#### INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

### 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), 3<sup>rd</sup> ed. In press, 2007
- Terminology and Nomenclature in Polymer Chemistry (Purple Book), 2<sup>nd</sup> ed. Still under revision. Publication expected late 2007or 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<sup>2+</sup> OH<sup>-</sup>, Cl<sup>-</sup>, CO<sub>3</sub><sup>2-</sup>, SO<sub>4</sub><sup>2-</sup> and PO<sub>4</sub><sup>3-</sup> 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 if 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, 3<sup>rd</sup> 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(butylenes terephthalate) and poly( $\epsilon$ -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.)