

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Minutes of the meeting in Beijing, China 16 and 17 August 2005

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

T Damhus (TM)
R Marquardt (TM)

J Corish (TM representing Div II)
J Kahovec (TM representing Div IV)
W Kutner (AM representing Div V)
Y Shiva (TM representing Div VI)
A McNaught (TM representing Div VIII)

Observers: A P Rauter (NR of Portugal, representative elect of Div III)
L Glasser (chairman CPEP)
A N Davies (secretary CPEP)
M L Bonardi (TM Div V)
A Jenkins (chairman task group revision of the Gold Book)
H Ogino (Science Council of Japan)
D Barden (RSC Young Observer)

1. Opening remarks and introduction of participants.

Prof Lorimer called to order the second plenary meeting of ICTNS. The agenda (Attachment 1), which had been previously circulated to all members, was approved unanimously.

Prof Lorimer presented the regrets of Dr W Val Metanowski (TM), Dr Patrick A.G. O'Hare (AM) Prof Reuben Jih-Ru Hwu (AM), Prof Jeremy G. Frey (TM, representative of Division I), Prof Gerrit-Jan Koomen (TM, representative of Division III, who asked to be replaced by Prof Amélia P Rauter), Prof Urban Forsum (TM, representative of Division VII), Dr Andrew Wallard, Bureau International des Poids et Mesures (BIPM), Mr Anders J. Thor, International Organization for Standardization (ISO / TC12), Prof Richard Cammack, International Union of Biochemistry and Molecular Biology (IUBMB), Prof André Authier, International Union of Crystallography (IUCr), Prof Michael Spedding, International Union of Pharmacology (IUPHAR) and Dr Leslie R. Pendrill, International Union of Pure and Applied Physics (IUPAP).

2. Minutes of Ottawa meeting

The following corrections to the minutes of the meeting in Ottawa 2003, previously circulated with the agenda were approved unanimously:

Errata already mentioned in the minutes of the “core” titular members in Lisbon 21 – 22 August 2004:

Front page, second title line:

Replace:

Interdivisional Committee Nomenclature and Symbols (IDCNS)

by

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Pg. 4, heading of last paragraph:

Replace

5.4 Macromolecular Chemistry Division

by

5.4 Macromolecular Division.

Pg. 4, last line:

Replace

Division VIII would be responsible in future for all nomenclature problems

by

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

Pg. 7, paragraph 9, line 3:

Replace

“Dalton”

by

“dalton”

Pg. 10, right column, line 4:

Replace

Dr. Anders Thor

by

Mr. Anders Thor

Erratum detected after the Lisbon meeting:

Headings of Items 9 – 13 lack a point after the number.

3. Minutes of meeting of core Titular Members, Lisbon

Draft minutes of the meeting of core titular members held in Lisbon 21 – 22 July 2004 were circulated to all members of ICTNS by e-mail on 12 December 2004, together with 12 attachments as a single pdf file.

A corrected version of the minutes was circulated together with the agenda. The corrected version of the minutes was approved unanimously (Attachment 2). This approval did not imply the ratification of the decisions, which are to be discussed under item 5 of the agenda.

4. Business arising from the Ottawa meeting not covered in Lisbon

It was commented that the question of whether to hold also plenary meetings in even years was not dealt with in Lisbon to the point of making a recommendation. The discussion was postponed to item 18 of the agenda.

5. Business arising from the Lisbon meeting. Ratification of decisions

Since the meeting in Lisbon was not a plenary one, the decisions were opened to renewed discussion on whether to ratify them or not.

5.1. Nomenclature in Technical Reports (Item 8 of the Lisbon minutes)

The discussion paper of Dr Metanomski and the comments of Prof Lorimer and Prof Herold on this discussion paper (Attachments 10 and 11 respectively of the Lisbon minutes) were reconsidered and the decisions recorded in the Lisbon minutes were ratified.

5.2. Freeman polemic on the mole (Item 3.1 and Attachments 2, 3 and 4 of the Lisbon minutes).

Prof Lorimer drew the attention of the meeting to four letters to the editor of Journal of Chemical Education with comments regarding the paper

R. D. Freeman, SI for Chemists: Persistent Problems and Solid Solutions, *J. Chem. Educ.* **2003**, *80*, 16-21.

The following three letters referred directly to the article of R. D. Freeman:

P. J. Karol, (with reply of R. D. Freeman), *J. Chem. Educ.* **2004**, *81*, 800

T. Cvitas, *J. Chem. Educ.* **2004**, *81*, 801

R. D. Freeman, *J. Chem. Educ.* **2004**, *81*, 802

A fourth letter, referring to the related problem of the redefinition of the kilogram:

P. J. Karol, The Kilogram and the Mole Redux, *J. Chem. Educ.* **2005**, *82*, 212

prompted the editor of that journal, J. W. Moore to add to the last letter a note, which ends as follows:

“Henceforth I will entertain manuscripts from official groups whose purview is defining and naming units, where the manuscripts inform readers and allow for input to said groups, but I will not entertain manuscripts that initiate proposals for defining and naming units.”

In view of what has been stated in the letters and in the note of the editor, it was considered that IUPAC should promote the publication of an article or a series of articles in Journal of Chemical Education, where the official position of IUPAC regarding questions like the adoption of SI units and the redefinition of the kilogram should be brought forward in a way, which would be adequate to the readership of that journal. It was also suggested that the collaboration of Prof Peter Atkins and Prof Ian Mills should be requested. This approach would thus avoid the character of a personal polemic and lend institutional weight to the statements. At the same time, the article(s) should have a didactic character, which would appeal to the readership of a journal that has an educational aim.

The chairman was asked study the possibility of submitting a specific project in order to allow a task group to carry out this idea with some financial support, as well as to start exploratory contacts with the editor of Journal of Chemical Education, and ask

Prof Peter Atkins and Prof Ian Mills for their collaboration. Prof Atkins had already expressed his support.

5.3. Inclusion of Chairman and Secretary as editors of PAC

Prof Lorimer informed the meeting that the position of ICTNS, as recorded in the minutes of the Lisbon meeting, regarding the roles as editors of the Chairman and Secretary of ICTNS, was accepted by the Secretary-General. The inside covers of *Pure & Applied Chemistry* mention since January 2005 the present chairman and secretary of ICTNS as “Editors, IUPAC Recommendations and Technical Reports”.

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.

Prof Lorimer informed the meeting that, when discussing with the editor of *Chemistry International* (CI) the view of ICTNS, that the period of public review of recommendations should be shortened to three months, the editor explained that, from the date CI receives the request to announce the public review of a provisional recommendation, until the printed copy of the next issue of CI can be mailed, at least two months will have passed by. In the ensuing discussion, the point was raised that in future there may perhaps be only an electronic edition of CI. It was argued, however, that in the near future this should not happen, because there are still too many regions in the world, where access to internet is not easy, and the hard copy of CI is important as the most effective way of disseminating information.

As a conclusion, the meeting decided to abstain from requesting a change of Bylaw B2.11.

6. Workshop on *Pure Appl. Chem.*, at IUPAC Secretariat

A report on the meeting of the Chairman and Secretary of ICTNS at the IUPAC Secretariat, Research Triangle Park, North Carolina on 2004-11-21 had been distributed with the Agenda of the present meeting for information (Attachment 3).

6.1. Editorial positions on *Pure Appl. Chem.*

See Attachment 3 and Item 5.3. of these minutes.

6.2. Establishment of Editorial Advisory Board (EAB) for *Pure Appl. Chem.*

Prof Lorimer reminded the meeting that he had been appointed to sit on the Editorial Advisory Board (EAB) for *Pure Appl. Chem* as Chairman of ICTNS. He also informed that there was not yet any agenda for the next meeting of the EAB.

6.3. Review of Manuscript Central

See Attachment 3, and Item 9.1 of these minutes.

7. Report to IUPAC Council

The Biannual Report of ICTNS to IUPAC Council had been distributed with the Agenda (Attachment 4). Prof Lorimer commented that the time available to write that report had been very short, but the meeting praised its conciseness. It was also commented that the activity of answering of queries from the public, which is mentioned in the report, contributes to the public image of IUPAC.

8. Current status of manuscripts: in the review cycle, completed, published

8.1. Technical Reports

8.2. Recommendations

Both aspects of the status, Technical Reports, as well as Recommendations are covered in Attachments 5 and 6, which were distributed previously together with the Agenda. The first one is a summary according to the records of the Chairman of ICTNS; the second one is the automatic output from the ManuscriptCentral system.

Prof Marquardt and Dr McNaught criticized the fact that the status reports do not specify which Division originated each manuscript.

The officers of ICTNS were asked by the members for specific information on several manuscripts to which they replied.

Prof Kutner mentioned that often, authors of IUPAC projects do not comply with instructions for authors on preparation of IUPAC documents to be published in *Pure & Applied Chemistry*. He suggested that the IUPAC-Secretariat, upon notifying authors of approval of their project proposals, should inform them about the exact location of these instructions on the web by including e. g. a link in the message of approval. Prof Lorimer reminded that he had written a memo to all Division Presidents about the recent changes in the Guidelines and Procedures and asked them to draw the attention of task group chairmen to these documents. He admitted, however, that Division Presidents have sometimes passed on manuscripts to ICTNS, without checking if they complied with the Guidelines.

9. Procedures for processing Technical Reports and Recommendations

9.1. Manuscript Central

Some members raised the possibility of exchanging reviews of particular manuscripts among members of ICTNS, in order to have a more widely shared responsibility, e. g. among all five core titular members for the final editorial decision concerning each manuscript. Others opposed the idea of having a panel to examine the reviewer's reports and deciding collectively, arguing that the mission of the editors and that of the reviewers should be kept separate from each other, and that there were advantages in knowing the opinions of reviewers independently from each other. In the ensuing discussion, the consequences for the administrative complexities and the length of the review process were also analyzed, in case an additional loop would be introduced in the process. A suggestion to have a WebBoard for discussion of manuscripts by ICTNS members was also suggested, but was opposed by others.

After lengthy discussion, the following procedures were approved.

1. For external reviewers (i. e., non-members of ICTNS) or for ICTNS members who do not wish to have their reviews read by others except by the officers of ICTNS and the authors, the usual procedures of review using Manuscript Central will apply.
2. For those who wish to exchange reviews, their reviews should be sent to the Secretary of ICTNS via ordinary e-mail (i. e., outside of Manuscript Central), including permission to exchange with others. When two or more such reviews have been received, the Secretary will circulate them to the appropriate members for comment within a two-week period. At the end of this time, each reviewer should submit an independent and final review to Manuscript Central.
3. This procedure is an experiment, which will be reviewed at the ICTNS meeting in 2006. The purpose of the experiment is to see if exchange of reviews will ultimately enhance the quality of the final versions of manuscripts.
4. The officers of ICTNS may, as occasion demands initiate exchanges of reviews among selected members to discuss controversial points involving terminology or nomenclature.

Prof Herold mentioned that, for a number of manuscripts, he had verified that the quality of the reviews was sometimes substantially improved by involving referees outside ICTNS and even IUPAC. The selection of outside reviewers has not always been easy. He asked for opinions on how the editors could have access to a database from which they could draw names and addresses of specialists for a variety of fields. Dr Damhus suggested that the Union Advisory Committee might be a way to get National Adhering Organizations to cooperate in the search for adequate referees for specific areas. Dr McNaught said, that the database used by the Royal Society of Chemistry might be consulted, subject to RSC permission. Dr Damhus expressed also his view that all members of ICTNS could be involved in the selection of referees. No immediate solution was found for these problems, but some of the members present suggested that they might help through their contacts to point out referees in those cases, where the officers of ICTNS had difficulties in finding adequate persons. Prof Lorimer offered to explore the possibility to set up a master list with the help of the Secretariat.

As a more technical aspect of ManuscriptCentral the question was asked about which are the built-in deadlines for referees uploading their comments. For Technical Reports it is one month. As for Recommendations, there were some doubts about the present situation. Prof Lorimer offered to ask Dr John Jost to change, if necessary, the system in a way that the deadline would be five minus one months, five months being the public review period.

9.2. Procedures for reviewing TRs and Recommendations

The Chairman reminded members that the procedures for reviewing Technical Reports and Recommendations as published in the 2004 – 2005 Handbook should be revised regarding some aspects. The deadline for submitting changes to the materials for the Handbook used to be end of December, but since this part of the Handbook may not be published in printed form, but only on-line, the deadline may become more flexible. He would propose some changes later this year and submit them to ICTNS member by e-mail for comment. Members are also invited to submit other changes, if they consider them necessary.

10. Reports from IUPAC Division Representatives

10.1. Division I, Physical and Biophysical Chemistry

Prof Marquardt presented orally a report of the representative of Division I, Prof Jeremy Frey, who had sent earlier his regrets for not being able to attend the meeting, and sent his report by fax to Beijing (Attachment 7).

10.2. Division II, Inorganic Chemistry

Prof John Corish, as representative and Vice-President of Division II apologized for not having been able to present a report of Division II prior to the meeting, because of the resignation of Prof Gerd Rosenblatt. He presented orally a report for the biennium 2004 – 2005.¹

Prof Marquardt asked about the status of the new Periodic Table, and the new atomic weights. Since no document had yet been presented to ICTNS, these data could not yet be published by IUPAC. Prof Lorimer pointed out that nevertheless the new atomic weights should be used in the preparation of the new Green Book.

10.3. Division III, Organic and Biomolecular Chemistry

Prof Rauter, replacing as observer Prof Gerrit-Jan Koomen, representative of Division III, highlighted some of the aspects of the report, which had been previously distributed together with the Agenda (Attachment 8). See also remarks of Dr McNaught under item 10.8.

10.4. Division IV, Polymer

The report of Division IV had been distributed previously together with the Agenda (Attachment 9). Dr Kahovec informed that the Sub-Committee on Macromolecular Terminology had been renamed “Sub-Committee on Polymer Terminology and Nomenclature”. In the ensuing discussion, it was commented that there might be an overlap between Divisions IV and VIII, regarding nomenclature.

10.5. Division V. Analytical Chemistry

Prof Kutner used the report of Division V to Council (Attachment 10) as a basis for emphasizing in his comments those aspects, which were of interest to ICTNS, mainly the publications of Division V. He pointed out that, although the report to Council mentioned the Recommendation “Terminology in Soil Sampling” (from Project 2005-033-1-500) as being under review, it had been published already in *Pure Appl. Chem.* **77**, 827–841 (2005).

Prof Kutner informed that a project proposal was recently submitted in Division V, entitled “Specific heat capacity functions of combustion gases and fuel gas components” with Prof. H. Gamsjaeger as the Task Group Chairman. He asked the meeting for an opinion on whether the document with the results of the project would be considered as a Technical Report rather than a Recommendation. The report would compile critically evaluated data and would recommend formulas, but neither terminology, nor nomenclature nor symbols. It was considered that such a document would indeed fall under the category of Technical Report.

¹ A report was sent to ICTNS after the meeting (see Attachment 21)

The part of the report concerning the Orange Book, in spite of this subject having been scheduled for Item 15.2, took place as follows:

Prof Kutner explained that the updating of the Compendium of Analytical Nomenclature would be made on the internet. He mentioned the poster display during the IUPAC General Assembly and a PowerPoint presentation on the Orange Book.

Some members pointed out that the term “Nomenclature” in IUPAC usage has a more restricted meaning than in general, and that one should replace it thus by “Terminology” in the title of the Orange Book.

It was also pointed out that in the Orange Book, as well as in other documents of Division V, the entries regarding the definition of pH needed to be reexamined, and that there should be no contradictions with the corresponding entries in the new web editions of the Green and Gold Books. In spite of this urgent question having been discussed in great detail, there were still some open question, which would have to be settled by e-mail after the General Assembly.

Some questions raising from paragraph 2.2.b of the Divison V report to Council, concerning the IUPAC Stability Constants Database (SCDB) were discussed. Some participants were concerned that there is no free access to SCDB, including for ICTNS officers and referees appointed by ICTNS. It was also pointed out that the names for ligands were very often outdated and not according to IUPAC nomenclature. Also terminology and units are in part obsolete. The question was raised, if it would be possible to use the period of three years, during which the company Academic Software transfers the responsibility for the management and maintenance of SCDB to IUPAC, to remedy this situation.²

² NOTE: Subsequent to this meeting, Prof K Powell, President of Division V, pointed out that, any further discussion about the concerns expressed by some ICTNS members about the SC-Database, should be based on the following information about the arrangements for publishing and maintaining the database in a sustainable manner:

1. The costs to users of the SC-Database only cover the current costs plus any involved in evolving a different or improved system for future users, and therefore the service, although not being free, is still non-profit. The Bureau and the Executive are fully aware that providing this service bears a significant cost (see below).
2. At the Bureau meeting in October 2004 a clear decision was made that SC-Database was a valuable resource for IUPAC and that the project should continue to be supported. The Bureau indicated quite explicitly that SC-Database should not be "given away". It asked for development of a Business Plan that would establish the cost-effectiveness of continued IUPAC support of the project (i.e. the project must be at least self-supporting). Considerable effort has gone into this Business Plan and there has been wide consultation. Regular reports have been made to the Executive. In this context one can comment that the Bureau views this exercise with SC-Database as very important because there are a number of other databases that will in future require IUPAC support on a commercial basis as and when their external sources of support terminate.
3. It is not necessary to go into all of the details regarding costs of providing SC-Database to users. However, at present IUPAC contributes around \$4,500 per year to support the data entry program. This does not cover the very significant voluntary contribution made by the President and other members of Division V. When their involvement is taken over by those who are currently paid to enter data, the costs will likely approach \$6-7,000. When the management of the database passes to IUPAC, there will be the cost of management of the master files and data conflation by a (yet-to-be-appointed) software expert at the secretariat (10-15% position); capital and depreciation costs for computer facilities required for management of Master files and source code; advertising; administration costs (registered mailing of CD's and manuals; etc). All of these costs must be covered by sales. With these costs alone, if one is considering, say, 40 sales per year, each item will cost several hundred dollars. If forward planning for a sustainable product involves placing the database on the web, when IUPAC moves to a secure server, conversion to web-compatible software will be a very significant cost, as the programming will have to be out-sourced. To effect the editing of terminology and nomenclature, considered as desirable by some members of ICTNS, there would be additional, significant costs incurred at the secretariat by the expert who alone has access to and exercises management of the master files (excluding any costs of an IUPAC project to guide this work). Adding these “projected” costs will double the price of the product to users. – This brief analysis overlooks the fact that

Dr Damhus referred in positive terms to a paragraph on page 5 entitled “Better Communication”, and recommended that, if one envisages enhanced involvement of IUPAC representatives at IUPAC-sponsored conferences, they should be given the opportunity to make a presentation of IUPAC. He considered that the existing material for a slide show would be too generic for that purpose. He considered the Division representations mentioned on page 8 of the same report as very important, and wished that such opportunities would also be used to increase the visibility of IUPAC nomenclature. This led to comments that most chemistry journals do not oblige the authors of submitted papers to use IUPAC nomenclature and terminology. Dr Barden confirmed that the Royal Society of Chemistry leaves it to the authors to comply or not to IUPAC rules, and that the referees usually do not pay much attention to such aspects. Prof Herold pointed out, that not many people are trained in applying IUPAC nomenclature rules, and that he was frequently asked whether there exists a directory with IUPAC names, which would allow to retrieve an IUPAC name for somebody who has no competence in that field.

Prof Sheva referred to the list of current projects of the report and asked what happens to projects as old as 1999, and if they could still be considered as relevant.

10.6. Division VI, Chemistry and the Environment

The report of Division VI had been distributed together with the Agenda (Attachment 11).

Prof Sheva highlighted some aspects of the report, and admitted, that IUPAC terminology, nomenclature and symbols were not always followed in documents resulting from IUPAC projects, also because not all were published in *Pure and Applied Chemistry*. mentioned that e. g. the editors of the IUPAC book series at J. Wiley did not make such demands. It was then recommended that, at least, project titles should be formulated according to IUPAC standards.

10.7. Division VII, Chemistry and Human Health

Academic Software has exclusive copyright over all of the software. When management passes to IUPAC, a significant royalty will be due to Academic Software, albeit on a diminishing scale with time. Any new copyright agreement will embody and preserve the intellectual property interests of Academic Software.

4. Regarding terminology and nomenclature: This is absolutely not the responsibility of Academic Software. On a most generous basis, they have committed to developing the software for database assembly and interrogation, for peripheral programs and for accepting new data for conflation into the database. Any matters related to “quality control” of data etc. are the responsibility of Division V. Division V have been aware of terminology matters, at least since the early 90's, but the work-load of accessing and abstracting the literature and verifying and validating the entered data, and correcting the thousands of errors transferred from the earlier book volumes, has been large enough. If the Division in the future sees editing of ligand names to consistent IUPAC format as a priority then it will have to find the funds to do so via the project system after management of master files is transferred to IUPAC. ICTNS is most certainly aware of some of the difficulties: Division V inherited over 1000 “old” ligand names from the book volumes; many current authors do not name their ligands but refer to them as L1, L2 etc. or they use trivial names; the field size for ligand names in the database must be limited to a realistic value; many new ligands have several names given in SciFinder (CAS naming), while some do not appear in SciFinder at all. One should note that most working chemists will search the database by trivial names as commonly used in the literature, by structure fragment, ligand class etc., not by full IUPAC name.

It is hoped that this information provides ICTNS with a more accurate picture of the nature and current status of the SC-Database project and demonstrates that the consultation team that is working with Academic Software on IUPAC's behalf are accurately carrying out the wishes of the Bureau and Executive.

A report had been attached to the previously distributed Agenda (Attachment 12). Since Prof Forsum was not be able to attend, no questions were raised. Prof Lorimer mentioned the Project no. 2000-014-1-700 - Recommendations for the use of nanotechnology in clinical laboratories referred tyo under paragraph 6.2.4 of the report, and pointed out that in the title one should replace “nanotechnology” by “microtechnology”. The manuscript would rather have to be considered as a Technical Report, than as a Recommendation.

10.8. Division VIII, Chemical Nomenclature and Structure Representation

The report of Division VIII had been previously distributed with the Agenda (Attachment 13). Dr McNaught added some comments and the following recent informations: An article on the IUPAC International Chemical Identifier InChI in *Chem. & Eng. News* is presently in print, and there will be a chapter on the InChI in the next edition of The ACS Style Guide.

The new Red Book is now scheduled for November 2005, and it is hoped that the new Blue Book will appear by middle 2006.

Prof Herold distributed a page with the comments of Prof Gerritt-Jan Koomen to the Recommendations on Graphical Representation of Stereochemical Configuration, which Prof Koomen wished to be read by the members of ICTNS (Attachment 14).

11. Reports from Representatives of Other International Organizations

11.1. Bureau International des Poids et Mesures BIPM

A report (Attachment 15) had been distributed previously to the meeting, together with the Agenda.

11.2. International Organization for Standardization ISO/TC12

No report has been received.

11.3. International Union of Biochemistry and Molecular Biology IUBMB

A report had been received, and was distributed together with the Agenda before the meeting (Attachment 16). Prof Lorimer informed that Prof Dietmar Schomburg has been designated successor of Prof Richard Cammack as representative in ICTNS.

11.4. International Union of Crystallography IUCr

No report has been received.

11.5. International Union of Nutritional Sciences IUNS

No report has been received.

11.6. International Union of Pharmacology IUPHAR

A report had been received, and was distributed together with the Agenda before the meeting (Attachment 17).

Prof Kutner pointed out that the work on a database for receptors mentioned in the report is of considerable interest to a project on biosensors listed in the report of Division V. He considered the task of giving systematic names to all ligands

interacting specifically with the receptors difficult to achieve, in view of its huge size.

11.7. International Union of Pure and Applied Physics IUPAP

A report had been received, and was distributed together with the Agenda before the meeting (Attachment 18). Prof Kutner mentioned that Division V was trying to avoid in their documents contradictions with the recommendations of IUPAP Commission C2: Symbols, Units, Nomenclature, Atomic Masses & Fundamental Constants (SUNAMCO).

12. Report of June meeting of BIPM/CCU Redefinition of the kilogram – pros and cons

A file with correspondence and publications from Prof Ian Mills, assembled by Prof Lorimer, had been distributed with the Agenda prior to the meeting (Attachment 19).

The question of the need to redefine the kilogram and other SI units was discussed, and the following resolution was approved:

Re: Possible changes to the definition of the kilogram, ampere, kelvin and Mole.

At its August 17, 2005 meeting in Beijing, the ICTNS adopted the resolution given below concerning changes to the definitions of several SI base units. This resolution shall be copied to the Executive Committee of IUPAC in accordance with the terms of reference of ICTNS, which include the requirement:

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

The ICTNS resolution is:

Given that the ICTNS agrees with the desirable qualities for the definition of a base unit, as paraphrased from I. M. Mills, *Molecular Physics* **103**, 15 July (2005):

1. Reference standards should be chosen that are believed, with good reason, to be stable and unvarying under translation in time and space on an astronomical scale (i.e., are “invariants of nature”).
2. Each definition of a reference standard should be able to be realized experimentally with a reproducibility and precision that are as good as those of the best measurements at the time, a requirement that suggests that revisions to standards will continue to be necessary as scientific skills increase.
3. Definitions should be simple, embracing concepts that are easy to comprehend and apparatus to realize the definition that is easy to construct and not excessively expensive.
4. Definitions should be available freely to anyone anywhere and at any time.

the ICTNS resolves that the resolution (appended below) of the Consultative Committee on Units (CCU) of the BIPM to the CIPM concerning possible redefinition of the kilogram, ampere, kelvin and mole be supported by IUPAC.
Beijing, China 2005-08-17

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 been 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.

13. New IUPAC Periodic Table

As had been already verified under Item 10.2, no submission of a new Periodic Table has been yet received by ICTNS.

14. Review of sections of the *IUPAC Handbook 2004-2005*:

14.1.

Procedure for Publication of IUPAC Technical Reports and Recommendations

See Item 9.2.

P

14.2. **Guidelines for Drafting IUPAC Technical Reports and Recommendations**

See Item 9.2.

15. Update on status of 'color' books

15.1. **Red Book – Nomenclature of Inorganic Chemistry**

Dr Damhus reminded that he had prepared a document after the Lisbon 2004 meeting of ICTNS core members, which explained in more detail than the preface, the changes made in relation to the 1990 edition. He reported that the second proofs would be sent by the Royal Chemical Society to the authors by mid September. He expressed his hope that publication will take place in November.

15.2. Orange Book – Compendium of Analytical Nomenclature

This subject had been already dealt with under Item 10.5.

15.3. Green Book – Quantities, Units and Symbols in Physical Chemistry

Prof Marquardt was asked to provide more information on the progress in updating the Green Book, than that contained in the fax of Prof Frey (Attachment 7). The urgency was justified by Prof. Davies when he reported on the current position of the XML Data Dictionaries project, in particular with regard to difficulties in cooperating with the compilers of the revised Green Book (see Item 15.6). A general discussion about the Green Book ensued during which it was revealed that a manuscript of the latest version of the Green Book could be made available in Beijing. During the meeting, photocopies of that manuscript were eventually distributed by Prof Roberto Marquardt who is a Green Book coauthor and who pointed out that this draft copy was only available in printed form and not as an electronic file. The draft is dated 3rd July. He said he believed that the earliest the full manuscript can be made available will be October as there is still significant revision taking place. Prof Lorimer requested some more details as to what work is still outstanding and Prof Marquardt replied that, although the basic page layout will not change some of the values for the fundamental constants have to be revised and with them all of the worked examples on around 150 pages. When this work is completed, the document index will need to be generated. Prof Davies pointed out that CPEP had passed a motion calling for the re-printing of the Green Book 2nd edition, should an electronic version of the completed Green Book 3rd Edition not be received by the Secretariat by the end of the General Assembly. With this in mind, and taking into account, that the earliest possible date for delivery is now the end of October 2005, Prof Davies asked Dr McNaught how long the RSC would require to bring the manuscript to print. Dr McNaught responded that they would need just under a year from receipt of the manuscript, so we would not see the 3d edition of the Green Book in print until late August, early September 2006.

Prof Lorimer pointed out that an ICTNS review would probably be required, and following a short discussion, the presence of new Recommendations in the Green Book will mean, that this will have to be a full ICTNS and public review of 5 months. This would delay the publication to early 2007. Taking this into account, John Jost would not be requested to proceed to a reprint of the 2nd edition. It was decided to wait for the 3rd edition to be sent to ManuscriptCentral and a clear deadline was established for this: 31 of October. The official review process would take 5 months. In order to try to speed up this process, it was also decided that ICTNS should start by reviewing unofficially the 3rd July Draft that was available. Prof Marquardt was requested to make sufficient copies available. The following 11 reviewers were nominated: Prof J Corish, Prof R Weir, Prof J Lorimer, Dr A Wallard, Dr L Pendrill, Dr T Damhus and Dr J Kahovec, Dr W Kutner, Dr M Bonardi, Prof B Herold, Dr A McNaught. Dr S Stein was to be requested to carry on as chairman of the Standard XML Data Dictionaries for Chemistry project while ignoring the next edition of the Green Book. Prof Lorimer pointed out, that there were Green Book entries, which may have to be

revised, but Dr McNaught explained, that these Green Book terms had been already added to the Gold Book 2nd edition, which is the basis for the XML version and as such had already undergone ICTNS review and approval. These 'Green Book' entries in the Gold Book, many of which were text equivalents of the original mathematical expressions, would be updated in the normal course of events following publication of the new Green Book.

15.4. Blue Book – Nomenclature of Organic Chemistry

Prof Herold pointed out, that the information on the status of the new Blue Book had been already given by Dr McNaught under Item 10.8 (Attachment 13). The question of whether the expected revised version would have to be submitted to a new period of public review or not, was not decided, and Prof Herold was asked to clarify some points by correspondence with the authors and Division VIII.

15.5. Silver Book – Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences

The report of Division VII, under "Revision of the Silver book" states that "no progress can be reported because a working group leader has been hard to find. The item has high priority and is not abandoned." Since Prof Forsum was unable to attend the meeting, there was no discussion.

15.6. Gold Book and XML Data Dictionaries

A report on XML data dictionaries by Dr S Stein and a report on the Gold Book by Prof A Jenkins had been distributed prior to the meeting together with the Agenda (Attachment 14).

The status report on the work on XML data dictionaries was the first to be discussed. The meeting congratulated Dr S Stein and his team for the impressive work already achieved, and expressed their concern over his resignation. The discussion of his complaints regarding the lack of cooperation from the authors of the Green Book revision has been already reported under Item 15.3. The meeting expressed their hope that Dr S Stein would accept, in view of the measures, which were decided, an invitation to reassume his responsibility as task group chairman.

Prof Davies clarified the decisions made at the CPEP meeting whereby the initial review of the XML version would be treated as a simple copy-editing task with Cheryl Wurzbacher being requested to carry out a comparison between the original printed recommendations and the XML version. Any corrections would be communicated to Miloslav Nic for correction. Once this copy editing review was completed only then would the Divisional Reps of ICTNS be requested to look at their respective contents and then as a review of the system rather than content. A fresh project proposal would then be considered when the final version of the Green Book 3d edition is available.

Prof Jenkins was also congratulated for the progress with the updating of the Gold Book. When asked to update the number of 104 terms already processed in March, he informed that the number was now 127. Prof Lorimer wished to know what was planned for the current Gold Book online version. Dr McNaught explained that there were actually two

versions, one hosted at the RSC and one on www.iupac.org with technically different search engines. It was planned to keep the versions alive and in place and their future would be part of the plans for the migration and update of the whole of the iupac.org website currently underway. Prof Lorimer pointed out that there were some incorrect definitions and symbols in the online version arising from mistakes in the original recommendations and proposed that the task group should collect these errors. ICTNS will be responsible for ensuring that the Divisions take appropriate action on error reports from any source. Prof Davies pointed out that the Colored Books also are used by the legal establishment and as such any changes in definitions must be audit-trailed, with the older versions remaining available online and being clearly flagged that they are now superseded with reciprocal links to the new version. Prof Kutner mentioned that Dr D Moore, Past President of Division V, Analytical Chemistry believed IUPAC would be publishing no more books. Prof Davies thought that this was not completely true. CPEP had been trying to raise the bar for projects which stated that they wanted to publish a book as we have a somewhat poor reputation in the past of bringing out books which nobody wants read at great cost to the Union, late and well over the agreed page limit. Many authors have been able to get a book deal with normal scientific publishers. Since the very successful move to self-publishing, IUPAC no longer has an “official” publisher.

The question was discussed whether the updated version of the Gold Book would be subject to ICTNS review. Prof Lorimer pointed out that there were definitions in the printed edition of the Gold Book, which were wrong, sometimes the symbols were wrong, and others have been superseded by definitions in Recommendations that are more recent. He also considered important that the traceability of definitions needed to be improved. It was understood, however, that this kind of revisions should be an ongoing long-term activity, which should not delay the current project of producing the XML versions but rather be introduced step by step at a later stage.

Concerning new data standards, Prof Davies pointed out that there were three new Recommendations from CPEP falling in the category of Scientific Data Standards. One was ThermoML: an XML Recommendation “XML-Based IUPAC Standard for Experimental, Predicted, and Critically Evaluated Thermodynamic Property Data Storage and Capture” as well as two JCAMP-DX standards, one on EPR/ESR JCAMP-DX for EMR, and one covering chromatography and mass spectrometry JCAMP-DX V.6.00 for Chromatography and Mass Spectrometry Hyphenated Methods. Prof Lorimer confirmed that these standards would undergo the shortened ICTNS three-month review, as they have been in the public domain for some time and already undergone extensive industrial review.

15.7 Purple Book – Compendium of Macromolecular Terminology and Nomenclature

Dr Kahovec informed that the Recommendations in the first edition of the Purple Book are still valid, and that the second edition would have no

substantial changes. The question was raised whether the title might be changed to read “Compendium of Terminology and Nomenclature of Polymers”, for the same reasons as the ones, which were given for changing the name of the Division. This suggestion was, however not further discussed during the meeting, and therefore nothing was decided about a possible change of the title, which would have to be agreed not just by ICTNS, but also by the editor and authors, as well as by Divisions IV and VIII.

It was considered that attention should be paid to consistency of the nomenclature used in the Purple Book with “A Guide to IUPAC Nomenclature of Organic Compounds (Recommendations 1993)”.

16. Meeting of JCGM Joint Committee for Guides in Metrology

Dr Ales Fajgelj was proposed to represent IUPAC at the meeting of JCGM Joint Committee for Guides in Metrology.³

17. Membership

See Attachment 20, which had been distributed together with the Agenda prior to the meeting. Prof Lorimer informed, that, according to the latest information, the Division Representatives would be probably the same as presently, with the exception of the following replacements:

Division I: Prof Ron Weir, Division III: Prof Amélia Rauter, Division VIII: Prof József Nyitrai. There were still no news about Division II, and Division VII.

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.

Because of poor attendance at Beijing, and the need to continue the discussion on several open projects, Prof Lorimer will try to arrange a plenary meeting in 2006.

19. Adjournment

The meeting was adjourned on the afternoon of August 17, 2005.

³ NOTE: Subsequent to the meeting, Dr Fajgelj considered that he had too many commitments, and Prof. Paul de Bièvre agreed to do this job.

List of Attachments

Attachment number	Referred to in Item(s)	Subject
1	1	Agenda
2	3	Minutes of the ICTNS Meeting of “Core” Titular Members in Lisbon, Portugal, 21 – 22 July 2004
3	6	Report of Workshops on Manuscript Central (MC) and Pure & Applied Chemistry (PAC) at IUPAC Secretariat, Research Triangle Park, North Carolina, 20 – 21 November 2004
4	7	Report of ICTNS to IUPAC Council 2005
5	8	ICTNS Chairman’s Status Summary of Recommendations and Technical Reports August 2005
6	8	Status Report on Technical Reports and Recommendations: 2004-5, Output from ManuscriptCentral on 2005-05-27
7	10.1 and 15.3	Division I Report to ICTNS
8	10.3	Division III Report
9	10.4	Division IV Report to ICTNS
10	10.5	Division V Report
11	10.6	Division VI Report
12	10.7	Division VII Report to ICTNS
13	10.8 and 15.4	Division VIII Report to ICTNS
14	10.8 and 15.6	Comments of Prof J.G Koomen on Provisional Recommendation J. Brecher, Graphical Representation of Stereochemical Representation
15	11.1	BIPM Report to IUPAC GA
16	11.3	IUBMB Report to ICTNS
17	11.5	IUPHAR Report to ICTNS
18	11.6	IUPAP Report to ICTNS
19	12	Ian Mills on Redefinition of the kilogram
20	17	Membership
21	10.2	Division II Report to ICTNS