

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Torino, Italy 2007-08-07 and 08
09:00 – 13:00 and 14:00 – 18:00

AGENDA

1. Opening remarks and introduction of participants.
2. Minutes of Beijing meeting Attachment item 2& 3
3. Business arising from the Beijing meeting Attachment item 2& 3
 - 3.1 Proposal for series of explanatory articles on IUPAC base units and their proposed revision. (Minutes Beijing, sect. 5.2)
4. Report to IUPAC Council Attachment item 4
5. Items for Editorial Advisory Board Meeting on 2007-07-08, a.m.
 - 5.1 Question of titles on references in PAC
 - 5.2 Style guide for Conference Reports and Special Issues
 - 5.3 Notice of changes in Guidelines in Handbook
 - 5.4 Review of manuscripts by Divisions before submission.
6. Current status of manuscripts: in the review cycle, completed, published
 - 6.1 Technical Reports Attachment item 6.1&2
 - 6.2 Recommendations Attachment item 6.1&2
 - 6.3 JCGM documents
 - 6.3.1 VIM: International Vocabulary of Metrology, Basic and General Concepts and Associated Terms. JCGM/WG2 (BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, OIML, ILAC). Publication status of 3rd edition – L Pendrill
 - 6.3.2 GUM: Guide to the Expression of Uncertainty in Measurement. Supplement 1. Propagation of Distributions Using a Monte Carlo Method - Publication status.
 - 6.4 Terminology and nomenclature in nanotechnology, status of IUPAP and ISO project – L Pendrill
 - 6.5 Responsibility of authors for internal consistency of glossary entries with existing Recommendations
 - 6.6 Nomenclature problems between IUPAC and IFCC (International Federation of Clinical Chemists) – J. Lorimer and J. Duffus Attachment item 6.6
7. Publicity for ICTNS
 - 7.1 Article for CI describing nature of ICTNS and its relation to PAC
8. Reports from IUPAC Division Representatives Attachment item 8
 - 8.1 Division I Physical and Biophysical Chemistry
 - 8.2 Division II Inorganic Chemistry
 - 8.3 Division III Organic and Biomolecular
 - 8.4 Division IV Polymer
 - 8.5 Division V Analytical Chemistry

- 8.6 Division VI Chemistry and the Environment
- 8.7 Division VII Chemistry and Human Health
- 8.8 Division VIII Nomenclature and Structure Representation
- 9. Reports from Representatives of Other International Organizations
 - Attachment item 9
 - 9.1 BIPM
 - 9.1.1 June Meeting of CCU at BIPM
 - 9.2 ISO/TC12
 - 9.3 IUBMB
 - 9.4 IUCr
 - 9.5 IUNS
 - 9.6 IUPHAR
 - 9.7 IUPAP
- 10. Review of sections of the *IUPAC on-line Handbook*:
 - 10.1 Procedure for Publication of IUPAC Technical Reports and Recommendations
 - 10.2 Guidelines for Drafting IUPAC Technical Reports and Recommendations
 - 10.2.1 Suggestion from D. Shaw
- 11 Update on status of 'color' books
 - 11.1 Green Book – R. Marquardt
 - 11.2 Blue Book – J Nyitrai and A McNaught
 - 11.3 Purple Book - J. Kahovec, J. Nyitrai
 - 11.4 Orange Book - W. Kutner
 - 11.5 Silver Book – J Duffus
 - 11.6 Gold Book and XML Data Dictionaries – A. Jenkins and S. Stein, by invitation
- 12 XML Gold Book:
 - Attachment item 12
 - 12.1 Strategy regarding approval of new terms from Royal Society of Chemistry.
 - 12.2 Procedure for modifying/correcting existing terms.
 - 12.3 Promotion of projects for new glossaries vs. new procedures for approving single terms not included in any glossary.
 - 12.4 Periodic Table in XML Gold Book?
- 13 Membership
- 14 Plans for future meetings
- 15 Adjournment

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Torino 2007-08-07 and 08

**Attachment to Agenda
Item 2 & 3**

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisonal 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)

6. 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 Metanowski 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.

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.

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

7.1. Technical Reports

7.2. 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.

8. Procedures for processing Technical Reports and Recommendations

8.1. 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.

8.2. 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.

9. 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

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

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.

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 Division 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 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.

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

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).

10. 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).

11. 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.

12. 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.

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

13.1.

P

Procedure for Publication of IUPAC Technical Reports and Recommendations

See Item 9.2.

13.2. Guidelines for Drafting IUPAC Technical Reports and Recommendations

See Item 9.2.

14. Update on status of ‘color’ books

14.1. 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.

14.2. Orange Book – Compendium of Analytical Nomenclature

This subject had been already dealt with under Item 10.5.

14.3. 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.

14.4. 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.

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.

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.

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

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Torino 2007-08-07 and 08

**Attachment to Agenda
Item 4**

**Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)
Biennial Report, August, 2005 to August, 2007**

1. Executive Summary

During the biennium August, 2005 to August 2007, ICTNS continued its activities on behalf of IUPAC in reviewing and approving Technical Reports and Recommendations submitted to IUPAC. Most of these Technical Reports and Recommendations were, or are about to be, published in *Pure and Applied Chemistry*. A few comprise what are essentially research papers containing new results but emanating from IUPAC projects, and these have been reviewed with publication recommended in research journals. A few others emanated from publications in preparation or prepared by international bodies of which IUPAC is a member; these were reviewed in the usual way. Finally, several of the “color” books have undergone revision during the biennium, and these have been reviewed by ICTNS. They include:

- Nomenclature of Inorganic Chemistry (Red Book), 2005
- Compendium of Chemical Terminology, on-line XML version (Gold Book), 2006
- Quantities, Units and Symbols in Physical Chemistry (Green Book), 3rd ed. In press, 2007
- Terminology and Nomenclature in Polymer Chemistry (Purple Book), 2nd ed. Still under revision. Publication expected late 2007 or 2008.

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

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

2. ICTNS Biennial Report, August, 2005 to 31 May, 2007 in Relation to Strategic Goals

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

The terms of reference of ICTNS include:

- (a) To be responsible for submission to the Bureau/Council,..., for publication or otherwise, any IUPAC document concerned with terminology, nomenclature, symbols, and other conventions.
- (b) Before recommending any material for publication as an IUPAC document, to ensure that full consultations have taken place, and the widest possible consensus has been reached among all Divisions and other bodies of the Union, and between IUPAC and other ICSU bodies, the international standardizing organizations, and the CGPM and its committees.

ICTNS is thus responsible for approving the content of IUPAC Recommendations and Technical Reports

for publication in *Pure and Applied Chemistry*, and also for approving, on behalf of IUPAC, publications emanating from international bodies on which IUPAC has representation. It carries out these tasks by very extensive review processes. For IUPAC Recommendations, a Public Comment Period of five months is required, with input from ICTNS members within four months. Both Recommendations and Technical Reports are carefully scrutinized for conformability with IUPAC-approved terminology and nomenclature, and are also edited carefully for scientific content. For documents whose source lies with international bodies, ICTNS also carries out careful reviews; editing in these cases is in the hands of the international body concerned. The overall goal in these activities is to continue and enhance IUPAC's reputation as a source of international standards in chemical terminology and nomenclature through publication of *Pure and Applied Chemistry* and continuing interaction with international organizations.

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

In its terms of reference, ICTNS is responsible for the official IUPAC comments on all documents on nomenclature, symbols, terminology and conventions sent to the Union for comment.

IUPAC Recommendations present traceable international standards for use by chemists or any scientist or engineer whose work involves chemistry. IUPAC Technical Reports present timely reviews of important subjects of general interest to scientists and engineers worldwide. Publication of the on-line version of the "Gold Book" provides an opportunity for almost continuous update of IUPAC-approved terminology, as well as corrections where necessary.

ICTNS also maintains up-to-date and detailed instructions of preparation of publications for *Pure and Applied Chemistry*.

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

See 2.2. This goal is addressed through internationally-recognized terminology and nomenclature.

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

The terms of reference require ICTNS to conduct, and advise the Executive Committee accordingly, all negotiations concerned with nomenclature and symbols with other ICSU bodies, with international standardizing organizations, and with CGPM and its committees. This measure ensures that IUPAC views carry the fullest possible weight among other international organizations. In practice, ICTNS maintains contact with IUPAC representatives on these organizations. For example, in 2005, ICTNS examined and sent a letter to BIPM in support of its efforts to re-define the kilogram in terms of atomic quantities. This action was also reported to the Executive Committee.

ICTNS membership includes representatives from Bureau International des Poids et Mesures

(BIPM), International Organization for Standardization (ISO), and the International Unions for Biochemistry and Molecular Biology (IUBMB), Crystallography (IUCr), Pharmacology (IUPHAR), and Pure & Applied Physics (IUPAP). Unfortunately, while there is a position available for a representative from the International Union of Nutritional Sciences (IUNS), this has not been filled for some years despite requests to that Union.

2.5 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.

ICTNS hopes to collaborate with the Committee on Chemical Education to prepare a series of articles on the science connected with the redefinition of the kilogram. ICTNS also acts as a consulting resource for the Secretariat in replying to queries from professionals and students on problems in terminology and nomenclature. ICTNS also deals with similar queries from other IUPAC bodies.

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.

Recommendations for membership on ICTNS by members to the President attempt to provide for a committee with broad scientific experience as well as good geographical and age distribution.

J. W. Lorimer, Chairman

B. J. Herold, Secretary

2007-05-28

APPENDIX

List of Publications for the Period August, 2005 to 31 May, 2007

Following the Manuscript Central reference number and the title, the name of the lead author(s) and the Division or other organization where the project originated are given.

3.1 Publications reviewed, edited and approved by ICTNS for publication in *Pure and Applied Chemistry*

Total pages published: 666

3.1.1 IUPAC Recommendations

Total pages published: 370

1. PAC-REC-04-12-04 Terminology of Polymers Containing Ionizable or Ionic Groups and of Polymers Containing Ions (Kubisa - Div. IV). PAC **78**, 2067-2074 (2006), 8 pp.
2. PAC-REC-05-03-01 Graphical Representation of Stereochemical Configuration (Brecher - Div. VIII). PAC **78**, 1897-1970 (2006), 73 pp.
3. PAC-REC-05-08-11 XML-based IUPAC~Standard for Experimental, Predicted and Critically Evaluated Thermodynamic Data Storage and Capture (ThermoML) (Frenkel - CPEP). PAC **78**, 541-612 (2006). 72 pp.

4. PAC-REC-05-09-13 JCAMP-DX for EMR (Lancashire - CPEP). PAC **78**, 613-631 (2006). 19 pp.
5. PAC-REC-06-01-01. Glossary of Terms Relating to Pesticides (Stephenson - Div. VI). PAC **78** , 2155-2168 (2006), 14 pp.
6. PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions. Part A. The Suspension Effect. (Oman - Div. V). PAC **79** 67-79 (2007), 11 pp.
7. PAC-REC-05-10-26 Glossary of Terms Used in Photochemistry (Braslavsky - Divs. I, III). PAC **79**, 293-465 (2007), 173 pp.
8. PAC-REC-06-01-06. IUPAC Explanatory Dictionary of Key Terms in Toxicology (Nordberg - Div. VII). For PAC **79** [9].
9. PAC-REC-06-04-02. IUPAC Glossary of Terms Used in Toxicology - Expanded and Revised (Duffus - Div. VII). For PAC **79** [7].
10. PAC-REC-06-02-01. Definitions of Terms Related to the Structure and Processing of Inorganic and Polymer Gels and Networks, and Inorganic-polymeric Materials (Jones - IV). For PAC **79** [10].

3.1.2 IUPAC Technical Reports

Total pages published: 296

11. PAC-REP-04-04-04 NMR for pKs (Popov - Div. V). PAC **78**, 663-675 (2006), 11 pp.
12. PAC-REP-04-05-06 The International Harmonized Protocol for the Proficiency Testing of Analytical Chemistry Laboratories (Ellison - Div. V). PAC **78**, 145-196 (2006), 50 pp.
13. PAC-REP-04-08-05 Standards, Calibration and Guidelines in Microcalorimetry. Part 2. Calibration Standards for Differential Scanning Calorimetry (Della Gatta - Div. I). PAC **78**, 1455-1476 (2006), 20 pp.
14. PAC-REP-05-05-03 Guidelines for Calibration in Analytical Chemistry. Part 3. Uncertainty Estimation and Figures of Merit for Multivariate Calibration (Olivieri - Div. V). PAC **78**, 633-661 (2006), 27 pp.
15. PAC-REP-05-09-16 Guidelines for Terminology for Microtechnology in Clinical Laboratories (Wilding - Div. VII). PAC **78**, 677-684 (2006), 6 pp.
16. PAC-REP-05-12-12. Cytokine Profiles in Human Exposure to Metals (Templeton - Div. VII). PAC **78** , 2155-2168 (2006), 14 pp.
17. PAC-REP-06-03-01. Atomic Weights of the Elements 2005 (Wieser - Div. II). PAC **78**, 2051-2066 (2006), 16 pp.
18. PAC-REP-06-05-06. Education, Outreach and Codes of Conduct to Further the Norms and Obligations of the Chemical Weapons Convention (Pearson, Mahaffy - CCE). PAC **78**, 2169-2192 (2006), 24 pp.
19. PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions. Part B. Guidelines for Practical pH Measurements in Soil Suspensions. (Oman - Div. V). PAC **79**, 81-86 (2007), 6 pp.

20. PAC-REP-04-10-25 Properties and Units in the Clinical Laboratory Sciences. Part XX. Properties and Units in Clinical and Environmental Toxicology (Duffus - Div. VII). PAC **79**, 87-152 (2007), 66 pp.
21. PAC-REP-06-05-09. Chemical Speciation of Environmentally Significant Ligands. Part 2. The Cu^{2+} - OH^- , Cl^- , CO_3^{2-} , SO_4^{2-} and PO_4^{3-} Systems (Powell - Div. V). PAC **79**, 895-950 (2007), 56 pp.
22. PAC-REP-06-04-09. Critically Evaluated Rate Coefficients for Free-radical Polymerization 6: Propagation Rate Coefficient of Methacrylic Acid in Aqueous Solution (Lacik - Div. IV). For PAC **79** [8].
23. PAC-REP-06-07-05. Representation of Configuration in Coordination Polyhedra and the Extension of Current Methodology to Coordination Numbers Greater than Six (Leigh - Div. VIII). For PAC **79** [10].
24. PAC-REP-06-01-06. Solute Movement in Soils with Potential Rapid By-pass Transport (Pesticide Movement in Soils) Actual title: Transport of Pesticides via Macropores (Kördel - VI). For PAC **80** [1].

3.2 Publications reviewed and approved by ICTNS for publication elsewhere than in PAC

3.2.1 Recommendations

25. PAC-REC-04-04-03. Nomenclature of Inorganic Chemistry (Revised “Red Book”) (Connelly). RSC Publishing (2005).
26. PAC-REC-04-05-02 International Vocabulary of Metrology (VIM) (JCGM - BIPM Joint Committee on Guides to Measurement). Accepted on behalf of IUPAC 2006-10-16 for publication by ISO.
27. IUPAC. Compendium of Chemical Terminology, 2nd ed. (the “Gold Book”). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: <http://goldbook.iupac.org> (2006-) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins.
28. PAC-REC-04-05-03 Guide to Expression of Uncertainty in Measurement (GUM), Supplement 1 (BIPM Joint Committee on Guides to Measurement - Working Group 1). Accepted on behalf of IUPAC 2007-04-26 for publication by ISO.
29. PAC-REC-05-11-10. Quantities, Units and Symbols in Physical Chemistry, 3rd ed. (“Green Book”) (Quack - Div. I). In press. RSC Publishing.

3.2.2 Technical Reports (reviewed, edited and approved as noted)

30. Reference Data for the Density and Viscosity of Liquid Aluminum and Liquid Iron (Assael - Div. I). JPCRD **35**, 285-300 (2006), 14 pp.
31. PAC-REP-06-01-07. Structure and Properties of Polyester Elastomers Composed of poly(butylene terephthalate) and poly(ϵ -caprolactone) (Takigawa - IV). Approved for publication elsewhere than in PAC 2006-10-30. (Contains new experimental work.)
32. PAC-REP-06-06-01. Structure and Properties of Polyamide-6 and 6/66 Clay Nanocomposites (Kim - IV). Approved for publication elsewhere than in PAC 2006-11-02. (Contains new experimental work.)

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Torino 2007-08-07 and 08

**Attachment to Agenda
Item 6.1 & 2**

Date: 2007-07-11 revised
To: All Members, ICTNS
From: Jack Lorimer
Re: Updated Summary of TRs and Recommendations to date (E&OE)

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

- (a) submitted before 2004-01-05 but not completed by that date;
- (b) submitted between 2004-01-05 and current date.

Sponsoring Division(s) in parentheses after name of principal author.

Summary

1.0 Recommendations and Technical Reports Submitted Before 2004-01-01 and Not Published by 2006-03-31 – total 5

1.0.1 Recommendations Submitted Before 2004-01-01 and Not Completed or Accepted, or Abandoned, by 2006-03-31 – total 2

1.0.2 Technical Reports Submitted Before 2004-01-01 and Not Completed or Accepted by 2006-03-31– total 3

2.0 Recommendations Submitted Between 2004-01-01 and Current Date– total 26

2.0.1 Recommendations Submitted, Accepted and Published in PAC Between 2004-01-01 and Current Date–total 7

2.0.2 Recommendations Submitted, Accepted and Published Elsewhere Between 2004-01-01 and Current Date-total 2

2.0.3 Recommendations Submitted and Accepted Between 2004-01-01 and Current Date but Not Published– total 5

2.0.4 Recommendations Submitted and Accepted Between 2004-01-01 and Current Date but Awaiting Final Manuscript or Final Review by ICTNS –total 5

2.0.5 Recommendations Submitted Between 2004-01-01 and Current Date and Not Accepted by Current Date– total 7

3.0 Technical Reports Submitted Between 2004-01-01 and Current Date– total 18

3.0.1 Technical Reports Submitted, Accepted and Published in PAC Between 2004-01-01 and Current Date– total 11

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

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

3.0.4 Technical Reports Submitted and Reviewed but Not Accepted for PAC (but acceptable for publication elsewhere) Between 2004-01-01 and Current Date-total 2

3.0.5 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Awaiting Final Manuscript or Final Review by ICTNS –total 1

3.0.6 Technical Reports Submitted Between 2004-01-01 and Current Date and Not Accepted by Current Date– total 0

**Published in PAC 77 (2005): 9 TR, 267 pp. (av. 30 pp.); 3 Rec., 147 pp. (av. 49 pp.)
Total: 12, 414 pp. (av. 35 pp.)**

**Published in PAC 78 (2006): 8 TR, 168 pp. (av. 21 pp.); 5 Rec., 186 pp. (av. 37 pp.)
Total: 13, 354 pp. (av. 27 pp.)**

Published in PAC 79 (2007): 3 TR, 128 pp. (av. 43 pp.); 2 Rec., 184 pp. (av. 92 pp.)

Total: 5, 312 pp. (av. 62 pp.)

1.0 Recommendations and Technical Reports Submitted Before 2004-01-01 and Not Published by 2006-01-01 – total 5

1.0.1 Recommendations Submitted Before 2004-01-01 and Not Completed or Accepted, or Abandoned, by 2006-03-31 – total 2

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

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

1.0.2 Technical Reports Submitted Before 2004-01-01 and Not Completed or Accepted by 2006-03-31 – total 3

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

877 Thermochemistry (da Silva - I). New ms being prepared. Reminder by JWL 2004-05-07. Author will prepare revision in September, 2005. No further information.

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

2.0 Recommendations Submitted Between 2004-01-01 and Current Date – total 25

2.0.1 Recommendations Submitted, Accepted and Published in PAC Between 2004-01-01 and Current Date – total 7

PAC-REC-04-12-04 Terminology of Polymers Containing Ionizable or Ionic Groups and of Polymers Containing Ions (Kubisa - IV). 9 reviews. Public comment period ends 2005-05-31. Letter 2005-04-20 major revision. Several stages of comments up to 2006-06, awaiting author's reply. Final acceptance 2006-07-20. Final acceptance with abstract 2006-09-13. PAC **78**, 2067-2074 (2006), 8 pp.

PAC-REC-05-03-01 Graphical Representation of Stereochemical Configuration (Brecher - VIII). Public comment period ends 2005-07-31. Letter of acceptance with minor revision (revised ms required) 2005-08-04. Revision under review September, 2005. Accepted with minor revision 2006-03-12. Final acceptance 2006-05-11. Published PAC **78**, 1897-1970 (2006), 73 pp.

PAC-REC-05-08-11 XML-based IUPAC~Standard for Experimental, Predicted and Critically Evaluated Thermodynamic Data Storage and Capture (ThermoML) (Frenkel - CPEP). Received 2005-08. ICTNS reviews due 2005-12. Accepted with major revisions 2005-12-18. Final acceptance 2005-12-29. Public comment ends 2006-01-31. ICTNS comments by 2005-12-31. Published PAC **78**, 541-612 (2006). 72 pp.

PAC-REC-05-09-13 JCAMP-DX for EMR (Lancashire - CPEP). Received 2005-09. ICTNS reviews due 2005-12-31. Recommended acceptance with minor corrections 2005-12-20. Revised ms

accepted 2005-12-30. Public comment ends 2006-01-31. ICTNS comments by 2005-12-31. Published PAC **78**, 613-631 (2006). 19 pp.

PAC-REC-06-01-01. Glossary of Terms Relating to Pesticides (Stephenson - VI). Rec'd 2006-01-05. Public comment period ends 2006-05-21. ICTNS comments by 2006-04-21. Accepted with major revision 2006-04-24. Final acceptance 2006-07-28. PAC **78**, 2155-2168 (2006), 14 pp.

PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions. Part A. The Suspension Effect. (Oman - V). Received 2005-07-18. Public comment period ends 2006-01-31. ICTNS comments by 2005-12-31. Subsequently, ms being reconsidered by Div. V. New ms received 2006-04-18. Accepted with minor revisions 2006-07-16. Revised ms accepted with minor revisions 2006-09-07. Final acceptance 2006-09-13. PAC **79** [1] 67-79 (2007), 11 pp.

PAC-REC-05-10-26 Glossary of Terms Used in Photochemistry (Braslavsky - I, III). Received 2005-10. Public comment period ends 2006-03-31. ICTNS comments by 2006-02-28. Accepted with major revisions 2006-03-07. Final version for review received 2006-07-25. Accepted 2006-11-02. PAC **79** [3], 293-465 (2007), 173 pp..

2.0.2 Recommendations Submitted, Accepted and Published Elsewhere Between 2004-01-01 and Current Date-total 2

PAC-REC-04-04-03. Nomenclature of Inorganic Chemistry (Revised Red Book) (Connelly). Final acceptance December, 2005. RSC Publishing (2005).

PAC-REC-05-11-10. Quantities, Units and Symbols in Physical Chemistry, 3rd ed. ("Green Book") (Quack - I). Rec'd 2005-11-10. Public comment period ends 2006-03-31. ICTNS comments by 2006-02-28. Accepted with revisions to come 2006-03-07. Hundreds of comments being processed 2006-06. In press May, 2007.

2.0.3 Recommendations Submitted and Accepted Between 2004-01-01 and Current Date- total 5

PAC-REC-04-05-02 International Vocabulary of 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 published. Revision VIM3 received 2006-05-17. Comments to de Bièvre from JWL on draft 2006-06-06. Final comments from ICTNS due 2006-09-30. Approved for IUPAC 2006-10-16. JCGM (BIPM Joint Committee on Guides to Measurement) reviewing final comments.

PAC-REC-06-01-06. IUPAC Explanatory Dictionary of Key Terms in Toxicology (Nordberg - VII). Rec'd 2006-01-24. Public comment period ends 2006-06-24. ICTNS comments by 2006-05-24. Accepted with major revision 2006-07-18. Accepted with minor revision 2006-11-08, 2006-11-15. For PAC **79** [5].

PAC-REC-06-04-02. IUPAC Glossary of Terms Used in Toxicology - Expanded and Revised (Duffus - VII). Received 2006-04-17. ICTNS review by 2006-08-17. Public Review ends 2006-09-17. Accepted with major revisions 2006-10-24. Final acceptance 2006-12-18. For PAC **79** [6].

PAC-REC-06-02-01. Definitions of Terms Related to the Structure and Processing of Inorganic and Polymer Gels and Networks, and Inorganic-polymeric Materials (Jones - IV). Received 2006-02-10. ICTNS comments by 2006-07-15. Accepted with major revisions 2006-07-16. Revised ms 2006-10-31 under review. More revisions requested 2007-01-25. Accepted 2007-03-19.

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 – but again under revision. ISO Document JCGM-WG1-SC1-N10. Status queried with A. Thor 2005-04-21 – reply not yet published. JCGM WG1 (Joint Committee on Guides to Measurement - Working Group 1) Final version reviewed by ICTNS and accepted on behalf of IUPAC 2007-04-26.

2.0.4 Recommendations Submitted and Accepted, but Awaiting Final Manuscript Between 2004-01-01 and Current Date or Final Review by ICTNS – total 5

PAC-REC-05-10-23 Compendium on Macromolecular Terminology and Nomenclature (The Purple Book), 2nd ed. (Wilks - IV). Received 2005-10. Reviewed by ICTNS. Accepted with minor changes 2005-12-18. Final ms 2006-03-22 under review by ICTNS and coordinating committee.

PAC-REC-06-12-04. Further Conventions for NMR Chemical Shifts (Harris - I). Received 2006-12-22. Accepted with minor revisions 2007-05-05.

PAC-REC-07-02-02 Glossary of Terms Related to Kinetics, Thermodynamics and Mechanisms of Polymerization (Moad - IV). Accepted with minor revision 2006-06-27.

PAC-REC-07-03-01 Glossary of Terms Related to Solubility (Shaw - V). Accepted with major revision 2007-06-27.

PAC-REC-07-02-0. Graphical Representation Standards for Chemical Structure Diagrams. (Brecher - VIII). Received 2007-02-10. Accepted with minor changes 2007-07-09.

2.0.5 Recommendations Submitted Between 2004-01-01 and Current Date but Not Accepted by Current Date– total 7

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

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

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

PAC-REC-05-12-09. Nomenclature of Rotaxanes (Yerin - VIII). Rec'd 2005-12-16. Public comment period ends 2006-04-30. ICTNS comments by 2006-03-31. Accepted subject to major revision 2006-09-11. Revision due 2006-11-10.

PAC-REC-06-04-06. Standard Definitions of Terms Relating to Mass Spectroscopy (Murray - V). Received 2006-04-23. Initial rejection 2006-04-25 because of lack of documentation. Revised ms received, under review. Accepted subject to major revision 2006-11-13.

PAC-REC-06-12-03. Structure-based Nomenclature for Cyclic Macromolecules (Mormann - IV). Received 2006-12-18.

PAC-REC-07-07-03 Isothermal Titration Calorimetry in Biology (Schwartz - I). Received 2007-07-11.

3.0 Technical Reports Submitted Between 2004-01-01 and Current Date– total 17

3.0.1 Technical Reports Submitted, Accepted and Published in PAC Between 2004-01-01 and Current Date– total 11

PAC-REP-04-04-04 NMR for pKs (Popov - V). Revised ms received 2005-07-28. New review September, 2005. Accepted 2005-10-21. Published PAC **78**, 663-675 (2006) (11 pp.)

PAC-REP-04-05-06 The International Harmonized Protocol for the Proficiency Testing of Analytical Chemistry Laboratories (Ellison - V). 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. Accepted 2005-09-20. Published PAC **78**, 145-196 (2006) (50 pp.).

PAC-REP-04-08-05 Standards, Calibration and Guidelines in Microcalorimetry. Part 2. Calibration Standards for Differential Scanning Calorimetry (Della Gatta - I). 4 reviews (3 ICTNS). Returned to author for minor revision 2004-11-25. Reminder 2005-04-21. Revised ms received 2006-03-07. Accepted 2006-03-22. Published PAC **78**, 1455-1476 (2006) (20 pp.)

PAC-REP-05-05-03 Guidelines for Calibration in Analytical Chemistry. Part 3. Uncertainty Estimation and Figures of Merit for Multivariate Calibration (Olivieri - V). Last rev. due 2005-05-03. JWL review complete. 2005-06-11. Revision under review, September, 2005. Accepted 2005-10-22. Published PAC **78**, 633-661 (2006) (27 pp.).

PAC-REP-05-09-16 (formerly PAC-REC-05-09-16) Guidelines for Terminology for Microtechnology in Clinical Laboratories (Wilding - VII). Rec'd 2005-10. Re-classified as a TR. Accepted with minor changes 2006-01-20. Published PAC **78**, 677-684 (2006) (6 pp.).

PAC-REP-05-12-12. Cytokine Profiles in Human Exposure to Metals (Templeton - VII). Rec'd 2005-12-22. Received 2005-12-22. Accepted with minor revisions 2006-03-14. Final version accepted 2006-07-19. PAC **78** , 2155-2168 (2006) (14 pp.).

PAC-REP-06-03-01. Atomic Weights of the Elements 2005 (Wieser - II). Received 2006-03-26. Accepted 2006-06-08. PAC **78**, 2051-2066 (2006), 16 pp.

PAC-REP-06-05-06. Education, Outreach and Codes of Conduct to Further the Norms and Obligations of the Chemical Weapons Convention (Pearson, Mahaffy - CCE). Received 2006-05-12. Accepted 2006-06-17. PAC **78**, 2169-2192 (2006), 24 pp.

PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions. Part B. Guidelines for Practical pH Measurements in Soil Suspensions. (Oman - V). Received 2005-07-18. Public comment period ends 2006-01-31. ICTNS comments by 2005-12-31. Subsequently, ms being reconsidered by Div. V. New ms received 2006-04-18. Accepted with minor revisions 2006-07-16. Revised ms accepted with minor revisions 2006-09-07. Final acceptance 2006-09-13. PAC **79** [1] 81-86 (2007), 6 pp.

PAC-REP-04-10-25 Properties and Units in the Clinical Laboratory Sciences. Part XX. Properties and Units in Clinical and Environmental Toxicology (Duffus - VII). Request for revised ms. showing what materials are to be archived on web site 2004-11-20, expanded 2005-01-25. Revised ms September, 2005. Accepted provisionally subject to major revision 2006-01-21. Revision received 2006-04-02, under review. Accepted with minor revisions 2006-07-14. Final acceptance 2006-10-13. PAC **79** [1] 87-152 (2007), 66 pp.

PAC-REP-06-05-09. Chemical Speciation of Environmentally Significant Ligands. Part 2. The Cu^{2+} - OH^- , Cl^- , CO_3^{2-} , SO_4^{2-} and PO_4^{3-} Systems (Powell - V). Received 2006-05-12; revision received 2006-10-26. JWL comments to author 2006-11-01. New revision 2006-12-28 under review. Final acceptance 2007-01-23. PAC **79**, 895-950 (2007), 56 pp.

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

Project (to be submitted to JPCRD) Reference Data for the Density and Viscosity of Liquid Aluminum and Liquid Iron (Assael - I). ICTNS review (JWL, R. Weir) sent to author 2005-04-24; final version accepted (with minor corrections) 2005-04-25. Published JPCRD **35**, 285-300 (2006) (14 pp.).

3.0.3 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Not Published by Current Date– total 4

PAC-REP-06-04-09. Critically Evaluated Rate Coefficients for Free-radical Polymerization 6: Propagation Rate Coefficient of Methacrylic Acid in Aqueous Solution (Lacik - IV). Received 2006-04-26. Returned 2006-06-26 for editorial corrections. Corrected ms received, accepted with minor revisions 2006-09-08. Final acceptance 2006-11-18. For PAC **79** [9].

PAC-REP-06-07-05. Representation of Configuration in Coordination Polyhedra and the Extension of Current Methodology to Coordination Numbers Greater than Six (Leigh - VIII). Received 2006-07-18. Accepted 2007-03-18.

PAC-REP-06-01-06. Solute Movement in Soils with Potential Rapid By-pass Transport (Pesticide Movement in Soils) Actual title: Transport of Pesticides via Macropores (Kördel - VI). Received 2006-01-30. Major revisions requested 2006-04-04. Reminder to author 2006-10-25. Revision received 2007-05-02. Accepted 2007-05-03.

PAC-REP-07-06-05 Chemists and the “Public” (Mahaffy - CCE). Final version received 2007-06-21. Accepted 2007-07-11.

3.0.4 Technical Reports Submitted and Reviewed but Not Accepted for PAC (but acceptable for publication elsewhere) Between 2004-01-01 and Current Date-total 2

PAC-REP-06-01-07. Structure and Properties of Polyester Elastomers Composed of poly(butylene terephthalate) and poly(ϵ -caprolactone) (Takigawa - IV). Received 2006-01-29. Revised ms received 2006-07. Rejected for PAC, OK for publication elsewhere 2006-10-30.

PAC-REP-06-06-01. Structure and Properties of Polyamide-6 and 6/66 Clay Nanocomposites (Kim - IV). Received 2006-06- Accepted but not for PAC 2006-09-07. Rejected for PAC, OK for publication elsewhere 2006-11-02.

3.0.5 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Awaiting Final Manuscript or Final Review by ICTNS– total 1

PAC-REP-07-03-03 Performance Evaluation Criteria For Preparation And Measurement Of Macro And Microfabricated Ion-Selective Electrodes (Lindner, Umezawa - V). Accepted with minor revisions 2007-06-20.

3.0.6 Technical Reports Submitted Between 2004-01-01 and Current Date and Not Accepted by Current Date– total 0

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisonal Committee on Terminology, Nomenclature and Symbols (ICTNS)

Torino 2007-08-07 and 08

**Attachment to Agenda
Item 6.6**

Date: 2007-09-03
To: Bernardo
From: Jack
Re: Agenda item 6.6

Problems between ICTNS and sub-committee SC-NPU (Nomenclature, Properties and Units) of IFCC (International Federation of Clinical Chemists)

1. There have been many criticisms among those members of ICTNS who have a more physical science outlook about the “Silver Book”, which is a joint IUPAC-IFCC publication. While the Silver Book does contain a few terms that are not acceptable to the IUPAC community in general, these are minimal in number, and on the whole the book presents systematic and useful rules for presenting data in clinical chemistry, and should continue as a standard reference for ICTNS.

2. The Silver Book, sect. 6.6.1, is very clear that IUPAC nomenclature is preferred except where the substances in question are too complex and require trivial names, and current practice in ICTNS follows the Silver Book plan. Unfortunately, SC-NPU has a large database (C-NPU) that does not use IUPAC names. Our irrevocable position is that, for publication in PAC, IUPAC names must be used.

3. In the most recent joint IUPAC-IFCC publication, PAC-REP-04-10-25 *Properties and Units in the Clinical Laboratory Sciences. Part XX. Properties and Units in Clinical and Environmental Toxicology* (Duffus - VII) PAC **79** [1] 87-152 (2007), ICTNS (especially Alan McNaught and Bernardo Herold) spent much time in assigning IUPAC names where necessary. This series of TRs is based on the C-NPU database, from which entries for a relevant sub-field are collected and coordinated.

4. Long after the above report had been well reviewed and accepted, the chair of SC-NPU, Prof. Françoise Pontet, sent the chairman of ICTNS two rather intemperate letters demanding on behalf of the whole SC-NPU that the manuscript be withdrawn from publication because “it was full of errors”, although not a single specific example of an error was given. This was disputed and the review procedures were described for her. Thanks to John Duffus, it was finally established that SC-NPU believed (incorrectly) that the original manuscript posted on the IUPAC web site was the version to be published. In the end, a few corrections supplied by one member of SC-NPU were incorporated by John before publication, but no actual final acceptance by SC-NPU was ever received.

5. Lack of formal acceptance of joint publications by IFCC or SC-NPU is nothing new. They have been asked in the past, but have not responded.

6. Conclusions

6.1 A small sub-committee of ICTNS (suggest Duffus, Herold, Lorimer, McNaught) should be set up to draw up some rules for facilitating joint IUPAC-IFCC publications.

- 6.2 The rules should include, but not be limited to:
- use of IUPAC names or trivial names for complex substances, with reference to the Silver Book
 - no approval for publication without approval by both Div. VII and IFCC (or one of its sub-committees)
 - obligation of authors to supply the Presidents of Div. VII and IFCC (or the chair of an IFCC sub-committee) with a copy of the final approved manuscript.
- 6.3 IFCC and SC-NPU be asked to agree to the above conditions
- 6.4 SC-NPU be encouraged to modify its database to include IUPAC names where practicable.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Torino 2007-08-07 and 08

**Attachment to Agenda
Item 8**

Division I Report to ICTNS for the Biennium 2006-07

A significant part of the five aims of Division I are realised via the project system for which dissemination of information is of paramount importance. These include recommendations on nomenclature, symbols, units, terminology and conventions in physical and biophysical chemistry, standards and reference materials, the compilation and documentation of critically evaluated physical chemical data. To place this activity of dissemination in context, the following statistics are provided.

1. Peer-Reviewed Publications for the period 2000-2007

Papers in peer-reviewed journals number **24** and occupy **2,610** journal pages for an average of **109** pages per paper. These include Pure App Chem (14 papers), Atmos Chem Phys (3 papers), J Chem Eng Data (1 paper), J Phys Chem Ref Data (6 papers).

2. Books

Three books have appeared in the year 2007. Most significant is the 3rd edition of the Green Book, the revision of '*Quantities, Units and Symbols in Physical Chemistry*' and the Appendices, July 2007, Royal Society of Chemistry/IUPAC.

3. Publications in process from nearly completed projects

The ICTNS has already provided helpful critiques from reviewers and accepted the Technical Report for the project '*Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies*'. The revisions are in progress. For another project, two peer-reviewed long papers are ready in draft form for submission to the J Phys Chem. Data.

4. Publications in process from 17 projects underway at various stages of completion

Papers from nine projects are drafted that deal with recommendations and technical reports. For three other projects, publications are ready for deposit to databases. Five projects are at an early stage and are not ready for publications.

REPORT FROM THE INORGANIC CHEMISTRY DIVISION TO ICTNS

IUPAC GENERAL ASSEMBLY - TURIN AUGUST 2007

The activities of Division II are grouped into three broad areas:

Atomic Weights and Isotopic Abundances;
Molecular Inorganic Chemistry;
Solid State Inorganic and Materials Chemistry.

The Atomic Weights and Isotopic Abundances activities are thriving, in part through continuation of the original IUPAC Commission II.I “Commission on Isotopic Abundances and Atomic Weights”, but also with a sequence of highly-focused and funded IUPAC projects in this area, leading to important publications such as Revision of the Table of Atomic Weights. The work of the Commission has recently been extended to include a joint Task Force involving the Geological Union, IUGS, concerning resolution of discrepancies in the half-lives of long-lived radioactive nucleides.

The molecular inorganic activities previously partly responsible for the creation of the new Division on Nomenclature are now going through a resurgence of activities including representation for the Division on the Federation of European Chemical Societies.

Solid state high-temperature materials chemistry, long an activity of Division II, is now broadened to encompass the much wider range of activities under the umbrella of Materials Chemistry. The sub-committee on Materials Chemistry is run largely from Division II, with representation from other Divisions and services an area that is evolving and expanding rapidly.

Validation of claims for discovery and naming of new elements

An important activity for Division II is the IUPAC- IUPAP Joint working Party which validates claims for the discovery of new elements. In recent years we have seen the authentication and subsequent naming of elements 110 and 111. The JWP was reconstituted by agreement between the Unions in 2006, again under the chairmanship of Professor Paul Karol, and is at present considering claims for six new elements with atomic numbers 112, 113, 114, 115, 116 and 118. These take claims to the widely-mooted ‘island of stability’ at $Z = 118$. The most recent call for documentation supporting these claims closed on June 30th last. The JWP has reported informally that its work has progressed well to date and it has reached the conclusion that it would be both most expedient and effective to split its next report into two sections. The first will deal with $Z = 112$ and the second with elements with $Z > 112$. The first section of the report is currently in draft form and is expected to issue

in the second half of this year. When this report has issued and has been accepted then, provided the claims for the discovery have been verified, the formal process of naming the new element can begin.

Translation of the Red Book into Spanish

Prof. Pascual Román Polo and Prof. Miguel A. Ciriano have translated the book *Nomenclature of Inorganic Chemistry* (the IUPAC “Red Book”) into Spanish.

It is expected that the book will be available from June 7, 2007.

http://www.ehu.es/proman/documents/20070417PortadaCastellanoRB_003.pdf

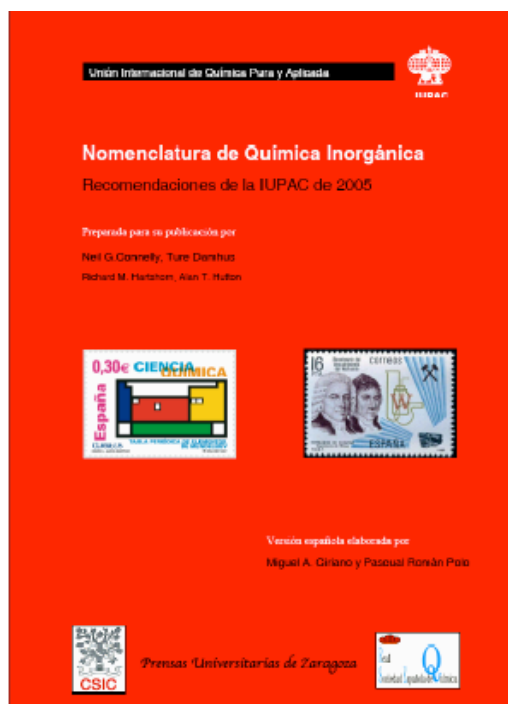


Fig. 2. Nomenclatura de Química Inorgánica. Translation to Spanish of the Red Book

The Green Book – Atomic Weights and the Periodic Table

Members of the Commission on Isotopic Abundances and Atomic Weights and other members of Division II have been in correspondence with the authors of the Green Book and are grateful for the clarifications that have been possible in the way in which the information on these subjects are now presented.

IUGS-IUPAC Task Group

The Inorganic Chemistry Division has established a link with geochemists via a joint Task Group (that was approved and funded in October 2006) between the International Union of Geological Sciences (IUGS) and IUPAC. The objective of this Task Group is to resolve discrepancies in the values of decay constants (reciprocals of radioactive half-lives) of long-lived radioactive nuclides that are used by geo-chronologists for the dating of geological materials with those decay constant values that were previously recommended by IUPAC.

In preliminary work to the major objectives, the Task Group has had an article accepted for publication in the journal, *Quaternary Science Review*, entitled "Convention on the use of Systeme International (SI) units in Earth Sciences" by Renne et al. This paper attempts to correct the inconsistent use of Systeme International (SI) units that deal with age determinations used in the geological sciences.

News and Articles of possible interest

The Periodic Table: Its Story and Significance by *Herbert D. Kaesz*, *Chemistry International* March-April 2007, pg 22, review of the book "The Periodic Table: Its Story and Significance" by Eric Scerri

The Periodic Table at a Glance by G.J. Leigh *Chemistry International* March-April 2007, pg 23. review of the book "The Periodic Table at a Glance" by Mike Beckett and Andy Platt

"Priority Claims for the Discovery of Elements with Atomic Number Greater than 111" by John Corish *Chemistry International* January-February 2007, pg 18

"Definitions of Terms Relating to the Structure and Processing of Inorganic and Polymeric Gels and Networks", *Chemistry International* July-August 2006, pg 23

Division II Projects of possible interest

2005-001-1-200 Day *Towards Defining Materials Chemistry*
Second Task Group meeting in Turin, August 2007.

2005-043-2-400 Ober *Terminology for self-assembly and aggregation of polymers*
No change since August 2006

2006-016-1-200 Renne *Recommendations for Isotope Data in Geosciences*
On schedule--recently funded.

2006-025-1-200 Holden *Assessment of fundamental understanding of isotopic abundances and atomic weights of the chemical elements*
On schedule--recently funded.

2006-028-1-400 Ober
responsive polymers
On schedule--recently funded.

Terminology for conducting, electroactive and field

2006-046-1-200 Karol
number greater than 111
On schedule.

Priority claims for the discovery of elements with atomic

The Materials Chemistry Sub-Committee has considered, and initiated, a project to produce a glossary of terms used in Materials Chemistry and nano-related terminology.

John Corish,
Trinity College Dublin,
July 2007.

**Report of the Division of Organic and Biomolecular Chemistry
(Division III) to the Interdivisional Committee on
Terminology, Nomenclature and Symbols (ICTNS)**

(December 2005-August 2007)

Division III aims at promoting the goals of IUPAC in the field of organic and biomolecular chemistry, areas where terminology, nomenclature and symbols are highly important. As representative of Division III, my participation at the ICTNS tasks resulted primarily in the extensive revision of the content of the following IUPAC Recommendations and Technical Reports:

PAC-REC-05-07-05.R1 Guidelines for Potentiometric Measurements in Suspensions A. THE SUSPENSION EFFECT (IUPAC Technical Report) B. GUIDELINES FOR PRACTICAL pH MEASUREMENTS IN SOIL SUSPENSION (IUPAC Recommendations 2006)

PAC-REC-05-12-09 Nomenclature for Rotaxanes

PAC-REP-05-12-12 Cytokine Profiles in Human Exposure to Metals

PAC-REC-06-01-06 IUPAC Explanatory Dictionary of Key Terms in Toxicology

PAC-REC-06-02-01 Definitions of terms relating to the structure and processing of inorganic and polymeric gels and networks, and inorganic-polymeric materials

PAC-REP-06-01-07 Structure and properties of polyester elastomers composed of poly(butylene terephthalate) and poly(ϵ -caprolactone)

PAC-REC-06-04-06 Standard Definitions of Terms Relating to Mass Spectrometry

PAC-REC-06-04-02 IUPAC Glossary of Terms Used in Toxicology - Expanded and Revised from “Glossary for Chemists of Terms Used in Toxicology”, 1993

PAC-REP-06-04-09 Critically Evaluated Rate Coefficients for Free-Radical Polymerization 6: Propagation Rate Coefficient of Methacrylic Acid in Aqueous Solution

PAC-REP-06-05-06 Education, Outreach and Codes of Conduct to Further the Norms and Obligations of the Chemical Weapons Convention

PAC-REC-04-05-02.R1 International Vocabulary of Basic and General Terms in Metrology (VIM)

PAC-REP-06-06-01 Structure and Properties of Polyamide-6 & 6/66 Clay Nanocomposites

PAC-REC-06-12-03 Structure-Based Nomenclature for Cyclic Macromolecules

PAC-REC-06-12-04 Further Conventions for NMR Chemical Shifts

PAC-REC-07-02-01 Recommendations for Graphical Representation Standards for Chemical Structure Diagrams

PAC-REC-07-02-02 Glossary of Terms Related to Solubility

PAC-REC-07-03-01 Glossary of Terms Related to Kinetics, Thermodynamics and Mechanisms of Polymerization

This revision was focused not only on the content of the manuscripts, but also on the correct use of IUPAC and other international standards. Efforts were made in order to harmonize organic and biomolecular chemistry terms and names with related ones from other research fields.

The following aspects of the activity of Division III deserve to be highlighted for ICTNS:

Division III fostered communication among chemists by promoting scientific discussions and by answering many questions arising from

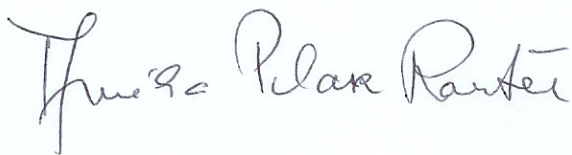
students and colleagues from around the world, concerning symbols, nomenclature and terminology in organic and biomolecular chemistry.

Advancement of research in these chemical sciences was also facilitated by Division III through discussions concerning new compounds' and concepts, among other scientific problems. In addition, this Division was particularly dedicated to the enhancement of organic and biomolecular chemistry education, motivation of the career development of young scientists in the field and the public appreciation of chemistry. Dissemination of IUPAC nomenclature and terminology, fostering its use among young students and researchers, and showing them the benefits thereof has been another well succeeded task of Division III.

As National Representative of Portugal in Division III I have also extended my contribution to the motivation of my students and colleagues at home in the fields of organic and biomolecular chemistry for nomenclature, in particular through the translations into Portuguese, namely of the IUPAC Carbohydrate Chemistry nomenclature recommendations, which will be soon available and very useful for the Portuguese speaking countries (Portugal, Brazil, Angola, Moçambique, Cabo Verde, Guiné, among others). In addition, in the courses which I lectured in Natural Products, Organic Chemistry and Carbohydrate Chemistry, I used IUPAC names and terms. I also recommended to authors and editors the use of IUPAC nomenclature when reviewing papers to be published in the following journals: Current Medicinal Chemistry, Journal of Carbohydrate Chemistry, Carbohydrate Research, Journal of Molecular Structure, Journal of the Science of Food and Agriculture, Journal of Chromatography A and Journal of Herbs, Spices & Medicinal Plants. My communication with the scientific community, students and society was focused on the dissemination of the proper IUPAC terms and names.

Division III, covering a broad area of multidisciplinary aspects, has dedicated its efforts to succeed in fulfilling the ICTNS goals in Organic and Biomolecular Chemistry.

Lisbon, August 2, 2007



Amélia Pilar Rauter

Representative of Division III on ICTNS

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Report to ICTNS by Division IV Representative.

The only available underlying materials for the present Report are:

Report to the IUPAC Council of the Polymer Division (Division IV) for 2006-2007 and

Report of the Subcommittee of Polymer Terminology (SPT) on current projects in 2005-2007.

The reports (see the Appendix) are not directly relevant to the ICTNS but they might indicate the types of IUPAC documents which will be submitted to PAC in near future.

IUPAC POLYMER DIVISION (DIVISION IV)

Report to Council for 2006 – 2007

Structure of Report

- 1. Objective**
- 2. Off – Year Meeting**
- 3. Subcommittees and New Responsibilities**
- 4. Projects**
- 5. Conferences**
- 6. Samsung-IUPAC Fund and Award**
- 7. Division Election**
- 8. Others**

1. Objective

The objective of this report is to highlight and summarize activities of the Polymer Division (Division IV) for the past two years. In particular, new developments in 2006 – 2007 will be updated. The division presently has six subcommittees besides the Division Committee.

2. Off – Year Meeting, August 2006

The Off – Year Meeting was held in Rio de Janeiro, Brazil, 15 – 16 August 2006. It was attended by 7 TMs, 4 AMs, 2NRs, 12 Subcommittee Members and 1 Observer. The minutes will be posted on the web after being approved by the next Division Committee meeting scheduled on 4 – 5 August 2007, Torino, Italy.

3. Subcommittees and New Responsibilities

During the past two years two new subcommittees were formed in addition to the existing four subcommittees. There are now six subcommittees in Division IV. All the TMs and AMs have been involved in the activities of the 6 Subcommittees. In addition there were small groups of Division members responsible for the initial evaluation of the Application of Sponsored Conferences, study of divisional Strategy and recruiting New Members, and Division Web Page and Electronic Publication. In light of the necessity to strengthen the Division's activities connected to Industrial and International

Relations, this new responsibility has been decided to be added. It also was agreed that after the next Division Election, either one TM or AM will be assigned for the initial evaluation of Project Applications. This responsibility will be combined with Strategy.

4. Projects

Division IV is one of the most active divisions in attracting and handling projects. Some of the projects are interdivisional especially with Division II and III. Presently, 16 projects (some of them are extensions of earlier projects) with 2005 –, and 2006 – numbers are proceeding (**Appendix I**). It is expected that several projects with 2007 – numbers will soon be included in the list.

DIVISION SUBCOMMITTEES (2006 – 2007)

1. Polymer Terminology

Chairman **R. G. Jones**

2. Structure and Properties of Commercial Polymers

Chairman **M. Buback**

Cochairman **S. C. Kim**

3. Modelling of Polymerisation, Kinetics, and Processes

Chairman **G. T. Russell**

Co-Vice Chairman **R. Hutchinson**

4. Developing Polymer Materials Systems

Chairman **C. K. Ober**

Cochairman **J. Stejskal**

5. Polymer Education

Chairman **J.-P. Vairon**

6. Molecular Characterisation of Polymers

Chairman **J. Pasch**

Cochairman

T. Chang

5. Conferences

In the last year 9 conferences including the World Polymer Congress – 2006 (41st IUPAC International Symposium on Macromolecules, earlier IUPAC MACRO) were sponsored by the division. This year 7 conferences have been granted sponsorship and some more are on pending.

In particular, Division is deeply involved in organizing the IUMACRO, New York City, 10 – 13 June 2007, which is the second international conference sponsored by IUPAC together with a local society. The meeting is coorganized by Division IV and the ACS Polymer Division and Polymeric Materials Engineering and Science Division with the theme of 'Macromolecules for a

Sustainable, Safe and Healthy World’.

The Division has been working very closely in finalizing the Congress Program of the Torino meeting related to polymer science. This was the first serious attempt by the Division to cooperate with the local organizers in formulating polymer sessions in IUPAC Congress.

The World Polymer Congress (Aug 2006, Brazil. Organizer: Prof. Ailton de Souza Gomes) attracted more than 1,200 participants from 50 different countries. The next WPC (WPC 2008) is scheduled on 29 June – 4 July 2008, Taipei, Taiwan. WPC – 2010 is going to be held in Glasgow, U.K., in 2010.

6. Samsung-IUPAC Fund and Award

The Samsung Total Chemical Co. (President: Mr. Hong-Sik Ko) donated additional USD 25,000 to IUPAC to increase the Fund to USD 150,000, for which we are very much thankful.

During the last World Polymer Congress (Aug. 2006, Rio de Janeiro, Brazil), the 2nd Samsung – IUPAC Young Polymer Scientist Award (USD 2,000 and award plaque) was given to Prof. Greg. Tew of the Polymer Science and Engineering Department, University of Massachusetts, Amherst, U.S.A..

The WPC – 2006 Organizing Committee was given USD 5,000 to help students of the economically disadvantaged countries to attend the conference and to defray the cost of plenary speakers. The short Course in Polymer Characterization associated with POLYCHAR – 15 (April, Brazil) was given USD 4,000 to help South American students to take the course.

7. Division Election

Division election is in progress to electronically elect 5 TMs and 6 TMs. Christopher K. Ober (Division VP) is chairing the Nominating Committee. The Division Secretary also has to be elected anew. It is expected that all the vacancies will be filled before the Torino GA.

8. Others

i) The DSM company of Netherlands approached IUPAC in order to establish a special program in Division IV by which we can award the DSM Performance Materials Award during each World Polymer Congress. Div. IV and DSM have been working out details and an agreement is expected to be signed soon. The first Award will be given in the next WPC, June 2008, Taiwan.

ii) The following Macromolecular Symposia volumes have been published as of May 1, 2007 by Wiley – VCH in 2006 – 2007, based on the presentations in the sponsored conferences.

- Volume 233 (2006), Fillers, Filled Polymers and Polymer Blends ed. By P. Dubois, G. Groeninckx, R. Jerome and R. Legras
- Volume 235 (2006), Recent Advances and Novel Approaches in Macromolecule – Metal Complexes ed. by R. Barbucci, F. Ciardelli and G. Ruggeri
- Volume 237 (2006), Molecular Mobility and Order in Polymer Systems ed.

by A. A. Darinskii

- Volume 239 (2006), Advanced Polymers, Composites and Technologies ed. by Giy. J. Marosi and T. Czigany
- Volume 240 (2006), Recent Trends in Ionic Polymerization ed. by D. Baskaran and S. Sivaram
- Volume 242 (2006), Polychar-14 World Forum on Advanced Materials ed. by M. Matsuo, K. Tashiro and Y. Bin
- Volume 245-246 (2006), World Polymer Congress – MACRO 2006 ed. by A. de Souza Gomes
- Volume 248 (2006), Radical Polymerization: Kinetics and Mechanism ed. by M. Buback and A. M. V. Herk
- Volume 249 – 250 (2007), Advanced Polymers for Emerging Technologies ed. by B. C. Kim and K. D. Ahn

Appendix I

Projects with 2005 – , 2006 –, and 2007 – numbers

2005-005-2-400

Definitions of terms relating to individual macromolecules, their assemblies, and dilute polymer solution (Chang, Planned end date: 31/12/08)

2005-007-1-400

Guide to macromolecular terminology and nomenclature (Wilks, Planned end date: 31/12/05)

2005-009-3-400

Efficiency and reproducibility of temperature rising elution fractionation (TREF) (Brüll, Planned end date: 01/07/08)

2005-011-3-400

Repeatability and reproducibility of sample preparation and analysis in hightemperature
SEC (Grumel, Planned end date: 31/12/08)

2005-021-3-400

Accuracy and reproducibility of functionality type analysis of Poly (ethylene oxide) homo and copolymers by LC-CC (Ritting, Planned end date: 31/12/07)

2005-023-2-400

Micro-Structural, melt processing and mechanical properties of compatibilised PA 6/ABS blends (Steiminger, Planned end date: 31/12/08)

2005-043-2-400

Terminology for self-assembly and aggregation of polymers (Ober and Jones, Planned end date: 01/04/09)

2006-002-1-400

Extension of 2002-006-2-400 (Jekins and Moad, Planned end date: 31/12/07)

2006-003-1-400

Short Course in Polymer Characterization associated with POLYCHAR-14 (Matsuo, Planned end date: 30/06/06)

2006-004-1-400

Recommendations on the abbreviated terms of polymers (He, Planned end date: 01/05/09)

2006-005-1-400

Extension of 2002-014-1-400 Glossary of class names of polymers based on their chemical structure and molecular architecture (Vohlidal, Planned end date: 30/06/07)

2006-006-1-400

Extension of 1999-051-1-800 nomenclature for chemically modified polymers (Kitayama, Planned end date: 30/06/09)

2006-007-1-400

Extension of 2003-019-2-400 Definitions of terms relating to crystalline polymers revision of IUPAC Recommendations 1988 (Allegra, Planned end date: 30/09/08)

Projects in Review

2006-018-2

Infrared spectroscopy of conducting polymer nanotubes (Trchova)

2007-007-1

Terminology Relevant to Biorelated Polymer Science and Applications (supplement to 2004-043-1-400) (Vert)

2007-008-1

Development of a multilingual encyclopaedia of polymer terminology (dos-Santos)

2007-004-1-

Guidelines for shear rheometer calibration and performance check (Ruellmann)

2007-009-1

Nomenclature for rotaxane polymers (Vohlidal)

Jung-II JIN

President of Div. IV

Report Subcommittee Polymer Terminology Summer 2005-2007

Submitted for publication:

2000-006-1-400 *Terminology of Polymers with Ionizable Groups and Polymers Containing Ions*

2000-007-1-400 *Glossary of Terms Relating to the Structure of Inorganic and Polymeric Gels and Networks, Inorganic Polymeric Materials and the processing thereof*

Final state of preparation:

2001-081-1-800 *Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Polymers* – Kahovec

2002-016-1-400 *Terminology for Kinetics, Thermodynamics and Mechanisms of Polymerization* – Penczek (this project was formerly **410/26/95**) Public review

2002-048-1-400 *Compendium of Macromolecular Nomenclature and Terminology (The Purple Book, 2nd. Edition)* – Wilks & Metanomski

2002-017-1-400 *Polymerization Processes and Polymers in Dispersed Systems*

In preparation:

2000-04-1-400 *Abbreviations*
No Project number *Dispersity*

2002-06-2-400 *New Radical Polymerization*
2006-002-1-400

2002-14-1-400 *Glossary of Class Names of Polymers Based on their Chemical Structure and Molecular Architecture*
2006-005-1-400

2003-19-2-400 *Definitions of Terms Relating to Crystalline Polymers* - revision of IUPAC Recommendations 1988
2006-007-1-400

2003-60-2-400 *Terminology on Separation of Macromolecules*

2004-043-1-400 *Terminology for Biomedical (Therapeutic) Polymers*

2005-05-2-400 *Definitions of Terms Relating to Individual Macromolecules, Their Assemblies, and Dilute Solutions* - revision of IUPAC Recommendations 1989

Interdivisional Projects:

1999-51-1-800 *Source-Based Nomenclature for Modified Polymer Molecules*

2004-46-1-800 *Structure-Based Nomenclature for Cyclic Macromolecules*

2002-37-1-800 *Nomenclature for Macromolecular Rotaxanes and Catenanes*

2003-42-1-800 *Source-based Nomenclature of Single Strand Polymers* formerly
Source-based Nomenclature of Organic Homopolymers and
Copolymers

New Projects:

2006-41-1-400 *Thermal Properties*

2006-028-1-400 *Macromolecular Assemblies*

2007-23-1-400 *Electric Field Responsive Polymers*

Report to ICTNS Analytical Chemistry Division (V) (January 2006 - June 2007)

**Włodzimierz Kutner, Associate Member ICTNS, ACD
based on**

a complete Report to Council (January 2006 - June 2007)
IUPAC Analytical Chemistry Division (V), prepared by Ryszard Lobinski, ACD
President, displayed on http://www.iupac.org/divisions/V/V_rpt2007.pdf

Contents

1. Tools for international standardisation
2. Projects of ACD and related bodies
 - 2.1 ACD projects published in 2006–2007
 - 2.2 Current projects of ACD
 - 2.3 Interdivisional Working Party on Harmonization of Quality Assurance (IWPHQA) projects
 - 2.4 Subcommittee on Solubility and Equilibrium Data (SSED) projects
 - 2.5 Interdivisional projects

1. Tools for international standardisation

This item addresses the IUPAC goal to facilitate advancement of research in the chemical sciences through the tools that it provides for international standardisation and scientific discussion.

The Analytical Chemistry Division 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 updating analytical terminology and making it readily available via the web.

1.1 The Orange Book: 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 radioanalytical 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.

1.2 The IUPAC Stability Constants Database (SCDB)

This is the most comprehensive compilation of stability constants available, covering the years 1877 to 2004+. 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 the 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 2008. To minimise risk the data collection team will be expanded from one site to involve experts in up to four countries (currently two).

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 2 years.

Division V formed a consultative team to work with Academic Software to achieve a successful transition of management of SCDB from Academic Software to IUPAC or an alternative external systems manager. Further, the Division was represented by Kip Powell on the Secretary-General's *ad hoc* committee that had as its Terms of Reference: "To explore requirements to achieve a modernized interactive IUPAC web site and an ability for IUPAC to provide large databases of value to chemists". The work of this committee led to the current developing arrangements with FIZ-Chemie.

1.3 Recommendations concerning quality assurance

The Working Party on Harmonisation of 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 WPHQA will make a major presentation at the GA on "Metrological Traceability of Measurement Results in Chemistry"

1.4 Critical evaluation of solubility and solution equilibrium data

The Division's Solubility and Solution Equilibrium Data sub-committee (SSED) has an active portfolio of projects. They embrace the critical evaluation of solubility data related to (a) mobility of metals in the environment, (b) industrial processes, and (c) human health. The outputs appear as review papers (Solubility Data Series) in the Journal of Physical and Chemical Reference Data and are thence transferred to the NIST-IUPAC Solubility Database: <http://srdata.nist.gov/solubility/>, or are published as book volumes, such as *Biomineralization – Medical Aspects of Solubility*, E. Königsberger and L-C. Königsberger (eds.), John Wiley & Sons, Chichester, England, 2006. Significant "umbrella" projects include a 25-chapter book volume on "*Solubility for industry*" and "*Chemical speciation of environmentally significant heavy metals with inorganic ligands*".

1.5 Tools of the Trade

The Division's Communications Team has worked with Dr Meyers to organise a new series of articles for CI that emphasises the advancement of research in the chemical sciences through the tools that IUPAC provides. This series commenced in September and features articles from several Divisions and Committees.

2. Projects of ACD and related bodies

2.1 ACD projects published in 2006–2007

Chemical speciation of environmentally significant metals with inorganic ligands Part 2: The Cu^{2+} -OH⁻, Cl⁻, CO_3^{2-} , SO_4^{2-} , and PO_4^{3-} systems (IUPAC Technical Report), *Pure Appl. Chem.* 79(5), 895-950, 2007.

Guidelines for potentiometric measurements in suspensions Part B. Guidelines for practical pH measurements in soil suspensions (IUPAC Recommendations 2006), *Pure Appl. Chem.* 79(1), 81-86, 2007.

Guidelines for potentiometric measurements in suspensions Part A. The suspension effect (IUPAC Technical Report), *Pure Appl. Chem.* 79(1), 67-79, 2007.

The International Harmonized Protocol for the proficiency testing of analytical chemistry laboratories (IUPAC Technical Report), *Pure Appl. Chem.* 78(1), 145-196, 2006.

Guidelines for NMR measurements for determination of high and low pKa values (IUPAC Technical Report)
Pure Appl. Chem. 78(3), 663-675, 2006

Uncertainty estimation and figures of merit for multivariate calibration (IUPAC Technical Report),
Pure Appl. Chem. 78(3), 633-661, 2006.

The International Harmonized Protocol for the proficiency testing of analytical chemistry laboratories (IUPAC Technical Report),
Pure Appl. Chem. 78(1), 145-196, 2006.

Parts 9-12 in IUPAC-NIST Solubility Data Series 81, Hydrocarbons with Water and Seawater – Revised and Updated, A. Mączyński, Volume Editor, 2006

C₁₀ Hydrocarbons with Water, *J. Phys. Chem. Ref. Data*, Vol. 35 (1), pp. 93-151, 2006
C₁₁ and C₁₂ Hydrocarbons with Water, *J. Phys. Chem. Ref. Data*, Vol. 35 (1), pp. 153-203, 2006

C₁₃–C₃₆ Hydrocarbons with Water, *J. Phys. Chem. Ref. Data*, Vol. 35 (2), pp. 687-784, 2006

C₅–C₂₆ Hydrocarbons with Seawater, *J. Phys. Chem. Ref. Data*, Vol. 35 (2), pp. 785-838, 2006

Book: T. M. Letcher (ed.), *Thermodynamics, Solubility and Environmental Issues*, Elsevier, Amsterdam, 2007.

2.2 Current projects of ACD

2.2.1 Recent ACD projects (started after Jan 1st, 2006)

2006-010-1-500 - Adjustment, estimation and uses of equilibrium reaction constants in aqueous solution.

2006-022-1-500 - Spectrochemical Analysis - Conversion of Orange Book Chapter 10 to Glossary Format.

2006-037-1-500 - Metal-focussed -omics: guidelines for terminology and critical evaluation of analytical approaches.

2006-032-1-500 - Solubility data related to industrial processes. Mutual solubility of ethers and ketones with water (**SSSED project**).

2006-033-1-500 - Solubility data related to industrial processes. Rare earth metal chlorides (Sc, Y, lanthanoids) in water and aqueous systems (**SSSED project**).

2006-034-1-500 - Solubility data related to industrial processes. The solubility of oxygen in all solvents (**SSSED project**).

2006-016-1-200 - Recommendations for isotope data in geosciences (**Interdivisional project**).

2006-039-2-600 - Extraction and fractionation methods for exposure assessment related to trace metals, metalloids and hazardous organic compounds in terrestrial environments (**Interdivisional project**).

2.2.2 Other ACD projects

1999-050-1-500 - Chemical speciation of environmentally significant heavy metals and inorganic ligands.

2001-041-2-500 - Recommendation on the use of countercurrent chromatography in analytical chemistry.

2001-072-1-500 - Low activation materials for fusion technology: State and prospects.

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.

2003-015-2-500 - Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry.

2005-014-1-500 - IUPAC stability constants database - completion of data collection up to 2006.

2005-017-1-500 - Glossary of terms related to solubility - updates and revisions to the Orange Book

2005-035-2-500 - Trace elements analysis: role of grain size distribution in solid reference materials.

2005-041-2-500 - Determination of selenomethionine in selenized yeast supplements.

2.3 Interdivisional Working Party on Harmonization of Quality Assurance (IWPHQA) projects

2001-010-3-500 - Metrological traceability of measurement results in chemistry.

2005-019-2-500 - Selection and use of proficiency testing schemes for limited number of participants.

2005-024-2-600 - Establishment of guidelines for the validation of qualitative and semi-quantitative (screening) methods by collaborative trial: a harmonized protocol.

2.4 Subcommittee on Solubility and Equilibrium Data (SSED) projects

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.

2002-035-1-500 - 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 halogenated aromatic hydrocarbons.

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.

2005-006-1-500: Mutual solubility of alcohols and water (update of SDS Vol 15).

2005-033-1-500 - Transition and 12 to 14 main group metals, lanthanide, actinide and ammonium halates.

2.5 Interdivisional projects

2003-060-2-400 - Terminology on separation of macromolecules.

- 2003-056-2-500 - Standard definitions of terms relating to mass spectrometry.
- 2004-021-1-300 - Reference methods, standards and applications of photoluminescence.
- 2004-023-1-700 - Internationally agreed terminology for observations in scientific communication.
- 2004-005-2-500 - Comparable pH measurements by metrological traceability.
- 2004-017-1-500 - Standardization of analytical approaches and analytical capacity building in Africa.



International Union of Pure and Applied Chemistry

A member of the International Council of Scientific Unions

Division of Chemistry and the Environment (DCE - VI)

Report of Activities

Abridged and Modified Version of DP - K. D. Racke Report

January 2006 – June 2007

1. HIGHLIGHTS

1.1 Terms of Reference

The Division of Chemistry and the Environment (DCE) objectives are to provide unbiased and timely authoritative reviews on the behavior of chemical compounds in food and the environment. The DCE is to undertake both fundamental and applied evaluations that contribute to solving environmental problems and enhancing the quality of food on a global scale.

Projects sponsored by the DCE generally fall into three broad categories, including:

- **State-of-the-art authoritative reviews** of specific areas of environmental chemistry which are developed and published in book form, under a working partnership with Wiley Press.
- **Technical evaluations**, critical assessment and development of specific recommendations for areas of interest of environmental or food chemistry, in an attempt to assist and influence research and public policy, including definitions, methodologies, and regulations.
- **Outreach** activities aiming on technology transfer to developing countries, including regional workshops and international congresses that maintain a high level of IUPAC involvement and serve to highlight ongoing and completed IUPAC projects.

1.2 DCE Committee composition and organization

The Division Committee (DC) is currently comprised of 24 members (10 TM's, 7 AM's, and 7 NR's), representing 20 different countries of wide continental coverage. In the recent election of officers, Prof. Nicola Senesi of Italy has been elected as the new Division President, as of January 2008, succeeding Dr. Kenneth Racke.

The work of the Division Committee is organised under several sub-committees, namely:

- Biophysico-Chemical Processes in Environmental Systems (Chair: Prof. Nicola Senesi)

- Chemistry of Environmental Compartments (Chair: Dr. Yehuda Shevah)
- Crop Protection Chemistry (Chair: Dr. Ken Racke)
- Food Chemistry (Chair: Open).

1.3 Projects

At the beginning of the 2006-2007 biennium there were 22 active projects, including 4 that were interdivisionally sponsored (Appendix I). Of these 22 projects, 7 have been completed with reports published or in-press, and 4 projects are nearing completion, while 2 moribund projects are to be abandoned. To the 9 ongoing projects, 10 new projects were approved over the biennium, and 2 project proposals are under review with a decision expected by the time of the Torino GA (Appendix II)

2. DIVISIONAL ACTIVITIES

2.1 Addresses global issues involving the chemical sciences.

- ***Remediation Technologies for Removal of Arsenic from Water and Wastewater*** (2003-017-2-600). The impetus for this project is the already apparent toxicity of water supplies in several regions through natural arsenic contamination affecting the health of millions of residents. There is an urgent need to reduce arsenic levels in drinking water supplies and, in some areas, irrigation waters. Although several technologies have been proposed, there has not been sufficient in-depth evaluation especially for routine treatment of large volumes of water, and agreement on assessment criteria is also lacking. This project is addressing these important issues and includes collaboration with WHO and other IUPAC initiatives in this area including CHEMRAWN. A final report outlining the issue, providing a critique of remediation technologies, and containing case studies for Bangladesh, Thailand, Hungary and Mexico has been completed and is soon to be published as a special volume in the series *Reviews of Environmental Contamination and Toxicology*.
- ***Impact of Transgenic Crops on the Use of Agrochemicals and the Environment*** (2001-24-2-600) and ***Evaluation of Food and Feed Safety Implications of Altered Residues of Pesticides Applied on Transgenic Crops*** (2006-015-3-600). Production of a sustainable global food supply has for the past 60 years relied upon a combination of cultural, biological, and chemical pest management tools. The recent introduction of transgenic crops containing genetic modifications for pest resistance or pesticide tolerance across millions of hectares of agricultural land has raised worldwide interests and significant differences of views between countries as relates to potential environmental and human health impacts. These two active projects are providing unbiased and authoritative international views to these areas of concern based on scientific assessment methodology, and provide an opportunity for IUPAC to take an important leadership role in promoting the importance of chemistry in applied molecular biology. The first project, emphasizing environmental impacts was initiated during 2002 and the report is in press in *Pest Management Science*. The second, follow-up project was initiated during 2007 to address primarily human health aspects.

- ***Air Pollution Models in Environmental Management and Assessment*** (2003-058-1-600). Air pollution models are considered to be a powerful and necessary tools in environmental management programs and allow predications. The aim of this project is to review and assess the application of mathematical models in assessment of air pollution and its impacts. The outcome of the project will be a technical guidance book describing key approaches and providing guidelines for correct application of mathematical models..
- ***XII International IUPAC Symposium on Mycotoxins and Phycotoxins, Istanbul, Turkey (May 2007)***. Although much scientific and public attention is directed at chemistry and human exposure aspects of synthetic chemicals in food, natural toxins are far more prevalent and potentially impactful for the majority of the world's population. IUPAC has had a long-standing interest in mycotoxins and phycotoxins, and this symposium was only the latest in a series that has become the premiere forum for exchange of research results and methodologies related to these important naturally occurring toxins. A report of the outcome of this XII symposium held in Istanbul, Turkey will be available by the time of the GA in Torino.

2.2 International standardization and scientific discussion.

- ***Glossary of Pesticide Chemistry*** (2004-002-1-600) and ***Global Availability of Information on Agrochemicals*** (2001-022-1-600). The recently published “pesticide glossary” provides an authoritative update of an IUPAC report of 10 years earlier, and it was developed with the collaboration of scientists from WHO, FAO, and OECD to ensure the broadest acceptance and applicability. The “global availability” project is aimed at increasing global availability of information on the chemistry of agrochemicals, including methods for testing and evaluation, summaries of properties for individual pesticides, and regulatory standards for pesticides. An internet-based approach developed in cooperation with the FAO-IAEA INFOCRIS program has been pursued, and a web-site launch is anticipated by the end of 2007.
- ***Terminology and Measurement Techniques of Starch Components*** (2004-022-3-400) and ***What are Dietary Fibres?*** (2007-017-1-000). 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. The proposed project is aimed at providing internationally needed guidance on the terminology for the complex carbohydrate class. The new “dietary fibres” project will characterize the nature of dietary fibres and how they are altered as a result of food processing, as well as clear set of internationally accepted definitions.
- ***Use of Reference Soils for Testing Fate and Effects of Chemicals*** (2001-026-1-600). This project aims to develop recommendations related to selection of standardized, reference soils, to allow greater comparability of tests conducted on different chemicals and laboratories.
- **Wiley-IUPAC book series on “Analytical and Physical Chemistry of Environmental Systems”**. The Division continues the 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 “*Environmental Colloids: Behaviour, Structure and Characterisation*” (2004-015-1-600) and No. 11 “*Biophysico-Chemistry of Fractal Structures and Processes in Environmental Systems*” (2003-014-2-600).

- **Wiley-IUPAC book series on “Physico-Chemical Processes in the Soil Environment”** an new series has recently been initiated and the first volume will be produced by the end of 2007 based on the project “*Biophysico-Chemical Processes of Heavy Metals and Metalloids in Soil Environments*” (2004-003-2-600). A second volume is now being initiated via the project “*Biophysico-Chemical Processes Involving Natural Nonliving Organic Matter in Environmental Systems.*” (2006-014-1-600).
- ***Combination of Chemical Analytical Measurements and Remote Sensing Techniques for Coastal Water Monitoring.*** (2006-049-2-600). The objectives of this recently initiated project are to record the state of the art in remote sensing techniques and methods used for marine environment monitoring, and to assess the potential combination of remote sensing data with in situ and laboratory analysis. Case studies based on the Eastern Mediterranean and Black Sea regions will be developed.

2.3 Addressing the needs of chemists in developing countries

- ***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.
- ***Development of Simplified Methods for Ecological Risk Assessment of Pesticides*** (2004-011-1-600) and ***Environmental Risk Assessments for the Registration of Pesticides used in Rice Paddy Fields*** (2006-044-2-600). The “simplified methods” project addresses a critical gap that now exists between the highly sophisticated and resource-intensive approaches to risk assessment practiced in some developed countries with the unreliable or non-scientific consideration of exposure and risk that plagues many developing countries. The recently initiated “pesticides in rice” project aims to develop a specific framework for assessment of pesticides for use in this highly important crop.
- ***IUPAC Regional Crop Protection Chemistry Workshops***. The workshops create a forum where IUPAC project outcomes as well as recommendations from other international bodies can be discussed and applied within the context of local environmental problem areas. Following successful sessions in China, Thailand, Taiwan, Brazil and Korea, the 6th workshop was held in San Jose, Costa Rica during February 2005 as part of the project *Crop Protection Chemistry in Latin America: Harmonized Approaches for Environmental Assessment and Regulation* (2003-013-1-600). The 7th workshop is planned for Beijing, China during October 2007 as part of the project “*Crop Protection Chemistry in Asia: Harmonized Approaches for Safety Evaluation, Regulation, and Protection of Trade*” (2006-017-2-600).
- ***Lecturers on Environmental Chemistry Topics***. Two IUPAC lecturers from Canada and New Zealand have been selected by the Division for presentation of plenary lectures at the *International Symposium of Interactions of Soil Minerals with Organic Components and Microorganisms* to be held in Pucón, Chile during November 2008. The lecturers will also visit local universities to provide more detailed presentations. Three IUPAC lecturers from Australia and USA have been proposed by the Division for presentation of plenary lectures at the *First International Conference on Agrochemicals Protecting Crop, Health, and Natural Environment* planned for Delhi, India during January 2008. Additional lectures at universities would follow.
- The ***11th IUPAC International Congress of Pesticide Chemistry*** was held during August 2006 in Kobe, Japan, and it was co-organized with the Pesticide Science Society of Japan (PSSJ). More than 1100 chemists from 52 countries participated in the Congress, which was organized around the theme “Evolution for Crop Protection, Public Health, and Environmental Safety”. The core of the scientific program consisted of welcoming speeches on behalf of PSSJ and IUPAC, 5 keynote addresses,

more than 100 invited lectures, and nearly 600 posters. The 12th IUPAC International Congress of Pesticide Chemistry is planned to take place in July 2010 in Melbourne, Australia in cooperation with the Royal Australian Chemical Institute.

APPENDIX I: EXISTING PROJECTS (active as of January 2006)

- 630/24/95 - Solute movement in soils with potential rapid by-pass transport (completed and report in-press)
- 1999-041-1-600 - Bioavailability of xenobiotics in the soil environment (nearing completion)
- 1999-014-2-600 – Airborne and remote monitoring of water quality: evaluation of remote sensing techniques for water quality control in surface water bodies (abandoned based on lack of progress)
- 2001-022-1-600 - Global availability of information on agrochemicals (ongoing – extension under consideration)
- 2001-023-1-600 - Agrochemical spray drift: Assessment and mitigation (nearing completion)
- 2001-024-2-600 - Impact of transgenic crops on the use of agrochemicals and the environment (completed and report in-press)
- 2001-026-1-600 - Use of reference soils for testing fate and effects of chemicals (ongoing)
- 2001-039-1-600 - Pest management for small-acreage crops: a cooperative global approach (nearing completion)
- 2002-013-2-600 - Determination of trace elements in oils and fats by inductively coupled plasma optical emission spectroscopy - evaluation of a method by collaborative study (nearing completion)
- 2003-011-3-600 - A critical compendium of pesticide physical chemistry data* (ongoing)
- 2003-013-1-600 - Crop protection chemistry in Latin America: Harmonized approaches for environmental assessment and regulation (ongoing)
- 2003-014-2-600 - Fractal structures and processes in the environment (completed and report in-press)
- 2003-017-2-600 - Remediation technologies for the removal of arsenic from water and wastewater (completed and report in-press)
- 2003-030-1-600 - Glossary of atmospheric chemistry (to be abandoned based on lack of progress)
- 2003-058-1-600 - Air pollution models in environmental management and assessment (ongoing)
- 2004-002-1-600 - Glossary of terms related to pesticides (completed and report published)
- 2004-003-3-600 - Biophysico-chemical processes of heavy metals and metalloids in soil environments (completed and report in-press)
- 2004-005-2-500 - Comparable pH measurements by metrological traceability* (ongoing)
- 2004-011-1-600 - Development of simplified methods and tools for ecological risk assessment of pesticides (ongoing – extension under consideration)
- 2004-015-1-600 - Environmental colloids: behavior, structure and characterization (completed and report published)
- 2004-017-1-500 - Standardization of analytical approaches and analytical capacity-building in Africa* (ongoing)
- 2004-022-3-400 - Terminology and measurement techniques of starch components* (ongoing)

* Interdivisional project

APPENDIX II: NEW AND PROPOSED PROJECTS (since January 2006)

- 2005-024-2-600 - Establishment of guidelines for the validation of qualitative and semi-quantitative (screening) methods by collaborative trial: a harmonized protocol* (continued as 2006-027-1-600)
- 2005-042-1-300 - Chemistry for Biology - an inventory for interdivisional and interdisciplinary activities within IUPAC in the field of biological chemistry*
- 2005-048-2-100 - Solubility and thermodynamic properties related to environmental issues*
- 2006-011-1-600 - Critical review of available methods to predict VOC emission potentials for pesticide formulations
- 2006-014-1-600 - Biophysico-chemical processes involving natural nonliving organic matter in environmental systems
- 2006-015-3-600 - Evaluation of food and feed safety implications of (altered) residues of pesticides applied on transgenic (GM) crops
- 2006-017-2-600 - Crop protection chemistry in Asia: harmonized approaches for safety evaluation, regulation, and protection of trade

2006-039-1 - Extraction and fractionation methods for risk assessment related to trace metals, metalloids and hazardous organic compounds in terrestrial environments*

2006-044-2-600 - Environmental risk assessments for the registration of pesticides used in rice paddy fields

2006-049-2-600 - Combination of chemical analytical measurements and remote sensing techniques for coastal water monitoring. The cases of Eastern Mediterranean and Black Sea

2007-015-1-000 - *Future energy: sustainable and clean energy alternatives for our planet**

2007-017-1-000 – *What are dietary fibres?**

* Interdivisional project or proposed interdivisional project

APPENDIX III: RECENT AND PENDING PUBLICATIONS

Technical Reports and Recommendations

Garelick, H. "Remediation technologies for the removal of arsenic from water and wastewater." *Rev. Environ. Contam. Toxicol.* (2007) in press.

Kleter, G.A.; Bhula, R.; Bodnaruk, K.; Carazo, E.; Felsot, A.S.; Harris, C.A.; Katayama, A.; Kuiper, H.; Racke, K.D.; Rubin, B.; Shevah, Y.; Stephenson, G.R.; Tanaka, J.; Unsworth, J.; Wauchope, D.; Wong, S.S. "Altered pesticide use on transgenic crops and the associated general impact from an environmental perspective." *Pest Manag. Sci.* (2007) in press.

Kördel, W.; Egli, H.; Klein, M.; "Transport of pesticides via macropores." *Pure Appl. Chem.* (2007), in press.

Stephenson, G.R.; Ferris, I.G.; Holland, P.T.; Nordberg, M. "Glossary of terms relating to pesticides." *Pure Appl. Chem.* (2006), 78:2075-2154.

Books

Ohkawa, H.; Miyagawa, H.; Lee, P.W. *Pesticide Chemistry: Crop Protection, Public Health, Environmental Safety.* Wiley-VCH, Berlin (2007) in press.

Senesi, N. *Biophysical Chemistry of Fractal Structures and Processes in the Environment.* John Wiley and Sons, New York (2007) in press.

Stephenson, G.; Solomon, K.; Carazo, E. *Pesticides in the Environment.* University of Costa Rica Press, San Jose (2007) in press.

Violante, A.; Huang, P.M.; Gadd, G.M. *Biophysico-Chemical Processes of Metals and Metalloids in Soil Environments.* John Wiley and Sons, New York (2007) in press.

Wilkinson, K.; Lead, J. *Environmental Colloids and Particles: Behavior, Separation, and Characterization.* John Wiley and Sons, New York (2007) 672 pages.

Other Reports

Kördel, W.; Klein, M. "Prediction of leaching and groundwater contamination by pesticides." *Pure Appl. Chem.* (2006) 78:1081-1090.

Loffredo, E.; Senesi, N. "Fate of anthropogenic organic pollutants in soils with emphasis on adsorption/desorption processes of endocrine disruptor compounds." *Pure. Appl. Chem.* (2006), 78: 947-961.

Racke, K.D. "Pesticide chemistry - report of the 11th IUPAC international congress." *Chem. Int.* (2007) 29: 30-32.

Chemistry and Human Health Division (VII)

IUPAC General Assembly Report to ICTNS

(August 2007)

Summarised from the Division VII (DVII) Report and submitted by John H Duffus

OVERVIEW

Division VII's technical diversity is organized within three Subcommittees, namely *Medicinal Chemistry and Drug Development* (MC), *Nomenclature, Properties and Units in Laboratory Medicine* (NPU), and *Toxicology and Risk Assessment* (SOT). The activities of these subcommittees relevant to ICTNS are listed below.

The critical need for standardization of properties and units associated with human toxicology assessment was recently addressed by DVII's NPU and SOT Subcommittees' report entitled "*Properties and Units in the Clinical Laboratory Sciences: Part XX. Properties and Units in Clinical and Environmental Human Toxicology* [PAC, **79**, 87-152 (2007)]. The NPU's generic database, published on the net under the URL: <<http://dior.imt.liu.se/cnpu/>>, represents an electronically available tool that can be used in a variety of clinical-related analytical settings.

The SOT's "*Glossary for Chemists of Terms Used in Toxicology*," "*Glossary of Terms Relating to Pesticides*" (primarily a project of Division VI, Chemistry and Environment) and "*Explanatory Dictionary of Terms in Toxicology*" were published in PAC or are in press, after being made available electronically for review on the IUPAC website. Several MC-sponsored glossaries are nearing completion: "*Combinatorial Chemistry Terms*;" "*Drug Metabolism Terms*;" "*Pharmaceutical Technology*;" "*Pharmaceutical Process Chemistry*;" "*Biomolecular Screening*;" and, an all encompassing "*Compendium of Glossaries*."

DETAILS OF INDIVIDUAL PROJECTS

SC Medicinal Chemistry Nomenclature and Terminology

2003-044-1-700 Glossary of Combinatorial Chemistry Terms.

The project leader has been changed because of his work commitments (from Derek Maclean to A. Ganesan). Derek stays on as a team member.

2000-009-1-700 Glossary of Drug Metabolism Terms. (Paul Erhardt)

Definitions are being adjusted to IUPAC format.

2002-001-1-700 Compendium of Glossaries. (Robin Ganellin)

Definitions are being adjusted to IUPAC format.

2001-049-2-700 Glossary of Terms in Pharmaceutical Technology. (Eli Breuer)

Definitions are being adjusted to IUPAC format.

2001-049-2-700 Glossary of Terms in Pharmaceutical Process Chemistry. (Mukund Chorghade)

Definitions are being adjusted to IUPAC format.

2005-050-1-700 Prototype Analysis of Molecular Biomarkers in Cancer. (Michael Liebman)

Molecular Biomarkers have become a major focus of disease management and drug development, particularly in oncology. This prototypic study will identify the existing biomarkers in breast cancer and classify them in terms of disease progression and also as to their clinical vs. research use. The project is underway.

2004-019-3-700 Glossary of Terms for Biomolecular Screening. (John Proudfoot)

Glossary sections were prepared by three sub-teams and recompiled into one document. This is undergoing internal review by the team members and contains draft definitions of approximately 150 terms related to biomolecular screening. Reviewers for the final glossary have been identified.

2005-049-1-700 Biological Context by Data Mining. (Michael Liebman)

To extend the usefulness and applicability of the glossaries, it would be worthwhile to explore methods for identifying the various contexts in which the terms appear in the scientific literature. In the ideal situation, this project can transcend the three Subcommittees of the Division to incorporate activities of each.

New Project under discussion:

Update of Glossary of Terms in Medicinal Chemistry.

The SC-NPU generic database

The SC-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, and to the Danish National Board of Health server. During the meeting in Wayne Pa USA with representatives of the CLSI (former NCCLS) it was agreed that the C-NPU and CLSI should seek a permanent hosting of the database probably as part of the CLSI website and server. Unfortunately, this collaborative project of hosting this database on the CLSI website had to be dropped because of CLSI board decision of declining the IFCC offer, the support of C-NPU database not being aligned with CLSI mission. The IFCC SD has thus proposed that the database be hosted on the IFCC website. The cost of such a management has been communicated to IFCC officers, so that IFCC SD could finalize its decision. A meeting in Amsterdam, at Euromedlab IFCC-FESCC congress was scheduled on June 6th, 2007.

Ongoing projects of SC-NPU

1. Properties and units for function examinations (IUPAC: 2001-067-1-700). An updating has been undertaken.
2. Properties and units for urinary calculi (IUPAC: 2001-070-1-700). A full reformatting of the manuscript is being done.
3. Internationally agreed terminology for observations in scientific communication. (IUPAC 2004-023-1-700) Chair : Françoise Pontet. Two drafts have been circulated and discussed during the last Sub-Committee meetings.
4. Mapping of IFCC-IUPAC laboratory coding system to SNOMED CT (IUPAC 2006-008-1-700) Chair : Ulla Magdal. Has just started on 2006-07-01. Abstract is on IUPAC website.

5. Securing and structural updating of information in the NPU coding system and its environment (IUPAC 2006-012-1-700) Chair : Ulla Magdal. Has just started on 2006-07-01. Abstract is on IUPAC website.
6. Recent advances in Nomenclature, Properties and Units : strategy for promoting SC-NPU achievements (2006-048-1-700) Chair : Françoise Pontet. Has just been accepted, budget pending.
7. Translation of SC-NPU database elements and properties into French (F. Pontet). Is being updated in 2007.
8. German translation of the SC-NPU data base (W Külpmann) done during 2005-2006 and is under review in the SC-NPU.
9. The Portuguese translation of the SC-NPU data base has been updated in 2005.
10. Paper on IFCC WG-HbA1c name and units (G. Nordin). This manuscript on the impact of systematic nomenclature on the naming of this particular important property has been agreed on by a ballot in IFCC. It is now submitted to Clinical Chemistry and Laboratory Medicine.
11. Revision of ENV 1614 has been done in collaboration with CENT C 251. It is now published.
12. The final draft of the 3rd edition of VIM is under editorial revision and will be sent to ISO in early June for final publication, due in the 2nd half of 2007.

SC Toxicology and Risk Assessment Nomenclature and Terminology

2005-047-1-700 - Glossary of Terms Used in Ecotoxicology

A list of appropriate terms was compiled and current definitions collected and compared. New definitions were prepared as appropriate. The draft glossary was reviewed at a meeting of the working group in Edinburgh. Professor Mike Schwenck attended this meeting and helped with this revision. Following the meeting a new draft has been prepared and is currently being circulated among the working group. Some problematic terms have been identified and are being given special attention.

Explanatory dictionary - part 2

A project proposal has been submitted and is currently still under consideration for funding. A contract for a subsequent book has been signed with the RSC. “*Explanatory Dictionary of Terms in Toxicology Part 1*” is in press with PAC.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Torino 2007-08-07 and 08

**Attachment to Agenda
Item 9**

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

Torino 2007-08-07 and 08

**Attachment to Agenda
Item 12**

Date: 2007-07-26
To: Division Presidents and Secretaries, ICTNS Members, Aubrey Jenkins
From: Jack Lorimer, Chairman, ICTNS
Bernardo J. Herold, Secretary, ICTNS
Re: 2007 List of Questionable Entries in Gold Book (including 2nd edition (printed), XML online version)

Introduction

ICTNS has become increasingly concerned with terms in the Gold Book that are in error according to current standards. The plan is to collect such terms on an annual basis, circulate them to the Divisions for comment and suggested revisions, then (although the details are still under consideration) make them the subject matter of new IUPAC Recommendations which will be submitted for Public Comment in the usual way. It is considered important to review any changes in as rigorous a way as that carried out for the original terms.

New terms that have not yet been incorporated into the Gold Book are not the subject of this exercise. These will be addressed in an ongoing current project and possible future projects.

ICTNS is therefore requesting that each Division examine the list below for any terms that have occurred in that Division's previous publications, decide if changes are necessary, and if so, propose new definitions. It would be appreciated if this task could be completed by September 30, 2007. You may add terms that are not on the list below. However, please do not add any new terms that have appeared in Recommendations published since 1997, the date of the last printed version of the Gold Book. Preparation of a list for 2008 will commence shortly.

(Note that preferred access to the XML online Gold Book is: <http://goldbook@iupac.org> and that the correct way to refer to it is:

IUPAC. Compendium of Chemical Terminology, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: <http://goldbook.iupac.org> (2006-) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins.)

1. absorption

Reported by: Several correspondents.

Gold Book: 1. The process of one material (absorbent) being retained by another (absorbate).

Problem: The words "absorbent" and "absorbate" are interchanged.

Suggested solution: Corrected in at least two current sets of Recommendations.
Correction can be made in Gold Book immediately.

2. acceptor number (AN)

Reported by: B. J. Herold , with comments by J. W. Lorimer

Gold Book: A quantitative measure of *Lewis acidity*

1994, 66, 1081

Problem: ‘AN’ as a symbol has to be replaced by ‘ A_N ’. ‘AN’ is however acceptable as an acronym.

Suggested solution: Replace in title line AN by A_N and add after ‘*Lewis acidity*’ ‘AN’ in upright characters is not acceptable as symbol, only as acronym.

3. donor number (DN)

Reported by: B. J. Herold , with comments by J. W. Lorimer

Gold Book: A quantitative measure of *Lewis basicity*

1994, 66, 1081

Problem: ‘DN’ as a symbol has to be replaced by ‘ D_N ’. ‘DN’ is however acceptable as an acronym.

Suggested solution: Replace in title line DN by D_N and add after ‘*Lewis acidity*’ ‘DN’ in upright characters is not acceptable as symbol, only as acronym.

4. electromotive force, E

Reported by: F. Meyers, with comments by J. Lorimer

Gold Book: Energy supplied by a source divided by the electric charge transported through the source. For a galvanic cell it is equal to the electric potential difference for zero current through the cell.

G.B. 58; ISO 31-4: 1992; 1996, 68, 971.

Related entries:

electric potential difference (of a galvanic cell), ΔV

Difference in the potentials of electrodes on the right and left of a galvanic cell. When is positive, positive charge flows from left to right through the cell.

1996, 68, 971

electromotive force, E

$$E = \int (F/Q) \square dr \quad V$$

Green Book, 2nd and 3rd eds. (section 2.3: Electricity and Magnetism)

See also: L. Landau and E. M. Lifshitz (transl. J. B. Sykes and J. S. Bell).

Electrodynamics of Continuous Media. Course of Theoretical Physics, Vol. 8, pp. 101-103. Pergamon, Oxford (1960).

Problem: Electromotive force is used in what appears to be two ways: (1) in electrostatics as defined above, which is a voltage, not a force; (2) for galvanic cells as the limiting value of the electric potential difference of a cell for zero current through the cell, which again is a voltage, not a force. However, Landau and Lifshitz (for example) show that the galvanic cell definition follows readily from the electrostatic definition, and define emf as: “work per charge done on a charged particle when it is carried reversibly along a closed circuit”, which corresponds to the definition in sect. 2.3 of the Green Book, 2nd or

3rd eds. (The 3rd edition, latest communication, uses correctly a line integral around a closed circuit.)

The new Green Book (3rd ed., sect. 2.13, note (14)) states:

"The limiting value of E_{cell} for zero current flowing through the cell, all local charge transfer and chemical equilibria being established, was formerly called emf (electromotive force). The name electromotive force and the symbol emf are no longer recommended, since a potential difference is not a force". However, the new Green Book (sect. 2.3) retains the electrostatic definition, which, as noted, also is not a force.

The most recent recommendation in which "cell potential" is used is: Measurement of pH. Definition, standards, and procedures. IUPAC Recommendations 2002. <<http://www.iupac.org/publications/pac/2002/7411/7411x2169.html>>

Suggested solution: Divisions I and IV should consider the above points carefully, and propose a solution that explains the connection between the electrostatic definition of emf and the electrochemical definition of the electric potential difference of a galvanic cell, possibly as a new project that clarifies the terminology surrounding potential differences in general. As a preliminary suggestion, in the Gold Book entry "electromotive force":

(1) the mathematical statement of emf could be given - $E = \oint_C (\mathbf{F} / Q) \cdot d\mathbf{r}$ or $\int_C (\mathbf{F} / Q) \cdot d\mathbf{r}$,

with the integral specified clearly as a line integral around a closed circuit. (ds would be preferable to $d\mathbf{r}$, to avoid confusion between a radius vector and a line element, but the new Green Book is keeping $d\mathbf{r}$.) (2) The second sentence could be modified to read: "For a galvanic cell, the term emf is no longer recommended, and should be replaced by the electric potential difference for zero current through the cell, $E_{\text{cell, eq.}}$." A Note could be added: "Alternatively, the emf is equal to the line integral of the electrical force per charge over a closed circuit."

5. energy

Reported by: Correspondents

Gold Book: In mechanics, the sum of *potential energy* and *kinetic energy*.

In thermodynamics, the *internal energy* or thermodynamic energy increase, ΔU , is the sum of *heat* and *work* brought to the system. Only changes in energy are measurable. For photons, $E = h\nu$ where h is the Planck constant and ν the frequency of radiation. In relativistic physics, $E = mc^2$, where c is the speed of light, and m is the mass.

Problems: (1) Energy in mechanics is defined in terms of two other energies. The definition of *kinetic energy* is OK (an equation is given), but *potential energy* is not. (2) Relativistic energy should use the rest mass and the speed of light in vacuum.

Suggested solution: Requires careful examination by Div. I.

6. fundamental physical constants

Problem: All need to be updated to the 2002 values from P. J. Mohr and B. N. Taylor. CODATA Recommended Values of the Fundamental Physical Constants: 2002. *Rev. Mod. Phys.* **77**, 1-108 (2005); <http://physics.nist.gov/constants>. The quantities found in the Gold Book and their recommended 2002 values should be:

Avogadro constant $L, N_A = 6.022\,141\,5(10) \times 10^{23} \text{ mol}^{-1}$

Boltzmann constant	$k (k_B) = 1.380\,650\,5\,(24)\,\text{H}\,10^{-23}\,\text{J}\,\text{K}^{-1}$
elementary charge (charge on a proton)	$e = 1.602\,176\,53\,(14)\,\text{H}\,10^{-19}\,\text{C}$
Faraday constant	$F = 9.648\,533\,83\,(83)\,\text{H}\,10^4\,\text{C}\,\text{mol}^{-1}$
gas constant	$R = 8.314\,472\,(15)\,\text{J}\,\text{K}^{-1}\,\text{mol}^{-1}$
permittivity of vacuum (electric constant)	
Planck constant	$h = 6.626\,069\,3\,(11)\,\text{H}\,10^{-34}\,\text{J}\,\text{s}$

These are the principal constants; others listed in the Green Book could be added as a table, as in the XML version of the Gold Book.

7. ground state

Reported by: T. Cvitaš

Gold Book: The state of lowest Gibbs energy of a system.

See also *excited state*.

Problem: Gibbs energy is inappropriate.

Suggested solution: State of lowest energy of a system.

See also *excited state*.

8. Haworth representation

Reported by: M. Peintinger m@peintinger.com

Gold Book: The Haworth representation of cyclic forms of monosaccharides can be derived from the *Fischer projection*, as follows. (Lengthy description follows.)

Problem: Below the two glucose molecules there is written both times glucopyranose. However, the right-hand one is glucofuranose (5 ring).

Suggested solution: As this is an obvious error, it is suggested that it be corrected immediately in the online and XML Gold Books.

9. Henderson-Hasselbach equation

Reported by: A. Baptista baptista@itqb.unl.pt; Instituto de Tecnologia Quimica e Biologica, Universidade Nova de Lisboa Av. da Republica, EAN, ITQB II, Piso 6, Apartado 127 2781-901 Oeiras, Portugal

Gold Book: See below.

Problems:

(1) Baptista: "There is a misspelling in the entry "Henderson-Hasselbach equation" which extends to other entries that cite this one. The second name should be spelled as "Hasselbalch" (with an additional "l"), after K. A. Hasselbalch, who included Sorensen's pH terminology into the equation introduced by L. J. Henderson for acid-base equilibrium. Unfortunately, the misspelled form is quite common (a quick search in Google or in the ACS Archives shows still some preference for the correct form), and I suspect that some of the incorrect occurrences were chosen after checking the 'correct' form in the Gold Book."

(2) Baptista: "The equation in the entry is, as usual, just the logarithmic form of the mass action law applied to acids. Now, it turns out that the mass action law (due to Gulberg and Waage) was known for some decades before Henderson proposed his equation,

which is actually an approximation to the exact mass action law. Thus, the so-called "Henderson-Hasselbalch equation" (which is exact) is not really due to Henderson or Hasselbalch. This issue has been clearly discussed by Robert de Levie (Chem. Educator 2002, 7, 132; J. Chem. Educ. 2003, 80, 146). Maybe IUPAC should discourage the usual designation, by adding a plus sign to the entry "Henderson-Hasselbalch equation", as done for some other entries.

Comment: Corrected in *Glossary of Terms Used in Toxicology*. 2nd ed. in press. Could be corrected immediately in Gold Book as a documented error.

10. isotope effect

Reported by: B.-L. Zhang benli.zhang@chimbio.univ-nantes.fr

Gold Book: The effect on the rate or equilibrium constant of two reactions that differ only in the isotopic composition of one or more of their otherwise chemically identical components is referred to as a *kinetic isotope effect* or a *thermodynamic* (or *equilibrium*) *isotope effect*, respectively.

Problem: Zhang: "The defined 'isotope effect' is only suitable for chemical reactions. In reality there are many isotope effects. For example, isotope effect on spectroscopic data, isotope effect on fusion point, etc. I propose to define 'isotope effect' as 'effects of isotope substitution on physico-chemical properties'."

Comment: This is a problem for Divs. I and III.

11. isotopomer

Reported by: B.-L. Zhang benli.zhang@chimbio.univ-nantes.fr; Danish colleagues of T. Damhus

Gold Book: Isomers having the same number of each isotopic atom but differing in their positions. The term is a contraction of 'isotopic isomer'.

Isotopomers can be either constitutional isomers (e.g. CH₂DCH=O and CH₃CD=O) or isotopic stereoisomers [e.g. (*R*)- and (*S*)-CH₃CHDOH or (*Z*)- and (*E*)-CH₃CH=CHD]. 1994, 66, 1132; 1996, 68, 2211.

Problem:

Zhang: "The definition of isotopologue and isotopomer is not sufficient for describing the isotope-substituted molecules of a compound. For example, are ¹²CH₃OH and ¹³CH₃OH two isotopologues or two isotopomers? In fact, in the literature the confusion of isotopologue and isotopomer is frequent. I propose to define "isotopomer" as follows: isotopomers of a compound are molecules that have the same chemical composition and configuration but differ in isotope substitution. The isotope substitution may differ by 1) element substituted by isotopes, 2) isotopes, 3) number of isotope atoms, 4) position of substitution. That means "isotopologue" is no more useful. The use of only "isotopomer" defined as above may avoid confusion and simplify the terminology. Thus, ¹²CH₃OH, ¹³CH₃OH, CH₂D¹⁸OH, CHD₂¹⁸OOD, etc. (including stereoisomers: *R*- and *S*-CHD¹⁸TOH) are all isotopomers of methanol. If it is necessary to classify the isotopomers, one can use monodeuterated, dideuterated, ¹³C-labelled, ¹⁸O-labelled isotopomer, etc.

12. lumen

Reported by: L. Glasser, J. Lorimer

Gold Book: SI derived unit of luminous flux, $\text{lm} = \text{sd sr}^{-1}$.

Problem: The units have been transcribed incorrectly from the Green Book, 2nd ed.

Corrected version: SI derived unit of luminous flux, $\text{lm} = \text{cd sr}$.

Notes: B. Kosata has corrected the entry in the XML Gold Book.

13. molecule

Reported by: K.-W. Huang hkw@bnl.gov (Brookhaven National Lab.) via A. McNaught

Gold Book: An electrically neutral entity consisting of more than one atom ($n > 1$).

Rigorously, a molecule, in which $n > 1$ must correspond to a depression on the potential energy surface that is deep enough to confine at least one vibrational state.

Problem: “In the kinetics of gases and some other fields, we often see that the term “monatomic molecule” is used to describe noble gases. This term has also been used in quite a few textbooks and literature. For your reference, please see:

<http://www.ac.wvu.edu/~vawter/PhysicsNet/Topics/Thermal/kinTheoryGas.html>

<http://en.wikipedia.org/wiki/Molecule>

[\[campus.com/engineering/electrical/fundamentals/atomic_theory1.html\]\(http://www.science-campus.com/engineering/electrical/fundamentals/atomic_theory1.html\)](http://www.science-</p></div><div data-bbox=)

<http://www.chemguide.co.uk/atoms/bonding/vdw.html>

Therefore, if IUPAC suggests that the term “molecule” can only be used to describe a compound that contains at least two atoms, might it be a good idea to make this point more clear by pointing out the misuse of the term “monatomic molecule”? Or maybe it would be better if the definition of “monatomic molecule” could be included in the IUPAC Compendium of Chemical Terminology as well?”

Suggested solution: Add a note to the definition that monatomic entities are excluded, as are ions (and free radicals??) ; i. e.,

“Electrically neutral entity consisting of more than one atom ($n > 1$). Rigorously, a molecule, in which $n > 1$ must correspond to a depression on the potential energy surface that is deep enough to confine at least one vibrational state.

“Note: Monatomic entities, ions and free radicals are excluded from the definition.”

14. pH

Reported by: J. Lorimer

Gold Book: In the restricted range of dilute aqueous solutions having *amount concentrations* less than 0.1 mol dm^{-3} and being neither strongly acidic nor strongly alkaline ($2 < \text{pH} < 12$).

$$\text{pH} = -\lg\{\gamma_{\pm}c(\text{H}^+)/\text{mol dm}^{-3}\} \quad \forall 0.02$$

where γ_{\pm} is the mean ionic *activity coefficient* of a typical univalent electrolyte on a concentration basis. The operational definition is based on the *electromotive force* measurement of the galvanic cell:

reference electrode | KCl(aq) || solution X | H(g) | Pt

where the KCl solution has a molality greater than 3.5 mol kg^{-1} relative to a standard solution S, replacing X in the scheme above [usually $\text{KH}_2\text{PO}_4(\text{aq})$ of molality 0.05 mol kg^{-1} which has a $\text{pH} = 4.005$].

$\text{pH}(\text{X}) = \text{pH}(\text{S}) + (E_{\text{S}} - E_{\text{X}})F/(RT \ln 10)$.
 G.B. 62; 1996, 68, 986; see also 1990, 62, 2205; 1984, 56, 569.

Problems: The entry: (1) uses amount concentration in the basic definition, but molality in the operational definition; (2) writes $\text{H}(\text{g})$ instead of $\text{H}_2(\text{g})$; (3) writes $\text{KH}_2\text{PO}_4(\text{aq})$ instead of $\text{KHP}(\text{aq})$ (potassium hydrogen phthalate). In addition, (1) the term electromotive force should be changed to cell potential; (2) there is a new pH recommendation from 1998.

Suggested solution (based on entry in the new Green Book):

pH

$$\text{pH} = -\lg[a(\text{H}^+)] = -\lg[m(\text{H}^+) (\gamma_{\text{H}^+}) / m^\circ]$$

where $a(\text{H}^+)$ is the activity of hydrogen ion (hydrogen 1^+) in aqueous solution, $\text{H}^+(\text{aq})$, (γ_{H^+}) is the activity coefficient of $\text{H}^+(\text{aq})$ (molality basis) at molality $m(\text{H}^+)$, and $m^\circ = 1 \text{ mol kg}^{-1}$ is the standard molality.

Note 1. pH cannot be measured independently because calculation of the activity involves the activity coefficient of a single ion. Thus it can be regarded only as a notional definition.

Note 2. The establishment of primary pH standards requires the application of the concept of “primary method of measurement”, assuring full traceability of the results of all measurements and their uncertainties. Any limitation in the theory of determination of experimental variables must be included in the estimated uncertainty of the method.

Note 3. The primary method for measurement of pH involves the use of a cell without transference, known as the Harned cell:



The equation for this cell can be rearranged to give:

$$-\lg[a(\text{H}^+) (\gamma_{\text{Cl}^-})] = (E - E^\circ)F/(RT \ln 10) + \lg[m(\text{Cl}^-) / m^\circ]$$

where E is the potential difference of the cell and E° is the known standard potential of the $\text{AgCl} \mid \text{Ag}$ electrode. Measurements of E as a function of $m(\text{Cl}^-)$ are made and the quantity $a(\text{H}^+) (\gamma_{\text{Cl}^-})$ (called the acidity function) is found by extrapolation to $m(\text{Cl}^-) / m^\circ = 0$. The value of (γ_{Cl^-}) is calculated using the Bates-Guggenheim convention based on Debye-Hückel theory. Then $-\lg[a(\text{H}^+)]$ is calculated and identified as $\text{pH}(\text{PS})$, where PS signifies primary standard. The uncertainties in the two estimates are typically 0.001 in $-\lg(a_{\text{H}^+} (\gamma_{\text{Cl}^-}))$ and ± 0.003 in pH.

Materials for primary standard buffers must also meet the appropriate requirements for reference materials, including chemical purity and stability, and applicability of the Bates-Guggenheim convention for the estimation of $-\lg[(\gamma_{\text{Cl}^-})]$. This

convention requires that the ionic strength be 0.1 mol kg^{-1} . Primary standard buffers should also lead to small liquid junction potentials when used in cells with liquid junctions. Secondary standards, H(SS), are also available, but carry a greater uncertainty in measured values.

Note 4. Practical pH measurements generally use cells with liquid junctions in which, consequently, liquid junction potentials, E_j , are present. Measurements of pH are not normally performed using the Pt|H_2 electrode, but rather the glass (or other H^+ - selective) electrode, whose response factor ($dE/d\text{pH}$) usually deviates from the Nernst slope. The associated uncertainties are significantly larger than those associated with fundamental measurements using the Harned cell. Nonetheless, incorporation of the uncertainties for the primary method, and for all subsequent measurements, permits the uncertainties for all procedures to be linked to the primary standards by an unbroken chain of comparisons.

Note 5. Reference values for standards in D_2O and aqueous-organic solvent mixtures exist.

G. B. 62; 1997, 69, 1007; 1996, 68, 986; see also 2002, 74, 2169; 1990, 62, 2205; 1984, 56, 569.

Note 1: The 2002 reference is: PAC 2002, 74, 2196 Measurement of pH. Definition, standards, and procedures (IUPAC Recommendations 2002). Older references must be included for legal reasons: changes in definitions must have a traceable history. The 1997 reference is: PAC 1997, 69, 1007. Reference values standards and primary standards for pH measurements in D_2O and aqueous-organic solvent mixtures: New accessions and assessments.]

Note 2: The above suggested entry is a slightly shortened version of that in the Green Book, 3rd ed., sect. 2.13.1 (viii) (in final stages of preparation), with two main exceptions: (1) addition of “(hydrogen 1⁺)” to conform with notation in the 2005 Red Book; (2) use of in-line parentheses instead of sub-subscripts for easier translation into web-compatible entries. It is also compatible with the 2002 IUPAC Recommendations on pH.

15. potential energy

Reported by: Correspondents.

Gold Book: Energy of position or orientation in a field of force.

Problem: Energy itself not defined; see *energy*.

Suggested solution: Careful consideration by Div. I.

16. rate of reaction, order of reaction

Reported by: Neo Wee-Koon weekoon@pmail.ntu.edu.sg

Gold Book: See entries *order of reaction*, *rate of reaction*.

Problem: “I would like to seek some clarifications on two entries in the IUPAC Compendium of Chemical Terminology, namely, rate of reaction and order of reaction. Please refer to the Word document for details.” (Word document available from A. McNaught.)

Comment: A. McNaught to Wee-Koon: “The Compendium entries in question are taken from the IUPAC Glossary of Terms in Physical Organic Chemistry (Pure Appl. Chem., 1994, 66, 1077), and I have passed on your questions to the Secretary of the IUPAC Division responsible for this glossary for comment.” Clearly a problem for Div. III.

17. redox, redox reaction

Reported by: Israel Agranat, Department of Organic Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904 Israel isria@vms.huji.ac.il

Gold Book and Glossary of Terms in Physical organic Chemistry: Missing.

Problem: “I have been looking at the IUPAC Compendium of Chemical Terminology (online version) and noticed that the terms ‘REDOX’ and ‘REDOX Reaction’ are missing. These terms also do not appear in the IUPAC Glossary of Terms in Physical Organic Chemistry. Please advise me how to overcome these omissions.”

Suggested solution: The Glossary was last updated in 1994, and perhaps should be revised under auspices of Div. III. As this qualifies as a new term for the Gold Book, it should be added through new Recommendations.

18. solubility parameter (of a polymer), δ

Reported by: J. Lorimer

Gold Book: A characteristic of a polymer used in predicting solubility of that polymer in a given solvent.

Notes:

1. For a substance of low molecular weight, the value of the solubility parameter is often estimated from the enthalpy of vaporization; for a polymer, it is usually taken to be the value of the solubility parameter of the solvent producing the solution with maximum intrinsic viscosity or maximum swelling of a network of the polymer.
2. The solubility parameter is usually expressed in $(\text{cal}/\text{cm}^3)^{1/2}$ or, preferably, $(\text{J}/\text{cm}^3)^{1/2}$ units. The units must always be given; $1(\text{cal}/\text{cm}^3)^{1/2} \cdot 2.05(\text{J}/\text{cm}^3)^{1/2}$.

Problem: The Gold Book entry is copied from the Purple Book. The entry asks the reader to accept rather odd-looking units without defining the physical quantity; it only gives some attributes of the quantity. The definition is useful for other substances besides polymers, so could be generalized.

Suggested solution:

solubility parameter, δ

Parameter used in predicting the *solubility* of non-electrolytes (including polymers) in a given *solvent*. For a substance B:

$$\delta_B = (\Delta_{\text{vap}} E_{\text{m},B} / V_{\text{m},B})^{1/2}$$

where $\Delta_{\text{vap}} E_{\text{m}}$ is the molar energy of vaporization at zero pressure and V_{m} is the molar volume [18].

Note 1: For a substance of low molecular weight, the value of the solubility parameter can be estimated most reliably from the enthalpy of vaporization and the molar volume.

Note 2: The solubility of a substance B can be related to the square of the difference between the solubility parameters for supercooled liquid B and solvent at a given temperature, with appropriate allowances for entropy of mixing. Thus a value can be estimated from the solubility of the solid in a series of solvents of known solubility parameter. For a polymer, it is usually taken to be the value of the solubility parameter of the solvent producing the solution with maximum intrinsic viscosity or maximum swelling of a network of the polymer. See [18] for the original definition, theory, and extensive examples.

Note 2: The SI units are $\text{Pa}^{1/2} = \text{J}^{1/2} \text{ m}^{-3/2}$, but units used frequently are $(:\text{Pa})^{1/2} = (\text{J cm}^{-3})^{1/2}$ or $(\text{cal cm}^{-3})^{1/2}$, where $1 (\text{J cm}^{-3})^{1/2} = 2.045 (\text{cal cm}^{-3})^{1/2}$.

Modified from [1, 18].

(The respective references are: [1] Gold Book; [18] Hildebrand & Scott, *Solubility of Non-electrolytes*.)

Notes: The problem has been brought to the attention of J. Kahovec and P. Kratochvil, both of whom have recommended a change in the entry to the executive of Div. IV and the committee in charge of revision of the new edition of the Purple Book. It could be corrected in the Gold Book.