition to the accuracy that the preceding definition could be realized. To this extent the revised definitions never changed the value of the unit. The third is that each definition of a base unit fixes – or defines – the value of the reference standard used in the definition. Thus the 1799 definition of the metre fixed the value of the distance from the pole to the equator to be ten million metres exactly; the 1889 definition fixed the distance between the scratches on the International Prototype to be one metre exactly; the 1960 definition fixed the wavelength of the red krypton line to be 605.780 311 nm exactly (this is equal to (1/1650 763.73) m); and finally the 1983 definition fixes the speed of light in vacuum to be 299 792 458 m/s exactly. Note however that the 1983 definition, which stands today, determines the metre in relation to the definition of the second.

The definition of the second as 1/86 400 of a mean solar day failed on criterion 1 in table 1, when it was realized that the rotation of the earth is slowing down by a few seconds a year due to tidal friction. The 'mean solar day' in the definition was then replaced by an appropriate fraction of the tropical year 1900. But it was the development of quartz crystal clocks, and then of atomic clocks, that revolutionized our ability to measure time intervals with high precision. The caesium beam

†The alloy is 90% platinum and 10% iridium. The International Kilogram is a cylinder about 39 mm high and 39 mm in diameter, and the metre is a stick with a tresca cross-section, an X with a central flat, and with two fine scratches at either end at right angles to its length between which the metre is measured.

clock was the first really reliable and relatively simple atomic clock, based on the frequency of the hyperfine transition in a caesium atom, at approximately 9.2 GHz in the microwave spectrum. Each caesium atom may be thought of as a perfect tiny clock, and in the caesium beam clock a stable microwave oscillator is locked on to the frequency of the hyperfine transition. Hence the 13th CGPM (1967–1968, Resolution 1; see also *Metrologia*, 1968, **4**, 43) revised the definition of the second as follows:

> 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.

At its 1997 meeting the CIPM† affirmed that:

> This definition refers to a caesium atom in its ground state at a temperature of 0 K.

This is still the definition at the time of writing (2005). It can be realized with a modern caesium beam clock with a relative standard uncertainty of less than 1 part in 10^{14} (which translates to about one second in 3 million years). Caesium fountain clocks give a more precise realization than caesium beam clocks, and these can now be used to realize the second to better than 1 part in 10^{15} (one second in 30 million years). The advantage of the caesium fountain clock is due to the longer time interval (of the order 1 second) over which the caesium oscillation is compared with the microwave oscillator; for the caesium beam clock this time interval is measured in milliseconds. However, it is likely that the definition of the second in terms of the caesium transition will be replaced at sometime in the next ten years by a definition based on an optical transition of an atom rather than a microwave transition, because the faster 'tick rate' of an optical transition leads to even more precise measurements of time intervals. Research in this field is proceeding at many laboratories around the world, but it is not yet clear which atomic transition or which technique for realizing it will be adopted. It is also important that the frequency of the new optical transition, when it is chosen, can be accurately related to the frequency of the microwave transition of the caesium atom, which is at present used to define the second. This also is the subject of much current research.

2. The kilogram

Returning to the kilogram, the present definition remains as the mass of the International Prototype, just as it was originally sanctioned in 1889. The International Prototype, denoted $\mathcal{K}$, and its six official copies (there are now six such copies), are still kept in the safe at the BIPM. The prototype kilogram has actually been taken from its safe and weighed against the various secondary standard kilograms only three times in the last 114 years, most recently in the late 1980s to the early 1990s. The artefacts are carefully solvent-cleaned, and then washed and dried, before weighing. Using the best modern balances, in which the knife edge suspension of the beam is replaced by flexure strips [3], it is now possible to compare two kilogram masses with a relative standard uncertainty of better than one part in 10^{10} (100 nanograms in a kilogram) [3]. The result of comparing the most recent experiments with previous measurements is that we find that the masses of the various kilogram artefacts are changing relative to each other at the level of several parts in 10^8, equivalent to more than 10 micrograms in a kilogram, over a period of the order 50 years. The conclusion is that we must regard the mass of the International Prototype, $m(\mathcal{K})$, (and indeed the masses of the whole ensemble of all its copies) as uncertain to at least a part in 10^7, and possibly as much as a part in 10^6. This is believed to arise from general wear and tear whenever it is handled, surface chemistry effects due to adsorption (it is stored and weighed in air), and the possible leaching out of gasses occluded within the artefact when it was made.

There is also a more general problem that arises with any definition of a base unit that uses a prototype artefact as a reference. If, for example, we were to accidentally damage the prototype and knock off a chip, it is tempting to say that its mass would be slightly reduced. However in saying that we are instinctively relating the mass of the kilogram to a reference that we believe to be invariant, such as the mass of an atom; but actually *by definition* the mass of the prototype, $m(\mathcal{K})$, always remains equal to 1 kg, so that in fact we are forced to conclude that the mass of all other objects, when expressed in the unit kg, would be slightly increased! This paradoxical situation is inherent in using a prototype to define a unit, and emphasizes the need to use truly stable references for our base units.

The conclusion is that we need a revised and improved definition of the kilogram, which is referenced

†The CIPM is the International Committee of Weights and Measures (Comité Interntaional des Poids et Mesures), which is responsible for running the BIPM between meetings of the CGPM, which occur only once every four years. The members of the CIPM are elected by the CGPM; they include representatives from many different countries, and the membership of the CIPM is rotated regularly.

to an 'invariant of nature', and satisfies the other desirable qualities listed in table 1. This problem has been evident for more than fifty years; it was remarked upon at the second verification of the kilogram around 1950, and confirmed by the third verification around 1990. The two most likely alternative new definitions are discussed below. But a new definition has not yet been implemented, because none of the suggested alternatives can yet be realised with an uncertainty that is significantly lower than the believed instability in the prototype kilogram.

The preceding discussion demonstrates that any definition of a base unit always fixes (or defines) the value of the reference standard that is used in its definition, and thus one approach to any suggested new definition is to ask: what is the quantity that it will fix? There are two possible revised definitions of the kilogram that have been under consideration for a number of years. One is to use the mass of an atom (such as the carbon 12 atom) as a reference; this would fix the value of the Avogadro constant. The other is to use the Planck constant as a reference in the manner described below; this would fix the value of the Planck constant. Both of these alternatives involve defining the kilogram in terms of an invariant of nature. Also both involve changing from a definition in terms of a macroscopic prototype to a definition in terms of a quantum reference on the microscopic scale, either the mass of an atom, or the value of one of the constants of quantum mechanics. This change from the macroscopic to the microscopic scale for the reference of mass has an important consequence discussed further in the next section and in [7]. First, however, we discuss the two alternative definitions.

2.1. *A definition to fix the Avogadro constant,* N_A

The first alternative is the easier to comprehend. At present the best direct experimental determination of N_A is through the X-ray crystal density experiment, in which one measures the lattice spacing d_{220} of a very pure, nearly crystallographically perfect, single crystal of silicon, and also the mass and volume of the crystal. Hence the number of silicon atoms in the crystal may be found, and hence the mean mass of a single silicon atom is determined. Then the Avogadro constant may be found from the mean molar mass of the silicon in the crystal, from the relation

$$N_A = \frac{M(\mathrm{Si})}{m(\mathrm{Si})} \tag{1}$$

where m denotes the mean atomic mass and M the mean molar mass of silicon. This experiment measures the Avogadro constant in terms of the kilogram used to determine the mass of the silicon crystal [4], and the suggestion is that we could reverse this process by fixing the value of N_A and then using the experiment to determine the mass of the international prototype. The uncertainty in our present ability to determine N_A this way would then become the uncertainty in our ability to realise the new definition of the kilogram.

Possible words for a definition of the kilogram to fix N_A might be as follows:

> The kilogram is the mass of a body at rest such that the value of the Avogadro constant N_A is exactly $6.022\,141\,527 \times 10^{23}$ inverse mole.

or alternatively:

> The kilogram is the mass of exactly $(6.022\,141\,527 \times 10^{23}/0.012)$ unbound carbon-12 atoms at rest and in their ground state.

The value of the Avogadro constant that appears in these draft definitions should be chosen to be the best estimate available at the time the definition is revised.

The present relative standard uncertainty in the best determinations of N_A by the crystal density method is about 4 parts in 10^7 [4], i.e. 0.4 ppm, and this would therefore be the uncertainty in the realization of a kilogram defined and realized in this way. Contributions to the uncertainty budget arise from many sources. In this experiment a single large silicon single crystal is grown in a zone refining apparatus, and is machined and polished into a sphere of mass around 1 kg. The sphericity achieved in polishing such silicon spheres is around ± 10 nm, and the volume of the sphere is then determined from its diameter, measured optically. The wavelength of X-rays used to determine the lattice spacing is determined by using an interferometer to compare with a visible laser of known wavelength. Corrections have to be made for the concentration of vacancies and for surface effects on the crystal. A major contribution to the overall uncertainty comes from our imperfect knowledge of the abundance of the isotopes silicon-29 and silicon-30 in the crystal, which enters into evaluating the mean molar mass M(Si). To reduce this contribution there is an international collaboration at present in progress to construct a silicon sphere of pure silicon-28 (for which the estimated budget is around one million euros). Results from this experiment will probably not be known for several years. Those who are working on the Avogadro project believe that they are going to reduce the relative standard uncertainty in the value of N_A determined in this way below 10^{-7},

but it is likely that this will not be achieved inside 5–10 years.

2.2. *A definition to fix the Planck constant, h*

The second alternative is the more difficult to describe. The SI unit of h is (J s) = (kg m^2 s^{-1}), and since the metre and the second are already defined in terms of invariants, if we fix the value of h the effect is to fix the kilogram.

The best direct determination of the Planck constant at present is through the watt balance experiment [5, 6], in which a kilogram standard is weighed against the electrical force generated by a coil in a magnetic field. The geometry of the coil and the magnetic field are difficult to measure with the necessary precision, but they may be eliminated from the analysis by measuring the voltage generated by moving the same coil through the same field at a known velocity, using an interferometer beam reflected off a mirror attached to the coil to measure the velocity. The gravitational acceleration at the position of the apparatus must also be measured. If all the electrical measurements are made using the Josephson effect to measure voltage and the quantum Hall effect to measure resistance, the result of this experiment is a measurement of the Planck constant in terms of the kilogram standard, and the suggestion is that we could reverse this process by fixing the value of the Planck constant and then using the apparatus to measure the mass of the international prototype [5], and to measure mass in general. Possible words for a definition of the kilogram to fix h might be as follows:

> The kilogram is the mass of a body at rest such that the Planck constant h is exactly $6.626\ 069\ 311 \times 10^{-34}$ joule second.

or alternatively:

> The kilogram is the mass of a body at rest whose equivalent energy corresponds to a frequency of exactly $(299\,792\,458)^2/(6.626\,069\,311 \times 10^{-34})$ hertz.

The value of the Planck constant that appears in these draft definitions should be the best estimate available at the time that the definition is revised. The above definitions make use of the Einstein relation $E = mc^2$, and the relation between the energy and frequency of a photon due to Planck and Bohr, $E = h\nu$. Note that the value of the speed of light c is fixed by the definition of the metre. Further details are discussed in [7].

The present relative standard uncertainty of the Planck constant determined from the watt balance experiment is believed to be about 8×10^{-8}, i.e. 0.08 ppm, and this is the most accurate source of information on the Planck constant at this time. Again there are many contributions to the uncertainty, most of which arise from the difficulty of aligning the position and the movement of the coil in the magnetic field [6]. It is also the case that there are at present only three watt balances operating in the world, one at NIST in Washington, one at the NPL in Teddington, and a new one at METAS in Bern which is at present just being commissioned. There are however three others at present planned or under construction, and as with the X-ray crystal density experiment there may be significant progress in this field during the next few years.

2.3. *Complications*

The Planck constant h and the Avogadro constant N_A are related by the equation below, which follows from the theoretical formula for the Rydberg constant expressed in the form developed by Mohr and Taylor [8]:

$$N_A = \frac{cA_r(e)\alpha^2 M_u}{2R_\infty h}. \qquad (2)$$

Here c is the speed of light in vacuum, $A_r(e)$ is the relative atomic mass of the electron on the scale in which $m(^{12}C) = 12$, α is the fine structure constant, M_u is the molar mass constant equal to 1 g/mol exactly, and R_∞ is the Rydberg constant. Apart from h and N_A all other factors in this relation are either exact or are known to a much higher accuracy than either h or N_A, so that (2) effectively becomes a relation between h and N_A. One can thus derive N_A from h, or vice versa. Unfortunately, however, the best current estimate of N_A from the X-ray crystal density experiment, when expressed as a measurement of h by using (2), differs from the best estimate of h from the watt balance experiment by a fractional amount of approximately 1 ppm, well outside the estimated uncertainty in either h or N_A. One of the two experiments is in error, and is being presented with an over-optimistic estimate of uncertainty. The situation is summarized in figure 1.

Partly because of this discrepancy, and partly because neither the X-ray crystal density experiment nor the watt balance has yet achieved the relative uncertainty of about 2×10^{-8} that has generally been considered desirable before a new definition is implemented, no decision has yet been taken on redefining the kilogram. The world is waiting for improved experimental results that would resolve the discrepancy and allow a new

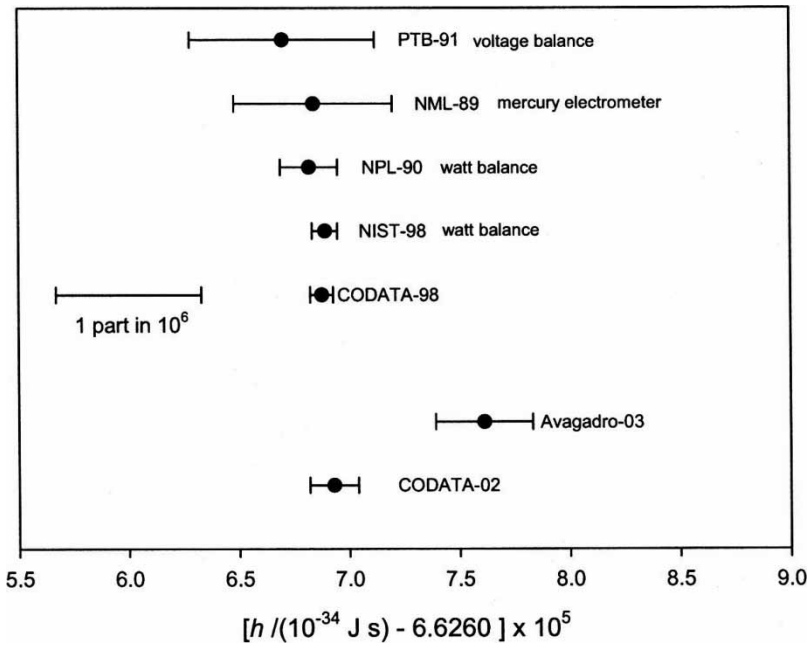

Figure 1. Experimental values of the Planck constant, with their associated uncertainties, obtained since 1989.

definition to be implemented with a relative uncertainty of measurement of perhaps a few parts in 10^{-8}.

3. A microscopic versus a macroscopic reference for the kilogram

A recent paper by Mills and co-workers [7] has drawn attention to an important further consideration involved in changing from a definition of the kilogram referenced to the international prototype, to a definition referenced to the mass of an atom or a fundamental constant such as the Planck constant. Mass metrology is divided into two fields of operation, the one involving the measurement of macroscopic masses, measured in grams and kilograms, and the other involving the measurement of microscopic masses, such as the mass of the electron, and other fundamental particles, and the atoms. The present situation is that relative mass measurements within either of these fields can be made with very much higher precision than that with which we are able to compare masses between the two fields.

For example, it is possible to compare the mass of two kilogram artefacts to better than a part in 10^9, a relative uncertainty of 0.001 ppm. Similarly the mass of an electron m_e can be measured against the unified atomic mass unit m_u (which is equal to one twelfth of the mass of a carbon-12 atom) with a relative uncertainty which is again of the order of a part in 10^9, 0.001 ppm. However when it comes to measuring the mass of any of the fundamental particles in terms of the present SI kilogram, which is the mass of the international prototype, we come back to the watt balance or the X-ray crystal density experiment, and we are only able to achieve about two parts in 10^7, 0.2 ppm, a relative uncertainty two orders of magnitude greater. For example the uncertainty in our best measurement of m_e/kg is at present 0.17 ppm [8], and there is a similar uncertainty in all atomic and particle masses when they are expressed in the present SI kilogram. If, however, we were to redefine the kilogram using an atomic or a quantum reference, for example by choosing the definition of the kilogram either to fix N_A or to fix h, then the uncertainty in all microscopic mass measurements would immediately be reduced by two orders of magnitude. However, there would be a price to pay: the uncertainty in the mass of the prototype, and all macroscopic mass measurements expressed in terms of such a redefined kilogram, would increase by two orders of magnitude.

The comparison goes further. The present best estimates of all the fundamental constants are revised at regular intervals by the CODATA Task Group on Fundamental Constants, established for this purpose, where CODATA denotes the Committee on Data for Science and Technology. The most recent such review is the 2002 review for which the results have been recently published [8], and the two previous such reviews were the 1998 review [9], and the 1986 review [10]. These reviews are based on a least squares adjustment of the constants to fit all available data, and it is a feature

of the results that the best estimates of many of the fundamental constants of physics are strongly correlated, and in particular many of them are correlated to the measurement of mass. For this reason, if we were to redefine the kilogram using an atomic reference the uncertainties of many fundamental constants, when expressed in SI units, would also be reduced by one to two orders of magnitude, in addition to the best estimates of the fundamental particle masses. The situation is illustrated in tables 3 and 4, which are taken from the data in reference [7]. Table 3 lists some of the fundamental constants that are strongly correlated to the measurement of mass, and table 4 lists the values and uncertainties of just a few such constants, by way of example, using (i) the present definition of the kilogram as the mass of the prototype, (ii) using a kilogram defined to fix the Planck constant h, and (iii) using a kilogram defined to fix the Avogadro constant N_A. It will be seen that the actual values of the constants do not change, but their uncertainties are dramatically reduced for either of the definitions based on a microscopic mass reference. It does not make a great deal of difference whether we choose a definition to fix h or to fix N_A, because h and N_A are strongly correlated with each other through the relation given earlier, equation (2). Furthermore, if the kilogram were to be redefined to fix either h or N_A, then future CODATA reviews of the values of the fundamental

Table 3. Some of the fundamental constants affected by redefining the kilogram.

h	Planck constant	μ_B	Bohr magneton
N_A	Avogadro constant	μ_N	Nuclear magneton
m_e	Electron rest mass	V_{90}/V	Conventional volt
m_p	Proton rest mass	A_{90}/A	Conventional amp
e	Elementary charge	W_{90}/W	Conventional watt
K_J	Josephson constant	$u = m_u$	Unified atomic mass unit
Φ_0	Magnetic flux quantum	c_1	First radiation constant
γ_p	Proton gyromagnetic ratio	eV in J	Conversion factor
F	Faraday constant	cm^{-1} in kg	Conversion factor

Table 4. Values, and relative standard uncertainties u_r, for a small selection of fundamental constants, for three alternative definitions of the kilogram, to fix $m(\mathcal{K})$, h, or N_A. Note that the values of the constants are essentially the same in all three cases (although they are quoted to more decimal places for the new definitions); only the uncertainties change.

Quantity $\times 10^8$	Symbol	Numerical value	Unit	u_r
$m(\mathcal{K})$ fixed (CODATA 2002)				
Mass of prototype	$m(\mathcal{K})$	1.000 000 00 (exact)	kg	0.0
Planck constant	h	$6.626\,069\,3\ (11) \times 10^{-34}$	J s	17
Avogadro constant	N_A	$6.022\,141\,5\ (10) \times 10^{23}$	mol^{-1}	17
Electron mass	m_e	$9.109\,382\,6\ (16) \times 10^{-31}$	kg	17
Elementary charge	e	$1.602\,176\,53\ (14) \times 10^{-31}$	C	8.5
Josephson constant	K_J	$483\,597.879\ (41) \times 10^9$	Hz V^{-1}	8.5
h fixed				
Mass of prototype	$m(\mathcal{K})$	1.000 000 00 (17)	kg	17
Planck constant	h	$6.626\,069\,311$ (exact) $\times 10^{-34}$	J s	0.0
Avogadro constant	N_A	$6.022\,141\,527\ (40) \times 10^{23}$	mol^{-1}	0.67
Electron mass	m_e	$9.109\,382\,551\ (61) \times 10^{-31}$	kg	0.67
Elementary charge	e	$1.602\,176\,532\,9\ (27) \times 10^{-31}$	C	0.17
Josephson constant	K_J	$483\,597.879\,13\ (80) \times 10^9$	Hz V^{-1}	0.17
N_A fixed				
Mass of prototype	$m(\mathcal{K})$	1.000 000 00 (17)	Kg	17
Planck constant	h	$6.626\,069\,311\ (44) \times 10^{-34}$	J s	0.67
Avogadro constant	N_A	$6.022\,141\,527$ (exact) $\times 10^{23}$	mol^{-1}	0.0
Electron mass	m_e	$9.109\,382\,5510\ (40) \times 10^{-31}$	kg	0.044
Elementary charge	e	$1.602\,176\,5328\ (80) \times 10^{-31}$	C	0.50
Josephson constant	K_J	$483\,597.879\,14\ (81) \times 10^9$	Hz V^{-1}	0.17

constants could only result in very small or zero changes in the values.

For these reasons Mills *et al*. advocate in their paper [7] redefining the kilogram to fix either h or N_A, as described in the preceding section. They do not make an explicit choice between these two alternatives, although they list the relative advantages of each. Not only would such a change define the SI unit of mass to an invariant of nature, but it would lead to a significant increase in the accuracy (or reduction in the uncertainty) of many of the fundamental constants. Because the uncertainty in the Josephson constant, K_J, would also be reduced, and because this is used in all precise electrical measurements today, electrical metrology would also be significantly improved. Further details are given in [7].

Finally we must consider the effect redefining the kilogram in this way on macroscopic mass metrology. The effect of such a change would be that the mass of the international prototype, $m(\mathcal{K})$, would no longer be 1 kg by definition, but would have to be determined by experiment. The watt balance and the X-ray crystal density experiment would become experiments to determine the mass of the prototype. The uncertainty of 0.17 ppm that previously applied to measurements of h and N_A would under the new definition apply to the experimental determination of $m(\mathcal{K})$. If the redefined kilogram were based on the best estimate of either h or N_A at the time of the redefinition, as suggested in the draft definitions in section 2, then initially the mass of the prototype $m(\mathcal{K})$ would still be exactly one kilogram, but subject to uncertainty. We would have $m(\mathcal{K}) = 1.000\,000\,00\ (17)$ kg, where the 0.17 ppm relative uncertainty that at present applies to many fundamental constants would be transferred to the mass of the prototype. A similar uncertainty would apply to all macroscopic mass measurements when expressed in terms of the new SI kilogram.

Although this may seem at first to be a disadvantage, in practice macroscopic mass metrology could continue exactly as at present by continuing to use the mass of the prototype as an intermediate reference. It is suggested by Mills *et al*. that the best estimate of the mass of the prototype should be called 'the conventional kilogram', with the symbol $m(\mathcal{K})_{07}$ if the change is made in 2007, just as the conventional values of the Josephson and von Klitzing constants that were established in 1990, $K_{J\text{-}90}$ and $R_{K\text{-}90}$, are at present used in electrical measurements. Alternatively the mass of the prototype could be described as part of the *mise-en-pratique* for realizing the new definition of the kilogram, so that macroscopic mass metrology could still be referenced to the mass of the prototype $m(\mathcal{K})$, which might be regarded as a secondary standard to be given an assigned value that might be revised if necessary as the experiments are improved.

In any case it will clearly always remain important to pursue research into watt balance and X-ray crystal density experiments in order to improve our knowledge of the relation between microscopic and macroscopic mass measurements. The importance of such research does not depend on whether the kilogram is redefined or not. If it is redefined, such experiments will be needed to maintain and improve our knowledge of $m(\mathcal{K})$; and if we retain the present definition they are needed to evaluate and improve our knowledge of all microscopic masses and the fundamental constants. If we do redefine the kilogram it is unlikely that future changes in the correction factor $[m(\mathcal{K})/\text{kg}]$, which will initially be equal to one, will ever be greater than 0.1 ppm, but in any case it will always be known for use in those cases where very precise macroscopic mass measurements are important. Thus macroscopic mass metrology could continue as at present, but its dependence on the mass of an artefact of questionable stability would be brought into the open.

4. Possible redefinitions for other base units

The kilogram is not the only base unit of the SI that may be considered for redefinition in the next ten years. The metre and the second have already been discussed in section 1. However, the ampere and the kelvin may also both be considered as possible subjects for redefinition.

The ampere is at present defined in terms of the force between two wires carrying electric currents, and the effect of this definition is to fix the value of the magnetic constant μ_0 (also called the permeability of free space). However, the realization of this definition can only be achieved indirectly, and at present all precise electrical measurements are made in terms of the conventional values of the Josephson and von Klitzing constants established in 1990, $K_{J\text{-}90}$ and $R_{K\text{-}90}$, using the Josephson and quantum hall effects. These conventional values are used because of the difficulty of determining the true values of these constants with a precision to match the repeatability of the experiments. An alternative way of defining the ampere, and hence all of our electrical units, would be in terms of a number of elementary charges per second. This would fix the value of the elementary charge e, at the expense of making the magnetic constant μ_0 a quantity to be determined by experiment. The uncertainty in our knowledge of e would be replaced by a corresponding uncertainty in our knowledge of μ_0, and it is to be considered which is the more convenient way of establishing the values of

these constants. The advantage of redefining the ampere to fix e is that, if this were done at the same time as redefining the kilogram to fix h, then the Josephson constant $K_J = 2e/h$ and the von Klitzing constant $R_K = h/e^2$ would both become exactly known constants, so that we could dispense with the conventional values $K_{J\text{-}90}$ and $R_{K\text{-}90}$, and precise electrical measurements would be simplified and significantly improved.

The Kelvin is at present defined in terms of the temperature of the triple point of water. Although this is not an 'artefact' definition, it does pose problems for its realization in obtaining pure water free from dissolved gases, and there is also uncertainty relating to the question of isotopic composition. An alternative would be to define the Kelvin to fix the value of the Boltzmann constant k_B. This may not immediately lead to an increased precision in our ability to measure temperature, but it would define the kelvin in relation to a fundamental constant, and if this change were made at the same time as redefining the kilogram to fix N_A, or to reduce the uncertainty in N_A if we were to fix h, then the molar gas constant $R = N_A k_B$ would become an exactly known constant. The possibilities of fixing e and fixing k_B are both discussed further in [7].

5. Conclusions

Definitions of the base units of the International System, the SI, need to be made with care, to achieve those desirable qualities listed in table 1. They should also be considered in the light of their effect on the uncertainties of the fundamental constants of physics. The present definition of the kilogram, in terms of a prototype artefact, dates from 1889, and is overdue for revision. The most likely way to redefine the kilogram is either to choose a definition to fix the value of the Avogadro constant, N_A, as considered in section 2.1 of this paper, or to fix the value of the Planck constant, h, as considered in 2.2. Although our ability to realize either of these definitions for macroscopic mass metrology would be no better, at present, than our ability to measure mass in terms of the prototype artefact, redefining the kilogram in this way would have two immediate advantages:

1. It would give us a definition of the SI unit of mass in terms of a true invariant, rather than an artefact of questionable stability;
2. It would lead to a significant reduction in the uncertainty with which many of the fundamental constants of physics are known. This would give a substantial improvement in the accuracy with which many measurements in science, particularly electrical measurements, can be made.

The price to be paid would be that the mass of the prototype would no longer be known by definition, but would have to be determined by experiment. However, macroscopic mass metrology could continue unchanged with masses still expressed in terms of the mass of the prototype, this being taken to be a secondary standard in the *mise-en-pratique* for realizing the new definition.

It may seem that redefining the kilogram as described here, with the objective of reducing the uncertainty in the values of the fundamental constants, is a book-keeping exercise, of no real significance, for of course it involves no experiment to obtain the increased precision in the constants. However, the reduced uncertainty of the fundamental constants would be a real and significant improvement in the basis of the International System of Units, in the sense that calculations involving the fundamental constants should really be related to the value of the Planck constant, or the mass of the carbon atom, rather than the mass of the prototype kilogram sitting in a safe at Sèvres.

The Comité International des Poids et Mesures (the CIPM) will consider proposals for the redefinition of the kilogram, and possibly other base units of the SI, in its future meetings, with advice from their various Consultative Committees. If it should so decide, a resolution to implement a new definition of the kilogram, and possibly other base units, could be put to the next General Conference on Weights and Measures (CGPM) which will take place in October 2007, or the following CGPM in 2011.

Acknowledgement

I am indebted to my colleagues who are the co-authors of reference [7] from whom I have learned so much of this subject. I am also indebted to Richard Davis at the BIPM, and to my colleague Catherine Deeley, for their comments on a first draft of this manuscript.

Dedication

This paper is offered in honour of Ben Widom, who is an inspiring scientist in the field of statistical mechanics and thermodynamics, an outstanding lecturer, and a valued friend.

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CCU/05-29
(With minor editorial changes added at the conclusion of the CCU meeting.)

On defining the mole so as to fix the value of the Avogadro constant N_A when the kilogram is defined so as to fix the value of the Planck constant h

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Introduction and Summary

The current SI definitions of the metre, second, and candela fix the values of the speed of light in vacuum c_0, the ground state hyperfine splitting of the Cs 133 atom $\Delta\nu(^{133}\mathrm{Cs})$, and the maximum spectral luminous efficacy K_m to have the exact values $c_0 = 299\,792\,458$ m s^{-1}, $\nu(^{133}\mathrm{Cs}) = 9\,192\,631\,770$ Hz, and $K_\mathrm{m} = 683$ lm W^{-1} for radiation of frequency $\nu = 540$ THz, respectively. Further, for the reasons given in the recent paper of Mills, Mohr, Quinn, Taylor, and Williams [Metrologia **42**(2), 71-80 (2005)] and some of the other documents submitted to the 17th meeting of the CCU, it is likely that the kilogram will be redefined so as to fix the value of the Planck constant h, the ampere will be redefined so as to fix the value of the elementary charge e, and the kelvin will be redefined so as to fix the value of the Boltzmann constant k. The purpose of this note is to show how even with definitions for the six SI base units metre, kilogram, second, ampere, kelvin, and candela that fix c_0, h, $\nu(^{133}\mathrm{Cs})$, e, k, and K_m, it is still possible to define the remaining SI base unit, the mole, so as to fix the value of the Avogadro constant N_A. If such a definition were also implemented, it would mean that five of the seven SI base units would be tied to well recognized fundamental physical constants and that some important additional constants would be exactly known, for example, the Faraday constant F, the molar gas constant R, and the molar volume of an ideal gas V_m at a specified reference temperature T_0 and pressure p_0. Looking to the future, it may also eventually be possible to redefine the second so as to fix the value of the Rydberg constant R_∞, thereby allowing six of the seven SI base units to be tied to universal constants that do not refer to properties of a particular particle or atom.

Our analysis is given in some detail in the Appendix, but its main conclusions can be summarized as follows: The mole can be defined so as to fix the value of the Avogadro constant

N_A even if the kilogram is defined so as to fix the value of the Planck constant h with negligible negative consequences and many positive benefits. Simply stated, this can be done by uncoupling the definition of the mole from the kilogram as in the current definition, with the result that the molar mass of carbon 12 is no longer defined to be 12 g mol^{-1}. Nevertheless, the current definitions of the unified atomic mass unit u (also called the dalton, Da) and atomic mass constant m_u, namely, 1 u = m_u = $m(^{12}C)/12$, where $m(^{12}C)$ is the mass of the carbon 12 atom, as well as the definition of the molar mass constant, M_u = g mol^{-1} = 10^{-3} kg mol^{-1}, can remain unchanged. The relative atomic mass $A_r(X) = m(X)/m_u$ of an entity X of mass $m(X)$ can also remain unchanged, in which case $A_r(^{12}C) = 12$ as at present, and existing compilations of relative atomic masses of atoms, of molecules, and of the elements as they naturally occur remain unchanged. Indeed, the new definition can be implemented in such a way that the only consequence of the change is that the relation between molar mass and relative atomic mass, which is presently given by $M(X) = A_r(X)M_u$, would become $M(X) = (1 + \kappa)A_r(X)M_u$. The additional multiplicative factor $1 + \kappa$, where κ is experimentally determined [see Eq.(12)], is irrelevant (i.e., it exactly cancels) for molar-mass ratios in chemical reactions. Moreover, the factor is initially equal to 1, since initially $\kappa = 0$ with an uncertainty of only about 2×10^{-9}, and κ may be expected to remain equal to 0 to within about this amount indefinitely and to have an even smaller uncertainty. This means that for all practical purposes, molar mass can continue to be calculated from the product $A_r(X)M_u$, because the only effect of the factor $1 + \kappa$ would be a possible shift in the product and an additional component of uncertainty that are significantly smaller than the uncertainty of (i) practical mass measurements involving the macroscopic kilogram with which molar mass values are used; and (ii) values of $A_r(X)$ of real substances, which depend on stoichiometry, isotopic composition, impurity content, etc. Finally, we note that the fact that F, R, and V_m would become exactly known constants as a consequence of defining the mole so as to fix the value of N_A means that, with the exception of the coupling constants of the basic forces of Nature, such as the fine-structure constant α (and those constants dependent upon them), all fundamental constants not related to a specific particle or atom would be exactly known.

Appendix

1. Current definitions and relationships. The current definition of the mole reads

1. 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; its symbol is “mol.”

2. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.

(In this definition, it is understood that unbound atoms of carbon 12, at rest in their ground state, are referred to.)

An important consequence of this definition is that one mole of any specified entity X contains the exact same number of entities. The Avogadro constant N_A is defined as this exact number of entities per mole, and its current recommended value is $N_A = 6.022\,1415(10)\times10^{23}$ mol^{-1} [1.7×10^{-6}]. [Here and throughout this note, all values of fundamental constants are 2002 CODATA recommended values—see P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **77**(1), 1-107 (2005).]

The molar mass M(X) of a specified entity X is the mass of one mole of X, and thus it follows from the above definition of the mole that the molar mass $M(^{12}\mathrm{C})$ of the carbon 12 atom is $M(^{12}\mathrm{C}) = 0.012$ kg mol^{-1} exactly. It is convenient to introduce the molar mass constant M_u, defined by

$$M_u = 10^{-3}\ \mathrm{kg\ mol^{-1}}, \tag{1}$$

in order to have the compact notation

$$M(^{12}\mathrm{C}) = 12M_u. \tag{2}$$

It also follows from the definitions of molar mass and N_A that for any entity X

$$M(\mathrm{X}) = N_A\, m(\mathrm{X}), \tag{3}$$

where m(X) is the mass of entity X. The molar mass of an entity is an important quantity, because it may be used to determine the amount of substance of the entity in a given sample.

The masses of atoms and molecules are most conveniently and accurately expressed not in the SI unit of mass, the kilogram, kg, but in the unified atomic mass unit u (also called the dalton, Da). A non-SI unit, it is defined according to

$$1\ \mathrm{u} = m_u = \frac{m(^{12}\mathrm{C})}{12}, \tag{4}$$

where m_u is called the atomic mass constant. The relative atomic mass A_r(X) of an entity X, which is a dimensionless quantity, is then defined as

$$A_r(\mathrm{X}) = \frac{m(\mathrm{X})}{m_u}, \qquad (5)$$

which together with Eq. (4) gives $A_r(^{12}\mathrm{C}) = 12$ exactly.

Equation (3) with X = ^{12}C, together with Eqs. (2) and (4), yield

$$M_u = N_A m_u, \qquad (6)$$

and Eqs. (3), (5), and (6) lead to the following well-known expression for the molar mass of an entity X:

$$M(\mathrm{X}) = A_r(\mathrm{X}) M_u. \qquad (7)$$

2. New definitions and relationships. Because the current definition of the mole depends on the kilogram, and we assume that the kilogram will be defined so as to fix the value of h and that the other SI base units will be defined as discussed in the Introduction and Summary, it is not possible to define the mole so as to fix the value of the Avogadro constant N_A while retaining its dependence on the kilogram. However, if one defines the mole so as to fix the value of N_A in a way that is independent of the kilogram, then there is no inconsistency between the definitions of the kilogram and mole. Such a definition of the mole might read

1. The mole is the amount of substance of a system that contains exactly $6.022\ 141\ 5\times10^{23}$ elementary entities; its symbol is "mol."
2. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.

Clearly, this definition (i) retains the basic definition of the Avogadro constant as the number of entities per mole; (ii) fixes the value of the Avogadro constant to have the exact value $N_A = 6.022\ 1415\times10^{23}\ \mathrm{mol}^{-1}$ without placing any restrictions on the kilogram; (iii) retains the basic relationship between the molar mass of an entity X and the mass of the entity as given in Eq. (3); and (iv) is more readily understood because of its simplicity than is the current definition while at the same time makes clear that the mole is a measure of a number of specified entities and has nothing to do with mass. Also, the new definition has no direct effect on the definitions of the molar mass constant, unified atomic mass unit, atomic mass constant, and the quantity relative atomic mass, as defined in Eqs. (1), (4), and (5). However, it does affect Eqs. (6) and (7), because they depend on the exact relation $M(^{12}\mathrm{C}) = 12M_u$, which is a consequence of the current definition of the mole but is not necessarily true for the new definition. Thus, since

Eqs. (6) and (7) are not necessarily consistent with both the current definitions of the quantities that appear in them and the new definition of the mole, it is necessary to reconsider the definition of molar mass, or relative atomic mass, or even in principle the molar mass constant, in order to obtain new expressions consistent with the new definition of the mole. We address this issue in detail in the following two sections, although for simplicity we do not consider the possibility of redefining more than one of these quantities at the same time. As we shall see, the issue can be resolved quite satisfactorily.

3. Preferred approach to the calculation of molar mass. Obviously, the new definition of the mole does not alter the relationship between the molar mass of an entity X, the Avogadro constant, and the mass of the entity as given in Eq. (3). However, because of the new definition, the molar mass in Eq. (3) is changed to $\tilde{M}(\mathrm{X}) = \tilde{N}_\mathrm{A} m(\mathrm{X})$, where $\tilde{M}(\mathrm{X})$ is the molar mass of X when the mole is defined so that the Avogadro constant has the fixed value $\tilde{N}_\mathrm{A}$. On the other hand, the Avogadro constant N_A in Eq. (6) cannot be replaced by the fixed value $\tilde{N}_\mathrm{A}$ without either changing the definition of M_u or m_u given in Eqs. (1) and (4), or including an additional correction factor in Eq. (6). We make the latter choice here and write

$$(1 + \kappa)M_\mathrm{u} = \tilde{N}_\mathrm{A} m_\mathrm{u}, \tag{8}$$

where

$$\tilde{N}_\mathrm{A} = (1 + \kappa)N_\mathrm{A}, \tag{9}$$

and so the updated version of Eq. (7) is

$$\tilde{M}(\mathrm{X}) = (1 + \kappa)A_\mathrm{r}(\mathrm{X})M_\mathrm{u}. \tag{10}$$

The factor $1 + \kappa$ can be evaluated from the definition of the Rydberg constant, $R_\infty = c_0\alpha^2 m_\mathrm{e}/2h$, where α is the fine-structure constant and m_e is the mass of the electron, and the exact relation $M(^{12}\mathrm{C}) = 12M_\mathrm{u}$ given above based on the current definition of the mole, which together yield

$$N_\mathrm{A} = \frac{c_0\alpha^2 A_\mathrm{r}(\mathrm{e})M_\mathrm{u}}{2R_\infty h}, \tag{11}$$

and hence

$$1 + \kappa = \frac{\tilde{N}_\mathrm{A}}{N_\mathrm{A}} = \frac{2R_\infty \tilde{N}_\mathrm{A} h}{c_0\alpha^2 A_\mathrm{r}(\mathrm{e})M_\mathrm{u}} = 1 + 0.0(1.9)\times 10^{-9}. \tag{12}$$

The numerical value of the multiplicative factor $1 + \kappa$ is based on the 2002 recommended values of the relevant constants under the assumption that the kilogram and mole are defined so as to fix the value of the Planck constant h and Avogadro constant $\tilde{N}_A$ to have their 2002 values but with no uncertainties, and also on the expectation that within the next year the relative standard uncertainty of the fine-structure constant $u_r(\alpha)$ will be reduced to about 9×10^{-10} from its present value of 3.3×10^{-9}. [If the latter value of $u_r(\alpha)$ is used, the relative standard uncertainty $u_r = 1.9\times10^{-9}$ in Eq. (12) becomes $u_r = 6.7\times10^{-9}$.] The important points concerning the factor $1 + \kappa$ are that it will initially be equal to one when the new definition of the mole is adopted, should never deviate from unity by more that a few parts in 10^9, and its uncertainty should be sufficiently small that it can be considered negligible in calculating molar mass for use in the determination of amount of substance, since amount of substance determinations in the real world rarely, if ever, have relative standard uncertainties that approach 1×10^{-6}. Thus, for all practical chemical measurements, which is where the mole is used, molar mass should still be obtainable from the product $A_r(X)M_u$ as in Eq. (7).

4. Other approaches to the calculation of molar mass. Equation (10), our preferred approach, is essentially one of three straightforward ways of adhering to a useful overall guiding principle, namely, that because Eq. (7) is so familiar and widely used, it would be helpful to retain an expression of the same general form for calculating molar mass when the mole is redefined so as to fix the value of the Avogadro constant. Although we prefer the solution offered by Eq. (10) for reasons that will soon become apparent, and therefore have included only it in the above Introduction and Summary, there are two other possible approaches that should be mentioned. In fact, all three possibilities may be summarized as follows:

Use a new equation for molar mass. This is the preferred approach as given by Eq. (10).

Define a new atomic mass constant. Equation (8) can be written in the form of Eq. (6) by defining a new atomic mass constant given by

$$m'_u = m_u/(1 + \kappa). \qquad (13)$$

However, in this approach all existing compilations of relative atomic mass $A_r(X)$ would no longer be valid and would have to be converted to compilations of $A'_r(X) = (1 + \kappa)A_r(X)$.

Further, the relative standard uncertainty $u_r = 1.9\times10^{-9}$ of the factor $1 + \kappa$ is larger than that of some values of $A_r(X)$ and thus would increase the uncertainties of these values, in some cases by more than an order of magnitude. Finally, the compilations would have to be revised every time CODATA issued a new set of recommended values, because the value of $1 + \kappa$ [see Eq. (12)] will likely change slightly from one least-squares adjustment to the next due to slight changes in the recommended values of R_∞, α, and $A_r(e)$. By way of comparison, such slight changes from unity are inconsequential in the first approach. Thus, we believe our preferred approach is the better of the two.

Define a new molar mass constant. Equation (8) can be written in the form of Eq. (6) by defining a new molar mass constant given by

$$M'_u = (1 + \kappa)M_u. \qquad (14)$$

However, as already noted above, since the molar mass constant is simply a special name and symbol for the unit gram per mole, symbol g mol^{-1} = 10^{-3} kg mol^{-1}, it would be inconsistent with the general practice in the International System of Units (SI), where there are 22 SI units with special names and symbols, to incorporate into the molar mass constant an experimentally determined multiplicative factor. Thus, we again believe that our preferred approach is advantageous.

Finally, we note that Eq. (8) can be written as 1 u = $m_u = (1 + \kappa)M_u/\tilde{N}_A$, which is to be compared to the corresponding relation from Eq. (6) based on the current definition of the mole, 1 u = $m_u = M_u/N_A$.

Attachment 20 Re Item 17

Date: 2005-08-08
To: Leiv Sydnes, President, IUPAC
cc Bryan Henry, David Black, John Jost, Bernardo Herold
From: Jack Lorimer
Re: Final Recommendations on Membership of ICTNS for 2006-2007

The recommendations resulting from consultation among the Officers and TMs of ICTNS, for your consideration, are:

Chairman:	John W. Lorimer	- continuing
Secretary:	Bernardo J. H. Herold	- continuing
Titular Members:	Ture Damhus	– continuing
	Roberto Marquardt	- continuing
	Alan D. McNaught	– new; has agreed to serve if approved
Associate Members:	Reuben J.-R. Hwu	– continuing
	Wlodzimierz Kutner	– new; has served as Div. V representative on ICTNS, and has been nominated by Div. V. Has not replied that he is wiling to serve, but I expect he will do so in Beijing.
	Patrick A. G. O'Hare	– continuing

Divisional Representatives

No information received

Representatives of Other Organizations

BIPM:	Dr. Andrew Wallard
ISO:	no confirmation to date – probably Mr Anders Thor
IUBMB	Dietmar Schomburg
IUCr	Prof. André Authier
IUNS:	to be named
IUPHAR:	no confirmation to date – probably Dr Michael Spedding
IUPAP:	Dr. Leslie Pendrill

Attachment 21
Re Item 10.2

Report to ICTNS from Division II

IUPAC General Assembly, Beijing, August 2005.

The Division Committee has completed a very successful meeting at Beijing with an average attendance of sixteen. It had proved impossible to complete the election process prior to the General Assembly but the results of the elections are now expected to be known by the end of September. The election will be used to strategically strengthen the Division by electing two in the area of molecules and one each in materials and atoms. The meeting considered five proposals for new projects and the approval of some of these will enable the funding for the current biennium to be fully committed.

The Red Book

The new edition of the Red Book, a project initiated in the Division and now coordinated by Division VIII is now in the very final stages of editing of proofs and is expected to be published before the end of this year.

Commission II.1

This Commission and some of its subcommittees met at Beijing prior to the General Assembly. The publication of some revised atomic weights is awaiting Council approval and a new project to continue this work during the next two years was discussed and approved in principle at the Division Committee meeting. The Commission continues to make substantial progress in the projects currently in its portfolio.

The naming of new elements

The name for the element with atomic number 111 was approved during the current biennium. The joint IUPAC/IUPAP Working Party with responsibility for the assignation of priorities for the discovery of new elements had decided that here was not sufficient new published data to justify a re-examination of claims for the discovery of elements above number 111 during the past twelve months but the Division Committee decided at Beijing to now invite it to carry out another review. This request

will be initiated immediately it is intended to again follow the new naming procedures, which have worked satisfactorily for elements numbers 110 and 111.

Sub-Committee on Materials Chemistry

This is an Interdivisional Sub-Committee and invitation to membership has been extended to all interested Divisions. The area of Materials Chemistry remains fast growing as is evident from the exceptional growth in interest in and contributions to the journals now dedicated to the area by both the ACS and the RSC. The editors of both of these journals attended the meeting of the Sub-committee held at Beijing.

Work has commenced on a project initiated by the sub-committee, under the leadership of Professor Peter Day, to define the area of Materials Chemistry. A second project aimed at producing a glossary of terms for nanotechnology has being formulated involving Divisions I, II and IV and will be initiated during this biennium. The Sub-Committee has also carried forward the series of Workshops in advanced Materials and WAM III, organised by a local committee led by Professor Ron Sanderson, will take place in Stellenbosch, South Africa, September 4th to 8th 2005. The Sub-committee will shortly set up a website linked to the IUPAC site.

John Corish,
August 15th 2005,
Beijing.