

International Union of Pure and Applied Chemistry

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Vice President: Prof. Bryan R. Henry (Canada)

Past President Prof. Pieter S. Steyn (South Africa)

Secretary General: Prof. David StC. Black (Australia)

Treasurer: Dr. Christoph F. Buxtorf (Switzerland)

Dr. John W. Jost

Executive Director:

All statutory actions necessary for convening the 43rd IUPAC General Assembly and Council Meetings in Beijing during the period 12-21 August 2005 have been taken through the following letters:

Re. Changes in Statutes and Bylaws 12 August 2004

re. Official invitations to National Adhering Organizations and Associate national Adhering organizations
16 November 2004

re. Official invitation to Associated Organizations 16 November 2004

re. Members of IUPAC Bodies 16 November 2004

re. Nominations of Candidates for Elections (Officers and Bureau) 12 November 2004

re. Items for Council Agenda 15 February 2005

re. Council Agenda 26 April 2005

re. Announcement of Candidates for Elections (Officers and Bureau) 21 June 2005

re. Documentation available for Council Agenda Items 5 July 2005

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* VOTING PROCEDURES IN IUPAC COUNCIL

(as of 27 June 2005)

There are 39 Delegations eligible to vote with a total of 133 assigned votes. The number of assigned votes may be changed on the day of the Council depending on the number of NAOs in arrears at that time.

1. Scientific Matters (Bylaw 2.11)

Voting by individual Delegates present at time of voting - simple majority on show of hands (67 if all assigned votes are cast).

2. Non-scientific Matters (Bylaw 2.2)

Voting by Delegation Cards - simple majority of votes cast is mandatory for all election matters, but see 2.4 below (67, if all assigned votes are cast).

(each Delegation must cast all of its votes in the same sense)

- 2.1 Admission and Removal of Members (Bylaw 2.21)
 - 2.1.1 Admission simple majority of Delegation Card votes cast (74, if all assigned votes are cast)
 - 2.1.2 Removal 75% of Delegation Card votes cast (100, if all assigned votes are cast)
- 2.2 <u>Election of Officers</u> (Bylaw 2.222)

Secret ballot by Delegation Voting Slips - simple majority of votes cast (67, if all assigned votes are cast)

(see second paragraph of Bylaw 2.222 for elimination procedure in case of lack of simple majority of votes)

2.3 Election of Bureau Members (Bylaw 2.222)

Secret ballot by Delegation Voting Slips - simple majority of votes cast per Bureau Member (67, if all assigned votes are cast)

^{*} BASED ON VOTING ASSIGNMENTS APPROVED AT GUILDFORD

VOTING PROCEDURES IN IUPAC COUNCIL

(see third paragraph of Bylaw 2.222 for elimination procedure in case of lack of simple majority of votes for necessary numbers of candidates)

2.4 Other Non-scientific Matters (Bylaw 2.23)

At the discretion of the Council, such matters may be adopted without a formal vote, for example, by a show of hands.

3. <u>Change of Bylaw</u> (Bylaw 6.2)

Voting by Delegation Cards – more than 50% of assigned votes (67)

4. <u>Change of Statute</u> (Statute 14.3)

Voting by Delegation Cards - 66.6% of assigned votes (89).

Note. Abstentions (Statute 5.32): In all Council voting procedures, abstentions shall not be recorded as votes.

Official Delegations of National Adhering Organizations at 43rd IUPAC Council Meeting 20-21 August, 2005, Beijing, China

(As of 28 June 2005)

<u>Argentina</u> (not available) (pending)

<u>Australia</u> 4 votes

Prof. Mary Garson

Prof. Robert G. Gilbert Delegation Leader, Elected Member of

Bureau, Former President of Polymer

Division

Prof. David B. Hibbert

Prof. Robert Lamb

Bureau Member Prof. David StC. Black, IUPAC Secretary

General

<u>Austria</u> 3 votes

Prof. Heinz Gamsjäger Delegation Leader

Bangladesh (not available) 1 vote

Belgium 5 votes

Prof. Paul de Bièvre Delegation Leader

Brazil (not available) (pending)

Bulgaria 1 vote

Prof. Christo Balarew Delegation Leader

Prof. Christo Kratschanov Non-voting Secretary

Canada 4 votes

Dr. Kelly Akers

Dr. Linda Johnston

Dr. Christopher I. Ratcliffe

Dr. Bernard West

Bureau Members: Prof. Bryan Henry – IUPAC Vice President

<u>Chile</u> (not available) (pending)

(As of 30 June 2005)

China - Beijing 6 votes Prof. Chunli Bai Leader of Delegation and Elected Member of Bureau Prof. Zhongfan Liu Prof. Xibai Qiu Prof. Yong Qiu Prof. Fu Xi Prof. Jiannian Yao China - Taipei 4 votes Prof. Kan-Nan Chen Prof. Teh-Chang Chou Prof. Ling-Kang Liu Dr. Cheng-Ching Wu Croatia 1 vote Prof. Leo Klasinc Czech Republic (not available) 2 votes 3 votes Denmark Dr. Ture Damhus Prof. Sven E. Harnung Egypt (not available) 2 votes Finland (not available) 3 votes 5 votes France Dr. Jean Claude Bernier Prof. Nicole J. Moreau Elected Member of Bureau

Dr. Jean-Marc Paris

Prof. Jean-Pierre Vairon

(As of 30 June 2005)

Germany 6 votes Dr. Michael J. Droescher Past-President of Chemistry and the Prof. Werner Klein **Environment Division** Prof. Wolfram Koch <u>Greece</u> (not available) 2 votes 2 votes Hungary Prof. George Horvai <u>India</u> 4 votes Prof. Sumit Bhadori Prof. B. Gopolan Non-Voting Secretary Dr. Javed Iqbal Prof. V. Krishnan Dr. J. P. Mittal <u>Ireland</u> (not available) 4 votes Israel 3 votes Prof. Shammai Speiser 5 votes <u>Italy</u> Prof. Giuseppe Della Gatta Prof. Franco Pavese <u>Japan</u> (not available) 6 votes Korea, Republic of 5 votes Prof. Jin Soon Cha Prof. Jun Il Jin

Prof. Heon Kang

Prof. Kook Joe Chin

(As of 30 June 2005)

1 vote

Kuwait

Dr. Khalidah Al-Dalama

Miss Sameera Al-Houli Non-voting Secretary **Netherlands** 4 votes Prof. Jan Reedijk Prof. Gus Somsen Elected Member of Bureau Dr. Iwan P. Thonus Prof. Rietje van Dam-Mieras New Zealand (not available) 2 votes Prof. H. Kipton Powell President of Analytical Chemistry Division Norway 2 votes Dr. Tore Benneche Prof. Nils Arne Jentoft Bureau Member: Prof. Leiv Sydnes, IUPAC President Pakistan 2 votes Dr. Din Mohammed Poland 3 votes Prof. Bogdan Marcineic Prof. Stanislaw Penczek Portugal (not available) 3 votes Puerto Rico 4 votes Dr. Gabriel A. Infante Dr. Ram Lamba Dr. Edgar Resto Dr. Carlos Tollinche Russia (not available) 4 votes Prof. Oleg M. Nefedov Elected Member of Bureau

(As of 30 June 2005)

Serbia and Montenegro 1 vote Prof. Teodor Ast Slovakia 2 votes Prof. Dusan Berek Slovenia (not available) 2 votes South Africa 3 votes Dr. Michael D. Booth **Delegation Leader** Prof. John D. Bradley Dr. Alufelwi Maxwell Tshavhungwe Bureau Member: Prof. Pieter S. Steyn, IUPAC Past President **Spain** 5 votes Prof. Luis A. Oro Giral Sweden (not available) 3 votes Switzerland 4 votes Dr. Reto Battaglia

Prof. Martin Quack

Bureau Member: Dr. Christoph F. Buxtorf, Treasurer of

IUPAC

Turkey 3 votes

Prof. Namik K. Aras

Prof. Nesrin Emekli

Prof. Mehmet Ali Gürkaynak

<u>United Kingdom</u> (not available) 5 votes

Dr. Alan Smith Elected Member of Bureau

(As of 30 June 2005)

<u>United States</u> 6 votes

Dr. Mark Cesa Secretary and Vice-Chairman of

Committee on Chemistry and Industry

Prof. Paul W. Erhardt President of Chemistry and Human Health

Division

Dr. Michael Jaffe Delegation Leader

Dr. John M. Malin Chairman of CHEMRAWN

Dr. Carolyn Ribes

Dr. David Schutt

Dr. Edwin P. Przybylowicz Elected Member of Bureau, Chairman of

Finance Committee

Observers of Other Organizations

(as of 30 June 2005)

Observers of National Adhering Organizations

Brazil: Prof. Salete Linhares Queiroz

Bulgaria: Dr. Elena Vassileva

Canada: Dr. Aicheng Chen

Ms. Megan Rosborough Dr. Yan Alexander Wang

Chile: Dr. Eduardo D. Pereira

France: Dr. Philippe Barthelemy

Germany: Dr. Wen-Wu Li

India: Dr. Govindasamy Mugesh

Dr. Sandeep Verma

Russia: Dr. Tamara Basova

Turkey: Dr. Sevgi Kocaoba

United Kingdom: Dr. David J. Barden

Dr. Victoria Cornelius Dr. Katherine Holt Dr. Andrea V. Jackson Dr. Richard Layfield Dr. Nicholas Walker

United States: Prof. Shaowei Chen

Prof. Christopher Gorman

Prof. Robert Hinde Dr. Igor Kozlov Prof. Yi Lu

Prof. Daniel Rabinovich Prof. Mark H. Schoenfisch

Dr. Angela Wilson Prof. Zhiping Zheng

Observers of Associate National Adhering Organizations

(To be named)

Observers of Associated Organizations

(To be named)

Observers of Other Organizations

(To be named)

Deceased IUPAC Colleagues (As of 17 June 2005)

Argentina	Prof. Eduardo J. Bottani – National Representative, Commission on Atmospheric Chemistry, 1998-2001
France	Prof. Roger Cohen-Adad – Member, Subcommittee on Solid Solubilities, 2000-2001; Task Group Member, Solubility Phenomena-Applications for Environmental Improvement.
Netherlands	Prof. Martin W. G. De Bolster – Associate Member, Commission on Nomenclature of Inorganic Chemistry, 1983-1987; Titular Member, Commission on Nomenclature of Inorganic Chemistry, 1987-1997; Member, Working Party on IUPAC Glossary of Terms in Inorganic Biochemistry (& Organometallic Nomenclature, 1991-1997.
Germany	Prof. Oskar Glemser – President, Inorganic Chemistry Division, 1969-1973.
Poland	Dr. Adam Skrzecz – Associate Member, Commission on Solubility Data, 1996-1997; Titular Member, Commission on Solubility Data, 1998-2001; Chairman, Subcommittee on Liquid Solubilities, 2000-2001; Task Group Chairman, Ternary Systems Containing Alcohols, Hydrocarbons, and Water; Task Group Member: Solubility Data Related to Industrial Processes, Mutual Solubility of Hydrocarbons in Water, A critical compendium of pesticide physical chemistry data, Mutual Solubility of Alcohols and Water.
Portugal	Prof. J. de Oliveira Cabral – National Representative, Commission on Nomenclature of Inorganic Chemistry, 1990-1991; Associate Member, Commission on Nomenclature of Inorganic Chemistry 1994-1999.
Spain	Dr. Enrique L. Madruga – Member, Subcommittee on Modeling of Polymerization Kinetics and Processes.
United States	Dr. John D. Bacha – Member, Subcommittee on Characterization of Carbonaceous Materials and New Carbons, 2000-2003. Dr. H. Steffen Peiser – National Representative, Commission on Isotopic Abundance and Atomic Weights, 1985-1991; Member, Subcommittee on Natural Isotopic Fractionation, 2000-2001; Member, Subcommittee for Isotopic Abundance Measurements, 2000-2005; Task Group Member: Element by Element Review of Atomic Weights to the Year 2000, A New Comprehensive Report on the Isoptopic Compositions of the Elements for Global User Communities, Determination of Atomic Weights Using New Analytical Techniques.

43rd IUPAC COUNCIL MEETING Beijing, China 20-21 August 2005 AGENDA

- 1. Introductory Remarks and Finalization of Agenda
- 2. Approval of Minutes of 42nd Council Meeting and Matters Arising
- 3. Ratification of Decisions Taken by Bureau and Executive Committee since 42nd General Assembly
- 4. Announcement of Nominations for Union Officers and Bureau Members
- 5. Announcement of Time of Elections
- 6. Statutory Report of President on State of the Union
- 7. Report of Secretary General
- 8. Adoption of Recommendations on Nomenclature and Symbols
- 9. Reports of Division Presidents (10 minutes each)
- 10. Reports of Standing Committee Chairmen (10 minutes each)
 - 10.1. Committee on Printed and Electronic Publications
 - 10.2. CHEMRAWN Committee
 - 10.3. Committee on Chemistry and Industry
 - 10.4. Committee on Chemistry Education
 - 10.5. Project Committee (written report only)
 - 10.6. Evaluation Committee (written report only)
 - 10.7. Interdivisional Committee on Terminology, Nomenclature and Symbols (written report only)
- 11. Report of the Vice-President: Critical Assessment of IUPAC
- 12. Proposal to Replace Executive Committee and Bureau with an Executive Board
- 13. Financial Reports
 - 13.1. Biennial Report of Treasurer
 - 13.2. Report of Finance Committee
 - 13.3. Accounts for 2003-2004
 - 13.4. Appointment of Auditors for 2005 and 2006

43rd IUPAC COUNCIL MEETING AGENDA

- 14. Budget Proposal
 - 14.1. Proposed Budget for 2006-7
 - 14.2. National Subscriptions for 2006-7
- 15. National Adhering Organizations in Arrears
- 16. Applications for National Adhering Organization Status
- 17. Proposals Formally Received from National Adhering Organizations
- 18. Organizational Changes in Existing IUPAC Bodies, Proposals for New and Reconstituted Bodies/Terms of Reference
 - 18.1. New Division Rules
 - 18.2. Standing Order and Membership of Editorial Advisory Board of PAC
- 19. Election of Union Officers and Bureau Members and Approval of Elected Officers of Divisions
- 20. Plans for 44th General Assembly and 41st Congress (Torino, 2007)
- 21. Approval of Dates and Sites of 45th General Assembly and 42nd Congress (2009)
- 22. Official Language of IUPAC (Statute 5.405)
- 23. Reauthorization of Commissions.
- 24. Important Matters Referred to Council by Bureau at 43rd General Assembly not Covered by Items on Council Agenda
- 25. Any Other Business (discussion only)
- 26. Closing Remarks, Adjournment

Guidelines for Discussion and Debate in Council

Most discussion in the Council meeting is informal, with decisions often made by voice vote or show of voting cards without an official count. However, for nonscientific matters that may require extended debate and a formal vote by delegations [Bylaw 2.2], the procedures for carrying out formal business have sometimes not been entirely clear. The Statutes and Bylaws do not prescribe detailed procedures for conduct of meetings, but they do assign to the President the responsibility for ruling on matters that are not clear or decisive. Under that authority, the President proposes to use the following guidelines for formal consideration of nonscientific matters in Council. The terminology and concepts in these guidelines are based on "Robert's Rules of Order, Newly Revised," a comprehensive and widely used authority on parliamentary procedure.

- 1. Business is formally brought before Council by a *motion*. A motion may be made by a delegation and seconded by another delegation, or made by an Officer or other individual presenting a report or recommendation from the Bureau or IUPAC committee. This latter type of motion does not require a second because the matter has already been formally considered and approved by the IUPAC body.
- 2. When a motion has been accepted by the President, it becomes the *pending business* and is considered the *main motion*. No other independent motion may be accepted until action on the pending main motion has been completed. However, *subsidiary motions*, such as amendments to the pending motion, may be considered. Also, under certain circumstances, the pending business may be interrupted to consider another, usually urgent, matter.
- 3. The motion should be clearly stated so that the intent is unambiguous. The wording of the motion may be modified by agreement with the maker of the motion before it is formally accepted by the President as pending business. After it becomes pending business, the wording may be modified by unanimous consent or through the amendment process.
- 4. In the course of debate on the motion, one or more *amendments* may be offered as motions that formally change the wording or even the intent of the pending motion. A motion to amend must be germane [relevant] to the main motion and must be stated clearly so that its effect on the main motion is clear. Usually the amendment will propose to make specific modifications in the language of the main motion or to substitute new language. The President will rule on the admissibility of an amendment in terms of clarity and relevance.
- 5. A proposed amendment requires a second. Once accepted by the President, the motion to amend becomes the pending business and must be debated and resolved before proceeding to consideration of the main motion. A *secondary amendment* may be offered to a pending *primary amendment*, but the secondary amendment may not be further amended because the parliamentary situation would become too confusing. [Normally, in such circumstances, it is preferable to quickly reject the amendments and main motion with the understanding that an alternative motion will be offered to handle the issue.]
- 6. The President will make efforts to ensure that all interested delegations have an opportunity to speak on a question and will attempt to avoid repetition or to recognize a given delegation several times. However, he may give the maker of a motion the

Guidelines for Discussion and Debate in Council

- opportunity to respond as often as necessary to questions or to explain points that are not clear.
- 7. When the President believes that debate has brought out the salient points, he will ask whether Council is ready to vote on the pending matter. Alternatively, any delegation may make a motion for the *previous question* [or "the question"]. This motion is *not* debatable but requires a 2/3 affirmative vote for approval. If approved, debate is terminated, and Council proceeds to vote on the pending motion or amendments in sequence.
- 8. Once a matter has been decided formally, it may normally not be brought up again for discussion and action. However, when subsequent actions or new information make it desirable to reconsider the matter, a motion [with second] may be accepted to *rescind* or *amend something previously adopted*. The motion is debatable and requires either a 2/3 affirmative vote or a majority of assigned votes for approval.
- 9. During debate on a main motion, a motion is in order to *refer* the matter to a standing or *ad hoc* committee, usually with instructions to carry out a particular analysis or to report at a specific time. Such a motion takes precedence over pending amendments. It is debatable. If approved, consideration of the main motion ceases, but the matter may be automatically raised again as specified in the motion to refer.
- 10. Debate on a motion may be interrupted by a *privileged motion*, such as a *point of order* that objects to the procedure or a *point of information*, raising an inquiry on a matter of fact.
- 11. The President will augment these guidelines as needed.

Ottawa, Canada, 16-17 August 2003

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42nd IUPAC COUNCIL MEETING Ottawa, Canada, 16-17 August 2003 Minutes

1. Introductory Remarks and Finalization of Agenda

President Steyn welcomed the delegates to the 42^{nd} Council meeting. He thanked the Chemical Institute of Canada for their generous hospitality and the excellent arrangements.

Prof. Steyn introduced Dr. S. Hofmann of the Gesellschaft für Schwerionenforschung mBH in Darmstadt, Germany, leader of the group that had synthesized the element of atomic number 110.

Prof. Steyn then asked the delegates to stand for a moment of silence in honor of deceased colleagues.

2. Approval of Minutes of 41st Council Meeting and Matters Arising

The Minutes of the 41st Council were approved with no changes and no matters arising.

3. Ratification of Decisions Taken by Bureau and Executive Committee since 41st General Assembly

Council ratified the decisions taken by the Bureau and Executive Committee since the 41st General Assembly.

4. Announcement of Nominations for Union Officers and Bureau Members

Dr. Becker reviewed the procedures as presented in the material provided to the delegates. He described in detail the procedures specific to the election of Officers and Bureau Members. He noted that if Prof. Gilbert or Prof. Henry were elected Vice President there would be as many candidates as vacancies for the Bureau. Dr. Becker also reported that the Bureau had made no recommendations for additional candidates and had not made any recommendations for or against any candidate.

Prof. Steyn reported that the Bureau had recommended the following persons to act as tellers for voting: Mr. S. Langer (UK) and Dr. C. I. Ratcliffe (Canada). The tellers were accepted unanimously by the Council.

5. Announcement of Time of Elections

Prof. Steyn announced that the elections would be held at 10 AM, Sunday, 17 August 2003.

6. Statutory Report of President on State of the Union

Prof. Steyn began his report by noting that this biennium had been the first in which IUPAC operated completely under the new project system. He then briefly reviewed the new Mission and Vision Statements. He noted that the Vision Statement emphasized the role of chemistry in improving the welfare of mankind, a role that has been emphasized by a number of recent reports published by groups such as the Federation of European Chemical Societies, the United States National Academy and the American Chemical Society. He then briefly described the changes to

the governance of the Union proposed by the Governance Structure Committee. This will be discussed in more detail in Item 13 of the Agenda.

He reported that the finances of the Union were in a strong position due to the work of the Treasurer and the Finance Committee, as would be seen when they reported in Item 8. He noted that the Finance Committee had prepared policy guidelines for the conduct of the Union's investments and for the handling of its endowment. He then described the proposal of the ad hoc Working Party on National Subscriptions to bill National Subscriptions in national currencies. This proposal addresses the concerns raised at the Brisbane Council meeting that many NAOs had difficulty in paying their National Subscriptions. Prof. Steyn then noted the proposal from the Working Party that the expenses of one delegate from each NAO be paid to attend the Council. He congratulated the Working Party on its work and thanked the members for their active participation in this important effort.

Prof. Steyn then reviewed the accomplishments of the Union as measured against the long-range goals as recently revised and approved by the Bureau. Some highlights of these accomplishments include:

- Advice to the Organization for Prevention of Chemical Weapons on the impact of scientific advances on the Chemical Weapons Convention.
- The International SCOPE/IUPAC Symposium on Endocrine Active Substances Yokohama, Japan.
- The naming of elements: name, darmstadtium, and symbol, Ds, of element 110.
- A Training Program for Safety and Environmental Protection.
- Workshops on Safety in Chemical Production.
- DIDAC Project, sponsored by COCI, CCE and UNESCO, for teaching of chemistry in developing countries.
- Conferences on New Directions in Chemistry:
 - Conference on "Biophysical complexity", April 2003, Southampton, UK
 - "CHEMRAWN on Innovation in the Chemical Industry:
 The Way from Pure to Applied Chemistry", August 2003, Ottawa.
- Four special topic issues and articles recently published in *PAC*:

 Natural Products, Nanostructured Advanced Materials, The Science of Sweeteners, and Medicinal Chemistry in the New Millennium.

Prof. Steyn then drew the attention of the Council to the improved content and appearance of *Chemistry International;* new design, better editing, more news, he emphasized that more input from members is needed, reminding the Council that *CI* is their newsletter. He then noted that the IUPAC web site had become not only a major means of communication within IUPAC but also with the wider chemical community and the public. He reminded the Council of the many new

features available on the web site, including: the *IUPAC Handbook*, the *Gold*, *Orange*, and *Purple* books, Minutes of Council, Bureau, and EC Meetings, and an on line naming service.

Prof. Steyn then reviewed the many programs the Union has initiated in the past few years to aid young scientists. These include: Young Scientists Program, IUPAC Young Observers Program, and the IUPAC Prize for Young Chemists. He noted that the Young Scientists Program had helped more than 85 young scientists from 45 countries to attend the Congress at Ottawa. He then mentioned the session at the Congress devoted to the Public Understanding of Chemistry. This session had been organized by the Committee on Chemistry Education in cooperation with the Canadian Society of Chemistry.

Prof. Steyn then listed the following challenges faced by IUPAC:

- to ensure the effective functioning of the new project system in IUPAC,
- to effectively involve the chemical industry in IUPAC,
- to improve the public understanding and perception of chemistry,
- to broaden the geographic base of the Union.

Prof. Steyn concluded by emphasizing that IUPAC takes enormous pride in the achievements of its members and their service to the discipline of chemistry. He then thanked all his colleagues in the Union and in particular the Officers, members of the Bureau and the Executive Director, Dr John Jost and his team at RTP. He especially thanked Dr Alan Hayes, Past President, Dr Ted Becker, Secretary General, Prof Leiv Sydnes, President-elect, and Dr. Christoph Buxtorf, Treasurer, for their assistance during his term as President.

7. Report of Secretary General

Dr. Becker in his remarks discussed a few highlights from his written report. He noted that while the Secretariat staff remained at five, as it was two years ago, three of the members are new. The Executive Director had used the opportunity given by the need to hire new staff to reorganize the work done so as to better handle the work, based on the experience gained since the original staff assignments were made in 1997 and 1998. He then noted the many contributions made to IUPAC by Dr. Fabienne Meyers, including the operation of the Project Approval system, the improved content and appearance of *Chemistry International*, and the continued development of the IUPAC web site as a resource not only for the IUPAC community but for chemists and those interested in chemistry around the world.

Dr. Becker commented on the successful operation of the project system, noting, however, that new projects continue to come from people who are familiar with the work of IUPAC. He urged the delegates to make IUPAC's interest in new projects from scientists not previously connected with IUPAC known to their colleagues. He noted that there had not been any financial constraints on funding new projects. He then went on to describe the project to provide advice to the Organization for Prohibition of Chemical Weapons. An initial allocation by IUPAC of USD 10,000 [much of it still unspent] was leveraged to a budget of USD 110,000 with support from foundations, government and industry, plus other cash and in-kind support from the US National Academies. The final report of the Workshop organized in Bergen has been widely distributed to interested parties.

Dr. Becker noted that the Fellows program, initiated at the Berlin General Assembly has been very successful, with the former members of IUPAC bodies very appreciative of the recognition that the program offers them. He then commented that the number of Affiliates in the Affiliate Membership Program has fluctuated over the past few years, mainly due to fluctuations in the number of Affiliates joining through the American Chemical Society. However, the number of Affiliates from other parts of the world has steadily decreased. He stressed that he felt that there is still untapped potential for growth of the program, but this will require continued efforts by the IUPAC Officers, the Secretariat, and especially the NAOs and national chemical societies. With the improved content and appearance of *Chemistry International*, we can provide a better tangible product to Affiliates.

Prof. De Bièvre (Belgium) asked two questions:

What actions have been taken to benefit developing countries?

Has the funding provided to one delegate from each NAO increased attendance at the Council?

Dr. Becker replied by noting that over 400 Affiliates are sponsored by IUPAC, that is, they pay no membership fee. He also noted the program to fund conferences in developing countries. It is too early to tell if the funding offered to delegates had had a significant effect on attendance of delegates at the Council.

Prof. Lamba (Puerto Rico) asked who should be contacted at IUPAC about chemical weapons.

Dr. Becker replied that the Secretary General should be contacted.

Prof. De Bièvre (Belgium) then asked if governments could address questions to IUPAC.

Dr. Becker replied that governments could address questions to IUPAC, even though IUPAC may not always be in a position to respond.

8. Financial Reports

8.1. Biennial Report of Treasurer

Dr. Buxtorf briefly reviewed his written report. The Union is on plan and the reserves are in good shape. He commented that he and the Finance Committee continue to be aware of the world economic situation, which remains difficult for many NAOs. He then discussed IUPAC's major sources of income: the National Subscriptions, publications, and grants and donations. He noted that publications income continues to be under pressure from the gradual decline in the number of institutional subscribers to IUPAC's journal, *Pure and Applied Chemistry*. Outside sources of funding while important, have not in the past been a significant factor in IUPAC's revenue. He urged that all those involved in IUPAC make greater efforts to generate funding from outside sources. This will require doing a better job of demonstrating the value of IUPAC's work to potential sources of funding. He then noted that he had asked the Divisions to adhere to a 25 % / 75 % split between operations and projects in the current and coming biennia. The reserves set aside in the budget have provided the flexibility to fund good projects when Divisions did not have the resources available.

Prof. De Bièvre (Belgium) asked if there was an "orange light" on the future financial position of the Union.

Dr. Buxtorf replied that there was no "orange light"; the proposed budget for 2004-5 is very moderate.

8.2. Report of Finance Committee

Dr. Przybylowicz noted that the financial environment had been difficult for the past two years; however, the Union's balanced portfolio has insulated the investments from major losses. The shift to a portfolio with a higher ratio of bonds to equities two years ago was a major factor in the good performance of the Union's investments as compared to the overall market. Dr. Przybylowicz pointed out that in order to hedge the Union's portfolio against currency fluctuations, part of the bond portfolio had been invested in Euro denominated bonds.

8.3. Accounts for 2001-2002

This item was for information only and there was no discussion.

8.4. Appointment of Auditors for 2003 and 2004

Council approved the appointment of Batchelor, Tillery & Roberts, LLP, of Raleigh, North Carolina, USA as IUPAC Auditors for 2003 and 2004.

9. Adoption of Recommendations on Nomenclature and Symbols

Council approved the Recommendations on Nomenclature and Symbols that had been published since the last General Assembly.

9.1. Approval of a Recommended Name of Element 110

Dr. Rosenblatt reviewed the procedure for assigning a name to a newly discovered element. He noted that the joint IUPAC-IUPAP (International Union of Pure and Applied Physics) Working Party (JWP) had confirmed the discovery of element number 110. In accord with IUPAC procedures the discoverers, at the Gesellschaft für Schwerionenforschung mbH (GSI) in Darmstadt, Germany, have proposed a name and symbol for the element. The Inorganic Chemistry Division Committee now recommends this proposal for acceptance. The proposed name is darmstadtium with symbol Ds. This is now a Provisional Recommendation, which has been available on the IUPAC web site for more than the five-month period specified in Bylaw 2.11. All comments received have been positive, and no controversy has arisen. He also noted that the Joint Working Party has issued a new report confirming the discovery of the element of atomic number 111 by researchers at the Gesellschaft für Schwerionenforschung mbH. The report also reviewed the evidence for the discovery of the elements of atomic number 112, 114, and 116; the discovery of these elements has not been confirmed. Dr. Rosenblatt thanked the member of the Joint Working Party, Prof. P. Karol (Chairman), Prof. H. Nakahara, Dr. B. W. Petley, and Dr. E. Vogt for their excellent and thorough work.

Council approved the recommended name darmstadtium and symbol, Ds unanimously.

Dr. Becker noted that the process of selecting and approving a name for the element of atomic number 111 would now begin. He requested that Council delegate to the Bureau the approval of the name and symbol for this element, if there is no controversy regarding the proposed name and symbol.

Prof. Koch (Germany) asked what is the definition of controversy in this case.

Dr. Becker replied that the judgment must be made by the Bureau.

Council approved the proposal unanimously.

10. Reports of Division Presidents

Physical and Biophysical Chemistry Division

Prof. Ralston reported that the Division has now moved into a project-based organization that is completely different from the past IUPAC structure. In September 2000 the name of the Division was changed to embrace Biophysical Chemistry, recognizing that many areas of bioscience are underpinned by physical chemistry. The Division was actively involved in an innovative conference on Biophysical Complexity, held in Southampton in April 2003. One successful aim of the meeting was to actively engage young researchers in the early stages of their research careers. An outstanding group of plenary speakers took part, drawn from Departments of Chemistry, Medicine, Bioengineering, Cell Biophysics, Anthropology and Human Genetics. A Report will be published in *Chemistry International* in the near future.

Another activity in the Biophysical Chemistry area is a major international workshop on the Physical Chemistry of Biointerfaces to be held in the Barossa Valley near Adelaide, South Australia from May 23 to May 26, 2004. This is a satellite workshop that will be held immediately following the Seventh World Biomaterials Congress [Sydney, Australia, May 17-21 2004]. This workshop is aimed at providing fundamental insights into topics such as interfacial forces and properties involved in protein/surface interactions and the molecular kinetics of drug delivery, to give just two examples. Advances in materials science, molecular biology, surface and interface analysis methods and theoretical and modeling approaches to biological systems will be key foci. It is intended that this workshop will be supported in part by IUPAC as an innovative conference under the banner of New Directions in Chemistry. Additional support is anticipated from private industry and from the Australian Government. It is expected that these conferences are the harbingers of future larger scale activities in the area of Biophysical Chemistry by the Division.

The Division's very important work in establishing databases in key areas continues. Of particular importance is the work on evaluated kinetic data for atmospheric chemistry. The website development has been very successful and there is now a mirror site at the IUPAC site at the University of North Carolina as well as the parent site in Cambridge. The site attracts about 2000 accesses per week, a very respectable figure indeed. Substantial numbers of downloads occur in areas covering heterogeneous reactions, thermodynamic data and guides to data sheets. There are over 300 subscriptions to the mailing list for announcements. All databases will in future be physically located at the server in North Carolina from the outset of the project. The Secretariat will

provide service whilst maintenance will be the responsibility of the Division; both will be addressed at the proposal stage for any project. Presently a significant proposal to develop a database for ionic liquids, whose development was actively encouraged by this Division, is being assessed for support.

The Division has been very active in chemical thermodynamics for many years. Following the restructuring of IUPAC at the end of 2001, the International Association of Chemical Thermodynamics [IACT] was established and, in April 2003, the IUPAC Executive recommended that the IACT be granted Associated Organization status within IUPAC, and that this recommendation be approved by Council at the August meeting in 2003 (see Item 19). The IACT has been very active, covering topics as diverse as electrolyte solution data and microcalorimetric standards to new areas such as the thermophysical properties of polymers.

Prof. Ralston reported that the Third Edition of the *Green Book* would be completed and sent to the publisher, the Royal Society of Chemistry, by the end of 2003. It is expected the revised *Green Book* will in part or in total be placed on the Web and also translated into foreign languages.

Prof. Ralston commented that there has been a conscious effort by the Division to complete projects and to focus on larger, better-resourced activities that can be completed within acceptable time frames. It is notable that seven projects are interdivisional, a clear demonstration of the central role that the Division plays in Chemistry.

Prof. Ralston then described the Advisory Group of 61 distinguished international scientists, a small proportion of whom are drawn from industry. The role of this Advisory Group is to act as a sounding board to the Division Committee, suggesting areas that might be dealt with by the Division, drawing attention to the need for experimental protocols in certain areas, taking part in IUPAC conferences and acting as one source of critical referees for IUPAC proposals. Networks of "IUPAC sensitive" scientists are invaluable in terms of support, as is the superb role played by the Secretariat. The membership of the Advisory Group will be reviewed on a biennial basis.

Prof. Collins (Brazil) asked when the new edition of the *Green Book* would be published.

Prof. Ralston replied that the Editor, Prof. Martin Quack of the ETH-Zürich, planned to send the manuscript to the publisher by the end of September.

Prof. De Bièvre (Belgium) asked if the Division had considered means to persuade editors of journals and books to promote the use of IUPAC recommendations regarding quantities, units, and symbols by their authors.

Prof. Ralston commented that the Division had worked on this issue and had had some success, but he agreed that there was much more to be done.

Prof. Kratochvil (Czech Republic) commented that it was important for important reference books such as the *Green Book* and the *Purple Book* to be available on the market.

Inorganic Chemistry Division

Dr. Rosenblatt's report discussed the following points:

- Generation of projects
 - o How can projects be generated?
 - o Where will they come from?
- Progress on projects
 - o What can be done to facilitate projects being completed in a timely and exemplary manner?
- People
 - o How can IUPAC locate and develop new volunteers and project participants?
- Workload
 - o 2-3 hours/day for Division President is not sustainable.
- Internal motivation and communication
 - o Gap between executive bodies and scientific volunteers.
- E-mail communication and the "reward" structure
 - o Is there a need for more face-to-face communication and interpersonal relations in motivating volunteers?
- Support of core efforts in atomic weights
 - o How can we fund meetings of Commission II.1?
- Communication with the inorganic chemistry and materials chemistry communities

Dr. Rosenblatt noted that the Division's work was in three areas, Elements, Molecules, and Materials. The work in Elements included the naming of new elements and the compilation of validated atomic weight and isotopic abundance data. The Molecules area was one that in the past had dealt mainly with nomenclature; this was now the responsibility of Division VIII. While the Division continues to participate in the work of Division VIII in this area, it is necessary to develop new projects that are not nomenclature related. To accomplish this the Division has been actively recruiting members for the Division Committee who are experts in relevant subjects. The Materials area has been active with a Subcommittee formed with members from Divisions I, IV, and V in addition to Division II. The Subcommittee has taken responsibility for the Workshops on Advanced Materials and is working towards the possible creation of a Materials Division. Dr. Rosenblatt noted that the series of Conferences on High Temperature Materials continues to be a major activity of the Division.

Dr. Rosenblatt concluded by emphasizing that if the project system is to work, ways would have to be found to generate new projects and to involve new people in the work of IUPAC. He urged the Bureau and especially the Officers to work on closing the perceived gap between those who do the work of IUPAC and those who manage IUPAC.

Prof. Collins (Brazil) asked why the naming of the elements was a responsibility of Division II and not of Division VIII.

Dr. Rosenblatt replied that the expertise on elements was in Division II. Dr. Becker then commented that Division VIII's mandate covered systematic nomenclature, the names of the elements being a good example of non-systematic nomenclature.

Prof. Shani (Israel) asked if there were any principles for choosing new names for the elements.

Dr. Rosenblatt replied that there were no principles; the only rule is that previously used names cannot be used again. Prof. Corish referred anyone who was interested in the details to an article by Prof. W. H. Koppenol. "Naming of new elements", Pure Appl. Chem. **74**, 787–791, (2002).

Prof. De Bièvre (Belgium) expressed his concern about the funding of the Commission on Isotopic Abundance and Atomic Weights. He commented that while the work of this Commission was important to IUPAC the uncertain funding situation under the project system was demoralizing the members of the Commission.

Dr. Becker replied that this was an issue that should be looked into to be sure that the Commission members understood the situation and to determine if any special arrangements needed to be made to facilitate the work of the Commission. Prof. Sydnes promised to investigate and discuss the issue with the Commission officers.

Organic and Biomolecular Chemistry Division

Prof. Tidwell noted that the work of the Division was managed by six Subcommittees:

- 1. Subcommittee on Organic Synthesis (Chair: David Black, Australia)
- 2. Subcommittee on Biomolecular Chemistry (Chair: Vadim Ivanov, Russia)
- 3. Subcommittee on Green Chemistry (Chair: Pietro Tundo, Italy)
- 4. Subcommittee on Photochemistry (Chair: Sylvia Braslavsky, Germany)
- 5. Subcommittee on Structural and Mechanistic Chemistry (Chair: Marek Krygowski, Poland)
- 6. Subcommittee on Biotechnology (Chair: In process of selection)

A major activity of the Division continues to be the organization of major conference series. In 2002, there were five such conferences with a major organizational role by the Division, in Physical Organic, Synthesis, Photochemistry, Natural Products, and Biomolecular, and their successors in 2004 are already being organized.

Prof. Tidwell then briefly reviewed the current projects of the Division. He commented that in common with other Division, Division III is concerned about the issue of generating new projects. He noted that it is clear that many potential proposers of projects are not sufficiently informed or motivated to present proposals, and better communication with our members and those outside IUPAC is needed to encourage the formulation of creative and worthwhile projects. The Division hopes to utilize IUPAC sponsored conferences more effectively to publicize its work and the opportunities for chemists worldwide to contribute to IUPAC. One way to do this is with a new brochure to be distributed at meetings describing the Division's work.

Prof. Tidwell reported that the Subcommittee on Organic Synthesis now coordinates the Thieme-IUPAC Prize in Organic Synthesis. He also commented that the IUPAC Prizes for the best Ph. D. theses have proven to be valuable for enhancing chemistry worldwide. It appears desirable to promote other comparable international awards, and the Division is seeking sponsors of IUPAC

awards in such areas as Structural and Mechanistic Organic Chemistry, Biomolecular Chemistry, and Green Chemistry.

Macromolecular Division

Prof. Stepto reported that, following the IUPAC restructuring, the Division took the opportunity to reorganize so that the Associate and Titular Members all have defined, coordinating roles to play. This approach has functioned well and all areas of activity are moving forward with vigor.

The areas of activity of the Division and the associated coordinators are:

- 1. Structure Property Characterization of Commercial Polymers (Coordinator H. M. Laun)
- 2. Molecular Characterization of Polymers (Coordinator D. Berek)
- 3. Polymerization Kinetics Characterization (Coordinator M. Buback)
- 4. Subcommittee on Macromolecular Terminology (Coordinators M. Hess (Chairman) and M. Barón (Secretary))
- 5. Developing Polymer Materials Systems (Coordinators J. Vohlídal and W. J. Work)
- 6. Education (Coordinators J.-I. Jin, A. R. Khokhlov, D. Tabak)
- 7. Conference Sponsorship (Coordinators P. Kubisa and S. Penczek)
- 8. Recruitment at Conferences (Coordinator R. G. Gilbert)
- 9. Electronic Publications and Communications (Coordinators R. G. Jones and W. J. Work)
- 10. Division Strategy (Coordinators K. Horie, J.-I. Jin, Wang Fosong)

Prof. Stepto noted that the Division web site has been changed so that the new structure and activities can clearly be seen. The Division is also actively pursuing a policy of having all its reports and recommendations available on the web site.

Prof. Stepto then reviewed the work of the various Subcommittees. He also reported that linked with its work in Education, the Division is pleased to announce a USD 125 000 endowment from the Samsung General Chemicals Company of South Korea. The interest from the endowment will be used for awards, prizes and bursaries for educational courses and young scientists. Prof. Jung-Il Jin, the Vice-President of the Division, was instrumental in obtaining the endowment.

Prof. Stepto reported that the Division has made a special effort to increase the number of sponsored Conferences. A total of 21 IUPAC-sponsored polymer conferences have been and will be held in 2002 and 2003. Every effort is being made to maintain this level during the coming biennium.

Eight conference volumes have resulted in 2002 and 2003 from this increased activity. More than half of the issues of *Macromolecular Symposia* are presently devoted to IUPAC-sponsored conferences, representing a significant income to IUPAC. This year, for the first time, the journal was unable to accommodate all the IUPAC conferences it was offered.

The IUPAC World Polymer Congress of 2002, organized through the Division, was held in Beijing. It is generally recognized that the biennial IUPAC World Polymer Congress, with over 1000 participants, is the main event in the international polymer conference calendar. The Division also helped to organize a very successful Strategic Polymer Conference in Kyoto in December 2002 and

a second is planned for New York in 2005. It has also launched a strategic study of future developments in polymer science.

Prof. Stepto noted that active steps are being taken in recruitment at Conferences. A Division Brochure has been prepared and is distributed at all IUPAC-sponsored conferences. In addition, the PowerPoint presentation issued by the Secretariat has been augmented to emphasize Macromolecular Division activities. Electronic versions of the brochure and the presentation are given to all conference organizers and IUPAC representatives.

Prof. Stepto concluded by noting that the Division will seek to expand its profiles in Molecular Characterization and Developing Polymer Materials Systems and maintain its high level of activity and throughput in all project areas and in Conference Sponsorship. The Division will seek to play a strategic role in defining the important areas of world polymer research through its strategic study and conferences.

Analytical Chemistry Division

Dr. Moore noted that the Division has completed the transition from a Commission-based to a Task Group-based project system, and has added several new managerial tools to enable efficient project acquisition and management. He reported that 14 projects had been published since January 2002; 17 projects are either with ICTNS or in the queue for publication.

Dr. Moore noted that the Division has the same concern as many other Divisions; new project proposals are not arriving at a high enough rate. At present, all the project proposals come from former Commission or Division members. To improve this situation, projects are being solicited via a four-pronged effort. First, the new Division web pages prominently display a call for proposals, with dates for selection and links to further information on the process. Secondly, each Division Committee TM has established a list of advisors to help them solicit new projects or identify needs for projects (although these have been difficult to establish and few results have been achieved to date). Thirdly, Division Committee members are presenting overviews of IUPAC with details on the project system at several international conferences. Fourthly, we have established plans for focus meetings with targeted industry groups, beginning with a focus meeting on Proteomics at the Ottawa GA.

Dr. Moore reported that the Division is using a competitive project approval system, with ranking of project proposals according to specific guidelines. The Division Committee has used this system twice in 2002 and once in 2003. Some projects that need more expedient action are approved outside the cycle via e-mail discussion and voting.

Internal and external communication deficiencies have been addressed via 1) a newsletter, "Teamwork," which has been implemented to keep Committee members and others apprised of their responsibilities, upcoming events, new project proposals, and deadlines, and 2) a new mechanism to oversee projects and their dissemination plans.

Dr. Moore reported that a major activity of the Division in past biennium was the development of an on-line version of the *Compendium of Analytical Nomenclature (Orange Book)*; this is now available on the IUPAC web site (http://www.iupac.org/publications/analytical_compendium). To judge the impact, according to "hits" on the directory, the *Orange Book* accounts for 1/6 (99432)

of the total hits (578399) on the IUPAC publication folder (during the first three months of 2003)! A process to update the *Orange Book* has been implemented, beginning with the electrochemical analysis and separation methods chapters, to be followed by the other chapters systematically over the next few years. The Division is involved in the IUPAC XML project to decide on a plan for eventual conversion of the *Orange Book to* XML.

Prof. Collins (Brazil) asked if the changes to the online edition of the *Orange Book* would be approved in the usual way.

Dr. Moore commented that no changes would be incorporated in the online *Orange Book* until they were part of an IUPAC recommendation or report published in *Pure and Applied Chemistry*.

Prof. Kratochvil (Czech Republic) commented that gel-permeation chromatography is a major analytical method but there is no mention of it in the *Orange Book*.

Dr. Moore replied that a Task Group with a Chairman had been set up to develop a project in this area.

Chemistry and the Environment Division

Prof. Klein noted that the work of the Division, projects and other activities, are targeted to provide authoritative information and judgments on issues of chemicals in the environment. The major part of the projects is directly customer oriented dealing with actual problems of several branches of industry and of international environmental and human health protection organizations and agencies. The second area of activity is on communicating advanced concepts and state of the art assessments by extension workshops and conferences between scientists, especially in developing countries.

He then noted that the Division's strategy for new projects is to further enhance customer orientation by consistently involving the parties interested in the work at the project development stage and by reacting proactively to issues raised by society within the mandate of the Division. Thus, dissemination of the outcome of the Division's projects is not only through the traditional scientific channels but also by direct transfer, i.e. workshops and seminars. This ensures optimal use of the work of experts and also gives them status and motivation.

In the reporting period, 10 projects were completed or terminated and 6 new projects were launched.

Prof. Klein noted that cooperation with other International Organizations is an important aspect of the Division's work. Cooperation is successful on a project basis (state of the art and workshop) and through eminent Division and sub-committees members with scientific organizations and customers. These include, for example: IOCD (International Organization for Chemical Sciences in Development), WHO (World Health Organization), Codex Alimentarius (Food and Agriculture Organization/WHO), the European Union Commission. In addition, there is a long-standing cooperation with ICSU/SCOPE (International Council for Science/Scientific Committee on Problems of the Environment) and SCOR (Scientific Committee on Oceanic Research) due to the partial overlap of interests. Activities have been initiated to increase this type of cooperation with OECD (Organization for Economic Cooperation and Development), IFCS (Intergovernmental

Forum on Chemical Safety) and with industry via ICCA (International Council of Chemical Associations).

Prof. Klein then described the extraordinary large project initiated by Division on "*Environmental Implications of Endocrine Disrupting Chemicals*". This is a joint IUPAC/SCOPE project, sponsored and co-financed by industry and several national and international organizations. The final report of the project will be published in *PAC* and a preliminary version of the Executive Summary has been distributed to the Council. Cooperation with OECD is at present mainly on Green Chemistry through the joint Subcommittee with Division III. However, the successful case-by-case interactions will be expanded and intensified as needed.

Prof. Klein commented that apart from the green chemistry activities with Division III, there is still insufficient interdivisional cooperation. The difficulties in expanding interdivisional work largely relate to different approaches and concepts of work, not in a lack of interest on either side.

Prof. Berek (Slovakia) asked if cooperation with other Divisions on environmental projects was still insufficient.

Prof. Klein replied that this was due to a shortage of people to provide the links. Meetings at this General Assembly had led to the initiation of a number of interdivisional projects.

Prof. De Bièvre (Belgium) asked if industry had contributed to the joint SCOPE/IUPAC project on *Endocrine Active Substances*.

Prof. Klein replied that industry had supported the project both financially and by encouraging its development and completion.

Dr. Wright commented that his perception was that industry appreciates the work that was done on this project.

Prof. Klein noted that this project was path breaking by finding consensus in what is viewed as a highly controversial subject.

Chemistry and Human Health

Prof. Kallner noted that the Division had formed by combining the former Clinical Chemistry Division and the Medicinal Chemistry Section. The Division had, since its formation, been making efforts to move beyond its traditional areas of activity to include chemistry involved in all aspects of human health. He pointed out that the Division had many international collaborations, including those with the IFCC (International Federation of Clinical Chemistry), the European Federation and ACS Division of Medicinal Chemistry. He especially noted its work on the ICSU Monograph on Genetically Modified Organisms as Food and an ICSU project on Health and Wellbeing. One of the Divisions objects is to promote the idea that when you "Think Chemistry – Think IUPAC". Prof. Kallner noted that the Division had formal representation on committees of the World Health Organization (WHO), ISO (International Standardisation Organisation), and CEN, the European Standardisation Committee.

Chemical Nomenclature and Structure Representation Division

Dr. McNaught explained that in setting up the new Division every effort had been made to ensure broad representation of all those who were interested in nomenclature. To accomplish this an Advisory Committee with 45 members had been created to provide advice to the Division Committee. He also emphasized that the work of the Division included activities other than traditional systematic nomenclature, especially in the area of computer recognition of chemical structure. He described a Web Discussion Board that was used to promote discussion of draft documents by all members of the Division. The Web Discussion Board was hosted by the Royal Society of Chemistry.

Dr. McNaught then discussed the IUPAC Chemical Identifier (IChI) project. This project has been very productive. The object of the project is to develop a unique ASCII text string that can be used to identify any chemical compound. He summarized the results of the project to date in the following table:

IUPAC Chemical Identifier

- Unique computerized representation of any chemical structure
- Test algorithm for organic structures March 2002
- Chemical Abstracts Service/IUPAC Conference July 2002
- Inorganic and organometallic structures included mid-2003
- Review meeting in Washington, November 2003
- Future work on polymer representation

The Division is working on three other major projects:

- Organic Preferred IUPAC Names (PINs)
 New Blue Book draft (1086 pages) undergoing expert review
 Publication expected late 2004
- Revision of "Nomenclature of Inorganic Chemistry" Revised Red Book undergoing expert review Publication expected 2004
- Alignment of Organic and Inorganic Preferred Names
 Rationale agreed; Inorganic Preferred Names project to be developed

The following six projects are also nearing completion: Rotaxanes, first draft under review, Fullerene nomenclature Part II, Extension of Part I (published) to larger and more complex molecules, approaching completion, Cyclic macromolecules, Macromolecular rotaxanes, Dendrimers, Chemically modified polymers.

Dr. McNaught commented that no project proposals had been received from the community and therefore the Division is developing proposals through scoping exercises to establish needs and feasibility in the following areas: stereochemistry, proposed book covering all chemical disciplines; structure representation, report under consideration; inorganic nomenclature, working group meeting April 2003, identified areas requiring development:

Preferred names for inorganics and organometallics

- Boron nomenclature
- Nomenclature of metallacycles
- Organometallic stereochemistry
- Stereodescriptors for seven-coordination +

Dr. McNaught reported that the Joint IUPAC-IUBMB Commission on Biochemical Nomenclature (JCBN) would be reconstituted from January 2004 (see item 18.1). The Number of Titular Members will be reduced from 8 to 4 and a mechanism for review and funding of proposals established. The principal activities of the Commission are:

- Advice on updating of the Enzyme List
- Maintenance of specialized naming systems (steroids, peptides, carbohydrates etc.)
- Advice on chemical names for compounds of biochemical importance

Dr. McNaught concluded by pointing out that the work of the Division had included publicizing its activities by publications in general interest magazines, both print and electronic, such as C&E *News*, *Nature*, and the *Alchemist*, in addition to the usual publication of reports in *PAC*.

11. Reports of Standing Committee Chairmen

11.1. Committee on Printed and Electronic Publications

Dr. Warr briefly reviewed her written report. She noted that CPEP is responsible for three projects:

- 1999-046-2-024 Data exchange standard for electron paramagnetic resonance data types (incl. ESR, EMR etc.) (Task Group Chairman: Prof. Lancashire, completion date 2003)
- 2002-020-2-024 Data exchange standard for near infrared spectra and general spectroscopic calibration data types (Task Group Chairman: Prof. Downey, completion date 2005)
- 2002-022-1-024 Standard XML data dictionaries for chemistry (Task Group Chairman: Dr. Stein, completion date 2005)

The first two projects continue the work of the previous Working Party on Spectroscopic Data Standards. A Subcommittee under Tony Davies (Secretary of CPEP) has been formed to act as the reporting body for Task Groups working in this field.

The third project will result in data dictionaries that can be used by chemists when developing XML documents so that the data in those documents can be easily searched using IUPAC definitions from the *Gold Book* or symbols as defined in the *Green Book*. The *Gold Book* has been converted to XML and the *Green Book* will be converted as soon as the revised edition is available.

CPEP represents IUPAC on ICSTI, the International Council for Scientific and Technical Information, an ICSU committee, and represents the views of IUPAC to the Committee on subjects such as electronic publishing and Open Access initiatives.

The subscription prices for the print edition of *PAC* were raised in 2003 from USD 1200 to USD 1300 for institutions and from USD 892 to USD 900 for the electronic-only service. The Bureau at Ottawa approved an increase to USD 1400 for print subscriptions for institutions while the electronic only subscription price remained at USD 900. The price increases for the print edition of *PAC* are in line with those of other publishers. The price of *CI* subscriptions and personal subscriptions to *PAC* remain the same, USD 45 and 99 respectively.

Dr. Warr noted that the ranking (27) and impact factor (1.758) of *PAC* improved between 1999 and 2002 and has now reached a level above that of the previous high in 1998. She also reported that Prof. James Bull had been appointed Scientific Editor of *PAC*, as one result of the report from the Conference Policy Development Committee.

Dr. Warr commented that Dr. Meyers was to be congratulated on the enhancements she has been able to make in *CI* within strict budget constraints. Her job would be made much easier if members of IUPAC Divisions and Committees (and others) were more willing to submit short articles to the Union's news magazine.

Dr. Warr pointed out that *PAC Online* has abstracts for all content and full text PDF versions of recommendations and technical reports. The full content of *PAC* for the volume before the current volume is freely available. Dr. Meyers has done excellent work in making the IUPAC Web site a significant source of information for the worldwide chemistry community. Her email news alerts are also much appreciated.

Dr. Warr concluded by thanking two long serving members of the Committee, Dr. Heller and Prof. Wolman, who will be retiring from the Committee at the end of 2003.

11.2. CHEMRAWN Committee

Dr. Norling reported that four conferences were in the planning stages, with one conference held in conjunction with the Ottawa General Assembly. These are:

- 1. CHEMRAWN XII—Senegal or South Africa (2005) Chemistry, Sustainable Agriculture, and Human Well Being in Sub-Saharan Africa
- 2. CHEMRAWN XIII–Pune, India (2003-2004) Cleaner Energy
- 3. CHEMRAWN XV–Paris, France (June 2004) Chemistry and Water
- 4. CHEMRAWN XVI–Ottawa, Ontario, Canada (August 2003) Forum: Innovation–from Pure to Applied Chemistry
- 5. CHEMRAWN XVII-Kingston, Ontario, Canada (2004-2005) Greenhouse Gas Mitigation

Dr. Norling emphasized that the Committee continues to deal with the issues of:

- obtaining funding of major conferences or finding less costly ways to carry out its mission
- 2. increasing the impact of conferences, workshops and studies through practical and actionable recommendations by the Future Actions Committee, many of

which can be implemented by the Committee or individuals and organizations that it can directly influence.

Dr. Norling urged Members of the Council and Bureau to help support the work of the CHEMRAWN Committee by:

- recommending individuals to serve on the Committee or act as "friends" in organizing conferences or carrying out a CHEMRAWN study or workshop,
- calling upon the Committee to provide a "Future Actions Committee" for IUPAC sponsored conferences where major issues are discussed and a set of findings and recommendations should be developed and disseminated, and
- urging the Committee to address a particular issue with a conference or workshop where there is broad interest throughout the chemical community.

11.3. Committee on Chemistry and Industry

Dr. Wright discussed the following highlights from the Committee's work in the biennium.

- The "Training Program for Safety and Environmental Protection", joint with UNESCO/UNIDO (United Nations Industrial Development Organization) and funded by COCI and UNESCO, was extended in 2002 to three trainees (including for the first time one from China) and the host base was extended from the U.S.A. to Company Associates in South Africa and Japan. In 2003, COCI plans to train five, including for the first time trainees from India and Uruguay. Host companies will include companies from Sweden and perhaps Belgium. A Poster Session in Ottawa featured recent trainees and the effects of their training on their countries.
- "Workshops on Safety in Chemical Production" continue their success with a
 workshop in Senegal in 2001 followed by a major one in Beijing in 2002. Cosponsored by COCI, UNESCO, and SINOPEC, the Chinese National
 Petrochemical Company, the workshop drew an audience of >150, including
 managers of "safety and environment" from SINOPEC plants throughout China.
- "DIDAC", a joint Project with CCE and UNESCO for the teaching of chemistry especially in developing countries, has been successful beyond all expectations. This Belgian-developed teaching tool has now been translated into many languages including Arabic, Japanese, Korean, and Russian and distributed to over 47 countries, with a UNESCO goal of > 100 by the end of 2003. The transparencies have been extended to color posters for use in countries with minimal electricity, and the system will soon be available in free CD ROMs and "books". This contribution to the developing world was reviewed in detail by all participants in Ottawa at a Special Session on Aug. 15th.
- Co-sponsorship of CHEMRAWN XVI, "Innovation in the Chemical Industry", in Ottawa, Aug. 9 and 12

Dr. Wright then reported that as result of a study of COCI new Standing Orders have been approved and would take effect in 2004, with a biennial budget to begin in 2004 as approved in Brisbane; Dr. David A. Evans of the U.K. has been appointed Vice-Chair and Chair-elect. The Committee expects an increasing emphasis on "Public Perception of Chemistry" along with greater efforts to involve the Company Associates in the work of the Committee.

Dr. Wright noted that the Committee had publicized its work in *CI* and expected to continue to provide news articles for *CI* on its work in the future.

11.4. Committee on Chemistry Education

Prof. Atkins reported that the Committee had established guidelines for the types of projects that it would seek to encourage in order to fulfill its terms of reference. It has decided to pursue the following criteria:

- 1. Projects that contribute to the flow of ideas.
- 2. Projects based on ideas that emerge within a country and are perceived to have regional or global significance.
- 3. Projects that encourage curriculum development within a region, where local requirements have indicated a demand.
- 4. Projects that contribute to the distribution of good practice and information within a region, using the appropriate language.
- 5. Projects strongly urged by Divisions and Standing Committees that have an educational dimension or are perceived as relevant to the public understanding of chemistry.
- 6. Projects that reach into regions that are currently under-represented in IUPAC activity.
- 7. Projects based on innovations within a country that are perceived by those outside the country as having potential regional or global significance.
- 8. Projects encouraging inter-Union collaboration.
- 9. Projects that are innovative in the realm of the public understanding of chemistry.
- 10. Projects that are a response to an explicitly demonstrable demand within a region or sub-region.
- 11. Projects that encourage collaboration between countries in a region or between regions (and sub-regions).
- 12. Projects where IUPAC seed money is helpful to gain access to other sources of funding.

Prof. Atkins noted that in order to facilitate the generation of projects, the CCE has established two subcommittees, the Subcommittee on Chemistry Education for Development (CED) and the Subcommittee on the Public Understanding of Chemistry (PUC), and appointed two chairmen, Prof. Bradley and Prof. Mahaffy, respectively. Projects are coordinated by Prof. Pestana, who is also Secretary of the CCE.

Prof. Atkins noted that the CCE is responsible for the program of the International Conferences on Chemical Education (ICCE). The 17th was held in Beijing in August 2002, the 18th will be in Istanbul in August 2004, and the 19th will be in Seoul in August 2006.

He then commented that special attention had been paid to the generation of links with other scientific unions and with COCI. There is now a representative of COCI on the CCE and COCI has established a small group to advise the CCE on items of mutual interest, particularly projects that COCI would regard as appropriate to its interests and which could be developed by the CCE.

Prof. Henry commented that a Symposium on the Public Understanding of Chemistry had been organized at the Congress with the cooperation of CCE. The Symposium was open to the public and had attracted over 200 people to the morning session.

11.5. Project Committee (written report only)

There was no discussion of this report.

11.6. Evaluation Committee (written report only)

There was no discussion of this report.

11.7. Interdivisional Committee on Terminology, Nomenclature and Symbols (written report only)

There was no discussion of this report.

12. Report of the Vice-President: Critical Assessment of IUPAC

Prof. Sydnes noted that the subject of the Vice President's Critical Assessment, as set forth in Statute 6.32, was "...the programs and the projects of all IUPAC bodies." This was obviously a major task and the three most recent Vice President's had chosen an area on which to focus. He had decided to focus on communication, especially with the National Adhering Organizations and the chemical societies that were not National Adhering Organizations. He then referred the Council to his written report for the details of what he had found and continued by discussing the five proposals made at the end of his report. These are:

- 1. Improve the Visibility of the Member Countries on IUPAC's Homepage
- 2. Make IUPAC News Stories More Useful for National Chemical Magazines
- 3. Appoint National Contacts (NCs) to all Divisions
- 4. Appoint National Contacts (NCs) to Project Task Groups
- 5. Establish the IUPAC Poster Prize

He noted that the Secretariat had begun to address this area by the appointment of Ms. Abernathy to be responsible for communications with IUPAC's various constituencies, including the NAOs and chemical societies. One immediate result has been the creation of an electronic newsletter, called e-Press, providing information suitable for publication by national chemistry magazines. This addresses point 2 above.

Point 1 requires both more attention by the Secretariat to the links for the NAOs and chemical societies on the IUPAC web site and more information from the NAOs as to what they would like to see in the way of links from IUPAC.

Points 3 and 4 are useful only if the NAOs make use of the opportunity. That is, they must appoint National Contacts who will be active both in following the work of the IUPAC Committees and Task Groups to which they have been assigned and in communicating that work to the members of their national chemical community. Point 5 requires that the NAOs and chemical societies take the initiative to create these Prizes.

Prof. Sydnes concluded by asking that the delegates send him, directly or via the Secretariat, their comments on these five proposals. Prof. Steyn asked that this feedback be provided by the end of October.

Prof. Shani (Israel) commented that the information on who is participating in IUPAC activities from a country is often not sent to the chemical society by the NAO. He suggested that lists of members of IUPAC bodies, by NAO, be made available on the IUPAC web site.

A general discussion followed Prof. Sydnes's report. The discussion covered a number of subjects that had been raised directly or indirectly in his report. The following is a summary of the suggestions and comments made during the discussion.

- While the web is a useful means of communication, access is difficult is some places, especially Africa.
- Communication with Company Associates should also be a priority.
- COCI has set up a Task Group to review the company Associates program.
- Should the number of National Representatives on Division Committees be increased?
 (Note: the Bureau approved an increase in the number of National Representatives on Division Committees from six to ten for the 2004-5 biennium.)
- To attract younger people, projects must be moved more rapidly to completion.
- Young Observers had positive comments about their experience but felt the need for mentoring.
- It takes energy on the part of the members of Division Committees to encourage Young Observers.
- It is important to enumerate for Young Observers the benefits to their career of participating in the work of IUPAC.
- Should chemical societies be automatically copied on all correspondence with NAOs?
- The recommendation for the formation of the Union Policy Committee (Note: the name of this committee was changed to Union Advisory Committee, see Item 13.) addresses the issue of the NAO as a black hole for communication.
- IUPAC could send a representative to each national chemical society meeting.

13. Report from Governance Structure Committee

Prof. Sydnes began by noting that the Governance Structure Committee was formed by the Bureau in response to a proposal from the Nordic countries that the governance of the Union be examined with the goal of improving the speed of decision making and increasing the involvement of the

NAOs. The Bureau in forming the Committee had charged it with providing a report for consideration by Council at Ottawa. The draft report had been widely circulated, including to all the NAOs. The responses received from the NAOs, although few, had been generally supportive. The final report of the Committee was discussed at the Bureau meeting on 13-14 August. The discussion was mixed with a number of members expressing reservations or serious concerns about the proposals of the Committee.

The proposals of the Committee are as follows:

- A new body, the Executive Board would replace the current Executive Committee and Bureau. The membership of the Executive Board would be the five Officers plus four members elected by Council.
- A new body, the Union Policy Committee would be formed to advise the Executive Board on policy issues facing the Union. Each NAO would be asked to name one member to this Committee.

The Executive Board would have the same responsibilities regarding the management of the Union as the current Bureau and Executive Committee without the confusion of the divided responsibilities of the current structure. The composition of the Executive Board is a compromise between the desire to have a small, efficient body and one that is representative of the various constituencies of the Union, especially the NAOs. The Committee feels that the creation of the Union Policy Committee addresses the issue of the representation of the NAOs and therefore felt that a small Executive Board was acceptable. The lack of representation of the Division Presidents on the Executive Board is addressed by requiring that the Executive Board meet jointly with the Division Presidents. This can easily be done be scheduling the fall meeting of the Executive Board to coincide with the annual meeting of the Division Presidents. The advantage to the Division Presidents in this arrangement is that the joint meeting can focus on subjects of common interest. The Bureau discussed the issue of the membership of the Executive Board, but did not arrive at a consensus.

Prof. Sydnes emphasized that for the Union Policy Committee to function properly, its members should be senior members of the chemical community in their NAO and would be expected to serve for a number of years so that they become familiar with IUPAC and its work. The proposed joint meeting of the UPC and the EB would occur during the General Assembly, either before or after the Council meeting. The meeting of the UPC and the EB would not be devoted to the issues before the Council, since these would have been discussed in advance by correspondence. The meeting would instead focus on issues to be considered in the coming biennium. That is, the joint UPC/EB meeting would be definitely oriented to the future, not the current issues before Council.

The Bureau has expressed its support of the proposal to create the UPC. The UPC can be established by Council as an ad hoc Committee without the need to modify the Statutes or Bylaws. If the decision is made to replace the Executive Committee and Bureau with the Executive Board, a committee to draft the necessary revisions to the Statutes and Bylaws would be appointed and the final decision on the new governance structure would be made at the 2005 Council meeting in Beijing.

Prof. Kallner commented that the proposals of the GSC were responsive to the original proposal made by the Nordic countries.

Prof. Steyn then suggested that the discussion of this important issue should be conducted in three phases, first a general discussion, then consideration of the proposal to create the Union Policy Committee, and finally consideration of the proposal to replace the Executive Committee and Bureau with an Executive Board.

The discussion that followed was wide ranging with a large number of delegates making comments in support of or in opposition to the two proposals. There were also a number of comments made of a general nature about the governance of the Union and requests for clarification of the two proposals. What follows is a summary of the discussion with no attempt to reproduce verbatim all the comments made.

One point of clarification was the relation between the UPC and the World Chemistry Leadership Meeting. The WCLM includes many representatives from organizations other than NAOs and is intended to discuss subjects of interest to the worldwide chemistry community, subjects not necessarily directly related to IUPAC and its work.

A number of delegates commented that the perceived problems with the operation of the current governance could be addressed by better management of the agendas of the EC and Bureau. It was pointed out that too much time is spent in reviewing reports that could be taken as read. By eliminating time spent on these reports the Bureau meetings could be made more productive. The comment was also made that the General Assembly is already too long and the addition of another meeting would make an already congested schedule even more so – the principal point being that the current structure is not incorrect, is only ill used.

A number of delegations expressed support for both proposals with some suggesting that the first assignment of the UPC should be to thoroughly study the proposal to create the Executive Board.

A number of delegations felt that the proposal to create an Executive Board diminished the influence of the NAOs and the Divisions in the governance of the Union. There was also a feeling that there had been insufficient time to study the proposal and its consequences. Some delegates suggested that the Executive Board should have more elected members, perhaps eight to ten.

A proposal was made to ask the candidates for Vice President to express their views on the two proposals. It was decided not to do this as it was against the traditions of the Union to have speeches by candidates for office.

Prof. Steyn then suggested that since there seemed to be general support for the creation of the UPC a motion be made to establish it as an ad hoc Committee for the coming biennium. He also suggested that the Council approve in principle the formation of the Executive Board with composition to be determined before the final proposal is presented to Council at Beijing.

The motion from the chair for the creation of the UPC was then put to the Council. The Australian delegation proposed an amendment changing the name of the Committee to Union Advisory Committee. The motion was seconded and in accord with the rules of procedure was voted on first. The amendment passed with 97 votes for, 22 against and 12 abstentions.

Prof. Koch (Germany) then asked if the Council should now agree on Terms of Reference for the UAC. Dr. Becker replied that it was the usual practice for the Executive Committee to write the Terms of Reference of Committees. The motion as amended was then voted on and passed with 118 votes for, 9 against and 6 abstentions.

Dr. Hayes then commented that there was no need for a motion regarding the Executive Board. The sense of the meeting was that further consideration of this proposal was necessary and that was a task for the Executive Committee and Bureau as part of their normal responsibilities. There was no further discussion of this issue.

14. Budget Proposal

14.1. Report of Working Party on National Subscriptions

Dr. Buxtorf reviewed the work of the Working Party on National Subscriptions. The Working Party had been established by Council at Brisbane in response to concerns raised by the Czech and French NAOs regarding the method of calculation of National Subscriptions and the ability of some NAOs to meet their obligations. He noted that of the three recommendations made by the Working Party, two had been implemented by the Bureau, while the third required Council action and was on today's agenda as Item 15. The two proposals that have been implemented are:

- 1. to calculate National Subscriptions using the average of the five most recent available years of chemical turnover data and
- 2. to provide travel support for one delegate from each NAO to attend Council.

Dr. Buxtorf expressed his thanks to members of the Working Party who had worked hard to develop these proposals.

14.2. Proposed Budget for 2004-5

Dr. Buxtorf reviewed the proposed budget for 2004-5. He noted that the National Subscriptions shown would be superseded by those proposed in Item 15 if that proposal were approved. There was no discussion of this Item and it was moved to approve the budget as presented and the National Subscriptions as calculated. The motion was approved with 129 votes for, none against, and 4 abstentions.

14.3. National Subscriptions for 2004-5

The National Subscriptions were approved by the same vote that approved the budget, see Item 14.2 above.

15. Proposal to Invoice National Subscriptions in National Currencies

Dr. Buxtorf described the proposal as presented in the Agenda Book. He noted that this proposal is intended to address two situations. The first occurs as a result of normal fluctuations in exchange rates when an NAO budgets for the National Subscription in its national currency, but when payment is made the budgeted amount is no longer sufficient to pay the amount due in USD. The second occurs when the currency of an NAO falls suddenly with respect to the USD and the

amount due in USD represents a much greater amount in national currency. The underlying concept of this proposal can be simply expressed as that the amount of National Subscriptions due is calculated and invoiced in each national currency. When payment is made it is made in USD at the then current exchange rate for the amount due in national currency.

There was no further discussion of this proposal. The motion was made to approve the proposal, and the motion was approved with 104 votes for, 11 against, and 12 abstentions.

16. IUPAC Programs

16.1. IUPAC Prize

16.1.1. IUPAC Prize 2002-3

Dr. Hayes thanked the members of the Prize Committee for their work in selecting the winners from so many worthy applicants. He commented that he was impressed by the overall high standard of work contained in the applications.

Prof. Collins commented that when introducing the winners at the Congress it would have been preferable to indicate the country in which the doctoral work was done since many of the winners had moved subsequent to finishing their degrees. This would have better indicated the diversity of the countries represented by the winners.

16.1.2. Reapproval of IUPAC Prize Program

Dr. Becker commented on the success of the program and noted that the original authorization of the IUPAC Prize program had been for a period of four years with reauthorization required by Council. He then asked that the Council reauthorize the program with no end date. This motion was passed by an overwhelming majority.

16.2. Conferences in Developing Countries and on New Directions in Chemistry

Dr. Becker reviewed the history of the Conferences in Developing Countries program and New Directions in Chemistry conferences. He commented that while the Conferences in Developing countries program had provided financial support for a number of conferences over the past four years, it was felt that the benefit to IUPAC from the program had been minimal. The conferences supported had in general been members of well-established conference series that happened to be held in a developing country. The Bureau had decided that in order to increase the benefit to IUPAC the program should be refocused in a number of ways.

- Try to relate the supported conferences to programs within the Divisions and Standing Committees. Applications for support will come from these IUPAC bodies, rather than conference organizers directly.
- Aim support to conferences that have some innovative aspect that relates to IUPAC interests and/or to benefits for the host country.
- Provide part of the support funds in the form of IUPAC Lecturers senior scientists who agree to speak at a conference and preferably also to visit nearby

- universities or other institutes for seminars, discussions and development of potential long-range collaborations.
- Expand eligibility to Associate NAOs, as well as NAOs, in order to broaden contacts with scientists in developing countries.

The refocused program will require additional proactive efforts on the part of IUPAC Divisions and Operational Committees, but there should be significant benefits to IUPAC in fostering a more coherent activity and in receiving greater recognition for its investment.

Dr. Becker noted that a pilot program, with a budget of USD 25,000 per biennium was established in 1999 at the initiative of President Jortner to permit IUPAC to initiate occasional conferences on cutting-edge research topics as a complement to the Union's sponsorship of a number of well-known series of conferences in established fields. Bureau approved the continuation of this program, but on a more formal basis with clear guidelines and with applications made by Divisions and Standing Committees for support of conferences in innovative areas.

Dr. Becker reported that the Bureau had approved consolidation of the funding for these two programs into a USD 65 000 allocation, as included in the proposed budget for 2004-2005. The Project Committee was charged with review of applications and funding decisions.

Dr. Becker concluded by noting that no action was required by the Council and this item had been placed on the agenda for information only.

17. Proposals Formally Received from National Adhering Organizations

The only proposal received was from the NAO of the United Kingdom. The proposal was as follows:

One of the most important issues for the future of chemistry and the long-term success and sustainability of the chemical industry, and therefore worldwide economic stability, is the decline in the number of young people being attracted into the subject. The importance of this issue has already been recognized by industry, trade associations, learned societies and academe. To address the problem, IUPAC should encourage and facilitate the coordination of the variety of initiatives proposed, with a view to enhancing the importance of chemical education at all levels, and to utilize younger chemists to promote the subject and its achievements. It is recommended that IUPAC collaborate with all these bodies to discuss how best to achieve these aims and, if considered appropriate, to solicit new financial resources to achieve them.

Prof. Atkins of the UK delegation then reviewed the intent of the proposal. He noted a two-stage program was envisioned:

1. The Union should establish a task Force to study the problem on a global basis.

2. The Task Force should raise funds from industry to finance the implementation of its proposals.

Prof. Atkins then suggested that the Task Force should include representatives from CCE, COCI, CHEMRAWN, CEFIC (Confederation of European Chemical Federations), and other industrial representatives.

A general discussion of this proposal followed. The discussion indicated that it was unclear what financial commitment from the Union was entailed by this proposal. Prof. Atkins clarified the proposal by noting that the intent was to provide funds for the initial study by the Task Force. Further discussion emphasized that approval of this proposal was not an open ended grant of funds and that funding would be determined by the Executive Committee.

Council then approved the proposal by a large majority.

18. Organizational Changes in Existing IUPAC Bodies, Proposals for New and Reconstituted Bodies/Terms of Reference

18.1. Continuation of the Joint Commission on Biochemical Nomenclature

Dr. Becker noted that the status of this Commission had been deferred pending discussions with the International Union of Biochemistry and Molecular Biology. These discussions had led to the proposal in the Agenda Book. He asked the Council to approve the continuation of the Joint Commission and its new Terms of Reference.

Council approved the motion by a large majority.

18.2. New Division Rules

Dr. Becker commented that the Division rules had become outdated and in many cases were no longer in agreement with the Statutes and Bylaws of the Union. He had developed, in cooperation with the Division Presidents a set of Model Rules that could be used as a basis for Division Rules. The Macromolecular and Analytical Chemistry Divisions had written new Division Rules and the Council was asked to now approve these rules. He also asked that Council authorize the Executive Committee to approve minor changes in the Division rules in future.

Prof. De Bièvre (Belgium) noted the use of the term nomenclature in the Terms of Reference of the Macromolecular Division. He commented that he understood that all work on nomenclature was the responsibility of the Chemical Nomenclature and Structure Representation Division.

Dr. Becker replied by noting that in this case nomenclature referred to work that was not the kind of systematic nomenclature as defined in the Terms of Reference of Division VIII, but was more akin to termininology.

Council approved the proposed Division Rules by a large majority.

19. Applications for Associated Organization Status

Dr. Becker referred the Council to the written material in the Agenda Book and asked for the Council's approval of the requests contained therein.

Prof. Schneider (Germany) noted with regret that the International Plasma Chemistry Society and the International Association of Chemical Thermodynamics were former IUPAC Commissions and commented that the Union should give them a home rather than an umbrella.

Council approved by a large majority the following requests:

- The new Constitution of the International Association of Catalysis Societies.
- Associated Organization status for: International Plasma Chemistry Society, International Association of Chemical Thermodynamics, Southern and Eastern Africa Network of Analytical Chemists.

20. Election of Union Officers and Bureau Members and Approval of Elected Officers of Divisions

Dr. Becker reviewed the voting procedures for officers and members of the Bureau.

The results of the first ballot for Vice President were as follows:

Prof. Gilbert: 32 votes
Prof. Henry: 60 votes
Prof. Ohtaki: 40 votes

The results of the second ballot for Vice President were as follows:

Prof. Henry: 85 votes
Prof. Ohtaki: 45 votes

There were no abstentions in either ballot, however, one delegation did not cast its two votes in the second ballot; Prof. Henry was declared the winner of the election for Vice President and President elect.

Dr. Becker reviewed the situation for the election of the Secretary General and the Treasurer.

The results of the ballot for Secretary General were as follows:

Prof. Black: 71 votes
Prof. Corish: 60 votes
Abstain: 1 vote

Prof. Black was declared the winner of the election for Secretary General.

The results of the ballot for Treasurer were as follows:

For: 125 votes Against: 0 votes

Abstain: 7 votes

Dr. Buxtorf was declared the winner of the election for Treasurer.

Dr. Becker then explained that with the election of Prof. Henry, there were now four candidates for four positions. He asked that the four candidates be approved by the Council by unanimous consent. Council approved this proposal by a show of cards with no negative votes and approved the election of the following Bureau members with no negative votes.

Prof O Nefedov (Russia)

Prof. A. Kallner (Sweden)

Prof. W. Klein (Germany)

Prof. N. Moreau (France)

Prof. Tidwell noted that a replacement for Prof. Black as President of the Organic and Biomolecular Chemistry Division would be named later.

21. Plans for 43rd General Assembly and 40th Congress (Beijing, 2005)

Prof. Bai reviewed the plans for the 40th Congress in 2005. The theme of the Congress was *Innovation in Chemistry*. The Congress will be held on 14-19 August 2005 and the General Assembly on 13-21 August 2005. The Congress and General Assembly will be held in the Beijing International Convention Center and the adjacent Beijing Grand Hotel.

Prof. Bai noted that the Division Presidents and Standing Committee Chairmen had been asked to suggest contributions to the planned program. He then pointed out that participants would need visa letters from the organizers to obtain visas at Chinese Embassies or Consulates. It was advisable to allow sufficient time to complete the paper work.

22. Approval of Dates and Sites of 44th General Assembly and 41st Congress (2007)

Prof. Della Gatta reviewed the proposal of the Italian National Adhering Organization to host the IUPAC Congress and General Assembly at Torino in 2007. The proposed theme of the Congress is *Chemistry Protecting Health, Natural Environment and Cultural Heritage*. The proposed dates are 5-11 August for the Congress and 4-12 August for the General Assembly. The proposed venue is the Lingotto Conference Centre. Prof. Della Gatta reviewed the facilities available, including the Agnelli auditorium with a capacity of over 2000, 14 meeting halls, and a large exhibit hall of over 46 000 m².

He then described the large number of hotel rooms available in the city of a wide range of price classes. The center of the city will be accessible by subway at the time of the Congress. Torino is readily accessible by air, train, and car. He noted the many sites of historic interest in the city and the proximity to both the Alps and the Mediterranean coast.

Prof. Nefedov (Russia) commented that the theme of the Beijing Congress and that proposed for the Torino Congress were very similar. He proposed adding Education and the Public Understanding of Chemistry to the proposed theme. Prof. Della Gatta noted that these topics fit well into the proposed theme for the Congress.

Council approved the application of the Italian NAO to host the 2007 Congress and General Assembly at Torino on the dates proposed by a large majority.

23. Important Matters Referred to Council by Bureau at 42nd General Assembly not Covered by Items on Council Agenda

Dr. Becker noted that the application of the Bangladesh Chemical Society for National Adhering Organization status had been received too late to be included in the Agenda Materials. While the Bureau had not discussed the application, it had discussed the general topic of the desirability of encouraging more countries joining IUPAC as NAOs. He moved that Council approve the application.

Council approved the application of the Bangladesh Chemical Society for National Adhering Organization status by a large majority.

Prof. Mosihuzzamann, President of the Bangladesh Chemical Society, was present at the Council meeting and expressed his appreciation of the Council action.

Dr. Becker then noted that the Mauritius Chemical Society had submitted an application for Associate National Adhering Organization status. This application was received too late for consideration by the Bureau and while Council approval was not necessary for ANAO status, he proposed that Council approve the application in order that approval not be delayed.

Council approved the application of the Mauritius Chemical Society for Associate National Adhering Organization status by a large majority.

24. Any Other Business (discussion only)

Dr. Przybylowicz briefly reviewed for the Council a project that had been approved by Bureau at Ottawa to investigate the feasibility of creating a web site on the *Contributions of Chemistry to Society*. The purpose of the project is to present in one location information on the contributions of chemistry to society. Much of the ground work has been done by various chemical societies, such as the American Chemical Society; but, there was a need for a centralized presentation of this information that was readily available to anyone searching for information on the internet and that was organized in such a way as to be useful for different groups of users, from students to decision makers to the press.

Prof. De Bièvre (Belgium) again raised the issue of the financial support of the Atomic Weights activity of the Union. He emphasized the importance of this work to the Union and his concern that it was not being properly supported. Prof. Steyn commented he would do his best to be sure that this activity is properly supported. Prof. Sydnes then noted that he would look into this issue and discuss their concerns with the Commission members. He had already asked the Commission Chairman to provide him with written comments.

Prof. De Bièvre (Belgium) noted that the IUPAP Commission SUNAMCO (Symbols, Units, Nomenclature, Atomic Masses and Fundamental Constants) included names and atomic masses in its terms of reference. He then moved to commend the Bureau on its implementation of the decision of Council on the creation of the Chemical Nomenclature and Structure Representation Division and

the new Division on its active program. The Council voted its appreciation to the Bureau and the Division.

Prof. De Bièvre (Belgium) then asked the Council to congratulate the Treasurer and the Finance Committee on their handling of the Union's financial matters. Council applauded this motion.

Dr. Sweeney (UK), a Young Observer, thanked the Union for the invitation to participate in the General Assembly and he suggested that other NAOs institute similar programs for their young scientists to encourage them to participate in IUPAC. He expressed the feeling of the other Young Observers that the time had been well spent and thanked the Royal Society of Chemistry for providing funding to enable him to participate.

Dr. Damhus (Denmark) commented that the CVs provided by the candidates for Officer and Bureau did not include a statement of policy if elected. Dr. Becker noted that this issue had arisen in the past and that oral presentations had been discouraged because of the language issue. Dr. Damhus made a motion that written statements from the candidates be included in the material for the Council. The motion was seconded by the US and approved by a large majority.

Dr. Damhus (Denmark) asked if the proposed plan for the governance of the Union would provide any financial savings. Dr. Becker commented that the Governance Structure Committee had considered the financial implications of the plan and concluded that there would be a small saving due to the smaller number of Elected Members, but that this was a minor consideration. There was no plan to fund the meeting of the Union Advisory Committee.

Prof. Cvitas (Croatia) commented that the work on databases seems to have been neglected. He asked that the Bureau address this issue.

Prof. De Bièvre (Belgium) asked if the Union was losing competence in this area. He then provided the Council with some information regarding the *International Vocabulary on Metrology*. The revised version of this document, VIM 3 includes for the first time terms from chemistry. The document will be mailed to IUPAC for comment in the near future and he asked that IUPAC approve VIM 3.

Prof. Shani (Israel) reported that there had been an increase of 40-50 % in chemistry students in Israel. Many computer science students have changed to chemistry as a result of the high tech bust. Israeli Universities are actively recruiting the best students.

25. Closing Remarks, Adjournment

Prof. Steyn congratulated the new Officers of the Union, new elected Members of the Bureau and the new Officers of Divisions and Standing Committees. He thanked the Council, Division Committees, Standing Committees, and Task Groups for their work in support of the Union. He also thanked all those who are ending their IUPAC service, especially Dr. Hayes the Past President and Dr. Becker the Secretary General for their work over the past years. Prof. Steyn then offered his best wishes to Prof. Sydnes and the new team leading IUPAC.

Prof. Sydnes thanked Prof. Steyn for his leadership as President and said that he looked forward to working closely with the NAOs to continue to make IUPAC an organization that made a valuable contribution to the global chemistry community and to society.

The meeting was then declared adjourned.



International Union of Pure and Applied Chemistry

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Item 3: Ratification of Decisions Taken by Bureau and Executive Committee

All decisions taken by the Bureau and Executive Committee, since those approved by the Council at Ottawa (Minute 3, 42nd Meeting), are contained in the following Minutes, which were distributed to National Adhering Organizations as shown:

78th Bureau 11 November 2003 79th Bureau 11 November 2003 80th Bureau 30 November 2004

131st Executive Committee 8 June 2004 132nd Executive Committee 21 June 2005



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Vice President:Prof. Bryan R. Henry (Canada)RTP, NC, 27709-3757 USAPast PresidentProf. Pieter S. Steyn (South Africa)Location:104 T. W. Alexander Drive, Building 19Secretary General:Prof. David StC. Black (Australia)Research Triangle Park, NC 27709 USA

Treasurer: Dr. Christoph F. Buxtorf (Switzerland) Phone: +1 (919) 485 8700
Fax: +1 (919) 485 8706
Executive Director: Dr. John W. Jost E-mail: secretariat@iupac.org

Item 4: Announcement of Nominations for Union Officers and Bureau Members

Nominations were to be received by the Secretariat at Research Triangle Park by 20 June 2005 (Bylaw 2.221). The list of nominees received is given below.

URL:

According to Bylaw 2.222, the Bureau has the right to make additional nominations for which information shall be provided. When the number of nominations exceeds the number of vacancies, the Bureau may make recommendations to the Council for filling the vacancies. These recommendations are not binding on the Council, either for Officers or for Elected Members of the Bureau. The procedures for conducting the election ballots are specified in Bylaw 2.222. The Officers and members of the Bureau are elected by Council. The situation for each position is set out below:

President – Prof. Bryan R. Henry (Canada), Vice-President and President-Elect, becomes President on 1 January 2006 (Statute 4.2).

Past-President – Prof. Leiv K. Sydnes (Norway), President, becomes Past-President on 1 January 2006 and remains an officer (Statute 6.1) and a member of the Bureau for a period of two years (Statute 7.2).

Vice-President – Vacancy.

The Vice-President to be elected at the 43rd Council will be President-Elect, and will become President on 1 January 2008.

The following Nominations have been received.

Prof. S. Chandrasekaran (India)

Prof. K. Matsumoto (Japan)

Prof. N. Moreau (France)

Secretary General – Prof. David StC. Black (Australia) was elected to a four-year term at the 42nd General Assembly and continues in office until the end of 2007.

Treasurer – Dr. Christoph F. Buxtorf (Switzerland) was elected to a second four-year term at the 42nd General Assembly and continues in office until the end of 2007.

Item 4: Announcement of Nominations for Union Officers and Bureau Members

Bureau - Six Vacancies (minimum).

According to Statute 7.2 the Bureau consists of the Officers, the Division Presidents, and no less than ten other members elected by Council, who are known as "Elected Members". Elected Members are elected for a four-year term, and are eligible for reelection to a second four-year term. No National Adhering Organization shall have more than one Elected Member on the Bureau. Statute 7.2 also states that "the principle of fair geographical representation of Members shall be taken into account".

At the conclusion of the 42nd Council in Ottawa, there were ten Elected Members on the Bureau. At the 43rd Council, the Bureau will make recommendations to Council as to the number of Elected Members (ten or more), who should be on the Bureau for the succeeding two years. At least six Elected Members will be elected at the 43rd Council in Beijing, *i.e.*, the minimum number of ten Elected Members (Statute 7.2) less the four Elected Members who continue in office until 2007.

Elected Members of Bureau whose terms end in 2007:

Dr. Anders Kallner (Sweden)

Prof. Werner Klein (Germany)

Prof. Nicole J. Moreau (France)

Prof. Oleg M. Nefedov (Russia)

Elected Members of Bureau, whose terms end in 2005 and who are eligible for reelection to a second four-year term:

Prof. Chunli Bai (China/Beijing)

Prof. S. Chandrasekaran (India)

Prof. Robert G. Gilbert (Australia)

Dr. Alan Smith (United Kingdom)

Elected Members of Bureau, whose terms end in 2005 and who are not eligible for reelection, but may be nominated for another office:

Dr. Edwin P. Przybylowicz (United States)

Prof. Gus Somsen (Netherlands)

The following Nominations have been received.

Prof. Chunli Bai (China/Beijing)

Prof. D. Berek (Slovakia)

Prof. S. Chandrasekaran (India)

Prof. P. De Bièvre (Belgium)

Prof. A. J. Mahmood (Bangladesh)

Prof. K. Matsumoto (Japan)

Prof. S. Penczek (Poland)

Dr. E. Reichmanis (USA)

Prof. I. Shopov (Bulgaria)

Dr. Alan Smith (United Kingdom)

Prof. M. C. E. van Dam-Mieras (Netherlands)

Item 4:Announcement of Nominations for Union Officers and Bureau Members

If Prof. Moreau is elected Vice President there will be an additional vacancy on the Bureau. If Prof. Chandrasekaran or Prof. Matsumoto is elected Vice President there will be one less candidate for the Bureau.

Biographical sketches of the candidates can be found on the following pages.

ASSIGNMENT OF VOTES TO DELEGATIONS

An updated basis for the assignment of votes was approved at Guildford (Minute 1/95, 38th Council, see table below), and it became operative at Geneva in 1997. The table on the following page lists votes as they will be assigned at Beijing, based on the assumption that all 2004 National Subscriptions will have then been paid. NAOs in arrears on their National Subscription for 2004 or earlier as of the time of the elections are not eligible to vote at the Council.

National Subscription	Votes
GTE USD 40 000	6
LT USD 40 000 and GTE USD 20 000	5
LT 20 000 and GTE USD 10 000	4
LT USD 10 000 and GTE USD 5000	3
LT USD 5000 and GTE USD 2000	2
LT 2000	1

 $\overline{GTE} = \overline{Greater Than or Equal to}$

LT = Less Than

Delegation Vote Assignments, IUPAC General Assembly 20-21 August, Beijing

	NS (2004)			
NAO	USD (1000s)	Votes		
Argentina	4.0	2		
Australia	10.4	4		
Austria	5.8	3		
Bangladesh	1.0	1		
Belgium	20.6	5		
Brazil	24.3	5		
Bulgaria	1.6	1		
Canada	15.8	4		
Chile	3.7	2		
China/Beijing	40.1	6		
China/Taipei	15.1	4		
Croatia	1.0	1		
Czech Republic	4.1	2		
Denmark	6.5	3		
Egypt	4.3	2		
Finland	5.7	3		
France	37.3	5		
Germany	52.9	6		
Greece	3.7	2		
Hungary	3.7	2		
India	19.6	4		
Ireland	13.2	4		
Israel	5.0	3		
Italy	32.0	5		
Japan	71.2	6		
Korea, Republic of	23.1	5		
Kuwait	1.0	1		
Netherlands	19.2	4		
New Zealand	4.3	2		
Norway	4.9	2		
Pakistan	3.1	2		
Poland	6.7	3		
Portugal	5.0	3		
Puerto Rico	16.2	4		
Russia	10.2	4		
Serbia & Montenegro	1.0	1		
Slovakia	2.9	2		
Slovenia	3.4	2		
South Africa	7.9	3		

Delegation Vote Assignments, IUPAC General Assembly 20-21 August, Beijing

	NS (2004)		
NAO	USD (1000s)	Votes	
Spain	21.6	5	
Sweden	9.3	3	
Switzerland	17.0	4	
Turkey	8.8	3	
United Kingdom	28.0	5	
United States	111.2	6	

IUPAC

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Nominee for Vice President and Member of the Bureau

Srinivasan Chandrasekaran (India)

Professor Chandrasekaran's research has been concerned with the development of new synthetic methodology for organic synthesis, synthesis of natural products, organometallic chemistry, catalysis, study of reaction mechanisms, and organic materials.



Sriniyasan Chandrasekaran

Education and Career

Chandrasekaran earned his B.S. (1965), M.S. (1967), and Ph.D. (1972) degrees at Madras University in Madras, India. His doctoral supervisor was Prof. S. Swaminathan in the Department of Organic Chemistry. He held postdoctoral fellowships/associateships in the laboratories of Prof. E.J. Corey at Harvard University, Cambridge, MA, USA (1973–1975 and 1976–1977) and Dr. J.A. Edwards at Syntex Research, Palo Alto, CA, USA (1975–1976).

He is currently the chairman, Division of Chemical Sciences and professor, Organic Chemistry at the Indian Institute of Science, Bangalore, India. He was earlier the chairman of the Department of Organic Chemistry (1996–2003) and Amrut Mody Chair Professor of Chemistry. From 1978 to 1989, he worked in the Department of Chemistry at the Indian Institute of Technology, Kanpur, India, where he served as lecturer (1978–1980), assistant professor (1981-1985), and professor (1985–1989). He has been a visiting professor at the Australian National University, Canberra (1985); University of Karlsruhe, Germany (1987); RWTH, Aachen, Germany (1992, 1996); University Paris Sud, France (1998, 2001), and Chinese Academy of Sciences, Beijing (2001).

Chandrasekaran has published over 170 research papers in national and international journals. Over the years he has supervised 26 Ph.D students, 60 M.S. students and 40 postdoctoral fellows. He is a consultant to a number of

chemical and pharmaceutical industries in India and abroad.

IUPAC Involvement

Chandrasekaran has been an elected member of the IUPAC Bureau since 2002 and has been a member of the Project Committee. He also served on the IUPAC Commission on Nomenclature of Organic Chemistry (1993–1995) and is currently on India's IUPAC National Committee.

Related Professional Activities

Chandrasekaran has been a member of many committees and organizations: associate editor, Proceedings of the Indian Academy of Sciences (Chemical Sciences, 1991–2000); member, Sectional Committee, Chemistry, Indian Academy of Sciences (1991–1998); editor, 10th International Conference on Organic Synthesis, Bangalore (1994); member, Editorial Board, Indian Journal of Chemistry (1995–2001); member, Program Advisory Committee in Organic Chemistry, Department of Science and Technology, New Delhi (1995–2001); member, Research Committee on Chemistry and Technology, Council of Scientific and Industrial Research, Govt. of India (CSIR, 1995–2001); member, Council of Indian National Science Academy (1998–2000); convener, National Symposium in Chemistry, Bangalore (1999); member, Task Force on Green Chemistry, Govt. of India; secretary, Indian Academy of Sciences, Bangalore; vice president, Chemical Research Society of India. He also serves as a member on the Research Councils of a number of CSIR laboratories and leading academic institutions in India. He has also served as a member on the Board of Studies of a number of universities in India. Chandrasekaran has delivered more than 180 invited lectures and seminars at various national and international meetings, universities, and research institutions in India and overseas.

Awards

Chandrasekaran received the Basudev Banerji Medal and Prize from the Indian Chemical Society in 1988 and the Shanti Swarup Bhatnagar Prize from CSIR in 1989. He was Prof. A.B. Kulkarni Endowment Lecturer at the University of Bombay in 1992; Prof. N. Venkatsubramanian Endowment Lecturer at the University of Madras in 1993; Prof. T.R. Seshadri Memorial Lecturer at Delhi University in 1998; Prof. Siddappa 60th Birthday Commemoration Lecturer at Dharward University in 1999; Professor O.P. Vig Endowment Lecturer, Panjab University, Chandigarh in 2000, Jawaharlal Nehru Birth Centenary Lecturer of the Indian National Science Academy in 2001; 125 Years-Indian Association for the Cultivation of Science, Kolkata—Commemoration Lecturer in 2002; and Prof. Sukh Dev Endowment Lecturer, Pune University, in 2004.

He received the Silver Medal of the Chemical Research Society of India (2002), Medal of the Material Research Society of India (2004), and the Alumni Award for Excellence in Research in Science (2004). Chandrasekaran was appointed research fellow of the Indian National Science Academy (1985–1987); fellow of the Indian Academy of Sciences (1989); and fellow of the Indian National Science Academy (1992); honorary professor of the Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore (2000–present); and fellow of the Third World Academy of Sciences, Trieste, Italy (2000).

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Nominee for Vice President and Member of the Bureau

Kazuko Matsumoto (Japan)

Professor Kazuko Matsumoto's research involves metal coordination chemistry and bioanalytical chemistry using metal complexes. She started her career as an inorganic chemist and has been expanding her expertise in designing and synthesizing new functional metal complexes such as fluorescent lanthanide labels for time-resolved detection in bioanalysis, and catalysis and electrical and magnetic properties



Kazuko Matsumoto

of nanowire metal complexes of metal-metal bonds.

Education and Career

Matsumoto received her B.S. in 1972 and Ph.D. in 1977, both from the University of Tokyo. She started her academic career in 1977 as a research associate working with Prof. Keiichiro Fuwa at the University of Tokyo, and then moved to Waseda University as an associate professor in 1984. She was promoted to a full professor at Waseda University in 1989, and has served there ever since. During these years, she spent two years (1991–1992) at the Institute for Molecular Science (Japan) as an adjunct professor, and spent half a year (1993) with Prof. Steve Lippard at MIT as a visiting professor. In addition, she visited and gave lectures at major Japanese and foreign universities (Bari, Florence, Dortmund, Leiden, Bazel, California Institute of Technology, Stanford) as a visiting professor. She also has given invited lectures at many internationally renowned academic meetings. (She will be a lecturer at the IUPAC Congress in Beijing in August 2005.) She has published more than 200 scientific papers in analytical and inorganic chemistry and holds 40 patents.

IUPAC Involvement

Matsumoto has been a titular member on the Analytical

Chemistry Division (2002–2005) and is preparing a project on the definition of concentrations of biomolecules. In Japan, she is a member of the chemistry division of the Science Council of Japan, which is the corresponding organization for IUPAC in Japan.

Related Professional Activities

Matsumoto is a member of the Engineering Academy of Japan, and is also a member of the Council for Science and Technology Policy, cabinet office. For more than 10 years, she has served on the advisory board of major scientific journals including the Bulletin of the Chemical Society of Japan and the European Journal of Inorganic Chemistry. She also served as the vice president of the Japan Society for Analytical Chemistry (2001) and is now the chairperson of the international relations committee of the Chemical Society of Japan. She has worked as the national representative in FACS (the Federation of Asian Chemical Societies) and organized the EurAsia conference (an international conference between Asia and Europe) in Asia.

Awards

Matsumoto has earned honors for her outstanding contributions to chemistry, which include the Award for Promotion of Young Researchers from the Japan Society for Analytical Chemistry (1984), the Division Award from the Chemical Society of Japan (1989), and the Ichimura Award (2000).

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Nominee for Vice President

Nicole J. Moreau (France)

After 10 years of research in organic synthesis, terpenes, steroids, and sugars, Professor Nicole J. Moreau successfully designed the first purification, using affinity chromatography, of enzymes that inactivate aminoglycoside antibiotics. Her research is at the interface of chemistry and life sciences, and she continues to study the mode



Nicole J. Moreau

of action of antibiotics and the ways bacteria can resist them. She developed a mean throughput screening system in order to find molecules able to be active against resistant bacteria, for instance inhibitors of efflux pumps or of inactivating enzymes. She has also researched molecular pharmacology, structure-activity relationships and synthesis of analogues of active compounds together with molecular modeling and docking calculations. In 2005, she launched, together with CNRS and Rhodia, a new program on fine chemistry using bioconversions.

Education and Career

Moreau received an M.S. in physical chemistry from the University of Paris (Sorbonne). She obtained a doctorate in physical sciences (chemistry distinction) in 1967 from Orsay University.

Since 1999, Moreau has been a professor at Ecole Nationale Supérieure de Chimie de Paris (ENSCP), where she is the leader of the Laboratory of Biochemistry. From 1994–1999 she was a professor in the Laboratory of Molecular Research on Antibiotics at the Paris 6 University (Pierre and Marie Curie). In 1973, she was a postdoctoral fellow in the laboratory of Dr. J. S. Pitton at the Medical Microbiology Institute in Geneva, Switzerland. Moreau began service with the Centre National de la Recherche Scientifique (CNRS) in 1962, where she was "directeur de recherche" from 1979 to 1992. In 1972, Moreau joined the chemistry laboratory of

Prof. Le Goffic at Ecole Normale Supérieure in Paris, where she worked until 1993.

Moreau has authored more than 80 publications, given more than 90 conferences or oral presentations, and supervised 25 Ph.D and 22 M.S. students and 10 post-doctoral fellows. She is responsible for teaching at the interface of chemistry and life sciences at the Ecole Nationale Supérieure de Chimie de Paris and is a member of the Administration Committee of the French Society of Biochemistry and Molecular Biology.

IUPAC Activities

Since 2000, Moreau has been an elected member of the Bureau and also a member of the Project Committee. She has served as vice president and currently is general secretary of the French National Committee for Chemistry. She has been a member of the French Delegation since 1995.

Related Professional Activities

Moreau has held a number of leadership positions with leading chemistry institutions. She has served as chargé de mission, State Department of Research (Ministère de la Recherche), deputy director of the Drugs department (1984–1989) and has been chargé de mission (1993–1997), then deputy director (1998–2003), at CNRS, Department of Chemical Sciences. Since 2003, she remained chargé de mission for natural substances for the CNRS Chemistry Department and International Relationships Direction.

She was secretary (1989–1997), then president (1997-1999) of EUCHEM, European Chemistry; president of GESA; Study Group of Structure-Activity Relationships (1990); vice-president of the French National Committee for Chemistry, CNC, IUPAC NAO (1994–2002). In addition, she is a long-time member of the French Chemical Society, French Microbiology Society, and the French Biochemistry and Molecular Biology Society.

Awards

Moreau was awarded the Prix de l'Académie de Pharmacie, Paris, in 1974, and the Chevalier de l'Ordre National du Mérite, awarded by the State Department of Research, in 2002. In 2004 she received the Silver Medal of the International Foundation of la Maison de la Chimie.

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Nominee for Bureau

Chunli Bai (China)

Professor Chunli Bai is the president of the Chinese Chemical Society and executive vice president of the Chinese Academy of Sciences. Bai's research has involved molecular nanostructures and nanotechnology, scanning probe microscopy, and molecular self-assembly on the liquid and solid interfaces.



Chunli Rai

Education and Career

In 1978, Bai graduated from the department of chemistry, Beijing University. He received his M.S. in 1981 and Ph.D. in 1985 from the Institute of Chemistry of the Chinese Academy of Sciences (CAS). From 1991 to 1992, he was a visiting professor at Tohoku University in Japan. He performed postdoctoral research from 1985–1987 at the California Institute of Technology. He is an academician of CAS and a fellow of the Third World Academy of Sciences (TWAS). He has more than 300 research papers to his credit, and has authored 11 monographs and several book chapters either in English or in Chinese.

IUPAC Involvement

Bai has been an elected member of the IUPAC Bureau since 2002 and a member of the Executive Committee since 2004.

Related Professional Activities

Bai is chief scientist of the National Steering Committee for NanoScience and Nanotechnology, director of China National Center for Nanoscience and Technology, president of Graduate University of the Chinese Academy of Sciences, vice-president of the China Association for Science and Technology, vice-president of the Western Returned Scholars Association, vice-president of the Chinese Materials Research Society, and president of the Chinese Association for Young Scientists and Technicians. In addition, he serves as a member of the Academic Degrees

Committee of the State Council.

Awards and Honors

Bai is a recipient of the "International Medal" given by the London-based Society of the Chemical Industry and the TWAS 2002 Medal Lecture in Chemical Sciences. As a project leader, Bai has won more than 10 national, CAS-awarded, or ministerial prizes. He has received the titles of "National Advanced Worker," "Young and Middle-Aged Specialists with Outstanding Contributions to the Country," and "Top 10 Outstanding Youths in China." He also has won National Awards for Young Chinese Scientists, Awards for Outstanding Young Scholars conferred by Hong Kong's Qiu Shi S&T Foundation, and Awards for Outstanding Chinese Visiting Scholars from the Hong Kong Polytechnic University.

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Nominee for Bureau

<u>Dušan Berek</u> (Slovakia)

Professor Dušan Berek has been active in the field of high-performance liquid chromatography of synthetic polymers, developing new types of column packings, as well as unconventional methods for their evaluation. He has worked out several original "coupled" procedures for liquid chromatographic separation and



Dušan Berek

characterization of complex polymer systems.

Education and Career

Berek graduated from the Faculty of Chemical Technology, Slovak Technical University in Bratislava in 1960. In 1966, he received his Ph.D. in physical chemistry from the Polymer Institute of the Slovak Academy of Sciences in Bratislava, Slovakia, and the Institute of Macromolecular Chemistry at the Academy of Sciences in Prague, Czech Republic. In 1991, he received his D.Sc. in Macromolecular Sciences from the Slovak Technical University and Slovak Academy of Sciences in Bratislava.

Since 1991, Berek has been head of the Laboratory of Liquid Chromatography Polymer Institute at the Slovak Academy of Sciences, where he has worked since 1960. Previously, Berek served as vice-director (1989–1990) and head (1980–1991) of the Department of Thermodynamics and Hydrodynamics of Polymer Systems. Prior to that he was head of the Department of Physical Chemistry (1966–1971).

He is author or co-author of two monographs, over 240 scientific papers in extenso, and chapters in books. He holds over 60 patents. Three of his patents were licensed to companies producing chromatographic materials and one to a company producing fillers for rubber. He has been an invited speaker at many universities and research institutions all over the world, and has delivered more than 300 lectures.

In addition, he has presented over 70 invited lectures and numerous regular contributions at international scientific meetings.

IUPAC Involvement

Since 1993, Berek has been chairman of the Slovak National Committee of Chemistry for IUPAC. From 1998–2003, he was the chair of the IUPAC Working Party on Molecular Characterization of Commercial Polymers. He has also been a member of the Commission on Chromatography (1998–2001) and a member of the Macromolecular Division Committee (2001–2003).

Related Professional Activities

Since 2005, Berek has been the vice president of the Slovak Chemical Society; he was president from 1997–1999 and from 2003–2004. In addition, he has been a member of the Board of the Federation of European Chemical Societies (1993–1996) and the Presidium of the Slovak Academy of Sciences (1992–1995). From 1991–1992 he was chairman of the Czecho-Slovak National Committee of Chemistry.

Berek has served on the organization committees of over 30 international conferences (14 times as chair) and on 12 international scientific boards of various symposia. Among the symposia he organized, four were under IUPAC auspices. He is a member of the editorial boards of four international journals: International Journal of Polymer Analysis and Characterization, International Journal of Polymeric Materials, Chemical Papers, and Current Analytical Chemistry.

Awards

Berek received the Gold Medal (1995) and Honorary Membership (2001) from the Slovak Chemical Society, Hanus Medal of Czech Chemical Society (2000), Commemorative Medal of the Polish Chemical Society (2003), and Gold Plaque of the Slovak Academy of Sciences (1998).

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Nominee for Bureau

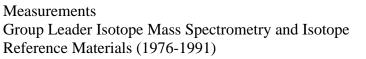
Paul De Bièvre (Belgium)

Education

PhD at Gent University (Belgium) 1959 Assistant, then Lecturer at Gent University 1959-1961

Professional Experience, Membership, and IUPAC Activities

Central Bureau for Nuclear Measurements (1961-1998) of the European Commission, called since 1993: Institute for Reference Materials and



Division Head, Adviser on Reference Materials (1991-1998) Adviser on Traceability (1994-1998) Adviser on "Metrology in Chemistry" (1998-2001)

Head of the Unit "Stable Isotope Measurements" at IRMM

(1991-1998).

Professor Antwerpen University (1972-1998) on Stable Isotope M.ass Spectrometry

Member, IUPAC International Commission on Atomic Weights and Isotope Abundances ICAW (1971-...), then CAWIA (...-...), now CIAAW (2001-...)

Chairman, IUPAC Subcommittee on the Assessment of the Isotopic Composition of the Elements SAIC (1975-1983) evaluating our present knowledge of the isotopic composition of the elements.

Member of the IUPAC Subcommittee on Isotope Abundance Measurements SIAM

Member of the IUPAC TICE project (Table of Isotopic Composition of the Elements)



Paul De Bievre

Member IUPAC Inorganic Division Committee (1985-1993)

Founder, then Chairman, then Member IUPAC Commission on Isotope-specific Measurements as References (in Div II) (1989-1998)

Project Leader of the IUPAC Project on 'Metrological Traceability of Measurement Results in Chemistry' (2001-...)

Chairman Annual Meeting of responsibles of European Nuclear Analytical Laboratories in the European Research and Development Association (ESARDA) (1976-1996).

Founder of the Regular European Interlaboratory Measurement Evaluation Programme (REIMEP) (1977) (the first Metrological International Interlaboratory Comparison for U and Pu measurements)

Founder & Chairman Joint European Project for Primary Isotopic Measurements (JEPPIM) (1998-...)

Member IAEA Advisory Groups on "Reference Materials for the Nuclear Fuel Cycle" and on the "Quality of Safeguards Measurements"

Member of the International Scientific Advisory Committee of the Belgian Nuclear Research Centre (SCK/CEN) in Mol and President of the Departemental Advisory Committee "Nuclear Chemistry and Fuel Cycle" at the same Centre (1988-1997)

President of the Belgian National Committee on Pure and Applied Chemistry of the Belgian Academies (1988-2005). Leader of the Belgian Delegation to IUPAC (1988-2005)

Member of the Comité Consultatif pour la Quantité de Matière (CCQM)) of the "Comité International des Poids et Mesures" (CIPM) at BIPM (1995-...)

Delegate of ISO/REMCO to CCQM (at BIPM)

Founder of the International Measurement Evaluation Programme (IMEP) (1986) (the first non-nuclear Metrological International Interlaboratory Comparison); IMEP programme leader 1988-1998

Co-founder of EURACHEM (1989); Chairman EURACHEM (1993-1995)

Co-founder (1992) and Member CITAC (Co-operation on International Traceability in Analytical Chemistry).

Founder of the Nuclear Signatures International Measurement Evaluation Programme (NUSIMEP) (the first Metrological International Interlaboratory Comparison for nuclear environmental measurements)

Editor-in-Chief "Accreditation and Quality Assurance" (SPRINGER Verlag) - Journal for Quality, Comparability and Reliability in Chemical Measurement (1996-...)

Member of the External Scientific Audit Team of the MiC Programme of the Physikalisch-Technische Bundesanstalt (PTB), the National Metrology Institute of Germany (July 2002),

both in Braunschweig and Berlin

External Adviser on Metrology in Chemistry in Mexico, Australia, Singapore, Chile, Brasil, Egypt, Japan, Slovenia, China, Croatia, (1996-...), Thailand

Member of the Council Committee on Reference Materials REMCO to ISO in Genève (1986-2005) (incl Chair Steering Group I: International Coordination & Harmonization)

Member of the Joint Committee on the Guides for Metrology at the BIPM (Bureau International des Poids et Mesures) in Paris, carrying out the revision of the "International Vocabulary of Basic and General Terms in Metrology" (1998-...)

Member of the Technical Advisory Group TAG 4 on Metrology to ISO (2001-...)

Over 400 published papers in all of the above fields.

Promotor of 10 PhD theses on Metrology in Chemistry by citizens of Belgium, France, Luxemburg, Germany, Hellas, Brasil.

Education & Training seminars on Metrology in Chemistry or VIM in Sydney (AU), Koebenhavn (DK), Zagreb (HR), Moskva (RU), Quito (EC), Singapore (SG), Maribor & Ljubljana (SI), Tallinn & Tartu (EE), Sao Paulo (BR), Helsinki (FI), Stockholm (SE), Teddington (UK), Santiago de Chile & Antofagasta (CL), Vilnius (LT), Praha (CZ), Warszawa (PL), Bratislava (SK), Beijing (CN), Al Qahera (Cairo, EG), Tel Aviv (IL), Torino (IT), Queretaro (MX), Daejon (KR in 2005), Bangkok (TH) (2004 & 2005), HongKong (HK) (2005)

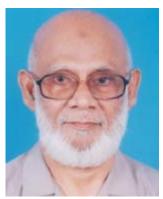
Adviser to the Journal of the Chinese Mass Spectrometry Society (2003-...)

43rd IUPAC Council Meeting

Nominee for Bureau

Abu Jafar Mahmood (Bangladesh)

Professor Abu Jafar Mahmood, president of the Bangladesh Chemical Society, has more than four decades of experience in the teaching and practice of chemistry. His research interests comprise chemical kinetics, photochemistry, surface chemistry and catalyst characterization, polymer chemistry, renewable energy sources, and environmental chemistry. Currently his major



Abu Jafar Mahmood

research emphasis is on zinc oxide mediated degradation by visible light of a number of reactive dyes used by the fabric dyers of the country. This process holds promise for removing residual dyes from factory effluent.

Education and Career

Mahmood received M.S. degrees from the University of Dhaka in 1960 and from the University of Leeds in 1965, and a Ph.D. from Cambridge University in 1972. He joined the Department of Chemistry at Dhaka as a teaching fellow in 1961 and has continuously served the department ever since. He was chairman between 1988–1991 and recently from June 2002 to January 2005.

Mahmood has produced 60 papers that were either published in national and international journals or presented at conferences, seminars, and symposia at home and abroad. In addition, he has supervised a large number of M.S. and some Ph.D and M.Phil. students.

Related Professional Activities

Mahmood has been elected as a lifetime member of numerous organizations: Bangladesh Chemical Society, Bangladesh Association for Advancement of Science, Asiatic Society of Bangladesh, Physical Society of Bangladesh, Bangla Academy, and Catalysis Society of India. In addition, he is a fellow of the Royal Society of Chemistry (London) and is a Chartered Chemist. Mahmood has played a leadership role in organizing many chemistry conferences in Bangladesh. Most recently he was chairman of the Organizing Committee for the Bangladesh Chemical Congress 2004. He was also chairman of the Organizing Committee for the National Workshop on Pesticide Residues, held in January 2003.

Since 2003, Mahmood has been editor of the Dhaka University Journal of Science, and since 1999 he has been one of the editors of (and contributors to) Bangla Academy Biggan Bishwakosh (Encyclopedia of Science in Bangla).

He has also held advisory or leadership positions on numerous committees and projects. From 1990–1997 he was chairman of the sectional committee on "Fine Chemicals" of the Bangladesh Standard Institution. In 1990, he worked out a plan of collaboration and formally signed a memorandum of agreement between Lamar University in Beaumont, Texas, USA, and Dhaka University for collaborative research in specific areas of chemistry. In 2000, he visited Utsunomiya University in Japan and initiated its collaboration with Dhaka University.

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43rd IUPAC Council Meeting

Nominee for Bureau

Stanislaw Penczek (Poland)

Professor Penczek's research activities have focused on kinetics, thermodynamics, and mechanisms of the polymerization processes, as well as on the synthesis of new polymer structures. Among his many accomplishments was establishing identical reactivities of ions and ion-pairs in cationic ring-opening polymerization at a time when the



Stanislaw Penczek

paradigm of higher reactivity of ions (free) was generally accepted as a dominating viewpoint. He also applied for the first time in macromolecular chemistry, dynamic NMR for studies of the ultra fast reactions of exchange between various ionic forms of active species. In addition, he developed a new general method of synthesis of soluble, highly branched (star shaped) polymers by catalytic reaction of macromolecular alcohols with bicyclic compounds (e.g., diepoxides) and methods of synthesis of simple, high molar mass phosphodiester chains with identical repeating units as in nucleic acids and teichoic acids.

Education and Career

Since 1974, Penczek has been a professor and head of the Department of Polymer Chemistry at the Polish Academy of Science in Lodz. He received his Ph.D. in 1963 from the Industrial Polymer Institute (Warsaw and Leningrad) of the USSR Academy of Science. From 1964–1968, Penczek was head of the Industrial Polymer Institute at the Laboratory of Polymerization. From 1966–1967, he was a post-doctoral fellow under Prof. M. Szwarc at Syracuse University, New York, USA.

Penczek has been a visiting professor at nine universities in Europe and the United States. He has given invited lectures at 80 international meetings and made over 290 printed contributions, including 8 monographs and textbooks and 15 chapters in books and monographs.

IUPAC Involvement

Penczek was a titular member of the Macromolecular Division from 1998–2001 and has been an associate member of IUPAC since 2002. He was also chairman of the World Polymer Congress 2000—38th IUPAC International Symposium on Macromolecules. He has also been chairman of two, and co-chairman of four, international symposia sponsored by IUPAC.

Related Professional Activities

In 1998, Penczek was elected a member of the Polish Academy of Science. He is also a longstanding member of the Polish Chemical Society, of which he served as chairman of the Division of Kinetics (1978–1988) and chairman of the Polymer Division (1988–1998). From 1997–1999 he was president of the European Polymer Federation and in 1993 he was a titular professor of the French Academy of Science.

Penczek is a member of the editorial boards of 11 international polymer journals, and is co-editor of e-Polymers, the first fully electronic polymer journal.

Awards

Over the course of his career, Penczek has received numerous honors: awards from the Polish Academy of Science (1974, 1985, 1988, 1989); Medal of the University of Jena (1988); M. Sklodowska-Curie Prize (1990); Medal of the French Academy of Science (1993); Chevalier dans l'Ordre de Palmes Académiques, France (1998); Biannual International Award of the Belgian Polymer Group (2001); Eminent Professor of RIKEN, Japan (2001); International Award and Personal Medal of the Society of Polymer Science, Japan (2002); Otto Warburg Foundation Award, Germany (2003); and the Biannual M. and P. Curie Joint Prize of the French and Polish Chemical Societies (2004). Penczek is Doctor of Honoris Causa of the University Pierre and Marie Curie in Paris (2003) and of the Russian Academy of Sciences (2004). The same year he was given a title of honorary professor of the Jagiellonian University in Krakow (Poland).

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Nominee for Bureau

Elsa Reichmanis (USA)

Dr. Reichmanis' research interests include the chemistry, properties, and application of materials technologies for photonic and electronic applications, with particular focus on polymeric and nanostructured materials for advanced communications technologies

Education and Career

Reichmanis is Bell Labs fellow and director of the Materials Research Department at Bell



Elsa Reichmanis

Laboratories, Lucent Technologies. She received her Ph.D. and B.S. degrees in chemistry from Syracuse University, and joined Bell Labs in 1978 after completing a post-doctoral fellowship program.

IUPAC Involvement

Reichmanis has been active in IUPAC throughout her career. She was a member of the U.S. National Committee for IUPAC for six years and has served on the U.S. delegation to the IUPAC General Assembly three times. She has been active in the Macromolecular Division of IUPAC, having served a term as a titular member.

Related Professional Activities

In 2003, Reichmanis was president of the American Chemical Society (ACS). She is past-chair of the ACS Polymeric Materials Science and Engineering Division and has served as a member of the executive committee of the division since 1986. She is a member of the ACS Committee on Science and has served on the ACS Publications Committee and the Chemical and Engineering News Editorial Board, and is associate editor of the ACS journal Chemistry of Materials.

In other technical capacities, Dr. Reichmanis has served as a

member of the Japanese Technology Evaluation Program Panel in Advanced Materials, the U.S. National Research Council (NRC) Committee to Survey Materials Research Opportunities and Needs for the Electronics Industry, and the NRC Committee on Policy Implications on International Students and Postdoctoral Scholars in the United States. She is also a former member of the NRC National Materials Advisory Board. Currently, she serves on the NRC Board on Chemical Sciences and Technology.

Awards

Reichmanis has received numerous awards, including the 1993 Society of Women Engineers Achievement Award. She was elected to the U.S. National Academy of Engineering in 1995 and named Bell Laboratories Fellow that year. She was the 1996 recipient of the ASM Engineering Materials Achievement Award, and was elected Fellow of the American Association for the Advancement of Science in 1998. She was awarded the 1999 ACS Award in Applied Polymer Science, the 2001 Society of Chemical Industry Perkin Medal, and the Arents Medal from Syracuse University. In 2004, she was elected as a Foreign Member of the Latvian Academy of Sciences. She is also a member of the American Physical Society, the Materials Research Society, the Institute of Electrical and Electronics Engineers, and the Society of Photo-optical Engineers.

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43rd IUPAC Council Meeting

Nominee for Bureau

Ivan Schopov (Bulgaria)

Education

1952-1958, M.Sc. Dipl. Eng. - Higher Institute of Chemical Technology, Sofia, Bulgaria

1968, Ph.D. - Institute of Organic Chemistry, Bulgarian Academy of Sciences

1982, D.Sc. - Institute of Organic Chemistry, Bulgarian Academy of Sciences



Ivan Schopov

Command of Languages: Bulgarian, English, German, French, Russian- fluently

Professional Experience

1958-1971, Research Fellow, Institute of Organic Chemistry, Bulgarian Academy of Sciences 1971-1983, Senior Research Fellow, Institute of Organic Chemistry, Bulgarian Academy of Sciences 1984-, Professor, Institute of Polymers, Bulg. Acad. Sciences

1989-2003, Director, Institute of Polymers, Bulgarian Academy of Sciences

Research Activities

Areas of Research Interests

- -Synthesis and structure properties relationship in conjugated polymers;
- -New synthetic methods in polymer chemistry carbonyl-olefin exchange reaction;
- -New electrically conductive polymers; Polymers for fuel cells membranes

Publications

More than 120 papers and 23 patents in the above fields

Visiting Professor

1983, 1990, 1993, 1994: Institute of Organic Chemistry, Free University, Berlin, Germany 1992: Institute of Organic Chemistry, Technical University

of Graz, Austria

1995: Max Planck Institute of Polymer Research, Mainz, Germany

Membership in Scientific Committees

since 1965 - member, Bulgarian National Symposia on Polymers (every 3 years)

since 1990 - President, Bulgarian National Symposia on Polymers (every 3 years)

1998, 2000, 2002, 2004 - member, International Conference of the Chemical Societies of the South-Eastern European Countries

1994, 1996, 1998, 2001, 2003, 2005 - member, European Polymer Federation Symposia on Polymeric Materials, European Polymer Congress 1995, 1997, 1999, 2003, 2005 - member, International Symposia on Macromolecule-Metal Complexes

Membership

since 1971 - member, Société Française de Chimie since 1992 - member, American Chemical Society since 1992 - President, Bulgarian Polymer Society since 1999 - President, Union of Chemists in Bulgaria

IUPAC Activities

1991-1993, 2002- National Representative on the Macromolecular Division

European Activities

1992-1995, National Coordinator of Programmes PECO, Copernicus 1999-2002, Programme Committee Member and National Contact Person, Improving Human Potential, Fifth Framework Programme of EU 2003, Programme Committee Member, Human Resources and Mobility, Sixt Framework Programme of EU

Plenary and Invited

Lectures on International Meetings and Seminars

Polymer Meetings: 1974 Leipzig, Germany; 1975 Frenstadt, Czechoslovakia; 1977 Varna, Bulgaria; 1977 Vilnius, USSR; 1984 Merseburg, Germany; 1988 Bucharest, Rumania; 1989 Potsdam, Germany; 1990 Gargnano, Italy; 1990 Pyongyang, North Korea; 1991 Lucerne, Switzerland; 1992 Hilton Head, USA;1994 Potsdam, Germany; 1995 Nancy, France; 1996 Agia Pelagia, Crete, Greece; 1997 Leipzig, Germany, 1998 Halkidiki, Greece; 1999 Calcutta, India; 2001 Zlatibor, Yugoslavia

Seminars at Universities and Research Institutes Austria (1988 Vienna, 1992 Graz); Czechoslovakia (1977

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Prague); China (1988 Beijing, Tianjin); Germany (1973, 1983, 1990, 1993, 1994 Berlin, 1981 Bremen, 1983 Freiburg, 1983, 1987, 1995, 2001 Mainz, 1985 Teltow, Dresden, 1994 Hamburg); Greece (1981 Thessaloniki, 1990 Iraklion, Athens); Japan (1986 Tokyo, Wako, 1988 Tsukuba, Osaka, Tokyo); Poland (1977 Warsaw); Spain (2003 Madrid); Thailand (1988 Bangkok); USA (2002 New York); Yugoslavia (1986 Belgrade).

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43rd IUPAC Council Meeting

Nominee for Bureau

<u>Alan Smith</u> (United Kingdom)

For more than 30 years, Dr. Smith has held leadership positions in the chemical industry. Most of his career was spent with Laporte, but he also worked for BDH/Merck for and started a consulting company.

Education and Career

Smith gained his B.Sc. (Hons.) in chemistry at Queen Mary College, University of London in 1965, during which time he had his first



Alan Smith

publication while still an undergraduate. He stayed on there and in 1968 received a Ph.D. in physical organic chemistry. He was then awarded a NATO Postdoctoral Fellowship for two years (1968–1970) and spent the first year on research into heterocyclic chemistry at the Technical University in Delft, Netherlands. The second year was spent in the School of Pharmacy, Nottingham University.

He joined the staff of the University of East Anglia (1970–1972), where he lectured and carried out research for the International Institute of Synthetic Rubber Producers. From 1972 to 1987, he worked at Laporte, during which time it became a leader in specialty chemicals. As Head of Research and Development, he had worldwide responsibilities for Laporte's technology, and he also looked after their laboratories for Interox, Laporte's joint venture with Solvay.

From 1987 to 1991, he was on the Board of BDH/Merck in the UK, where he was technical director and ran their Advanced Materials Business. From 1991 to 1996, he returned to Laporte as the head of Group Technology, with responsibilities for worldwide technical matters, especially relating to their extensive program of acquisitions.

In 1996, he set up AZTECH Consultancy, which advises on

scientific technical matters and acquisitions and mergers, and included the post of part-time technical director for BIP, Ltd. He is currently actively involved in UK government projects, the main one is their initiative on nanotechnology. He also carries out roadmapping strategies for the South African government.

IUPAC Involvement

Smith is a titular member of the Committee on Chemistry and Industry, which he has been a part of since 1994. From 1995 to 1999, he was on the Editorial Advisory Board for Chemistry International. He is also a titular member of the CHEMRAWN Committee, which he has been a member of since 1998. From 1997 to 2001, Smith was a delegate for the UK's National Committee, and in 2001 he was chairman of the UK delegation. Since 2002, he has been a member of the Bureau and a member of the Project Committee. He is also currently chairman of the Future Actions Committee for the Chemistry for Water CHEMRAWN conference held in Paris in 2004.

Related Professional Activities

Smith served on the Chemical Industry Association's Science, Education, and Technology Committee from 1986 to 1996. He is past president of the Industrial Affairs Division of the Royal Society of Chemistry, and is also on the following RSC committees: Annual Conference Committee, Innovation Team Award Committee, and the Research Fund Committee. He is a member of the Industrial Advisory Boards for Chemistry at Imperial College and Bristol University, and lectures at the University of Strathclyde and Nottingham University. He was on a CBI task force to obtain industrial input for the next Research Assessment Exercise for UK universities. He is on the Board of the latest Faraday Partnership on Colloids, established by the UK Government. From 1995 to 1999, he was on the Chemicals Panel of the Government's Foresight exercise. From 1999 to the present, he has been on the Materials Panel, and continues to lecture extensively on foresight. He is a fellow of the Royal Society of Chemistry and a fellow of the Linnean Society.

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43rd IUPAC Council Meeting

Nominee for Bureau

Maria C.E. (Rietje) van Dam-Mieras (The Netherlands)

Since 1993, Professor Maria C.E. van Dam-Mieras has been chair of Natural Sciences at the Open University of The Netherlands in Heerlen. In this position and other leadership roles, her activities have involved higher education in sustainability and globalization, chemistry curriculum in secondary education, biotechnology, environmental science, and knowledge transfer.



Maria van Dam-Mieras

Education and Career

Prof. van Dam-Mieras studied biochemistry and inorganic chemistry at the University of Utrecht in The Netherlands and received her Ph.D. from the same university in 1976. She started her academic career at the Limburg University in Maastricht, where her research was focused on blood coagulation and vascular pathology.

In 1983 she joined the Faculty of Natural Sciences at the newly founded Open University of The Netherlands in Heerlen, where she developed course materials in biotechnology, pollution prevention, and sustainable development. Also she was involved in several research programs of the European Union (COMETT, TEMPUS, PHARE, and SOCRATES). In 1992 she was appointed to the chair of Natural Sciences at the Open University.

In 1996, van Dam-Mieras became rector of the Open University. In 1997, she was appointed chair of the Copernicus Task Group of the European Association of University Rectors. The work of the Task Group led to the formation of "Copernicus-campus," a network of European Universities dealing with the role of higher education in sustainability and globalization. From 1995-2001 she was a member of the Scientific Advisory Board of the "Deutsches Institut für Fernstudien Forschung" at the University of

Tübingen in Germany. In 2000, she became a member of the Supervisory Board of the Institute of Environmental Science of the University of Antwerp in Belgium, and since 2003, she has been a member of the Board of Trustees of Lüneburg University in Germany.

IUPAC Involvement

Prof. van Dam-Mieras is a member of the joint ad-hoc Committee for IUPAC of the Royal Netherlands Chemical Society (KNCV) and the Royal Netherlands Academy of Sciences. Since 2003, she has been a board member of the KNCV and was previously president elect, president, and immediate past president.

Related Professional Activities

From 1998 until 2003 van Dam-Mieras was a member of the national "Scientific Advisory Council for Government Policy" in The Netherlands. Since 1997 she has been a member of the Board of Commissioners of the "Akzo Nobel Nederland" concern. In 2000 she joined the Board of Trustees of the Dutch organization TNO (Applied Scientific Research) and since 2001 has held a position on the societal advisory board of the Division on Chemical Sciences of the organization NWO (Netherlands Scientific Research). In 1995 she was a member of the working group that developed the outline for the new natural sciences program in Dutch Secondary Education, and since 2002, has been a member of the working group developing the outline for a new chemistry curriculum in secondary education. Since 2003, she has been chairperson of the Dutch-Flemish Association of Science Centres.

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Report on the General State of the Union

Introduction

According to the Union's statues (S6.23) the "President shall submit to each regular meeting of the Council a report on the general state of the Union." The accurate meaning of the words "general state" is not evident, but it is natural that this report takes into account the contents of two related reports presented at this meeting, *viz.* the Secretary General's report which focuses on the administrative aspects of the Union (agenda item 7), and the Vice President's Critical Assessment (VPCA), which this time contains a most thorough review, assessment, and analysis of our project system (agenda item 11). The "general state" of the Union should therefore be assessed with the Union's stakeholders in mind.

IUPAC's stakeholders constitute an extremely complex group of people, nations, regions, governmental institutions, professional societies as well as national, regional and international organizations. Within this group there are significant differences in the understanding of chemistry and the awareness of the needs for and the purpose of chemical products, secure handling of chemicals, and chemical management. As a result the Union has to be sensitive and responsive to

- formal requests and expectations from its members,
- professional expectations from the scientific community,
- adequate requests and questions from practicing chemists,
- regulations and legal aspects in societies at different levels of development,
- curious as well as biased questions from lay people and the general public,
- unarticulated needs caused by natural processes, accidents, and disasters involving chemicals.

Thus, the general state of the Union should be judged on the basis of the organization's ability

- to maintain an active, fruitful and democratic interaction between its leadership (at all levels) and its membership,
- to disseminate the results of the scientific and educational activities as well as conclusions reached in discussions related to science policy,
- to address and get engaged in important global issues, which involve application of chemistry in the service of Mankind.

Interaction with the members

The abilities summarized above are certainly interdependent; our contributions in solving global issues require efficient dissemination of the results of our activities, which again rests on transparent and efficient communication within the organization. But in this context, at the Council meeting, it makes sense to focus on the two first items, where the NAOs play an important role.

The interaction and communication within the Union were of significant concern at the General Assembly (GA) in Ottawa in August 2003, but in spite of the ideas and proposals put forward in the discussion there, the improvements in the internal interaction have been minor in the current biennium. It is still true that the written correspondence with the National Adhering Organizations (NAOs), which is an important part of the formal structure of the

Union, is characterized by a low reply percentage. It is still true that when all NAOs are contacted by mail regarding a matter of importance to the Union, it is rare to receive more than five replies. It is also true that when all the NAOs are asked and encouraged to nominate national representatives to various groups, the feedback is usually not much better. Therefore, it is still true that although IUPAC's officers are consulting the Union's members for advice, very few people are in fact involved in the decision-making process.

This democratic deficit is of course regrettable in itself, but it also hampers the scientific work of the Union. Experience shows that chemists are more likely to engage in IUPAC activities and projects when they feel included and are well informed about what is going on in the Union. Consequently, IUPAC will only be able to fulfil its objectives and live up to global expectations if the relationship with all NAOs is characterized by active involvement and creative interaction. In my honest opinion that is far from the case yet, so in this perspective the general state of the Union leaves quite a lot to be desired.

Two concrete matters support this conclusion. At the GA in Ottawa two measures were proposed and gained support, viz. a national contact from each member country to each of the eight divisions should be appointed, and a new body, named the Union Advisory Committee (UAC), should be formed with one member chosen by each NAO. The idea with the national contacts was that they will be informed by mail about the work being done in the Division to which they belong, and have the right to give feedback to the relevant Division Committee. This interaction should improve the quality of the work carried out in the divisions, and help to disseminate the results of IUPAC's scientific work. In addition this arrangement should give chemists from all member countries IUPAC experience that may, eventually, lead to an elected position in the organization.

As for the UAC, the idea was and still is that UAC will give each member country a direct role to play in the governance of the Union. Without the UAC the NAOs have limited opportunity to influence Union policy since the Council meets only every two years. Furthermore, the Council delegates are often new to IUPAC and unfamiliar with the issues before the Council meeting. The existence of the UAC gives an opportunity for greater continuity because its members would become familiar with the issues facing IUPAC since they would see all the material provided to the proposed Executive Board and would be asked to advise and provide comments on policy aspects of issues being considered.

Appointment of UAC members was solicited from all the NAOs, and by January 1st 2005, almost all member countries had appointed their members. The members have been kept informed by e-mail of selected matters being considered by the Executive Committee, and several significant issues have been referred for comments, assessment, and feedback. To say that the response from the committee members has been good, would be an exaggeration, although the reply frequency has been more than twice of that achieved regularly when comments are solicited from the NAOs and is increasing. The UAC has therefore not yet become the instrument within the organization that the committee could and should have, but when it has, I am sure the general state of the Union will have improved.

On several occasions representatives from various NAOs have said to me that they would like to discuss bigger issues at the Council meeting. I agree, that could be both interesting and very useful, but at the same time I believe that the format of the Council meeting and the size of the audience make such discussions too difficult to manage. That was in fact an important reason for establishing the UAC. I therefore urge the NAOs to raise such issues either through their UAC representative, or via the President, or through the IUPAC Secretariat, so that

important challenges recognized by the NAOs can become part of the IUPAC agenda. Such interactions will absolutely improve the general state of our Union.

Dissemination

Within IUPAC the importance of interaction and communication with the global chemical community has been recognized for some time, and it has been realized that extensive internal exchange of ideas and opinions is required if the Union is going to reach its goals. But that does not imply that the Union has experienced such a situation; in fact, in my critical assessment (presented in Ottawa in August 2003) it was pointed that we have challenges and a long way to go before we can be satisfied.

Some improvements have been made during the current biennium. It has been encouraging to see that *Chemistry International* (CI) continues to develop in the right direction and has become increasingly interesting (partly due to talented use of colors). The range and diversity of topics have grown, and this development has contributed to increase the impact of *CI*. There is no doubt that the chemical community, also outside IUPAC, views the magazine as more informative and more useful than before. However, there is room for improvements; for instance, more information about on-going projects will definitely attract readers if the presentations are of good quality.

Furthermore, the frequency of the *e-News* has increased and so has the quality. Many of the news pieces are such that they can be used more or less directly in national news magazines. This news service is therefore a considerable resource for the NAOs, but so far it is fairly little utilized. I therefore urge the NAOs to follow the *e-News* and extract material for use in the national magazines for the benefit of the national chemical community.

Finally, the brochures, which a few years ago suffered from a somewhat dubious reputation, have partly been overhauled. Rewriting and design brush-up have made the appearance more attractive and the contents far more relevant. This, combined with the fact that the material has been more broadly distributed, at conferences and meetings and to the chemical industry, seems to have contributed to improve the profile of IUPAC.

Conferences

The biennial IUPAC Congress and a large number of IUPAC symposia and conferences are well established as an important and authoritative means of communication with the global chemical community. However, with the exception of the former, the IUPAC profile has traditionally been rather low at most of the other meetings. With the improved brochures and posters being developed by the IUPAC staff (in interaction with the appropriate people), the Union has become better prepared to inform about its activities and results. This should be utilized to promote IUPAC better and increase the organization's visibility at all IUPAC meetings. Perhaps it should be considered compulsory to include an IUPAC presentation, with focus on the scientific activities, in the program at all IUPAC-supported conferences; for instance could there be a session during the meeting, dedicated to discuss the need for standardization or critical assessment of quantitative data within the conference theme, or to explore if new, exciting scientific topics related to the conference theme and beyond, are about to emerge. I know some of the Divisions have tried this and been satisfied.

In a very short time the IUPAC Prize for Young Chemists has become an important award in chemistry. An important reason for this success is the solid reputation and the high standing IUPAC has globally. In order to further promote IUPAC and chemistry, the IUPAC Poster Prize was established. The prize consists of a diploma, which is given to the best posters (up to three) at one national meeting in each member country. The scheme is administered by the

NAOs, but so far very few NAOs have taken advantage of this opportunity. All NAOs are therefore urged to include the IUPAC Poster Prize in their national activity plan. That will indeed increase the profile of IUPAC and the standing of the Union and thus, the general state of IUPAC.

Public appreciation

Our societies are heavily influenced by media, and rating, standing and reputation have become important issues that have to be taken into consideration. In doing so we realize that the chemical enterprise suffers from a dubious public image; chemicals are associated with bad things happening to people and in the environment. The positive contributions from chemistry and chemical engineering on a daily basis, to society and every one of us, are barely publicized, in spite of the fact that these sciences are instrumental in feeding us, clothing us, housing us, and healing us.

This situation is an enormous challenge that industrial and chemical organizations and enterprises have made efforts to meet in the past and continue to meet today. IUPAC has also been involved, the idea being that IUPAC, with a global reputation of providing authoritative and unbiased information in the field of chemistry, would have added value and be regarded as more trustworthy than facts and figures furnished by others. In the current biennium a feasibility study entitled "Chemistry's Contributions to Humanity" was carried out. A task group with a wide membership was engaged, and the group interacted with all the NAOs and the UAC. Unfortunately, the conclusion was that IUPAC at this point in time is unable to carry through such a project at a reasonable cost. This is a situation I strongly regret, and in this perspective it is reasonable to conclude that the state of Union leaves a lot to be desired. But we are not going to give up, and we have to continue to work, with the "Subcommittee on Public Understanding of Chemistry" as the driving force.

Conclusion

If we are critical, this report shows that the general state of the Union can be improved to a considerable extent. More involvement from many NAOs is requested, but also more imagination from the leadership. Let us use this Council meeting to start the work that has to be done.

Bergen/RTP, June 2005

Leiv K. Sydnes President

Item 7: Report of Secretary General

According to the Statutes, the Secretary General "shall carry out the business of the Union as specified by the Council, by the Bureau, by the Executive Committee, or by the President, and be responsible for keeping its records and for the administration of the Secretariat". As this is my first report, I shall try to comment on all those aspects of IUPAC that impinge in particular on the Secretariat staff, and to give an overview of the developing policy areas. This might also be useful for those Council delegates attending their first meeting.

The Secretariat

The current staff consists of six persons, but since the last General Assembly there have been some changes. Laura Abernathy and Lucinda Kelly have resigned and been replaced by Erin Slagle and Enid Weatherwax respectively. Many members will already be familiar with both of these new staff members, through their particular roles. Also Fabienne Meyers has moved to Boston and continues her work for the Secretariat from an office generously provided by the Boston University Department of Chemistry, whose support is gratefully acknowledged. The management of the Secretariat continues in the very capable and experienced hands of the Executive Director, John Jost, who also carries a wide range of specialist administrative and financial tasks. In particular, since the last Council meeting, John has masterminded the introduction of the Manuscript Central submission and refereeing process for *Pure and Applied Chemistry*. Fabienne Meyers is responsible for all electronic publishing, and will guide the implementation of website improvements, following recommendations from the Committee on Printed and Electronic Publications (CPEP). However, the description of Electronic Publishing Manager does not adequately reflect the wide range of Fabienne's activities. Her role as editor in the transformation of *Chemistry International* will already be widely appreciated, and she is also largely responsible for a range of new brochures and publicity material. Fabienne is involved in many aspects of IUPAC work, including the Young Chemist and Young Observer awards programs. In conjunction with the Committee on Chemistry and Industry (COCI) and the relevant National Adhering Organizations (NAOs), Fabienne has initiated a pilot program to grant complimentary Company Associate status for one year to companies financially supporting IUPAC conferences. It is hoped that such companies would then see the benefit of this association with their NAO and IUPAC and continue the link and the subscription. Fabienne also administers, with efficiency and sensitivity, the operation of the project system, IUPAC's major work area. Paul LeClair continues to maintain and develop a wide range of databases that provide information about all those people who interact with IUPAC in any way. His contribution is no less valuable for being perhaps a little less visible to most members. Erin Slagle has taken over as the communications specialist and is also responsible for the administration of the conference sponsorship and financial support programs. Both of these programs are quite complex, and are characterized by a need for careful and discretionary handling: current discussions are seeking to clarify some ambiguous aspects. Linda Tapp and Enid Weatherwax smoothly handle a wide variety of administrative matters, the most visible of which are concerned with the monitoring of projects and their finances and the processing of financial claim forms. Despite an increasing array of tasks, the Secretariat continues to function well within its budget, and recent steps have been taken to build a more cohesive structure by giving each member a clearer idea of the overall operation. I should like to thank all the

Item 7: Report of Secretary General

Secretariat members for their capacity and dedication, and also their patience in helping to educate a new Secretary General.

The Project System

IUPAC's major output is generated by the Project System, through which the Union's unique global perspective can be put to work: modest amounts of money can be used to great effect through the efforts of many volunteers. As this is the major topic of the Vice President's Critical Assessment, I shall make just a few brief comments here about its operational process. Most projects are initiated through the activities of Divisions and Standing Committees, but can be submitted by anyone, anywhere in the world. Completion of the web-based form indicates those relevant Divisions and Standing Committees which are then able to comment on the merits of the proposal. External reviews are also sought. Frequently, a Division or Standing Committee commits its own budgeted funds to provide full support to a project. Larger or inter-Divisional projects are sent to the Project Committee for evaluation, and funding can then be compiled from Division or Standing Committee input as well as additional support from the Project Committee budget. There is also a project reserve fund at the discretion of the Secretary General and Treasurer, and this can also be called on as a last resort. The efficient operation of the Project System requires a great deal of cooperation from Divisions and Standing Committees to return frank and balanced responses to project proposal questions. Input from reviewers, both internal and external, is frequently mixed and contradictory, so an overall balance needs to be achieved. It is also important that successful applications are monitored by the leading Division or Standing Committee, so that projects can be completed in a timely manner. Clearly different Divisions and Standing Committees are able to generate different kinds of projects, and there are many opportunities still available to be developed. While there will always be the highly technical areas such as nomenclature and standardization of data, it is important that areas involving the educational promotion of chemistry, and the stimulus of newly emerging fields are not overlooked. As the Vice-President's Critical Assessment has focused extensively on the Project System, it can safely be assumed that this area will receive considerable attention during the next biennium to strengthen its benefit to worldwide chemistry.

Sponsorship of Conferences

Traditionally this is one of IUPAC's most important roles and results in much of its current visibility. It should be immediately clarified that IUPAC sponsorship is not financial, but simply an accreditation of quality. However, the granting of IUPAC sponsorship generally leads to an increase in attendees, and a concomitant increase in the conference revenue accruing to the host country. There are quite clear guidelines relating to both quality and the international character of a conference, but frequently the issues are not entirely clear cut. On the one hand, it is important that the quality remains high, while on the other hand there is value in being reasonably generous in the granting of sponsorship in order to raise the profile and influence of IUPAC. There are different categories of IUPAC conferences, as outlined on the web, in *Chemistry International* articles and in the guidelines on recently revised sponsorship application forms. The Union is seeking to maximize the impact of those conferences (category 1) promoted by Divisions and Standing Committees. These are the core "IUPAC conferences" as

Item 7: Report of Secretary General

opposed to other conferences that are just "sponsored by IUPAC". The initiation of prestigious IUPAC Poster Prizes for these core conferences should help to highlight the differentiation. Again, Divisions and Standing Committees can be proactive in promoting a good range of high-profile core conferences. It should also be noted that IUPAC Poster Prizes are also available to National Adhering Organizations for one national conference each year.

Financial Support of Conferences

This aspect of IUPAC support has undergone some change as a result of discussions at the Bureau meeting in October 2004. Typically for IUPAC, quite small amounts of money are involved to add value to a conference already adequately financed. There are two criteria for support, the provision of stimulus for scientifically emerging regions, and for very new developments in chemistry. Applications must be submitted in the first instance to the President of the most relevant Division. This will then be forwarded to the Secretariat for consideration by the Project Committee only if the Division seriously supports it. The Project Committee is currently discussing the suggestion that funding decisions be made only several times each year, so that comparative and competitive evaluations can be made for the allocation of limited funds.

The Company Associates Program

Through the Committee on Chemistry and Industry (COCI), the Union is making a concerted attempt to build stronger connections with the chemical industry. The Company Associates program is actually coordinated by the Secretariat on behalf of the various National Adhering Organizations (NAOs), who benefit directly in the funding provided by the Company Associates. Each Company Associate unit is USD450, of which USD50 go to IUPAC as an administrative fee, and the remaining USD400 are entirely under the control of the NAO. Funds derived in this way can then be used by the NAO to support Young Observer programs, provide support for young chemists to attend IUPAC conferences, or even to offset some or all of the annual dues.

The Affiliate Membership Program

This program has operated since 1986 to serve the needs of individual chemists who wish to be actively connected to the international chemical enterprise. Members come from major chemical nations as well as those which currently might lack strong official links to the rest of the chemical world through IUPAC. In addition to paid Affiliate Members, IUPAC sponsors a limited number of additional Affiliate Members, usually young chemists from scientifically emerging countries. In 2006, the fee will be increased from the current USD16 to USD20. This fee covers the cost of distributing *Chemistry International*, information about projects and recommendations, and a 25% discount on all IUPAC publications. Moreover, Affiliates are entitled to a 10% reduction of registration fees for many IUPAC sponsored conferences. Most countries that are involved in the program charge an extra amount to cover their local expenses.

The Union Advisory Committee

The Union Advisory Committee (UAC) has already been dealt with by the President in his report. However, I simply add that I should be very pleased to hear from any UAC member with any point of view that can help the Union be more effective in promoting wordwide chemistry.

Item 8: Recommendations on Nomenclature and Symbols

The recommendations approved by the Interdivisional Committee on Terminology, Nomenclature, and Symbols and published in *Pure and Applied Chemistry* in 2003, 2004, and through June 2004 are listed below.

Name and symbol of element of atomic number 110,

Pure Appl. Chem. 75(10), 1613-1615, 2003

J. Corish and G. M. Rosenblatt

Terminology for analytical capillary electromigration techniques,

Pure Appl. Chem. 76(2), 443-451, 2004

M.-L. Riekkola, J. A. Jönsson, and R. M. Smith

Definitions of terms relating to reactions of polymers and to functional polymeric materials,

Pure Appl. Chem. 76(4), 889-906, 2004

K. Horie, M. Báron, R. B. Fox, J. He, M. Hess, J. Kahovec, T. Kitayama, P. Kubisa, E. Maréchal, W. Mormann, R. F. T. Stepto, D. Tabak, J. Vohlídal, E. S. Wilks, and W. J. Work

Glossary of terms used in toxciokinetics,

Pure Appl. Chem. 76(5), 1033-1082, 2004

M. Nordberg, J. Duffus, and D. M. Templeton

Quantities, terminology, and symbols in photothermal and related spectroscopies,

Pure Appl. Chem. 76(6), 1083-1118, 2004

M. Terazima, N. Hirota, S. E. Braslavsky, A. Mandelis, S. E. Bialkowski, G. J. Diebold,

R. J. D. Miller, D. Fournier, R. A. Palmer, and A. Tam

Definition of terms related to polymer blends, composites, and multiphase polymeric materials,

Pure Appl. Chem. 76(11), 1985-2007, 2004

W. J. Work, K. Horie, M. Hess, and R. F. T. Stepto

Name and Symbol of the Element with Atomic Number 111,

Pure Appl. Chem. 76(12), 2101-2103, 2004

J. Corish and G. M. Rosenblatt

Terminology in soil sampling,

Pure Appl. Chem. 77(5), 827-841, 2005

P. de Zorzi, S. Barbizzi, M. Belli, G. Ciceri, A. Fajgelj, D. Moore, U. Sansone, and M. Van der Perk

Numbering of fullerenes,

Pure Appl. Chem. 77(5), 843-923, 2005

F. Cozzi, W. H. Powell, and C. Thilgen

PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION REPORT FIRST YEAR OF THE BIENNIUM 2004-2005

JUNE 2005

REPORT TO THE IUPAC BUREAU: MEETINGS IN BEIJING, P.R.CHINA, AUGUST 2005

Professor Ron D. Weir President, Division of Physical and Biophysical Chemistry

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I. Executive Summary and Highlights

Initiatives to promote projects from those working in the Biosciences subject area continued to be made during the biennium following the change in name of Division I in autumn 2000 to Physical and Biophysical Chemistry Division (PBPCD). A major international workshop on the Physical Chemistry of Bio-interfaces was held near Adelaide, South Australia 23–26 May 04 in series with the Seventh World Biomaterials Congress in Sydney, Australia 17-21 May 04. IUPAC was well represented with the Past President of Division I being one of the organisers of the workshop attended by the current President of the Division. Time was allocated for these two individuals to address the attendees about the IUPAC system that provides funding support for projects and to encourage their submission. The workshop was aimed at providing fundamental insights into topics such as interfacial forces and properties involved in protein/surface interactions and the molecular kinetics of drug delivery. It is clear that there is a need for standardisation of terminology and agreement on calibration protocols, both areas where IUPAC can play an important role as the catalyst. The workshop itself was very successful and we wait to see its success in encouraging IUPAC participation. One immediate result is the emergence of a TM nominee representing the field of biophysical chemistry.

The Division continues with its important work of **establishing databases in specific subject areas**. A significant advance has been achieved with one of our several projects on databases, namely that of the evaluated kinetic data for atmospheric chemistry by setting up a website at the University of North Carolina, USA, to mirror the parent site in Cambridge, UK. The site continues to attract some 4000 accesses per week and for the eleven of the publications that have resulted from this database to date, there have been 2599 citations in RED. A substantial number of downloads continues in areas of heterogeneous reactions, thermodynamic data and in guides to the data sheets. The positive spin off is being realised from the decisions taken at the Bureau meetings in Paris to locate all the databases at the University of North Carolina with service support from the IUPAC secretariat and maintenance from the Division. It is at the stage of submission of a project proposal that these matters are to be defined clearly.

The Division remains active with its **chemical thermodynamics** component. You will recall that as a result of the IUPAC restructuring beginning in 2002, the International Association of Chemical Thermodynamics [IACT] was set up. The IUPAC Council at its meeting in Ottawa in August 2003 granted the IACT Associated Organisation status within IUPAC. The IACT has held its biennial meeting, the 18th IUPAC International Conference on Chemical Thermodynamics, in Beijing, P.R. China, during August 2004 with an especially large attendance by scientists from within Asia, many not reachable when the ICCT Conference is held in Europe or the Americas. Topic areas included electrolytes and non-electrolytes, new materials, supercritical fluids, biological applications, medical applications, interfaces, molecular simulation, energetics, industrial thermodynamics and databases, and frontiers in thermodynamics.

The Division is contributing to the final stages of the revision of the Third Edition of the Green Book [Quantities, Units and Symbols in Physical Chemistry], through its membership in the ICTNS. The third edition is to be placed in whole or in part on the Web as well as to be translated into several languages. It is unfortunate that its publication has been delayed. For the biennium 2004-05, the Division has 28 projects underway, which include five nearing completion and seven interdivisional. This total of 28 compares with 35 for the 2003-04 biennium as the Division attempts to focus its efforts on fewer projects but with more financial support for each.

The initiative by the Division to establish the Advisory Subcommittee of 61 international distinguished scientists and engineers, some of whom are drawn from industry, is bearing fruit. The members of the subcommittee are listed on the IUPAC website and in the IUPAC Handbook (p29) and all are IUPAC Fellows. The role of the subcommittee is to serve as a sounding board for the Division Committee, suggesting areas that may by dealt with by the Division, drawing attention to the need for experimental protocols in specific subject areas, taking part in IUPAC conferences, and acting as one source of expert referees for IUPAC proposals. The immediate benefit realised from the subcommittee is the reduction of the period needed for the assessment of project proposals to a period of weeks rather than months. It is important to realise that the responsibility for leading and guiding the Division to include encouraging and supporting all its growing activities lies on the shoulders of a relatively few individuals,

who also have heavy responsibilities in their work place and who undertake IUPAC work for public service and service to their profession. The network created by the establishment of our Advisory Subcommittee has been helpful in this regard as well as by the IUPAC Secretariat. The membership of the subcommittee is to be reviewed biennially.

II. Activities of Division I within the IUPAC Framework and its Goals

In their totality, the projects of Division I embody all of the five long-range goals of IUPAC. Some projects support certain goals more strongly than other projects depending on the nature of the project. In terms of **leadership**, the Division continues to exert a strong role through the Interdivisional Committee on Terminology, Nomenclature and Symbols. Its current major project is the production of the new edition of the Green Book, whose influence is very significant in education, research, industry, and publishing through the world. The Division's work with the Chemical Education Committee serves both goals of **leadership** and **chemical education**. Its projects through the International Association of Chemical Thermodynamics promotes connections to **chemistry-related industry** via workshops, **communications** among individuals and the addressing needs of chemistry and applied chemistry in **developing countries** via the rotation of conferences to include these countries with special financial incentives to assist attendance. Several of the Division's current projects are devoted to **advancing research in the chemical sciences** via international **standardisation**, while simultaneously promoting **scientific discussion**.

Scientific **leadership** is further realised by the Division's IUPAC-sponsored projects. One excellent example is the introduction of thermodynamic networks that is changing the way evaluated data will be obtained in the future where experimental redundancies exist. In those cases, a thermodynamic parameter such as the standard heat of formation of an intermediate of transient molecular species may be deduced using different experimental data from various experimental methods. Consistent thermodynamic networks will minimise the individual errors and optimise the fit to all existing data at the same time. The formalism is in the process of being worked out and applied in the near future. Specific examples are the free radical projects 2001-015-1-100 (Standard potentials of radicals) (see Sections III A 3 and IV A 3) and 2003-024-1-100 (Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment) (see Sections III A 12 and IV A 12). It is clear that this procedure applies to "mature" fields where there is large bank of existing data.

The creation of the 61-person Advisory Subcommittee has **broadened the membership base** of the Division significantly with a geographic balance and with an attempt to address the gender and age imbalance.

III. Project List with Updated Progress Reports

This section contains the list of all projects underway together with their current brief progress reports. These include the 16 Current Projects, the five projects nearing completion, the seven other interdivisional projects and the single project in review at the time of preparing this report. The funds awarded for support to the 17 current projects amount to \$205.7k, which compares with the Divisional budget of about \$55k. The large difference has originated from the IUPAC Projects Committee.

PROJECT LIST WITH UPDATED PROGRESS REPORT

A. CURRENT PROJECTS

1. 1999-016-3-100 - Recommendation for the use of AFM in the direct measurements of colloidal forces

This project for the use of the Atomic Force Microscope (AFM) is nearing completion. The manuscript was submitted July 2004 to the IUPAC ICTNS, is accepted for publication and is in the final stage for printing. The abstract of the paper follows by J. Ralston, I. Larson, M.W. Rutland, A.A. Feiler, and M. Kleijn.

The atomic force microscope (AFM) is designed to provide high-resolution (in the ideal case atomic) topographical analysis, applicable to both conducting and non-conducting surfaces. The basic imaging principle is very simple: a sample attached to a piezoelectric positioner is fastened beneath a sharp tip attached to a sensitive cantilever spring. Undulations in the surface lead to deflection of the spring, which is monitored optically. Usually a feedback loop is employed which holds the spring deflection constant and the corresponding movement of the piezoelectric positioner thus generates the image. From this it can be seen that the scanning AFM has all the attributes necessary for the determination of surface and adhesion forces: a sensitive spring to determine the force, a piezo electric crystal to alter the separation of the tip and surface, which if sufficiently well-calibrated also allows the relative separation of the tip and surface to be calculated. One can routinely quantify both the net surface force (and its separation dependence) as the probe approaches the sample, and any adhesion (pull-off) force on retraction. Interactions in relevant or practical systems may be studied and, in such cases, a distinct advantage of the AFM technique is that a particle of interest can be attached to the end of the cantilever and the interaction with a sample of choice can be studied, a method often referred to as colloid probe microscopy. The atomic force microscope, or, more correctly the scanning probe microscope, can thus be used to measure surface and frictional forces, the two foci of this article. There have been a wealth of force and friction measurements performed between an AFM tip and a surface, and many of the calibration and analysis issues are identical to those necessary for colloid probe work. We emphasise that this article confines itself primarily to elements of colloid probe measurement using the AFM.

2. 1999-037-2-100 - Evaluation of kinetic data for atmospheric chemistry

The objectives of this project are to enhance the accessibility and availability of the evaluated kinetic database, to develop and implement a way to update material on the website to include various linkages and the creation of a mirror website at IUPAC in North Carolina. All the data sheets for reactions of Ox, HOx, NOx, SOx, organic reactions, the inorganic halogen reactions, and most of the inorganic halogen reactions have now been added. Additional supplementary material has also been posted on the site. The remaining work includes data sheets for the halogen species, heterogeneous reactions and any updates created since June 2005. The current number of accesses is about 4000 per week with 370 subscribers to the mailing list for announcements, which represent an increase of 10% since 2003-04. The mirror site at UNC continues to be operational and is automatically updated when changes are made to the Master site in Cambridge, UK. For 11 of the publications that have flowed so far from this project, there have been 2599 citations in RED.

3. 2001-015-1-100 - Standard potentials of radicals*

The aim of this project is to evaluate critically the standard potentials of inorganic and organic radicals in the literature, to recommend values, and to identify reduction potentials for further experimentation.

Currently, one set of evaluations and seven summary tables have been prepared, including: Inorganic Standard Potentials, Gibbs Energies of Formation for Radicals, Inorganic Radical pK_a s, Hemicolligation Equilibrium Constants, Organic Standard Potentials, Radical Henry's Law Constants, and Inorganic Radical Equilibrium Constants. Linked to these tables are the 140 individual evaluation sheets. The Technical Report was accepted for publication in February 2005.

One particularly challenging task is to obtain a least-squares optimisation for a thermo-chemical network that links the properties of about 50 radicals, primarily inorganic. Evaluations are complete for about half of these radicals and a robust method has been developed for performing the least-squares optimisation.

4. 2001-028-1-100 - <u>Electrochemical impedance spectroscopy -</u> terminology, nomenclature and data exchange formats

The aim is to summarize, standardize and disseminate the nomenclature of fast developing new fields of application of electrochemical impedance spectroscopy. It seeks to standardize conventions of formats for experimental data exchange and analysis.

The work is complete and the paper written for two of the three items, namely the aspects of nomenclature and data exchange formats. The first

draft of the paper for terminology or definitions aspect resulted in 70 pages, which is currently being reduced to about 20 pages.

5. 2001-030-1-100 - Recommendations on the measurement and analysis of results obtained on biological substances with isothermal titration calorimetry

The aim is to prepare recommendations for measurement procedures for isothermal titration calorimetry applied to biological substances, the calibration procedures. The recommendations will include analysis and reporting of the results in order to facilitate universal comparability of ITC data from different laboratories.

Measurements are complete for a working standard NAD/NADH binding to a protein, lactate-dehydrogenase for checking the performance of isothermal titration calorimeters. The first draft of the report is will be complete by December 2005. The 'round-robin' ITC results from 12 laboratories on the binding of 4-carboxybenzene sulfonamide to carbonic anhydrase are complete and they are being evaluated for inclusion in the IUPAC Recommendations.

6. 2001-035-1-100 - <u>Measurement and interpretation of electrokinetic</u> phenomena

The aim is to prepare recommendations to standardize definitions of the different electrokinetic phenomena, names for the physical quantities, the use of the different experimental methods phenomena and the applicability of the various experimental techniques.

The Technical Report was accepted by the ICTNS on February 2005 for publication in PAC.

7. 2002-005-1-100 - Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems

The aims of this project are to initiate systematic studies of thermodynamic and thermo-physical properties of Ionic Liquids (IL) based on the needs of industrial chemical processes, to establish a reference system of IL's and (IL + liquid mixtures) with reliable stability and purity and well defined thermodynamic properties, and to define guidelines regarding where research activities and future cooperation should be directed.

At ten different laboratories around the world for the standard reference materials, extensive measurements have been completed for the viscosity, density, thermal conductivity, heat capacity, electrical conductivity, enthalpy of dilution, gas solubility at high pressure, and speed of sound over the temperature range from 238 K to 378 K. The target date for completion of all experiments is July 2005 and final report is anticipated July 2006.

8. 2002-063-1-100 - Chemical thermodynamics in industry

The book was published in September 2004 by the Royal Society if Chemistry, Cambridge. It contains 23 chapters that cover 276 pages.

9. 2003-005-1-100 - Recommended values of the viscosity of molten iron and aluminium

The aims of this project are to reach agreement about the equations used to determine the viscosity by the oscillating cup method, to review critically the widely different data that exist in the literature, and to recommend standard values to ne used by the international community.

The round-robin experiments have been completed and the goals of the work are realised. The final manuscript for this Technical Report and IUPAC Recommendation has been approved by ICTNS for publication in PAC and for submission to J Physical Chemical Reference Data.

10. 2003-006-1-100 - NMR chemical shifts: updated conventions*

The objectives are to update IUPAC Recommendations 2001: NMR Nomenclature, Nuclear Spin Properties and Conventions for Chemical Shifts [*PAC* 73, 1795 (2001)] by addressing several issues in setting standards for chemical shifts, including temperature variation of the NMR signals of reference compounds, the use of magic-angle spinning for both solutions and solids, solvent effects, and magnetic susceptibility corrections.

Fundamental measurements of the temperature variation of proton chemical shifts versus the signal for He-3 gas are complete and the manuscript is in draft form. The draft paper has also been prepared on shape factors for use with magnetic susceptibility corrections and on high-precision chemical shift measurements. These articles will form the backbone of the final IUPAC Report.

11. 2003-020-2-100 - Ionic liquids database

The aim is to create an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structure, properties, and uses.

The collection of data has been assigned among the seven participating laboratories along with the assignment of the development of the WEB outlet for the system and the storage and retrieval system. The database, storage and retrieval systems have been developed at the Thermodynamics Research Centre at NIST. These systems have been successfully deployed and are undergoing testing. The external launch is planned for December 2005 at which time the collection of data will be interfaced. A meeting of the Task Group is planned for Beijing, P.R. China in August 2005.

12. 2003-024-1-100 - <u>Selected free radicals and critical intermediates:</u> thermodynamic properties from theory and experiment

The objective of this project activity is the compilation and critical evaluation of published thermodynamic properties, including the computation of accurate thermo-chemical data for selected free radicals that are of importance in atmospheric and combustion chemistry.

A substantial part of the work has been completed and 12 papers have appeared or are in press during 2004-05. See Section IV below. Additional papers are being written as the work progresses. While the scope of this project was originally targeted to perform a systematic critical evaluation of the thermochemistry of important radicals, the scientific problems that are being encountered and formulated as the evaluation effort progresses, have become a unique *spiritus movens*, motivating ground-breaking research and development of new general methods. Thisis especially the case in the areas of electronic structure calculations (W3 and HEAT), and of dealing efficiently with complex interrelationships inherently present in thermochemistry (ATcT).

Given the fact that the funds originally allocated for this project are being utilized more slowly than planned, and that the scope of the project has expanded beyond the initial intent (both by expanding the target list of radicals and by developing new generalized approaches related to the needs of the project), the project requests a no-cost extension.

13. 2003-036-2-100 - <u>Thermodynamics and non-equilibrium criteria for development and application of supplemented phase diagrams</u>

The aim of the project is to establish rational links between thermodynamic aspects of phase diagrams supplemented by the non equilibrium curve of the glass transition temperature for mixtures of water with vitrifying agents used in the cryo- and dehydro- preservation of natural (foods, seeds, etc.) and synthetic products (pharmaceuticals).

The update and literature classification on supplemental phase diagrams for relevant aqueous systems for food and pharmaceuticals has been completed. The initial critical evaluation of this database to include the

shortcomings of current practice is to be finished by July 2005. The Technical Report is expected during December 2005.

14. 2004-010-3-100 - <u>Heat capacity of liquids: critical review and recommended values for liquids with data published between 2000 and 2004</u>

The aims are to update and to extend two publications that contained recommended data on liquid heat capacities for almost 2000 mainly organic compounds, "Heat Capacity of Liquids: Critical Review and Recommended Values", and its "Supplement I" by M. Zábranský, V. Ruzicka, V. Majer (1st work only), and E.S. Domalski published in *Journal of Physical and Chemical Reference Data* in 1996 and 2001. The publications were the product of IUPAC Projects 121/11/87 and 2000-031-1-100.

The new literature search has located about 150 papers that report results for calorimetric measurements of liquid heat capacities of about 300 compounds having their melting temperature below 573 K. The existing database for experimental results is being expanded to include these new results and will be complete during November 2005. Their critical assessment and correlation is expected to be complete by April 2006 and manuscript destined for J Physical Chemical Reference Data to be ready for ICTNS by September 2006.

15. 2004-026-2-100 - <u>Categorizing hydrogen bonding and other</u> intermolecular interactions

The aims are to provide a modern definition of the hydrogen bond by examining comprehensively the various intermolecular interactions in the light of all current experimental and theoretical information. Hydrogen bonded systems both in gaseous and condensed phases in chemical and biological systems will be examined.

The first meeting of the Task Group is scheduled for a workshop in September 2005, where all members will present a summary of their recent work.

16. 2004-036-1-100 - <u>Establishing recommended data on thermodynamic properties of hydration for selected organic solutes</u>

The objectives are to establish a database of thermodynamic properties of hydration for approximately 200 selected organic solutes at reference conditions of T = 298.15 K and 0.1 MPa and as a function of temperature and pressure up to the near critical region of water, to calculate from the reliable experimental data the values of hydration properties for solutes

covering different molecular structures, to use the established database as a standard for testing and deriving new physico-chemical models and methods of molecular simulation to include the development of semi-theoretical prediction schemes for chemical engineering, environmental chemistry and geochemistry.

The work has just begun.

* Interdivisional project

B. PROJECTS NEAR COMPLETION OR IN PRESS

1. 110/2/81 - Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition)

The objective is to revise the 2^{nd} edition of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices.

Progress: Its sole project the *Revision of the Green Book: Quantities, Units and Symbols in Physical Chemistry* consists of preparation of the third edition planned. The draft version was circulated at the GA held in Brisbane in 2001. No progress has been reported since that date.

2. 120/15/95 - Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies

The Technical Report describing this project has been submitted, reviewed and accepted by the ICTNS with recommended change in the organisation of the report to reflect both Recommendations and content of a Technical Report. The approved revised title is 'Thermochemistry of Chemical Reactions: I. Terminology and Symbols IUPAC Recommendation 2003, II. Experimental Methods for the Determination of Bond Energies IUPAC Technical Report'. The revisions are being incorporated and the project should be complete by the close of this biennium.

3. 120/16/97 - New Edition of Experimental Thermodynamics Vol II

The aim of this project is to prepare an updated version of Experimental Thermodynamics. The enormity of the task led to dividing it into two separate volumes. Volume VI appeared in 2003 and Volume VII is due out from the printer in late 2005 or early 2006.

Volume VI. Measurement of the Thermodynamic Properties of Single Phases

Editors: A.R.H. Goodwin, K.N. Marsh and W.A. Wakeham *published* - Elsevier, 2003 [ISBN 0-444-50931-3]

Volume VII. Measurement of the Thermodynamic Properties of Multiple Phases

Editors: Th. de Loos and R.D. Weir

The 16 chapters that make up the edition are in the hands of the production department of Elsevier Publishers. Some 24 authors from nine different countries contributed material. This book contains descriptions of recent developments in the techniques for measurement of thermodynamic quantities for multiple phases of pure fluids as well as mixtures over a wide range of conditions. The precision and accuracy of results obtained from each method was regarded as an essential element in each description. Throughout the text, the quantities, units and symbols are those defined by IUPAC for use in the international community. *Anticipated publication date*: late 2005 or early 2006.

4. 150/24/95 - <u>Spectroscopy under extreme conditions of temperature and pressure</u>

The objectives are to obtain international agreement on methods and standards and to prepare documents to guide workers in the field of spectroscopy under extreme conditions. Initially vibrational and electronic spectroscopy will be considered, but the project may be extended to NMR, Mossbauer, and other spectroscopies if the early work reveals interest in these areas. The main issues to be pursued come under the three general headings Instrumentation, Pressure Calibration, and Temperature Calibration. Instrumentation includes the consideration of cell design, the use of membranes with diamond anvil cells, the properties of optical windows under extreme conditions, the design of spectrometers and microscopes, the use of optical fibres for safe access to difficult experimental situations, and the simultaneous generation of high pressure and low temperature in an optical cell. The calibration issues include methods and standards for the calibration of hydrostatic and very nonhydrostatic pressures. Emphasis will be on calibration through the spectroscopic properties, with the intention to make recommendations in the final report of standard substances, inorganic, organic and biological, whose spectroscopic properties can be used for calibration and for establishing the performance of apparatus.

Progress:

A progress report has not been received and the status of this project is unknown.

5. 2000-026-1-100 - <u>Critical compilation of vapour liquid critical</u> properties

The objective is to review all measurements of vapour-liquid critical properties for pure organic compounds containing **nitrogen**, **halogen**(s), and **sulphur** and **silicon** and to recommend values for critical temperature, critical pressure and critical densities, with uncertainties.

To date, the project has resulted in eight review papers (Parts 1 to 8) published in the *Journal of Chemical and Engineering Data*. See Section IV below.

Part 9 (nitrogen compounds) has completed the IUPAC review process and will be submitted for publication in June 2005. Part 10 (halogen compounds) will be sent to IUPAC review in June 2005. Part 11 (miscellaneous compounds) is 95% written.

6. 140/6/93 - <u>Evaluated Chemical Kinetics Data for Combustion</u> <u>Chemistry</u>

This project ended formally several years and was coordinated by Don Baulch and Michael Pilling. It is appropriate at this point of this divisional Report to note that following a fairly long delay, the extensive article regarding the database for chemical reactions is about to be published by Journal of the Physical and chemical Reference Data.

C. OTHER INTERDIVISIONAL PROJECTS

- 1. 2000-012-1-300 Single molecule spectroscopy (Division III)
- 2. 2001-036-1-300 Glossary of terms in photocatalysis and radiation catalysis (Division III)
- 3. 2002-024-1-300 Glossary of terms used in photochemistry (3rd version) (Division III)
- 4. 2003-056-2-500 <u>Standard definitions of terms relating to mass</u> spectrometry (Division V)
- 5. 2004-005-2-500 <u>Comparable pH measurements by metrological traceability</u> (Division V)
- 6. 2004-035-1-100 A database of water transitions from experiment and theory (Division V)

7. 2004-021-1-300 - Reference methods, standards and applications of photoluminescence (Divisions III and V)

D. PROJECTS IN REVIEW

1. 2005-016-1- Solubility for Industry

* Interdivisional project

IV. PROJECT DESCRIPTIONS

This section contains a detailed summary of all projects currently underway.

A. CURRENT PROJECTS

1. Number: 1999-016-3-100

Title: Recommendation for the use of AFM in the direct measurements of colloidal forces

Task Group Chairman: John Ralston

Members: A.A. Feiler, R. Horn, I. Larson, M. Rutland, and J.M. Kleijn

Objectives: To recommend:

- Procedures for the measurement of the inter-particle distance dependence of colloidal force data using the atomic force microscope colloid probe technique
- Methods by which the force-distance data can be compared with existing models of inter-particle forces.

Description:

The colloid probe AFM technique is a promising new method to determine the interactions between colloidal bodies. The technique is based on the general AFM and this equipment is, in principle, available for many research groups (not excessively expensive). In order to avoid confusion in the literature about the use of the AFM equipment for colloid stability measurements (and consequently about the interpretation of

results) recommendations for the use of this equipment for this type of measurement are needed.

Project Contents:

- Principles of atomic force microscopy
- Attachment of colloidal probe to cantilever
- Force measurement Attachment of colloidal probe to cantilever
- Distance separation
- Determination of spring constant
- Determination of colloid probe radius
- Interaction geometry
- Inter-particle forces
- Non-deformable and deformable surfaces
- Symmetric and asymmetric interactions

Progress: Review/update published in <u>Chem. Int. Nov 2003</u> In July 2004, a technical report was submitted for publication in *Pure and Applied Chemistry*

Last Update: 12 July 2004

2. Number: 1999-037-2-100

Title: Evaluated kinetic data for atmospheric chemistry

Task Group Chairman: R.A. Cox

Members: R. Atkinson, J.N. Crowley, R.F. Hampson, R.G. Hynes, M.E. Jenkin, M. J. Rossi, and J. Troe

Remarks: Continuation and expansion of 141/3/89

Objective

The primary objective of this project is to enhance the accessibility and availability of the evaluated kinetic database, which has been assembled by the IUPAC Subcommittee for Gas Kinetic Data evaluation for Atmospheric Chemistry, by placing the material on an interactive site on the www. A second objective is to develop and implement a scheme for updating the material on the website.

Background

The IUPAC Subcommittee (formally the CODATA Task Group on Chemical Kinetics) was originally tasked to produce an evaluation of the existing chemical kinetics data in 1977, in response to the need to provide an internationally judged data set for modelling the depletion of

atmospheric ozone due to man made pollutants. Since that time the Subcommittee has continued to expand and update the evaluations to aid modelling of a wide range of issues involving Atmospheric Chemistry. The evaluations have been published in a series of nine peer-reviewed articles in J. Phys. Chem. Ref. Data. These articles contain two elements: Firstly a summary table which contains a list of recommended rate parameters giving the best available values for rate coefficients for use in models representing atmospheric chemistry explicitly as a system of elementary chemical reactions: Secondly each reaction is discussed in a separate data sheet, in which the key experimental data are summarised and the basis of the recommendation together with its uncertainty is given. These data sheets provide details that are of interest to atmospheric modellers and experimental scientists conducting investigations of kinetics and mechanisms of atmospheric reactions, and chemical kinetics generally. In order to further publicize the accessibility of this web-based material to the scientific community, the evaluation is also being published as a series of journal articles in Atmospheric Chemistry and Physics.

Description

In 1998 the IUPAC Subcommittee created a website at the Centre for Atmospheric Science in the Department of Chemistry, University of Cambridge, UK, (http://www.iupac-kinetic.ch.cam.ac.uk). This site has attracted very significant interest since its creation, and has now been expanded, and a mirror site has been created at the IUPAC HQ website in N. Carolina, US. Currently there are approximately 4000 connections to the website per week and over 370 subscriptions to the web mailing list for announcements.

The main purpose of the ongoing IUPAC project is to extend the content of the website to include the remaining datasheets for the 850 gas phase reactions, the photochemical reactions (absorption cross sections, quantum yields), and heterogeneous reactions (kinetic uptake coefficients for atmospheric gases on a range of surfaces), for which the data have been evaluated since the first publication by the Group in 1980. In addition to expansion, the website is continually being modified to give improved access, including a simple search facility and implemented hyperlinks between the summary table and the data sheets.

Progress: The database covers over 600 reactions relevant to the chemistry of the stratosphere and the troposphere. The data sheets are grouped in a series of categories that include:

1. Gas phase and photolysis reactions of Ox, HOx, NOx and SOx species.

- 2. Gas-Phase and photolysis reactions of organic species (including reactions with HOx, NO3 and halogen radicals.
- 3. Reactions of organic peroxy radicals, organic alkoxy radicals and other organic radicals with oxygen.
- 4. Gas Phase and photolysis reactions of inorganic FOx, ClOx, BrOx and IOx species.
- 5. Gas Phase and photolysis reactions of organic halogen species.
- 6. Uptake coefficients for non-reactive and reactive heterogeneous processes.

In the future the efforts of laboratory kineticists will continue to provide new data in response to new scientific and societal issues in the field of Atmospheric Chemistry. The IUPAC Group is seeking a more effective way of updating and extending the portfolio of recommended rate coefficients, which will be necessary to maintain an effective and ongoing communication between laboratory scientists and atmospheric modellers. The establishment of web-based material allows for the first time the opportunity of near continuous update of the evaluation. The development and implementation of protocols for the updating of the evaluation, both web-based and archived hard copy will also be carried out.

Publications listing (including latest supplements)

The number of citations are shown at the end of each entry and are in the sequence of the time history as follows: 3 Mar 2000/3 Nov 2000/16 Apr 2001/20 Nov 2001/19 Apr 2002/11 Jun 2003/16 Jun 2004/9 Jun 2005.

R.Atkinson, D.L.Baulch, R.A.Cox, J.N.Crowley, R.F.Hampson, Jr., R.G. Hynes, M.E. Jenkin, M.J. Rossi, and J. Troe, Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II - reactions of organic species, *Atmos. Chem. Phys.Discuss*, in open review (2005).

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R.Atkinson, D.L.Baulch, R.A.Cox, R.F.Hampson, Jr., J.A.Kerr, M.J. Rossi, and J. Troe, Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry; Supplement VIII, Halogen Species, *J. Phys. Chem. Ref. Data*, 29, 167-266, (2000). 0/0/1/7/12/37/57/74

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Atkinson R, Baulch DL, Cox RA, Hampson RF, Kerr JA, Troe J, Evaluated kinetic and photochemical data for atmospheric chemistry: Supplement III – IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry, INT. J. CHEM. KIN. 1989, Vol. 21, pp. 115-150 (only Summary Table). 44/46/47/48/49/50/50

R.Atkinson, D.L.Baulch, R.A.Cox, R.F.Hampson, Jr., J.A.Kerr, J.Troe, Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry; Supplement III, *J. Phys. Chem. Ref. Data*, 18, 521-1012, (1989). 491/504/510/516/519/534/557/565

D.L.Baulch, R.A.Cox, R.F.Hampson, Jr., J.A.Kerr, J.Troe, R.T.Watson, Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry; Supplement II, *J. Phys. Chem. Ref.Data*, 13, 1259-1380, (1984). ?/?/?/?/292/296/300

D.L.Baulch, P.J.Crutzen, R.A.Cox, R.F.Hampson, Jr., J.A.Kerr, J.Troe, R.T.Watson, Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry; Supplement I, *J. Phys. Chem. Ref.Data*, 11, 327-496, (1984). ?/?/?/?/385/393/401

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Last Update: 11 November 2004

3. Number: 2001-015-1-100

Title: Standard potentials of radicals

Task Group Chairmen: David M. Stanbury

Members: D. Armstrong, J. Butler, R. E. Huie, W.H. Koppenol, Sergei V. Lymar, G. Merényi, Pedi Neta, S. Steenken, and P. Wardman

Objective:

To evaluate critically the standard potentials of inorganic and organic

radicals in the literature, to recommend values, and to identify reduction potentials for further experimentation.

Description:

Radicals play an important role in many chemical transformations. There are presently two fields where more detailed knowledge of the thermodynamic properties of radicals would be extremely useful. The first is biomedicine. The discovery of superoxide dismutase and nitrogen monoxide as a messenger has led to an explosive growth in articles in which one-electron oxidations and reductions are explored. Organic radicals play an important role in the treatment of cancers. The other is atmospheric chemistry where modelling of reactions requires accurate reduction potentials. There are presently two compilations (1,2) which are now both more than ten years old and in need of updating. We plan to compile new data that has been published since 1989, set up a thermodynamic network and develop in this fashion values for standard potentials that are internally consistent. Per radical we will prepare a data sheet as found in the JANAF tables. The relation of a particular radical to neighbouring (+/- one electron) stable compounds will be shown in oxidation state diagrams. We will start with radicals for which accurate data are known in water and then extend our studies to radicals that have been studied in organic solvents, or for which only estimated data are available.

References

(1) Stanbury, D.M. (1989) Reduction potentials involving inorganic free radicals in aqueous solution. *Adv. Inorg. Chem.*, **33**, 69-138.

⁽²⁾ Wardman, P. (1989) Reduction potentials of one-electron couples involving free radicals in aqueous solution. *J. Phys. Chem. Ref. Data*, **18**, 1637-1755.

Progress:

Feb 2005 - So far, a set of evaluations and seven summary tables have been prepared, including: Inorganic Standard Potentials, Gibbs Energies of Formation for Radicals, Inorganic Radical pK_a s, Hemicolligation Equilibrium Constants, Organic Standard Potentials, Radical Henry's Law Constants, and Inorganic Radical Equilibrium Constants. Linked to these tables are the individual evaluation sheets. At present we have prepared about 140 evaluation sheets.

One particularly challenging task is to obtain a least-squares optimization for a thermo-chemical network that links the properties of about 50 radicals (primarily inorganic). We have completed evaluations for about half of these radicals and found that we have a robust method for performing the least-squares optimization.

Last update: 24 February 2005

4. **Number**: 2001-028-1-100

Title: Electrochemical impedance spectroscopy – terminology,

nomenclature and data exchange formats

Task Group Chairman: Z. Stoynov

Members: C. Brett, M. Orazem, and J. Vogelsang

Objective:

The aim of this project is to summarize, standardize and disseminate the nomenclature of fast developing new fields of application of electrochemical impedance spectroscopy. It is also targeted to standardizing conventions of formats for experimental data exchange and analysis.

Description:

The IUPAC recommendations "Impedances of electrochemical systems: terminology, nomenclature and representation. Part I. Cells with metal electrodes and liquid solutions" M. Sluyters-Rehbach (*Pure Appl. Chem.*, **66** (1994) 1831-1891) covered the basic knowledge of the field. Since that time electrochemical impedance (often now known as Electrochemical Impedance Spectroscopy (EIS)) has been developed very actively and now a large variety of systems are investigated by this method. In addition, new types of impedance analysis are being developed - multiple transfer function analysis, local impedance measurements, differential impedance analysis etc.

Many scientists from many different fields - chemistry, physics, biology, materials science, corrosion - are now using EIS as a research tool owing to the ready availability of instrumentation. This is made clear through the success of the triennial series of symposia on Electrochemical Impedance Spectroscopy (the 5th held 17-22 June 2001 in Italy with 200 participants). It is important that conventions and a common data format are implemented in order to facilitate application and understanding of electrochemical impedance data by scientists with different backgrounds and training, including for dissemination through Internet and Virtual Laboratories. These conventions should include: programming of the experiments and obtained data, recommended algorithms for data preprocessing and analysis, and representation of final numerical and graphical results. Such guidelines are important for the chemistry community as a whole.

It is expected to incorporate these recommendations in future ISO standards. A working group has already been formed for this purpose regarding the application of impedance to measurement of the effectiveness of organic coatings (ISO DC35 SC9 WG29, chairman J. Vogelsang).

Progress:

Last update: 11 September 2001

5. **Number**: 2001-030-1-100

Title: Recommendations on the measurement and analysis of results obtained on biological substances with isothermal titration calorimetry

Task Group Chairmen: Frederick P. Schwarz and Hans-Jurgen Hinz

Objective: Recommendations for isothermal titration calorimetry measurement procedures on biological substances, calibration procedures, and procedures for testing the performance of isothermal titration calorimeters (ITCs) with a biological test solution are described. Recommendations for the analysis and reporting of the results will be presented to facilitate universal comparability of ITC data from different laboratories.

Description:

Isothermal titration calorimeters (ITCs) have been widely used in the biotechnological and pharmaceutical industry and in academia to determine the thermodynamics of binding reactions of biological substances, including DNA-DNA, DNA-RNA, protein-protein, protein-ligand, and DNA-intercalating drug interactions. ITCs monitor the power exchanged between a reference vessel and a solution vessel as aliquots of a titrant solution are injected into the solution vessel, isothermally. The change in enthalpy, binding affinity, and the stoichiometry for the binding reaction are obtained from an analysis of the power exchanged per each injection and the total concentrations of the reactants in the solution vessel. In addition, the temperature dependence of these quantities can be determined in terms of a heat capacity change for the binding reaction. Thus, the thermodynamics of the binding reaction can be completely characterized over a wide temperature range.

Published results sometimes lack a systematic reporting and analysis of the data and often employ a variety of notation inconsistent with IUPAC recommendations. An important aspect of this project is the fabrication of a test solution for determination of ITC binding data. ITC test solutions will be distributed to members of the working party to run in their ITCs so that a consensus set of binding data can be developed on a particular system under a specified set of operating conditions. This consensus data can then be used to determine if a particular ITC is being operated properly. This is particularly important for new and in-experienced researchers employing ITC for the first time. The results will also be shared with the MIRG committee of the Association of Biomolecular Research Facilities (ABRF). MIRG is involved in evaluating how well binding affinities determined by ITC, Biacore SPR, and Ultra-analytical centrifugation are in agreement.

Progress:

Last update: 20 November 2002

6. Number: 2001-035-1-100 (previous 160/5/98)

Title: Measurement and interpretation of electro-kinetic phenomena

Task Group Chairmen: F. Gonzalez-Caballero and Á. Delgado Mora

Members: A.S. Dukhin, S.S. Dukhin, K. Furusawa, C. Grosse, R.J. Hunter, R. Jack, M. Kaszuba, L.K. Koopal, M. Kosmulski, J. Lyklema, R. Noremberg, V. Ribitsch, V.N. Shilov, F. Simon, C. Werner, A. Zhukov, and R. Zimmerman

Objective:

- Discuss the various electro-kinetic phenomena and give recommendations on the use of the different techniques.
- Discuss briefly the theories of electro-kinetic phenomena.

Description:

Collect and spread the available and updated scientific information about the main electrokinetic phenomena. This includes:

- fundamental background and clarification of notions used in electro-kinetics
- discussion of theoretical models, with emphasis on the validity and usefulness of the various models
- critical evaluation of experimental methods with their ranges of applicability and limitations (electrophoresis, streaming potential/current, electro-osmosis, dielectric dispersion, electroacoustics)

- description of model systems that can be used as standards for each technique
- elucidation of the physicochemical information that can be obtained from the use of a given method and the corresponding theoretical models

Progress:

The project was first discussed in the Electro-kinetic Phenomena Conference held in Salzburg (1998). A significant number of specialists in the field agreed to contribute and sent their chapters to the coordinator during 1999-2000.

A meeting of the Task Group took place during the Electro-kinetic Phenomena Conference in Dresden, October 2000. The discussion made clear that the project is ambitious with many difficulties that have to be settled. After the workshop, written comments were sent to the coordinator by several members of the task group and a preliminary list of recommended symbols was produced. Restructuring of the draft has been demanding and the second draft was completed just before the GA in Brisbane (July 2001).

A final period is required to produce a document that gives balanced guidelines for the use of electro-kinetic methods and the correct interpretation of the results. There is a

This project was presented at a <u>poster session</u> at the IUPAC Congress/GA July 2001 ><u>view pdf - 95KB</u><

large number of electro-kinetic techniques that all need attention including their theoretical background (which is complicated even for ordinary surfaces).

The 3rd draft will be prepared before July 2002. The working party will meet at the EKP Conference, August 2002, in Cracow (Poland) to discuss the progress and advise on open questions. A final draft is planned for end 2002, resulting in a technical report to be submitted to *PAC*.

Last update: 29 August 2001

7. **Number**: 2002-005-1-100

Title: Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems

Task Group Chairman: Kenneth N. Marsh

Members: Joan F. Brennecke, Michael L. Frenkel, Andreas Heintz, Joe W. Magee, Cor J. Peters, Luis P.N. Rebelo, and Kenneth R. Seddon

Objective:

- 1. To initiate systematic studies of thermodynamic and thermophysical properties of Ionic Liquids (IL) based on the needs of industrial chemical processes.
- 2. To establish a reference system of IL's and (IL + liquid mixtures) with reliable stability and purity and well defined thermodynamic properties.
- 3. To define guidelines which research activities and future cooperation should be directed to.

Description:

Ionic liquids (IL's) represent a new class of liquid solvents having the character of molten salts. Recently synthesised compounds are moisture, air and temperature stable. Their melting points are distinctly below room temperature. Most of these IL's consists of cations such as different Alkyl-Imidazolium or Alkyl-Pyridinium ions and anions such as BF_4^- , PF_6^- , $N(CF_3SO_2)_2^-$, $CF_3SO_3^-$. Chloroaluminate anions are also important provided moisture can be excluded. A large number of ionic combinations is possible for designing special properties.

IL's have gained large interest during the last years. They have no detectable vapour pressure and therefore exhibit an ideal system of solvents for new homogeneous catalytic reactions and other chemical production processes with respect to a "green chemistry". An increasing number of successful applications are described in the literature. The utilization of IL's in industrial chemistry requires a systematic study of their thermodynamic and thermo-physical properties that are of considerable interest for chemical process design. The most important properties are:

- a) solubilities of gases in IL's
- b) miscibility gaps of organic liquids and water with IL's
- c) densities, activity coefficients and excess properties of
- IL + organic substances (or water) mixtures
- d) viscosities, diffusion coefficients, and electric conductivities of IL + organic substance (or water) mixtures
- e) There is also a strong interest in IL's from the side of theoreticians dealing with statistical mechanical theories and/or computer simulation methods of concentrated electrolyte solutions.

There have been a number of workshops and special sessions at conferences on ionic liquids but they have been specifically directed towards their use as solvent systems for chemical reactions with emphasis on kinetics and homogeneous organometallic catalysis. There has been minimal emphasis on thermo-physical property information.

Three workshops are planned to be held within a period of 3-4 years. Each workshop (2 days) should include at least 4 invited lectures, short oral and poster contributions, and a panel discussion. The aim of the workshop series is to stimulate the discussion and cooperation concerning items a) to e) between chemical engineers, thermodynamicists, organic chemists active in the research field of IL's and those who are dealing with IL's in technical and industrial applications. Standardized IL's and IL + liquid mixture should be developed which can be used as reference systems.

Progress:

Last update: 15 November 2004

8. Number: 2002-063-1-100

Title: Chemical thermodynamics in industry

Task Group Chairman: T.M. Letcher

Members: Theo de Loos, John Dymond, and Ron Weir

Objective:

To bring to the attention of a wide audience, the pivotal role that Chemical Thermodynamics plays in the Chemical Industry of the 21st century.

Description:

The book is to be written for chemical engineers and industrial chemists, agencies and groups that fund chemical research, and research students and general chemists.

Draft outline

- 1. Multi-phase thermodynamics of pulp suspensions scale-up and reactor design with thermochemical models (combining reaction rates with Gibbs energy models)
- 2. Use of multi-phase thermodynamics in slag metallurgy and steelmaking
- 3. Metastable coating structures in PVD-coatings

- 4. Properties of nano-size particles by using multi- phase thermodynamics
- 5. Distillation (more in particular reactive distillation) (Arlt, Germany)
- 6. Thermo properties from *ab initio* quantum chemistry (Sandler, USA)
- 7. Molecular modelling (Cummings, USA)
- 8. Bioseparations/downstream processing (Van der Wielen, Holland)
- 9. Fine particle production (Reverchon, France)
- 10. Polymer synthesis in ScFl's (Beckman, USA)
- 11. Sustainability (De Swaan Arons, Holland)
- 12. Ionic liquids (Heintz, Germany)
- 13. Reactions in ScFl's (Eckert, USA/Poliakoff, UK)
- 14. Polymer recycling (Kleintjens, Holland)
- 15. Non-equilibrium thermo (Ratkje, Norway)
- 16. Process simulation
- 17. Non-classical critical phenomena (Sengers/ Anisimov, USA)
- 18. Self-ordering systems
- 19. CO₂ sequestration
- 20. Clathrates (Dendy Sloan)
- 21. Reactive Distillation
- 22. Molecular Thermodynamics (Prausnitz)
- 23. Thermodynamic Properties of new materials (Manfred Martin, Aachen)
- 24. Thermodynamic Properties of Polymers for Industry (Ralf Dohrn, Bayer, Germany)
- 25. Thermodynamic Properties of Mixing for Industry (Chris Wormold, Bristol)
- 26. Calorimetric Measurements for Industry (Jean-Pierre Grolier, U of Blaise Pascale)
- 27. Flow Microcalorimetry measurements and Industry (Tony Beezer, U of Greenwich)
- 28. Transport Properties and Industry (Bill Wakeham or Hartmut Brueschke, Germany)
- 29. Viscosity of Refrigerants in Industry (Bill Wakeham)

Progress:

Last update: 29 January 2003

9. **Number**: 2003-005-1-100

Title: Recommended values of the viscosity of molten iron and aluminium

Task Group Chairman: W.A. Wakeham

Members: Marc Assael, Michael Banish, Ivan Egry, Ken Mills, Akira Nagashima, Tony Overfelt, Peter Quested, John Redgrove, and Yuzuro Sato

Objective:

The widely different data obtained for the viscosity of molten iron and aluminium will be critically reviewed via an inter-laboratory comparison and recommended values will be proposed.

Description:

Wide ranges of values of viscosity of both molten iron and aluminium are reported in the literature. The most widely used method is some form of oscillating vessel. For the oscillating cup a number of analytical techniques have been used to convert the measurements (logarithmic decrement and time period) to viscosity.

The Roscoe equation (1958) was recommended as providing the most accurate data for molten metals. Ferriss *et al* (2002) have pointed out there is a missing numerator in one of the expansions and a number of workers and standard texts have quoted "1/2" but expansion shows it to be "3/2".

In a parallel development chemical engineers have adopted a set of equations for oscillating cup viscometers by Kestin and Newell, which have been rarely used for molten metals.

There are two challenges:

- 1. Agreement about the equations used to determine the viscosity by the oscillating cup method. At present the modified Roscoe equation by Ferriss and the Kestin and Newell appear to give similar results with one laboratory's data.
- 2. The widely different data obtained for the viscosity of aluminium and iron need to be critically reviewed and recommended values suggested. This may result in the need for an inter-laboratory comparison.

The project should lead to a consistent, internationally approved set of values for the viscosity of these two metals, as an exemplar for the field.

- Roscoe, R (1958), *Proc. Phys. Soc.* **72**, 576
- Ferriss, D H; Quested, P N; Chapman, L A; and Day, A P (2002) "The Choice of Equations for the Measurement of Viscosity by the Oscillating Cylinder Method". Presented at ECTP, London. Kestin, J and Newell, GF (1957) ZAMP VIII, 433

Progress:

The available experimental data for the density and viscosity of liquid aluminium and iron have been critically examined with the intention of establishing a density and a viscosity standard. All experimental data have been categorized into primary and secondary data according to the quality of measurement specified by a series of criteria. The proposed standard reference correlations for the density of the aluminium and iron are characterized by standard deviations of 0.65 and 0.77% at the 95% confidence level respectively.

A full report is being prepared and will be submitted for publication in *JPCRef Data*.

Last update: 19 April 2005

10. Number: 2003-006-1-100

Title: NMR chemical shifts: updated conventions

Task Group Chairman: Robin K. Harris

Members: Edwin D. Becker, Sonia M. Cabral de Menezes, Pierre Granger, Roy E. Hoffman, and Kurt Zilm

Objective:

To update IUPAC Recommendations 2001: NMR Nomenclature, Nuclear Spin Properties and Conventions for Chemical Shifts [*PAC* 73, 1795 (2001)] by addressing several issues still to be resolved in setting standards for chemical shifts, including temperature variation of the NMR signals of reference compounds, the use of magic-angle spinning for both solutions and solids, solvent effects, and magnetic susceptibility corrections.

Description:

Nuclear magnetic resonance [NMR] has long been an invaluable technique for determining molecular structure and for investigating a wide variety of chemical phenomena. The cornerstone of such applications is the *chemical shift* - a quantity that must be measured relative to an agreed reference. For many years, common practice [endorsed by IUPAC in the 1970s] was to use a separate reference for each nuclide. However, as a result of the above-cited publication, IUPAC is now on record as recommending that chemical shifts for all nuclides be expressed on a unified scale relative to the proton [¹H] resonance of tetramethylsilane [TMS] in a 1 per cent solution in CDCl₃. Since its publication only a year ago, this recommendation has been well received by the international NMR community; has been widely disseminated by republication in NMR

journals and presentations at NMR conferences, as detailed below; and has been publicized by one of the three major NMR equipment manufacturers.

The IUPAC publication in 2001 included extensive tables of data on NMR properties, chemical shift values of secondary references for each nuclide, and detailed explanations of factors affecting measurements of chemical shifts. However, in the interest of bringing that work to closure and publishing the Recommendations, the task group was forced to defer detailed consideration of several important matters:

- The temperature dependence of the primary standard, TMS in CDCl₃, should be established on the basis of data in the literature and possible new measurements.
- Changes of solvent or concentration are known to have major effects on chemical shifts. These effects should be evaluated for selected systems by use of an external reference, physically separated from the sample being studied.
- An external reference, in turn, requires correction for effects of the magnetic susceptibility of the sample. Methods for measuring magnetic susceptibility and applying the correction in a reliable manner must be analyzed.
- The use of magic-angle spinning [MAS] can, in principle, eliminate the need for magnetic susceptibility corrections, but this method must be evaluated more carefully.
- MAS is widely used for the study of solids. IUPAC has thus far made no recommendations for referencing in solids, a matter that should be rectified.
- Various conventions have been suggested in the literature for shielding and/or chemical shift tensor parameters, and a preferred nomenclature needs to be decided on and recommended.

This project is designed (1) to solicit the views of a broad segment of the relevant NMR community on these and possibly other important matters to be addressed, and (2) to bring together a task group of experienced NMR spectroscopists to analyze the theory and literature data, make experimental measurements where feasible, and prepare a Recommendation that will extend and broaden IUPAC's previous statements.

Progress:

(1 May 2005)

Following a Discussion Forum held during the International Meeting on NMR organised by the Royal Society of Chemistry in Cambridge (England) in the summer of 2003, each of the six task group members was assigned one of the relevant topics and was asked to prepare a briefing paper on it. Progress has been made with all of these, with comments

sought from all members of the task group and from some other experts in the field. The task group concluded that for several areas - temperature variation of chemical shifts, shape factor for magnetic susceptibility correction, and solvent effects - new data or calculations would be needed.

In the case of temperature variations of chemical shifts, it was decided to undertake some new measurements with respect to the He-3 nuclide, and one of the task group members (Dr. Roy Hoffman) has been doing this. The funds supplied by IUPAC for the project sufficed to obtain the necessary helium-3 gas. Fundamental measurements of the temperature variation of proton chemical shifts (vs. the signal for He-3 gas) are now complete, and he has submitted a paper (with Dr. Ted Becker) on this topic for publication in an NMR journal (with acknowledgment of the IUPAC project). Draft papers have also been written on shape factors for use with magnetic susceptibility corrections (Dr. Hoffman) and on high-precision chemical shift measurements (Prof. Pierre Granger). It is intended to use these articles as reference material for the eventual IUPAC report on the project. The briefing paper on shielding tensors has been sent to several experts for comment before recommendations are drawn up and some responses have been received.

At the 46th Experimental NMR Conference, held in Providence (Rhode Island) 10-15 April 2005, four members of the Working Party held a discussion on the progress and future direction of the project. A synopsis for the final report has been agreed, but several matters need to be concluded before a full draft can be produced. It was agreed to add a short section on the vexed question of referencing for nitrogen chemical shifts (to be addressed by Dr. Sonia Cabral de Menezes). The need for new data and calculations has delayed completion of the overall project beyond the initial target date, but the quality of the resultant IUPAC document will be markedly improved by inclusion of these results.

Last update: 4 May 2005

11. **Number**: 2003-020-2-100

Title: Ionic liquids database

Task Group Chairman: K.R. Seddon

Members: <u>Andrew Burgess</u>, <u>Michael Frenkel</u>, <u>Marcelle Gaune-Escard</u>, <u>Andreas Heintz</u>, <u>Joseph Magee</u>, <u>Kenneth Marsh</u>, and <u>Roger Sheldon</u>

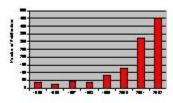
Objective:

Create an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including

their syntheses, structure, properties, and uses; lack of this information is impeding progress in a burgeoning field of significant current interest.

Description:

Ionic liquids are expanding dramatically in popularity (see inset figure), and the first industrial application (the BASF BASIL process) was announced at the end of March 2003. Crucial to their implementation on a wider scale (and these are green solvents) is



universal access to their physical properties. As there are potentially over one million simple ionic liquids (although fewer than one thousand have yet been reported), the need for a living database, with continuous updating is paramount. This project brings together some of the world leaders in ionic liquid technology with leading thermodynamicists and database technologists.

A task group, that wishes to work under the auspices of IUPAC, has been formed to address the need for international scientific cooperation to implement the design and development of a web-based free-access database for ionic liquids. Taken as a whole, the task group has acquired a critical mass to make the goal of this project a reality. The task group members represent broad interests by organisational type (academic, governmental, and industrial) and geographical location, as well as a wide range of expertise (measurement science, synthesis, enzyme catalysis, data management, structure, and industrial application). To the extent possible, sharing of data and exchange of proposed ideas among group members will be carried out electronically. A total of two in-person meetings of this group will be arranged, preferably around international conferences or at venues provided gratis by a host member's organization, such that expenditures will be held to an absolute minimum. Personal meetings will be used to iron out detailed issues that are crucial to the design of the database, and to divide the larger tasks into those that are more manageable.

The task group is expected to decide on the format of the new database, including its root language, its structure, and the means by which various information types will be stored and retrieved. Seven types of information will be compiled, namely: synthesis; structure; thermodynamic, thermochemical and transport properties; solvent properties and reactions; catalytic properties; and, reviews and bibliography. To ensure that a uniform assessment of each type of information is made, the task group chair will assign primary responsibility for each information type to subgroups. The task group chair will expect each subgroup to take responsibility to assess the available data for its quality and reliability, compile this data, and make regular reports to the full task group. Frequent

interchanges of information among subgroups will prevent repetition of work. Task group members will be expected to provide their own organisation's existing data holdings for the benefit of the project, according to their specialised knowledge and assets. To ensure compatibility of the information coming from various data sources, the output and input formats for each record will be agreed upon in advance. For example, NIST-Thermodynamics Research Centre will extract ionic liquid data for more than 120 properties from its SOURCE data archival system that currently contains over 1.3 million data points on over 17,000 substances and 12,000 mixtures. It is searchable by several means, including CAS registry numbers, chemical name or chemical formulae. In addition to property values in SI units, it stores estimated uncertainties for practically all the stored numerical data, citations of original documents, as well as detailed information about the samples such as their source, method of purification and final reported purity. This information derived from the original sources will contribute to the assessment of overall uncertainties of the data, and will facilitate reports of recommended values. Software has been prepared that will automatically extract ionic liquids data from the SOURCE system. Making this unique tool for automatic data evaluation available to this project will streamline the assessment and compilation of thermodynamic, thermo-chemical and transport properties of ionic liquids.

When each subgroup's data has been compiled into agreed-upon formats, the parts will be combined into a beta version of the entire database. It then will be tested by a wide range of users, whose comments will be solicited to improve the product. When the improvements have been implemented and tested, IUPAC Ionic Liquids Database version 1.0 will be released to the public. NIST will provide web space with a single-entry point for all users of this database, and provide the tools to measure usage and compile a monthly statistical report for the website. As part of an ongoing commitment, NIST will maintain this database on a NIST server and update its holdings on a regular basis. Our long-range operating plan, built upon continuous exchange and cooperation with both data generators and users, will streamline the process of adding new results and making further improvements better to serve the needs of the international chemistry community.

Progress:

Last update: 25 July 2003

12. Number: 2003-024-1-100

Title: Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment

Task Group Chairman: Branko Ruscic

Members: <u>Tibor Bérces</u>, <u>J. E. Boggs</u>, <u>A. Burcat</u>, <u>A. Császár</u>, <u>J. Demaison</u>, <u>R. Janoschek</u>, <u>J.M.L. Martin</u>, <u>M. J. Rossi</u>, <u>J. Stanton</u>, <u>P. Szalay</u>, <u>P.R.</u> Westmoreland, and F. Zabel

Objective:

The main objective of this project activity is the continued compilation and critical evaluation of published thermodynamic properties, including the computation of accurate thermo-chemical data for selected free radicals that are of importance in atmospheric and combustion chemistry. A distinguishing feature of the critical data evaluation is the systematic utilization of all available kinetic, spectroscopic and ion thermo-chemical results as well as high-level computations.

Description:

Knowledge of accurate thermo-chemical properties of free radicals is of great importance in many branches of chemistry, in particular atmospheric and combustion modelling. Thermo-chemical kinetic estimations provide sometimes the only possibility for obtaining rate coefficients and branching ratios for reactions of short-lived intermediates such as free radicals. Thermodynamic quantities for stable molecules are relatively well established. These are typically obtained from calorimetric determinations, while heat capacities and entropies are derived from the results of spectroscopic measurements. For free radicals and other shortlived intermediates, direct calorimetric measurements are (in most cases) not possible, while spectroscopic investigations require more skill and sophisticated instrumentation. Consequently, thermo-chemical data for a number of free radicals have a higher uncertainty than the corresponding values of closed shell species. However, computational chemistry has made great progress in reliability and accuracy. A solid basis of thermochemistry now comprises the optimized combination of experimental and computational results.

Such type of work has been initiated in our <u>IUPAC project 2000-013-1-100</u> which comes to a preliminary conclusion at the end of the year 2003. Within this project the critical evaluation of thermodynamic properties of 36 free radicals has been carried out.

The success of this work so far suggests an extension of data evaluation beyond the initial goal to cover an increased number of key radicals that play important part in atmospheric chemistry and combustion. This requires the development of datasheets for about 25 further radicals.

Progress: extension of project #2000-013-1-100

Last update: 21 October 2003

The following publications have appeared from this project.

W. M. F. Fabian and R. Janoschek

Thermochemical Properties of the Hydroxy-formyl Radical HO-CO, and the Formyloxy Radical, HC(O)O, and their Role in the Reaction OH + CO \rightarrow H + CO2: Computational G3MP2B3 and CCSD(T)-CBS Studies. *J. Mol. Struct. TheoChem* **713**, 227 (2005)

- P. G. Szalay, A. Tajti, and J. F. Stanton Ab Initio Determination of the Heat of Formation of Ketenyl (HCCO) and Ethynyl (CCH) Radicals. *Mol. Phys.* **103**, xxx (2005) *in press*
- B. Ruscic, J. E. Boggs, A. Burcat, A. G. Császár, J. Demaison, R. Janoschek, J. M. L. Martin, M. L. Morton, M. J. Rossi, J. F. Stanton, P. G. Szalay, P. R. Westmoreland, F. Zabel, and T. Bérces. IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals: Part I. *J. Phys. Chem. Ref. Data* 34, xxx (2005) *in press*
- X. Tang, Y. Hou, C. Y. Ng, and B. Ruscic Pulsed Field Ionization Photoelectron-photoion Coincidence Study of the Process N2 + hv \rightarrow N⁺ + N + e⁻: Bond Dissociation Energies of N₂ and N₂⁺ *J. Chem. Phys.* **123**, xxx (2005) *in press*

R. Janoschek and M. J. Rossi

Thermochemical Properties of Free Radicals from G3MP2B3 Calculations, Set-2: Free Radicals with Special Consideration of CH₂=CH-C=CH₂, *cyclo*-C₅H₅, CH₂OOH, HO-CO, and HC(O)O. *Int. J. Chem. Kinet.* **36**, 661 (2004)

- A. D. Boese, M. Oren, O. Atasoylu, and J. M. L. Martin W3 Theory: Robust Computational Thermochemistry in the kJ/mol Accuracy Range. *J. Chem. Phys.* **120**, 4129 (2004)
- B. A. Flowers, P. G. Szalay, J. F. Stanton, M. Kállay, J. Gauss, and A. G. Császár. Benchmark Thermochemistry of the Hydroperoxyl Radical. *J. Phys. Chem. A* **108**, 3195 (2004)

A. V. Marenich and J. E. Boggs

Vibrational Spectrum and Thermochemistry of the Formyl (HCO) Radical: A Variational Study by the Coupled Cluster CCSD(T) Method with Complete Basis Set Extrapolation. *J. Phys. Chem. A* **108**, 5431 (2004)

- M. Oren, M. A. Iron, A. Burcat, and J. M. L. Martin Thermodynamic Properties of C₁ and C₂ Bromo Compounds and Radicals: A Relativistic ab Initio Study. *J. Phys. Chem. A* **108**, 7752 (2004)
- B. Ruscic, R. E. Pinzon, M. L. Morton, G. Von Laszevski, S. J. Bittner, S. G. Nijsure, K. A. Amin, M. Minkoff, and A. F. Wagner. Introduction to Active Thermochemical Tables: Several "Key" Enthalpies of Formation Revisited *J. Phys. Chem. A* **108**, 9979 (2004)

B. Ruscic

Active Thermochemical Tables in: 2005 Yearbook of Science and Technology, McGraw-Hill, New York, 2004, pp. 3-7

P. G. Szalay, L. S. Thøgersen, J. Olsen, M. Kállay, and J. Gauss Equilibrium Geometry of the Ethynyl (CCH) Radical. *J. Phys. Chem. A* **108**, 3030 (2004)

A. Tajti, P. G. Szalay, A. G. Császár, M. Kállay, J. Gauss, E. F. Valeev, B. A. Flowers, J. Vázquez, and J. F. Stanton

HEAT: High Accuracy Extrapolated Ab Initio Thermochemistry. *J. Chem. Phys.* **121**, 11599 (2004)

A. G. Császár, M. L. Leininger, and A. Burcat Enthalpy of Formation of ${}^2\Pi_{3/2}$ SH. J. Phys. Chem. A **107**, 2061 (2003)

J. Demaison, L. Margulès, and J. E. Boggs Equilibrium Structure and Force Field of NH₂. *Phys. Chem. Chem. Phys.* **5**, 3359 (2003)

A. V. Marenich and J. E. Boggs

Structural and Thermochemical Properties of the Hydroxymethyl (CH₂OH) Radical: A High Precision Ab Initio Study. *J. Chem. Phys.* **119**, 10105 (2003)

A. V. Marenich and J. E. Boggs

Coupled Cluster CCSD(T) Calculations of Equilibrium Geometries, Anharminic Force Fields, and Thermodynamic Properties of the Formyl (HCO) and Isoformyl (COH) Radical Species. *J. Phys. Chem. A* **107**, 2343 (2003)

A. V. Marenich and J. E. Boggs

A Variational Study of Nuclear Dynamics and Structural Flexibility of the CH₂OH Radical. *J. Chem. Phys.* **119**, 3098 (2003)

R. Janoschek and M. J. Rossi

Thermochemical Properties of Free Radicals from G3MP2B3 Calculations. *Int. J. Chem. Kinet.* **34**, 550 (2002)

A. G. Császár, P. G. Szalay, and M. L. Leininger The Enthalpy of Formation of ²Π CH. *Mol. Phys.* **100**, 3879 (2002)

J. Demaison, L. Margulès, J. M. L. Martin, and J. E. Boggs Anharmonic Force Field, Structure, and Thermochemistry of CF₂ and CCl₂. *Phys. Chem. Chem. Phys.* **4**, 3282 (2002)

13. **Number**: 2003-036-2-100

Title: Thermodynamics and non-equilibrium criteria for development and application of supplemented phase diagrams

Task GroupChairman: Horacio R. Corti

Members: <u>C. Austen Angell, Tony Auffret, Harry Levine, María del Pilar Buera, David S. Reid, Yrjo Roos, and Louise Slade</u>

Objective:

The aim of the project is to establish rational links between thermodynamic aspects of phase diagrams supplemented by the non equilibrium curve of the glass transition temperature for mixtures of water with vitrifying agents used in the cryo and dehydropreservation of natural (foods, seeds, etc.) and synthetic products (pharmaceuticals). It will contribute to improve processing and conservation practices of these important materials. It intends not just to compile information that already exists, but to consider all the sort of basic and applied problems that one should consider when managing these phase/state diagrams.

Description:

The present proposal is prepared as to have a very broad and interdisciplinary scope for impacting on many fields related to chemistry and biophysical chemistry. It would permit promoting IUPAC activities and competence to a wider non-chemistry scientific community. It is largely inspired in early activities of the International Symposia on the Properties of Water (ISOPOW). The applicability of state diagrams is recognized in food chemistry and related areas. However, many basic questions are still open and more precise definitions are needed for a correct interpretation of the involved phenomena. The practical aim of the project is to give solid basis to develop supplemented state diagrams of aqueous glassy formers, such as saccharides, polyols, etc., in order to describe the influence of water content, nature of the vitrifying agent and temperature on the physico-chemical stability of natural and synthetic products.

To fulfil this goal this study proposes to analyze:

- 1. The areas of food and pharmaceutical processing in which theoretical basis are needed for a better definition of the involved phenomena.
- 2. The practical/theoretical applicability of equations extensively employed to predict transition temperatures.
- 3. Which is the best standard procedure to determine the glass transition curve over the water content scale.
- 4. Differences between methods based on thermodynamics and kinetics to determine the phase/state transitions, and how could they be standardized.
- 5. What is the effect of water content on the kinetics of phase/state transitions (glass temperature, crystallization temperature) in biomaterials.
- 6. How can be state diagrams applied to analyze the stability of biomolecules under extreme conditions (i.e. frozen systems, high or low pressures).

7. How can multi-dimensional (ternary systems, pressure coordinate) diagrams be managed. The project will aim to give scientific-based definitions in the detected critical areas.

Progress:

Last update: 5 August 2004

14. Number: 2004-010-3-100

Title: Heat capacity of liquids: critical review and recommended values

for liquids with data published between 2000 and 2004

Task Group Chairman: Vlastimil Rùžièka

Members: Eugene Domalski, Zdenka Kolská, Milan Zábranský

Objective:

To update and extend two publications that contained recommended data on liquid heat capacities for almost 2000 mostly organic compounds, "Heat Capacity of Liquids: Critical Review and Recommended Values", and its "Supplement I" by M. Zábranský, V. Ruzicka, V. Majer (1st work only), and E.S. Domalski published in *Journal of Physical and Chemical Reference Data* in 1996 and 2001. The publications were the product of IUPAC Projects 121/11/87 and 2000-031-1-100.

Description:

Experimental data on heat capacities of pure liquid organic and some inorganic compounds published in the primary literature between 2000 and 2004 will be compiled, critically evaluated and recommended values provided. Recommended data supplemented with an assessment of their uncertainty and presented in terms of parameters of correlating equations for temperature dependence of heat capacities will be developed by critical assessment of literature calorimetrically determined heat capacities. The work will be an update of a two-volume monograph that was published in 1996 as a Monograph No.6 of the Journal of Physical and Chemical Reference Data, and of its Supplement I, published in J. Phys. Chem. Ref. Data 30, 1199-1689 (2001). The updated and extended database will contain data for about 250 compounds taken from more than 120 literature references. The whole work consisting of the monograph and of its two supplements will also provide an exhaustive survey of the literature for all isobaric and saturation heat capacities for pure organic and inorganic compounds in the liquid state having a melting point below T = 573 K. The literature survey includes references to the original paper and to the description of the experimental equipment used for heat capacity data determination and serves as a valuable source of references. The overall

number of compounds in the whole database of recommended data will exceed 2000.

Progress:

Last Update: 2 September 2004

15. Number: 2004-026-2-100

Title: Categorizing hydrogen bonding and other intermolecular

interactions

Task Group

Chairmen: Elangannan Arunan and Steve Scheiner

Members: Ibon Alkorta, David C. Clary, Robert H. Crabtree, Joseph J. Dannenberg, Gautam R. Desiraju, Henrik G. Kjaergaard, Roger A. Klein, Karl Kleinermanns, Anthony C. Legon, Benedetta Mennucci, David J. Nesbitt, and Joanna Sadlej

Objective:

To take a comprehensive look at intermolecular interactions and classify them and to give a modern definition of the hydrogen bond, taking in to account all current experimental and theoretical information, and including hydrogen bonded systems both in gaseous and condensed phases as well as in chemical and biological systems.

Description:

Hydrogen bonding has fascinated chemists and biologists for several decades now and it is central to chemistry and biology. The original definition of hydrogen bonding invoked two electronegative atoms (X and Y) interacting through a hydrogen atom as in X-H --- Y. Initially X and Y were found to be mostly N, O and F which led to the mentioning of these atoms as part of the definition of hydrogen bonds in various sources (including the Gold book of IUPAC). Hydrogen bonding was inferred by the difference in physical properties between otherwise chemically similar systems such as found between H₂O and H₂S. However, now it is well known that both H₂O and H₂S form a hydrogen bonded (H₂X)₂ dimer in the gas phase. Spectroscopic red shift in XH stretching frequency was among the first experimental evidence used for inferring hydrogen bonds. Now there are several hydrogen bonded systems that appear to show blue shift in XH stretching frequency. More interestingly, these systems have CH as the hydrogen bond donors, which was against conventional wisdom. The CH --- O interactions have been well established now in organic and biological systems by crystal structure analysis and NMR methods. Traditionally, hydrogen bond acceptors interact through a lone

pair or bonded pair electrons. However, optically active hydrogen bonded complexes involving radicals have been found in the atmosphere. Matrix experiments and theoretical studies have shown that CH₃ radical could form a complex with H₂O, which could be represented as C --- HO? Are these one-electron hydrogen bonds with C as the acceptor? There have been reports on X-H --- interactions where electrons act as hydrogen bond acceptors. Dihydrogen bonds have been observed in which H in XH (X=electronegative) interacts with another hydrogen in MH (typically a metal hydride) with partial negative charge. Moreover, there have been numerous reports on H₂ molecular complexes in the literature - should these be regarded as containing hydrogen bonds?

Electrostatic interaction was identified as the dominant factor for hydrogen bonds. Recent NMR and Compton scattering experiments have given evidence for partial covalency in hydrogen bonds. Dispersion forces have been shown to dominate hydrogen-bonded complexes of second row hydrides (HCl and H₂S). Chlorine monofluoride (ClF) has been shown to form weakly bound complexes with bases very much like HF and these have been identified as chlorine bonded complexes. Such chlorine bonding interactions have been observed in crystal structures as well. Hydrogen bonding, electrostatic interactions and van der Waals interactions are all loosely and interchangeably used in the field. Often van der Waals forces are equated to dispersion forces, though the origin of van der Waals forces (from the equation named after him) should include all intermolecular forces. Should rare gas complexes such as Ar-Ne be called London molecules instead of van der Waals molecules, as only London dispersion forces contribute to stabilization of Ar-Ne? Should Ar-HF be called hydrogen bonded or van der Waals complex? This project will attempt to give a modern definition of a hydrogen bond that is as inclusive as possible. Also, intermolecular interactions will be categorized logically considering the physical forces involved.

Progress:

The Task Group will be having a meeting in Pisa during the week of 5th to 9th September 2005 in the form of a workshop. All the participating members of the Task Group will be presenting a summary of their recent work in the area of hydrogen bonding and molecular interactions and will also give their views about the classification of inter- and intra-molecular interactions. The Task Group will have several rounds of discussion during the Workshop and it is intended that a provisional position paper will be produced at its conclusion. There will also be sufficient place for an additional 25-30 non-task group participants to take part in the Workshop (anyone interested in participating should contact either Elangannan Arunan arunan@ipc.iisc.ernet.in or Roger Klein klein@institut.physiochem.uni-bonn.de.

The Workshop details are available at the URL address: http://institut.physiochem.uni-bonn.de/IUPAC_Pisa2005/Workshop.html

Last update: 7 April 2005

16. Number: 2004-036-1-100

Title: Establishing recommended data on thermodynamic properties of hydration for selected organic solutes

Task Group Chairman: Vladimir Majer

Members: V. Dohnal, R. Fernandez-Prini, M. Frenkel, A.H. Harvey, J. Sedlbauer, and E.L. Shock

Remark: This project is co-funded by the International Association for Properties of Water and Steam (IAPWS) www.iapws.org>

Objective:

The objective of the project is to establish a database of thermodynamic properties of hydration for approximately 200 selected organic solutes at reference condition of T = 298.15 K and 0.1 MPa and as a function of temperature and pressure up to the near critical region of water. The values of hydration properties for solutes covering different molecular structures will be calculated from the reliable experimental data for aqueous and pure solutes. The established database will be used as a standard for testing and establishment of new physico-chemical models and methods of molecular simulation as well as for developing semitheoretical prediction schemes of interest for chemical engineering, environmental chemistry and geochemistry.

Description:

Thermodynamic properties of hydration (TPH) covered in the project are: the Gibbs energy of hydration and its temperature and pressure derivatives (the enthalpy of hydration, the heat capacity of hydration and the partial molar volume at infinite dilution), other TPH result from their combinations; for exact definitions and inter-relationship see Appendix 1 (pdf).

TPH express the difference between the property of a solute in the standard state of infinite dilution at a given temperature and pressure and that of an ideal gas at the same temperature and reference pressure of 0.1 MPa. Thus they characterise the transfer of a solute from a state where molecules are not interacting to the state where the solute molecules

interact solely with the water solvent. Due to this definition they can be used conveniently in testing and conception of theoretical models and simulation approaches for dilute aqueous solutions developed by physical chemists. At the same time, TPH allow an easy calculation of partition coefficients (such as the Henry's law constant, air-water partition coefficient, relative volatility, etc.) and of the thermodynamic reaction constants for aqueous systems. Therefore they also have a practical value of interest for chemical engineers and environmental chemists. In addition, the high temperature / high pressure TPH are required to characterize phase and chemical equilibria in hydrothermal systems and to guide the development of geochemical prediction schemes for aqueous fluids.

TPH cannot be directly measured but are calculated from the experimental data characterising aqueous and pure solutes, which result from phase equilibrium, calorimetric and volumetric measurements. Appendix 1 (pdf) summarises equations used to calculate TPH and lists types of experimental data that can be exploited.

The task group will select from the primary literature the best available experimental results for establishing a database of reliable values of TPH for 100 - 200 organic solutes and several common gases. In selecting the solutes, three main criteria will be observed:

- i) coverage of the widest range of molecular structures, indispensable for the development of theoretical models and group contribution prediction schemes,
- ii) availability of reliable experimental data, particularly with regard to the HT/HP region,
- iii) technological and environmental importance of individual solutes.

The database will comprise values at the reference condition for about 200 solutes and at elevated temperatures (T < 673 K) and pressures (p < 40 MPa) for about 100 solutes. For several solutes the recommended TPH will be given up to the critical region of water where they undergo remarkable changes. A tentative list of the classes of solutes covered and their respective numbers are given in Appendix 2 (pdf). Every effort will be made to supply a database that will not be biased by use of any particular correlation model for interpolating or extrapolating the data. This project requires collaboration of researchers having complementary knowledge in data evaluation and in different experimental techniques used for obtaining data for aqueous and pure solutes.

Progress:

Last update: 8 February 2005

B. Projects Nearing Completion or in Press

1. Number: 110/2/81

Title: Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition)

Coordinator(s): I.M. Mills, H.L. Strauss, M. Quack, and T. Cvitas

Remarks: Commissions within Division I, ISO/TC12, SUNAMOCO, CIPM

Progress: Its sole project the *Revision of the Green Book: Quantities*, *Units and Symbols in Physical Chemistry* consists of preparation of the third edition planned for 1999. The typing of the whole text into a standard computer-readable format (Revtex) is taking time. It is being carried out under the supervision of M. Quack and a meeting of I.1 is planned for January 1999 in order to finalize the text and get it to the printers. The main changes with respect to the <u>second edition</u>, except for producing the book on a computer, involve extensions in the field of surface chemistry and the treatment of uncertainties of measurement.

Last update: 6 June 2000

2. Number: 120/15/95

Title: Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies

Coordinator(s): M. Ribeiro da Silva

Objective:

Nomenclature and symbolism for bond energies are, at the moment, somewhat confusing although these quantities are widely used to estimate the thermo-chemistry of species for which the enthalpies of formation are unknown. The proliferation of designations and symbols for quantities variously known as bond strengths, bond enthalpies, bond energies, bond dissociation enthalpies, bond enthalpy terms, stepwise bond dissociation energies, intrinsic bond energies, BDE, D etc clearly requires some standardisation. Several experimental techniques are available to

determine the parameters named above but can only be used to study the thermo-chemistry of long-lived molecules. However, modern techniques have made possible the study of these species. The correct relationship between the quantities measured with some of these new techniques and thermodynamic functions are often not straightforward and deserve a careful analysis. It is therefore proposed that this project considers in the first stage a comprehensive list of methods that have been used to derive energetic data. A second stage will involve a description of each method with an analysis of its basic assumptions and how thermodynamic data can be derived. In addition recommendations of standard nomenclature and symbols for bond energetics would be prepared.

Progress:

Progress in the first two years has been very good. A draft of the basic information to be included in the report has already been circulated for approval. In the next period comments will be incorporated and the descriptive material added.

A draft of the paper has been now prepared and is awaiting final comments before being submitted for publication.

A manuscript is being prepared for publication in *Pure Appl. Chem.* A final document is submitted to public review comments until 30 September 2002.

> see provisional recommendations

Last Update: 17 April 2002

3. **Number**: 120/16/97

Title: New Edition of Experimental Thermodynamics Vol II

> View Series Titles

Coordinator(s): W.A. Wakeham, R.D. Weir, T.W. deLoos and A.

Goodwin

Remarks: Industrial contact to provide rationale for the task and as authors

Objective:

Experimental Thermodynamics prepared by the Commission in 1970 has been an archival book for nearly 30 years on Thermodynamic Measurement Techniques. It is now out of date; many new techniques have been developed. At the same time many industrial organisations have reduced their expertise in the field. Industrialists and Academic Research

Workers have argued that the volume needs to be updated to provide a reference for the world expertise before it is lost and has to be reinvented. It is proposed to update the volume by including only what is new and relevant. It will comprise two volumes on single and multiple phase separately.

Progress:

- Volume VI. <u>Measurement of the Thermodynamic Properties of Single</u> Phases

Editors: A.R.H. Goodwin, K.N. Marsh and W.A. Wakeham *published* - Elsevier, 2003 [ISBN 0-444-50931-3]

- Volume VII. Measurement of the Thermodynamic Properties of Multiple Phases

Editors: Th. de Loos and R.D. Weir

The 16 chapters that make up the edition are in the hands of the production department of Elsevier Publishers. Some 24 authors from nine different countries contributed material. This book contains descriptions of recent developments in the techniques for measurement of thermodynamic quantities for multiple phases of pure fluids as well mixtures over a wide range of conditions. The precision and accuracy of results obtained from each method was regarded as an essential element in each description. Throughout the text, the quantities, units and symbols are those defined by IUPAC for use in the international community.

Anticipated publication date: late 2005 or early 2006.

Last Update: 19 April 2005

4. Number: 150/24/95

Title: Spectroscopy under extreme conditions

of temperature and pressure

Coordinator(s): A..M. Heyns

Remarks: Collaboration with Commission V.4, Max Planck Institute (Stuttgart) and AIRAPTS organisers of Conference series on High Pressure Science

Objective:

To obtain international agreement on methods and standards and to prepare documents to guide workers in the field of spectroscopy under extreme conditions. Initially vibrational and electronic spectroscopy will be considered, but the project may be extended to NMR, Mossbauer, and

This project was presented at a <u>poster session</u> at the IUPAC Congress/GA July 2001

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other spectroscopies if the early work reveals interest in these areas. The main issues to be pursued come under the three general headings Instrumentation, Pressure Calibration, and Temperature Calibration. Instrumentation includes the consideration of cell design, the use of membranes with diamond anvil cells, the properties of optical windows under extreme conditions, the design of spectrometers and microscopes, the use of optical fibres for safe access to difficult experimental situations, and the simultaneous generation of high pressure and low temperature in an optical cell. The calibration issues include methods and standards for the calibration of hydrostatic and very non-hydrostatic pressures. Emphasis will be on calibration through the spectroscopic properties, with the intention to make recommendations in the final report of standard substances, inorganic, organic and biological, whose spectroscopic properties can be used for calibration and for establishing the performance of apparatus.

Progress:

Much progress has been made on this project. A 6-page summary was presented to the Commission in Berlin, accompanied by a detailed report on the scope of the project.

The final report is submitted for publication in *PAC*.

Last update: 25 January 2002

5. **Number**: 2000-026-1-100 (continuation of 121/10/87)

Title: Critical compilation of vapour liquid critical properties

Task Group Chairman: Kenneth N. Marsh

Members: C.L. Young, C. Tsonopoulos, J.H. Dymond, and D. Ambrose

Objectives:

Values of vapour-liquid critical properties are essential in correspondingstates treatments of equilibrium thermodynamic and transport property data. The objective is to review all such measurements for pure organic compounds containing **nitrogen**, **halogen**(s), and **sulphur** and **silicon** and to recommend values for critical temperature, critical pressure and critical densities, with uncertainties.

Progress:

The current project is the continuation of <u>project 121/10/87</u> which has to date, resulted in 7 review papers published in the *Journal of Chemical and Engineering Data*. These include an introductory survey (which covers experimental methods and effects of impurities and decomposition on the

results; Normal alkanes; Aromatic hydrocarbons: Aliphatic alkanols; Branched alkanes and cyclo-alkanes; Unsaturated aliphatic hydrocarbons and Oxygen compounds other than alkanols and cycloalkanols.

Eight papers in the series "Vapour-Liquid Critical Properties of Elements and Compounds" were published in the *Journal of Chemical & Engineering Data*:

- Part 1. An introductory survey, Vol. **40**, 345-350 (1995)
- Part 2. Normal alkanes, Vol. **40**, 531-546 (1995)
- Part 3. Aromatic Hydrocarbons, Vol. **40**, 547-558 (1995)
- Part 4. Aliphatic Alkanols, Vol. 40, 1025-1036 (1995)
- Part 5. Branched Alkanes and Cycloalkanes, Vol. 41, 365-372 (1996)
- Part 6. Unsaturated Aliphatic Hydrocarbons, Vol. 41, 645-656 (1996)
- Part 7. Oxygen Compounds other than Alkanols and Cycloalkanols, Vol. 46, 457-479 (2001).
- Part 8. Organic Sulfur, Silicon and Tin Compounds, Vol 46 (3), 480-485 (2001).
 - > View earlier references in this series

Papers in preparation: Part 9 - nitrogen compounds Part 10 - halogen compounds Part 11 - miscellaneous

Last Update: 14 May 2001

This project was presented at a poster session at the IUPAC Congress/GA July 2001 ><u>view pdf - 40KB</u><

Item 9: Reports of Division Presidents

The Report from Division II, Inorganic Chemistry, was not available at the time the Agenda Book was printed.

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

August 2005

Minoru Isobe, President

I. Executive Summary and Highlights

The Mission of Division of Organic and Biomolecular Chemistry is to promote the goals of IUPAC in the field

of organic and biomolecular chemistry in the broadest sense. To this end the Division consists of a Division

Committee and 6 Subcommittees. Together these promote the formulation and execution of Projects on

relevant chemical problems, the staging of chemical conferences on important areas of chemistry, the

education and professional development of chemists worldwide, the advancement of chemical industry, and

the application of chemistry to meet the world's needs. The Division is committed to utilizing the talents of

chemists from around the world in these activities, and promoting diversity in our membership.

The Division covers such a broad area of multidisciplinary aspects, and stimulates the fundamental and applied

organic synthesis as the top edge science. It includes asymmetric synthesis of Natural products, Process

chemistry with Molecular catalysts, and still explosively expanding Organometallic chemistry. Chemical

biology or Post genomic chemistry is the key sciences for the biomolecules in this century, and it is also close

to Biotechnology. Physical chemistry has been the fundamental mechanistic science, and it is also important in

the spectroscopy and/or organic analysis. Photochemistry is of worldwide significance in the standardization

for analytical chemistry as well. Green and sustainable chemistry are increasingly recognized as important

environmental and limited organic materials from the global scale. The Division coordinates these subjects to

be interdivisional activities as well as among the following Subcommittees.

Subcommittee on Organic Synthesis (Chair: Frank McDonald, USA)

Subcommittee on Biomolecular Chemistry (Chair: Vadim Ivanov, Russia)

Subcommittee on Green Chemistry (Chair: Pietro Tundo, Italy)

Subcommittee on Photochemistry (Chair: Silvia Braslavsky)

Subcommittee on Structural and Mechanistic Chemistry (Chair: T. Marek Krygowski)

Subcommittee on Biotechnology (Chair: Romas Kazlauskas)

The Subcommittees have been dealing with the IUPAC sponsored conferences in the various location of the

world with quite success. Some of them are recognized as the conference series and planned long time in

advance with adjusting the period of time and place for the similar conferences to be held.

The following report style is slightly different from the instruction, since the subcommittees are differently

active to fit making this report for the six Goals in the current IUPAC Strategic Plan.

1

II. An overall report of Division activities during 2004 and the first part of 2005

- a) IUPAC will provide leadership as a worldwide scientific organization that objectively address global issues involving the chemical sciences. Organic Synthesis Subcommittee has long time the tradition as the worldwide leadership in the synthetic chemistry communities; thus, asymmetric synthesis of natural products, new reactions catalyzed by organometallic compounds. In the Biomolecular Subcommittee, it is also recognized as the world leading level for the elucidation of the molecular structures in trace amount and/or complexity and/or biochemical mechanism. These have been indicated in the division-supported series of conferences as Organic Synthesis and Natural Product Chemistry.
- b) IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion. Photochemistry is a good example for the standardization since it has been widely applied to various kind of spectroscopy on the basis of physical chemistry such as NMR, Photoluminescence, and Chemical Actinometry. It should be noted that Photochemistry Subcommittee is in good collaboration with major photochemical societies in the world.
- c) IUPAC will assist chemistry-related industry in its contribution to sustainable development wealth creation, and improvement in the quality of life. Green Chemistry Subcommittee has contributed to this subject in worldwide starting from South East Asia, India, Arab region, Latin America, Russia, Africa in the strong connection with the economical growth and chemical industry activity.
- d) IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries. Biomolecular Subcommittee has been achieving the Biodiversity project, which has been completed in the form of IUPAC recommendation (*Pure Appl. Chem. 74*, 697-702, **2002**). It was discussed in Thailand, Brazil, China, and Turkey before the recommendation. Further workshop was held in New Delhi in 2004 during the 4th IUPAC Conference on Biodiversity proposed for a Natural Product Center in Bangladesh.
- e) IUPAC will utilize its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists and the public appreciation of chemistry. IUPAC prizes have been awarded to young chemists in the ICOS meeting as well as Poster Prize to 3 presentators. Many conferences have similar award system to give presentation awards to young chemists.
- f) IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender, and age. The Division has been committed to these goals for some time, as witnessed by our current 31 members (11 TM, 6 AM, 12 NR, 2 PR), who are from 29 countries (Asia 8), (Europe 15), (North America 3), (South America 3),

and (Africa 2). Only 4 are female but we expect to increase this representation. We are always conscious of the need to recruit younger chemists, but recognize their carriers; In addition our Subcommittee include 73 additional individuals, many of them younger chemists.

SUBCOMMITTEES:

Subcommittee on Organic Synthesis

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

IUPAC International Conference on Organic Synthesis (ICOS-15) was held in Nagoya, Japan from Aug. 2004, which was quite successful with nearly 1000 participants. IUPAC Prize was awarded to Prof. Hartwig, and next Prize nomination has just opened since June 20 by co-sponsor with Theme. It will be awarded in ICOS-16, which will be held in Merida, Yucatan, Mexico during June 11-15, 2006 by organizer Eusebio Juaristi. Further ICOS-17 was proposed to be held at Daejeon in Korea during Aug 17-23, 2008; ICOS-18 (2010) in Bergen, Norway; ICOS-19 (2012) in Taiwan.

Heterocyclic Chemistry (FHC-5) was held in Florida, USA in March 2004, and will be held in 2006.

Organometallic Chemistry (ICOMC-21) was held in Vancouver, Canada in July 2004.

There are 2 more conferences planned in 2005; thus, Heterocyclic Chemistry (ICHC) in Palermo, Italy in July-Aug, and Organometallic Chemistry (OMCOS-13) in Geneva in July.

Subcommittee on Biomolecular Chemistry

The Subcommittee will seek to deliver the long-range goals of IUPAC, particularly within the vital interfacial area of molecular science that lies between organic chemistry and biology. It will support the application of the powerful methods of chemistry to current and emerging problems in biology to achieve understanding and, where appropriate, modification of the systems of living organisms at the molecular level. To that end, the Sub-Committee will provide a focus for the dissemination of current knowledge and the development of future directions in the following fields: 1) Structure, function and applications of biomolecules and their analogues; 2) Molecular mechanisms of biological processes and their modulation; 3) Molecular engineering via chemo-enzymatic processes; 4) Analysis, manipulation and application of biomolecular information systems. International Conference on the 4th Biodiversity and 24th Natural Products: Chemistry and Medical

Applications was held in New Delhi, India in January 2004 by organizer V. S. Parmar with ca. 1000 participants. A Satellite symposium on Bioresources toward drug discovery and development was held in Mauritius in Feb. 2004 (Org. Am. G. Fakim). The next joint symposia (5th and 25th) will be held in Kyoto, Japan (D. Uemura) in July 2006; (6th and 26th) will be held in Australia (Mary Garson).

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

Subcommittee on Photochemistry

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

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

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

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

Subcommittee on Structural and Mechanistic Chemistry

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

The 17th IUPAC Conference on Physical Organic Chemistry (ICPOC-17) was held in Shanghai, China in August 2004 (Guo Zhen Ji). The next ICPOC-18 is planned in Warsaw in Aug 2006; and ICPOC-19 will be in Santiago, Spain (Galicia) in 2008. Next group conference will be held in Essen, Germany in 2007 (Roland Boese). CAIC-10 was held in Bussan, Korea in August 2004 (Dae Dong Sung).

Subcommittee meeting in Shanghai approved the name of "Correlation Chemistry" to change to "Correlation and Modeling in Chemistry). This change aims at fostering research in all aspects of the modeling of the structure-property quantitative relationship (SPQR); thus, between structural variations and measurable properties as equilibrium constants, (enzyme catalyzed) reaction rates, etc.

Subcommittee on Green Chemistry

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

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

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

Subcommittee on Biotechnology

The International Biotechnology Symposium and Exhibition (IBS-12) was held in Oct. 2004 in Santiago, Chile

(J. A. Asenjo). The program included 10 sections with newer areas of Molecular tools, Cellular tools, Genomic tools, applied genome research, Cultivation technology, downstream processing, Biocatalysis, Health care, Plant and food biotechnology, and Environmental Biotechnology.

III. Any other substantive information

Budget of Division III for 2004-2005 is allocated to the 6 Subcommittees in part, and the rest are available for projects. Further funding is available for good proposals. The generation of new projects remains the most urgent business of the Division.

Many potential proposals have been discussed among the subcommittee meetings to generate most important and timely projects.

IV. Tabular material

List of publications

Current Projects

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

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

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

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

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

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

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

2002-029-1-300 - A IUPAC coordinated web page on Green/Sustainable Chemistry

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

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

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

2004-021-1-300 - Reference methods, standards and applications of photoluminescence*

OTHER INTERDIVISIONAL PROJECTS

2001-014-1-800- Fullerene nomenclature - part II

2001-031-1-800 - Alignment of nomenclature in areas of overlap between the preferred names for

^{*} Interdivisional project

organic nomenclature and the revision of the nomenclature of inorganic chemistry

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

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

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

PROJECTS NEAR COMPLETION / IN PRESS

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

Recently Completed

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

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

2002-008-1-300 - Chemical actinometry

Representation on other IUPAC Bodies

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

Interdivisional Committee on Nomenclature, Terms, and Symbols (ITCNS) Gerrit Koomen.

Subcommittee on Materials Chemistry Shunichi Fukuzumi and Istvan Horvath.

Division VIII Nomenclature Warren Powell.

Recent Reports from ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION (III)

Chemical actinometry (IUPAC Technical Report)

Pure Appl. Chem. 76(12), 2105-2146 (2004)

Phane nomenclature. Part II. Modification of the degree of hydrogenation and substitution derivatives of phane parent hydrides (IUPAC Recommendations 2002) (III)

Pure Appl. Chem. 74(5), 809-834 (2002)

Molecular basis of biodiversity, conservation, and sustained innovative utilization

Pure Appl. Chem. **74**(4), 697-702 (2002)

Nomenclature for the C60-Ih and C70-D5h(6) fullerenes (IUPAC Recommendations 2002) (III.1)

Pure Appl. Chem. 74(4), 629-695 (2002)

Critical evaluation of proven chemical weapon destruction technologies

Pure Appl. Chem. 74(2), 187-316 (2002)

Organic photochromism (IUPAC Technical Report) (III.3)

Pure Appl. Chem. **73**(4), 639-665 (2001)

Figures-of-merit for the technical development and application of advanced oxidation technologies for both electric- and solar-driven systems (IUPAC Technical Report) (III.3)

Pure Appl. Chem. 73(4), 627-637 (2001)

Synthetic Pathways and Processes in Green Chemistry. Introductory Overview (III.2)

Pure Appl. Chem. 72(7), 1207-1228 (2000)

That is the *Introductory Overview* to the <u>PAC special topic issue on Green Chemistry</u>.

Revised Section F: Natural products and related compounds (III.1)

Pure Appl. Chem. **71**(4), 587-643 (1999)

+ Errata, *Pure Appl. Chem.* **76**(6), 1283-1292 (2004)

IUPAC POLYMER DIVISION (IV)

Report to Council for 2003 - 2005

Structure of Report

Section I highlights and summarises key points in terms of achievements and developments. **Section II** describes Division IV's activities according to the goals of the IUPAC Strategic Plan

Section III summarises the levels of work and output in Division IV's areas of activities **Section IV** lists collected data detailing the projects, conferences and publications with which Division IV has been involved.

I. Highlights and Executive Summary

- ◆ To reflect the continuing expansion of its work to include polymers as substances and materials as well as individual macromolecules, the Division has changed its name from Macromolecular Division to **Polymer Division**
- ♦ Associate and Titular Members have defined, co-ordinating roles to play in the activities of the Division.
- ◆ Two more areas of activity, namely, the **Structure and Properties of Commercial Polymers** and the **Modelling of Polymerisation Kinetics and Processes**, are now structured as **Sub-Committees**
- The areas of activity of the Division and the associated co-ordinators are:

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

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

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

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

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

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

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

Electronic Publications and Communications

(Co-ordinators R.G. Jones (TM), W.J. Work (TM))

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

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

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

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

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

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

♦ The projects in the area of polymerisation are now run by the **Sub-Committee on the Modelling of Polymerisation Kinetics and Processes.** The work is related to polymerisations of industrial relevance. The Chairman of the S-C and the person coordinating the projects is Michael Buback. The S-C has 28 members from 12 countries, with 2 members from industry. It has had 1 meeting since Ottawa.

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

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

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

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

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

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

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

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

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

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

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

- ◆ Linked with its work in Education, the first awards from the interest on the endowment from the Samsung General Chemicals Company of South Korea, were made in 2004. An IUPAC-Samsung Young-Scientist Award was presented at the IUPAC World Polymer Congress in Paris and Bursaries were given to help 12 students attend the Congress. The first IUPAC-Samsung Education Award (2005) will be presented shortly.
- ◆ A successful **Symposium on Polymer Education** was held as part of the 2004 IUPAC World Polymer Congress in Paris. This was a new venture that the Division hopes to continue at future WPCs.
- ♦ At the IUPAC-sponsored Polymer Networks 2004 Meeting, in Bethesda, USA, the first **IUPAC Poster Prizes** were awarded for posters from young scientists.
- ◆ As with Education, the Division continues to place particular emphasis on **Conference Sponsorship**. Largely through the efforts of the Co-ordinators for Conference Sponsorship, Przemyslaw Kubisa and Stan Penczek, and other Division Members, a total of **31 IUPAC-sponsored polymer conferences** have been and will be held in 2003-5, maintaining the high level of conference sponsorship from the previous biennium.
 - **16 conference volumes** of Macromolecular Symposia have been published in 2003-5. See publications [1-16]. In fact, more than half of the issues of Macromolecular Symposia are devoted to IUPAC-sponsored conferences, representing a significant income to IUPAC, some of which is now used to supplement the budget of Division IV.
- ♦ The IUPAC World Polymer Congress of 2004, organised through the Division, was held in Paris. It is generally recognised that the biennial IUPAC World Polymer Congress, is the main event in the international polymer conference calendar. This year's Congress, with about 2500 participants, was the largest ever.
 - The future WPCs presently planned are 2006 Rio de Janeiro, 2008 Taipei and 2010 Glasgow.
- ♦ Regarding Recruitment at Conferences, the Division Brochure is distributed at all IUPAC-sponsored conferences. In addition, the Powerpoint presentations issued by the Secretariat have been augmented to emphasise Macromolecular Division activities. Electronic versions of the brochure and the presentations are given to all conference organisers and IUPAC representatives.
- ♦ The consideration of **Polymer World and Division Strategies**, started during the last biennium, has continued. As recognised in the change of name of the Division, polymer science and technology is no longer based primarily on the macromolecule but it is central to many modern functional and structural materials. The Division's aims and activities need to change continually and to grow in order to reflect the new emphasis and increasing diversity. The work is co-ordinated by Kazuyuki Horie and Jung-Il Jin.

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

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

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

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

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

♦ Future Plans and Structure

- ◆ The Division intends to maintain its existing project areas, Structure-Property Characterization, Molecular Characterization, Polymerization Modelling, Terminology and Nomenclature, Developing Polymer Materials Systems and Education and also its efforts in Conference Sponsorship.
- It will seek to expand its profiles in Molecular Characterization and Developing Polymer Materials Systems and maintain its high level of activity and throughput in all project areas and in Conference Sponsorship.
- ◆ The Division will seek to play a strategic role in defining the important areas of world polymer research through its strategic study and conferences.
- ♦ In order to give continuity to the Division's structure and range of activities, the elections to the Division Committee in 2005 have been to positions designated for particular responsibilities, essentially those listed at the beginning of this report.

II. Division Activities and the IUPAC Strategic Plan

(a) World Leadership

The Division has a **Strategic Study** into the needs and directions of World Polymer Science (project 2002-057-1-400).

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

The **IUPAC World Polymer Congresses** organised biennially under the auspices of Division IV are the largest and the most important conferences in the international polymer conference calendar. The WPC in 2004 took place in Paris, that in 2006 will take place in Rio de Janeiro, in 2008 in Taipei, and in 2010 in Glasgow.

(b) Advancement of Research through International Standardisation and Scientific Discussion

The Division is active in several areas under this heading, as witnessed by the work of the Sub-Committees on the Structure and Properties of Commercial Polymers, the Modelling of Polymerisation Kinetics and Processes, and Macromolecular Terminology, as well as its work on the Molecular Characterisation of Polymers and on Developing Polymer Materials Systems. Overall, 10 projects have been completed, 14 new projects have been launched and 18 other projects have been active during 2003-5. 34 reports and papers have been published or are in press (publications [7,17-49]). In addition, a total of 8 meetings has been held by the three Sub-Committees.

(c) Assistance to Chemistry-Related Industry

The Division's work in the four areas of Structure and Properties of Commercial Polymers, Molecular Characterization of Polymers, Modelling of Polymerisation Kinetics and Processes and Developing Polymer Materials Systems is directly related to the needs of chemistry-related industry. Of the detailed figures given under (b), this work accounts for 7 of the new projects, 4 of the continuing projects, 27 of the publications and 7 of the meetings of the Sub-Committees.

In addition, the 31 sponsored conferences and the 16 volumes of Macromolecular Symposia resulting from sponsored conferences deal with topics relevant to chemistry-related industry.

Most of the 19 projects on Macromolecular Terminology are of industrial relevance as well as the two publications in this area [47,48].

(d) Fostering Communication between Individual Chemists and Scientific Organisations

The **strategic study and strategic conferences** described under (a) are definite attempts to foster communication between individual chemists and scientific organisations.

The **Symposium on International Collaboration**, organised in conjunction with the latest World Polymer Congresses brought together representatives from Chemical and Polymer Societies from across the world and fostered scientific discussion and the exchange of ideas.

A booklet giving details of all World Polymer Organisations was prepared for the symposium by the Society of Polymer Science, Japan under the auspices of Division IV.

The **31 conferences sponsored** in 2003-5 and the **16 volumes of conference papers** published so far [1-16] in the same period represent attempts to foster communication between individual chemists.

The **5 educational courses, workshops and conferences** partially sponsored and supported by the Division and IUPAC (Project Committee) have been aimed specifically at reaching young chemical scientists from educationally hindered countries.

The development of a polymer-education web site and the new project (in conjunction with the CCE) on preparing educational material for French-speaking countries will also improve communication.

(e) Enhancement of Chemistry Education, Development of Young Scientists and Public Appreciation of Chemistry

As just stated under (d), the 5 educational courses, workshops and conferences partially sponsored and supported by the Division and IUPAC (Project Committee), the polymereducation web site and the new project for French-speaking countries were and are aimed at young chemical scientists from educationally hindered countries.

Students on one of the courses, the postgraduate course based in Prague, have published numerous papers in journals (publications [50-104]). The other workshops and conferences have led and will lead to material being issued as booklets and in electronic format, some of which will appear on the Division web site.

The IUPAC-Samsung Young-Scientist Award and Student Bursaries were presented at the 2004 World Polymer Congress. The first IUPAC-Samsung Education prize will be awarded in 2005. The first IUPAC Poster Prizes were presented at Polymer Networks 2004.

(f) Breadth of National Membership

Scientists involved with Division IV are spread worldwide. For example, the Division Committee, numbering 26, has members from 18 countries, the Sub-Committees on Macromolecular Terminology, Structure - Property Characterization of Commercial Polymers, and Modelling Polymerization Kinetics and Processes have members from 15, 17 and 12 countries, respectively.

III. Summary for 2003-5 of Levels of Work and Output in the Division's Areas of Activities

(The detailed lists of projects, sponsored conferences and publications are given in Section IV.)

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

- 3 projects completed this biennium
- 4 projects completed earlier and awaiting publication
- 2 continuing projects
- 3 new projects
- 5 feasibility studies for new projects
- 6 meetings (Ludwigshafen, Stonefield Castle (Scotland), Paris, Kyoto, Zürich, Beijing)
- 19 reports and papers published, in press, submitted or prepared for publication [21-39]

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

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

- 1 project completed
- 2 new projects (1 interdivisional)
- 3 submitted proposals for new projects
- 3 reports and papers published or in press [40-42]

Sub-Committee on Polymerisation Kinetics and Process(Co-ordinator M. Buback):

- 2 projects completed
- 2 projects continuing
- 2 new projects
- 1 meeting (Paris)
- 4 reports and papers published or in press [43-46]

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

- 2 projects completed
- 13 continuing projects (5 interdivisional)
- 4 new projects (2 interdivisional)
- 8 feasibility studies for new projects
- 2 meetings (Paris, Beijing)
- 2 recommendations published [47,48]
- 4 recommendations under ICTNS and public review

Developing Polymer Materials Systems (Co-ordinators: C. Ober, J. Vohlidal, W.J. Work)

1 project completed (on conducting polymer colloids)

Feasibility studies for new projects in the areas of new polymer-based materials, biopolymer materials and biodegradability.

1 report published [49]

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

1 UNESCO/IUPAC postgraduate course (Prague) completed (project)

1 new UNESCO/IUPAC postgraduate course (Prague) (project)

1 new characterisation course (Minho) (project)

1 new project on Educational Materials for French-Speaking Countries (joint with the CCE)

All the courses have led or will lead to the publication and distribution of educational materials. For the postgraduate course in Prague, numerous published papers have been an outcome (see publications [50-104]).

Financial support (via Project Committee) for UNESCO/IUPAC conferences in South Africa (2004) and Mauritius (2005) and for a conference in St. Petersburg (2005); all related to the IUPAC programme for disadvantaged countries.

IUPAC-Samsung Young-Scientist Award and Student Bursaries (2004) and IUPAC-Samsung Education Prize (2005) distributed.

Conference Sponsorship (Co-ordinators P. Kubisa and S. Penczek):

The Division has been active in seeking out conferences for IUPAC sponsorship. The following figures summarise the results of its activities (see Section IV for details of the conferences):

10 conferences sponsored in 2003

10 conferences sponsored in 2004

11 conferences sponsored to date for 2005

3 conferences are sponsored so far for 2006 and 1 conference for 2007

- \approx 100% of the sponsored conferences result in journal or book publications of conference proceedings (see publications [1-16])
- \approx 50% of the volumes of Macromolecular Symposia are proceedings from IUPAC sponsored conferences approved through Division IV

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

The Polymer Summit is held biennially as part of World Polymer Congresses, and brings together representatives from Polymer Societies worldwide to discuss matters of strategic importance and future initiatives. A meeting was held in Paris, in 2004, as part the World Polymer Congress there and the next will be held in Rio de Janeiro in 2006.

To maintain a sense of world polymer community, a database and booklet of World Polymer Organizations is compiled, in conjunction with the Division, by The Society of Polymer Science, Japan. A new booklet was published in July, 2002.

Publications [7,17-20] have resulted the first IUPAC Strategic Conference on the Mission and Challenges of Polymer Science and Technology, held in December 2002 in Kyoto. The next strategic conference will be held in New York in 2007.

A project on the strategic study of world polymer science is underway.

R.F.T. Stepto Manchester 1st August, 2005

IV. Collected Data

Projects

Structure and Properties of Commercial Polymers

Completed Projects

421/20/87 Characterisation of flow behaviour and properties of Liquid Crystal and Aromatic Polymers

Task Group Leader: J.L.S. White

421/31/93

Structure and Properties of Hydrogenated NBR Task Group Leaders: T. Kobatake and T. Masuda

421/33/95

Rheological and Mechanical Properties of $P\alpha MSAN/PMMA$ Blends in Miscible and Phase Separated Regimes of Various Morphologies

Task Group Leaders: H.M. Laun, L. Lyngaae-Jörgensen and V. Altstädt

421/34/95

Property Improvement via Interfacial Chemical Reaction - Reactive Extrusion of EVOH/SMA and Polyamide/MAH-EPR

Task Group Leaders: J.E. Curry, J.G. Bonner, and P.S. Hope

421/35/97

Effects of Side-Chain Branching on Processability of Commercial Polycarbonates Task Group Leaders: M. Takahashi, K. Sato, T. Masuda

1999-020-1-400

Quantifying scratch resistance of commercial polymers

Task Group Leader: R.S. Bailey

1999-039-1-400

Structure and Properties of Cyclic Olefin Copolymers

Task Group Leader: S.C. Kim

Continuing Projects

2002-052-1-400

Structure and Properties of polyester elastomers composed of poly(butylenes terephthalate) and poly(ϵ -caprolactone)

Task Group Leader: T. Takigawa

2003-009-1-400

Recommendations for data presentation, applicable to mechanical and rheological measurements of polymers.

Task Group Leader: E. Wassner

New Projects

2003-051-1-400

Structure and Properties of polymer/clay nano-composite materials.

Task Group Leader: S. C. Kim

2004-009-1-400

Guideline for rheological characterisation of polyamide melts.

Task Group Leader: D. Dijkstra

2003-038-4-400

Structure and Properties of Linear and Crosslinked Structural PVC Foams

Task Group Leader: V. Altstädt

Molecular Characterization of Polymers

Completed Project

1999-021-1-400

Round-Robin Test on the Molecular Characterization of Epoxy Resins by Liquid

Chromatography

Task Group Leader: S. Podzimek

New Project

2003-023-2-400

Data treatment in size exclusion chromatography of polymers

Task Group Leader: G. R. Meira

New Interdivisional Project

IV/VI/VII

2004-022-3-400

Terminology and Measurement Techniques of Starch Components

Task Group Leader: M. Fitzgerald

Modelling of Polymerization Kinetics and Processes

Completed Projects

2000-001-1-400

Critically Evaluated Propagation Rate Ccoefficients for Free-Radical Polymerizations of Methacrylic Acid Esters with Functional, Cyclic and Branched Ester Groups

Task group Leader: Sabine Beuermann

2002-023-1-400

Critically Evaluated Propagation Rate Coefficients for Free-Radical Polymerizations: Acrylic

Acid Alkyl Esters

Task group Leader: Robin Hutchinson

Continuing Projects

2000-028-1-400

Critically Evaluated termination Rate Coefficients for Free-Radical Polymerization Task Group Leader: G.T. Russell

2002-053-1-400

Establishment of Quantitative Reliability of Electron Spin Resonance Techniques for Polymerization Kinetics

Task group Leader: B. Yamada

New Projects

2004-034-1-400

Critically Evaluated Propagation Rate Coefficients for Free-Radical Polymerization of Water-Soluble Monomers Polymerized in the Aqueous Phase Task group Leader: I. Lacík

2004-040-1-400

Towards a Holistic Mechanistic Model for Reversible Addition Fragmentation Chain Transfer (Raft) Polymerizations: Dithiobenzoates as Mediating Agents Task group Leader: P. Vana

Macromolecular Terminology and Nomenclature

Completed Projects

410/24/93

Terminology Related to Polymer Composites and Blends

Task Group Leaders: K. Horie, W.J. Work

1999-048-1-400

Definition of Terms Relating to Reactions of Polymers and Functional Polymers

Task Group Leader: K. Horie

Continuing Projects

410/22/93

Guide to Polymer Terminology and Macromolecular Nomenclature Task Group Leader: E.S. Wilks

2000-006-1-400/2004-008-1-400

Terminology of Polymers Containing Ionizable Groups and Polymers Containing Ions

Task Group Leader: P. Kubisa

2000-014-1-400

Glossary of Class Names of Polymers Based on their Chemical Structure and Molecular Architecture

Task Group Leader: J. Vohlidal

2000-016-1-400

Terminology for the Kinetics, Thermodynamics and Mechanisms of Polymerizations

Task Group Leader: S. Penczek

2000-017-1-400

Polymerization Processes and Polymers in Dispersed Systems

Task Group Leader: S. Slomkowski

2002-006-2-400

Terminology for Radical Polymerizations with Minimal Termination – the so-called "Living"

and "Controlled" Radical Polymerizations

Task Group Leaders: A.D. Jenkins, R.G. Gilbert, G. Moad

2002-048-1-400

Purple Book, 2nd Edition

Task Group Leader: E.S. Wilks

2003-021-1-400

Definitions of Terms Relating to Crystalline Polymers

Task Group Leader: G. Allegra

Continuing Interdivisional Projects

IV/II

2000-007-1-400

Glossary of Terms Relating to Polymeric Gels and Networks, Hybrid Inorganic Polymer Materials and the Processing thereof

Task Group Leaders: R.G. Jones, M. Hess

VIII/IV

1999-051-1-800

Source Based Nomenclature for Modified polymer Molecules

Task Group Leader: T. Kitayama

2000-037-1-800

Nomenclature for Macromolecular Rotaxanes

Task Group Leader: A. Yerin

2000-081-1-800

Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Polymers

Task Group Leader: J. Kahovec

2000-082-1-800

Terminology and Nomenclature of Macromolecules with Cyclic Structures

Task Group Leader: W. Mormann

New Projects

2004-043-1-400

Terminology for Biomedical (Therapeutic) Polymers

Task Group Leader: M. Vert

2005-005-2-400

Definitions of Terms Relating to Individual Macromolecules, their Assemblies and Dilute

Polymer Solutions

Task Group Leader: T. Chang

New Interdivisional Projects

IV/V

2003-060-2-400

Terminology for the Chromatographic Separation of Molecules

Task Group Leader: T. Chang

VIII/IV

2003-042-1-800

Source-Based nomenclature of Single-Strand Organic Polymers

Task group Leader: T. Kitayama

Developing Polymer Materials Systems

Completed Project

2002-019-1-400

Conducting Polymer Colloids and Nanofilms

Task Group Leader: J. Stejskal

Education

Completed Project

2002-047-1-400

UNESCO/IUPAC Postgraduate Course in Polymer Science

Task Group Leader: P. Kratochvíl

New Projects

2003-041-1-400

UNESCO/IUPAC Postgraduate Course in Polymer Science

Task Group Leader: P. Kratochvíl

2003-021-2-400

12th Annual Course on Polymer Characterization

Task Group Leader: A. Cunha

2004-037-1-400 (with the support of CCE)

Design of Polymer Education Material for French Speaking Countries

Task Group Leader: G. Froyer

Strategy

Continuing Project

2002-057-1-400

Strategic Study of World Polymer Science

Task Group Leader: M. Sawamoto

Conference Sponsorship

2003 (10 conferences)

11th International Conference on Polymer Characterization (POLYCHAR-11), Denton, Texas, USA, January 6-10, 2003

6th Annual UNESCO School/IUPAC Conference on Polymer Properties, Mpumalanga, South Africa, April 14-17, 2003

Xth International Symposium on Macromolecule Metal Complexes (MMC-X), Moscow, Russia, May 20-24, 2003

International Symposium on Ionic Polymerization, Boston, USA, June 30 - July 4, 2003

Degradation, Stabilization, and Recycling of Polymers, Prague, Czech Republic, July 14-17, 2003

Spectroscopy of Partially Ordered Macromolecular Systems, Prague, Czech Republic, July 21-24, 2003

17th Bratislava International Conference on Macromoleculaes. Molecular Characterization of Polymers, Bratislava, Slovakia, August 24-28, 2003

Interfaces and Interphases in Multicomponent Materials, Balatonfüred, Hungary, Oct 5-8, 2003

1st International Conference on Bio-based Polymers (ICBP 2003), Saitama, Japan, Nov 12-14, 2003

8th Pacific Polymer Conference, Bangkok, Thailand, Nov 24-27, 2003

2004 (10 conferences)

12th Annual Polychar World Forum on Advanced Materials, Guimaraes, Portugal, Jan. 5-9, 2004

7th Annual UNESCO School/IUPAC Conference on Polymer Properties, Stellenbosch, South Africa, April 5-8, 2004

8th World Conference on Biodegradable Polymers and Plastics, Seoul, Korea, June 1-4, 2004

2nd International Symposium on Macro- and Supramolecular Architectures and Materials (MAM-04), Missoula, MT, USA, June 13-17, 2004

World Polymer Congress 2004 - 40th IUPAC 40th Int. Symposium on Macromolecules, Paris, France, July 4-9, 2004

43rd PMM Microsymposium: Polymer Biomaterials; Biomimetic and Bioanalogous Systems, Prague, Czech Republic, July 12-15, 2004

11th International Conference on Polymers and Organic Chemistry, Prague, Czech Republic, July 18-23, 2004

Polymer Networks 2004, Bethesda, MD, USA, August 15-19, 2004

Biological Polyesters (ISBP2004), Beijing, China, August 22-28, 2004

5th International Symposium on Natural Polymers and Composites, Sao Pedro, Brazil, September 12-15, 2004

2005 (11 conferences)

Joint Meeting of the 8th European Symposium on Polymer Blends and Fillers 2005, Bruges, Belgium, May 9-12, 2005

8th Annual UNESCO School & IUPAC Conference on Macromolecules, Reduit, Mauritius, June 4-9, 2005

5th International Symposium on Molecular Mobility and Order in Polymer Systems, St. Petersburg, Russia, June 20-24, 2005

23rd Discussion Conference PMM, Current Trends in Polymeric Materials, Prague, Czech Republic, June 26-30, 2005

67th Prague Meeting on Macromolecules, Polymer Gels and Networks, Prague, Czech Republic, July10-14, 2005

ERPOS 10 – Electrical and Related Properties of Organic Solids and Polymers, Corsica, France, July 11-16, 2005

8th Society of Polymer Science, Japan International Polymer Conference (IPC 2005),Fukoka, Japan, July 26-29, 2005

8th International Symposium: Polymers for Advanced Technology, Budapest, Hungary, September 13-16, 2005

11th International Symposium on Macromolecule-Metal Complexes, Tirrenia, Italy, September18-22, 2005

15th International Symposium on Fine Chemistry and Functional Polymers (FCFP-XV), Shanghai, China, October 17-20, 2005

International Symposium on Ionic Polymerisations and Related Processes, Goa, India, October 23-28, 2005

2006

12th International Conference on Polymers and Organic Chemistry (POC'06), Okazaki, Japan, July 2-7, 2006

World Polymer Congress MACRO 2006, 41st IUPAC International Symposium on Macromolecules, Rio de Janeiro, Brazil, July 16-21, 2006

International Symposium on Radical Polymerisation Kinetics and Mechanism, Il Ciocco/Castelvecchio Pascoli, Italy, September 3-9, 2006

2007

Polymer Conference on the Mission & Challenges of Polymer Science and Technology II, New York, June, 2007

2008

World Polymer Congress MACRO 2008, 42nd IUPAC International Symposium on Macromolecules, China/Taipei, 2008 (provisional)

2010

World Polymer Congress MACRO 2010, 43rd IUPAC International Symposium on Macromolecules, Glasgow, U.K. (provisional)

Publications

Conference Publications

1. 10th International Symposium on Macromolecule-Metal Complexes Moscow, Russia, May 20-24 *ed. T. M. Birshtein* Macromol. Symp. **191**, 1-200 (2003)

2. 5th Annual School and IUPAC Conference on Macromolecules and Material Science, Stellenbosch, South Africa, March 2002 *eds. H. Pasch, R. D. Sanderson*

Macromol. Symp. 193, 1-304 (2003)

3. 39th International Conference on Macromolecules-IUPAC World Polymer Congress (MACRO 2002), Beijing, China, July 2002 *ed. M. Xu*Macromol. Symp. **195**, 1-327 (2003)

4. Metal and Metalloid Containing Macromolecules, Ottawa, Canada, August 10-15, 2003 ed. A.S. Abd-El-Aziz

Macromol. Symp. 196, 1-353 (2003)

 $5.\,7^{th}$ World Conference on Biodegradable Polymers and Plastics, Tirenia, Pisa, Italy, June $4\text{-}8,\,2002$

eds. E. Chellini, R. Solaro Macromol. Symp. **197**, 1-466 (2003)

6. 16th Polymer Network Group Meeting, Polymer Networks 2002, Autrans, France, 2-6 Sept. 2002

ed. E. Geissler

Macromol. Symp. 200, 1-296 (2003)

7. Mission and Challenges of Polymer Science and Technology, Kyoyo, Japan, 2-5 Dec. 2002, *eds. K. Horie, A, Abe* Macromol. Symp. **201**, 1-325 (2003)

8. Polymer-Solvent Complexes and Intercalates, 63rd Prague Macromolecular Meeting, Prague, Czech Republic, July 21-25, 2002 *eds. J. Spevacek, J. Kahovec* Macromol. Symp. **203**, 1-338 (2003)

 $9.\ 10^{th}$ International Symposium on Macromolecule-Metal Complexes, Moscow, Russia, May $18\text{-}23,\ 2003$

eds. E. Karakhanov, A. Maksimov Macromol. Symp. **204**, 1-294 (2003) 10. Electrical and Related Properties of Polymers and Other Related Solids, Prague, Czech Republic, July 14-18, 2002

ed. J. Kahovec

Macromol Symp. 212, 1-580 (2004)

11. 6th Annual UNESCO School/IUPAC Conference on Polymer Properties, Mpumalanga, South Africa, April 14-17, 2003

eds. R.D. Sanderson, H. Pasch

Macromol. Symp. 214, 1-379 (2004)

12. International Symposium on Ionic Polymerization, Boston, USA, June 30 - July 4, 2003 eds. J. W. Mays, R. F. Storey

Macromol. Symp. 215, 1-383 (2004)

13. 8th Pacific Polymer Conference, Bangkok, Thailand, Nov 24-27, 2003 eds. S. Supaphol, S. Tantayanon

Macromol. Symp. 216, 1-306 (2004)

14. Spectroscopy of Partially Ordered Macromolecular Systems, Prague, Czech Republic, July 21-24, 2003

ed. J, Kahovec

Macromol. Symp. 220, 1-175 (2005)

15. 8th World Conference on Biodegradable Polymers and Plastics, Seoul, Korea, June 1-4, 2004

eds. S. S. In, Y. H. Kim. J. S. Yoon, I.-J. Chin

Macromol. Symp. 224, 1-376 (2005)

16. 7th Annual UNESCO School/IUPAC Conference on Polymer Properties, Stellenbosch, South Africa, April 5-8, 2004

eds. R. D. Sanderson, H. Pasch

Macromol. Symp. 225, 1-237 (2005)

Strategy

17. The Missions and Challenges of Polymer Science and Technology R.F.T. Stepto, K. Horie, T. Kitayama and A. Abe

Pure and Applied Chemistry **75**, 1359-69 (2003)

18. Molecular Structure and Dynamics of Proteins in Solution: Insights Derived from High Resolution NMR Approaches

D. A. Torchia, R. Ishima

Pure and Applied Chemistry **75**, 1371-81 (2003)

19. Rotaxanes and Catenanes as Prototypes of Molecu;lar Machines and Motors *C. Detrich-Buchecker, M. C. Jimenez-Molero, V. Sartor, J. P. Sauvage* Pure and Applied Chemistry **75**, 1383-93 (2003)

20. Challenges in Polymer Physics *M.Doi*

Pure and Applied Chemistry 75, 1395-1402 (2003)

Structure - Property Characterization of Commercial Polymers

21. Melt Rheology and Concomitant Morphology of a Model Binary Mixture of Polyethylene and Polystyrene (Polyblend)

A. P. Plochocki

Pure and Applied Chemistry, *resubmitted 2005* (Project 421/15/86)

22. Characterisation of Flow Behaviour and Properties of Liquid Crystal and Aromatic Polymers

J. L. S. White, L. Dong, P. Han and H.M. Laun Pure and Applied Chemistry, *submitted 2001* (Project 421/20/87)

23. Blends Containing Core-Shell Impact Modifiers. Part 4: Fatigue Behaviour *C. B. Bucknall* Plastics Rubber & Composites **33**, 234-241 (2004) (Project 421/29/91)

24. Blends Containing Core-Shell Impact Modifiers. Part 5: Fracture in Dart-Drop and Notched Bending Tests

C. B. Bucknall

Plastics Public & Compositos 33, 241, 248 (2004)

Plastics Rubber & Composites **33**, 241-248 (2004) (Project 421/29/91)

- 25. Structure and Properties of Hydrogenated Acrylonitrile-Butadiene Rubber (HNBR). Part I. Relation between Viscosity and Intermolecular Interaction in Dilute Solution States *T. Kobatake, A. Yoshioka, K. Nakayama, J. He, Y. Aoki, T. Masuda* Pure and Applied Chemistry, *in preparation* (Project 421/31/93)
- 26. Structure and Properties of Hydrogenated Acrylonitrile-Butadiene Rubber (HNBR). Part II. Relation between Viscosity and Intermolecular Interaction in Condensed States *T. Kobatake, A. Yoshioka, K. Nakayama, J. He, Y. Aoki, T. Masuda* Pure and Applied Chemistry, *in preparation* (Project 421/31/93)
- 27. Rheological and Mechanical Properties of Poly(α-methylstyrene-co-acrylonitrile)/poly(methylmethacrylate) Blends in Miscible and Phase Separated Regimes of Various Morphologies. Part 4. Influence of the Morphology on the Mechanical Properties *V. Altstädt, L. de Lucca Freitas & D. W. Schubert* Pure and Applied Chemistry 76, 389-413 (2004) (Project 421/33/95)

28. Property Improvement via Interfacial Chemical Reaction - Reactive Extrusion of Polyamide 12 and Maleic Anhydride Grafted Ethylene Propylene Copolymer Rubber *J. E. Curry, P. S. Hope and J. G. Bonner* Pure and Applied Chemistry 2004, *in press* (Project 421/34/95)

29. Influence of Long Chain Branching on Linear Viscoelastic Flow Properties and Dielectric Relaxation of Polycarbonates *C. Liu, C. Li, P. Chen, J. He and Q. Fan* Polymer **45**, 2803-2812 (2004)

(Project 421/35/97)

30. Characterisation and Rheological Properties of Three Polycarbonates with Side-Chain Branching

M. Takahashi, K. Sato, P. Tas, J. He, M. Lecomte and T. Masuda Pure and Applied Chemistry, in preparation 2002 (Project 421/35/97)

31. Characterisation, Rheological Properties and Processability of Three Polycarbonates with Side-Chain Branching

M. Takahashi, K. Sakai, K. Sato, J. He, P. Tas and T. Masuda Pure and Applied Chemistry, in preparation (Project 421/35/97)

32. Quantifying Scratch Resistance of Commercial Polymers *R. Bailey, et al.*Pure and Applied Chemistry, *in preparation*(Project 1999-020-1-400)

33. Thermal Degradation Studies on Cyclic Olefin Copolymers *C. Liu, J. Yu, X. Sun, J. Zhang and J. He*J. Polymer Degradation and Stabilty **81**, 197-205 (2003) (Project 1999-039-1-400)

34. Chemical Structure and Physical Properties of Cyclic Olefin Copolymers *J. Y. Shin, J. Y. Park, C. Liu, J. He and S. C. Kim*Pure and Applied Chemistry **77**, 801-814 (2005)
(Project 1999-039-1-400)

35. Morphology and Micromechanical Behaviour of Ethylene Cycloolefin Copolymers V. Seydewitz, M. Krumova, G. H. Michler, J. Y. Park and S. C. Kim Polymer **45**, 5608-5614 (2005) (Project 1999-039-1-400)

36. Dependence of Zero-Shear Viscosity and Steady-State Compliance on Molecular Weight between Entanglements for Ethylene-Cycloolefin Copolymers *T. Takigawa, H. Kadoya, T. Miki, T. Yamamoto and T. Masuda* Rheologica Acta, *submitted* (Project 1999-039-1-400)

37. Dynamic Birefringence of Cyclic Olefin Polymers

O. G. Kyo and T. Inoue

Rheologica Acta, in press

(Project 1999-039-1-400)

38. Rheological Properties of Cyclic Olefin Copolymers

T. Takigawa, D. Dijkstra and J. He

Pure and Applied Chemistry, in preparation

(Project 1999-039-1-400)

39. Mechanical and Dynamic Mechanical Properties of Cyclic Olefin Copolymers

K. Nitta, K. Nakayama and G. Michler

Pure and Applied Cemistry, in preparation

(Project 1999-039-1-400)

Molecular Characterization of Polymers

40. Characterization of Polyamides 6, 11 and 12; Determination of Molecular Weight by Size Exclusion Chromatography

E.C. Robert, R. Bruessau, J. Dubois, B. Jacques, N. Meijerink, T.O. Nguyen, D.E.

Niehaus and W.A. Tobisch

Pure and Applied Chemistry (2004)

(Project 422/6/98)

41. Molecular Characterization of Epoxy Resins by Liquid Chromatography

S. Podzimek et al.

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IUPAC Analytical Chemistry Division (V)

Report to Council, 2003 - 2005

I. Executive Summary

- The Division has made significant moves to build partnerships with
 - organizations that have experience in developing countries (IAEA, UNIDO, IOCD, SEANAC),
 - other unions and expert bodies (IUPAP, BIPM, IUGS).
- The Division is coordinating a series of articles for Chemistry International on the topic of "Emerging needs of developing countries". This series should run for 8-10 issues and will carry contributions from several Divisions.
- The Division has started a significant number of inter-Divisional projects. These link us with Divisions I, III, IV, VI and VII, and with COCI.
- To ensure attention to critical areas it has identified a limited number of "priorities" for the biennium. It has focused its energy on these.
- To cultivate a spirit of "collective responsibility" it has formed seven Teams, each with responsibility for one priority area. All NR, AM and TM are assigned to one or two teams. The Team structure should facilitate continuity of effort into the next biennium.
- Communication within the Division and with other officers of the union is maintained through the electronic newsletter "Teamwork".
- The Division is working on the maintenance and updating of two key IUPAC publications, The Compendium of Analytical Nomenclature (Orange Book) and the IUPAC Stability Constant Database (SCDB).
- To facilitate the development of new projects the Division involved external experts in a mini-symposium on "*Metrological traceability*" held at the IAEA in conjunction with its even-year meeting.

II. Report on Division activities in relation to IUPAC goals

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

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

Core Activities:

Communication

Project initiation and management in the areas of:

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

Emerging issues in analytical chemistry:

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

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

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

Communication.

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

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

Global issues.

One global issue being addressed is the measurement of pH, through the project: Comparable pH measurements by metrological traceability. Part I: Water quality monitoring and assessment; Part II: Clinical and biochemical matrices. This project sees a continuation of work by the "pH task group" [Measurement of pH. Definition, Standards and Procedures. 2002] and it has the financial and professional backing of three Divisions and COCI.

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

- (a) A successful joint project proposal with IOCD which includes two Division V members, titled: "Standardisation of analytical approaches and analytical capacity building in Africa". This project involves a melding of IUPAC technical expertise with IOCD appreciation of geopolitical issues in developing countries.
- (b) Division V support for the WPQA in the preparation of an ICSU proposal on "Measurement traceability a fair basis for trade". This application for funds was not successful but the process of preparing the proposal generated very positive interactions with project partners UNIDO and IUPAP (including their participation in a WPQA/Division V workshop).

Symposia and Workshops.

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

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

At the even-year meeting in Vienna 2004 a mini-symposium on "*Metrological traceability*" was held jointly with IAEA staff and the WPQA. It attracted speakers from IUPAP, UNIDO, BIPM, IAEA and WPQA. The meeting identified several areas in which IUPAC expertise might be applied. We now try to identify possible 'concrete' outcomes from that meeting - IUPAC projects that could be crafted

around the ideas and concerns that were shared. IUPAC will benefit through any projects that link it with agencies that are working much closer to the geopolitical coal-face.

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

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

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

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

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

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

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

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

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

- (c) **The Working Party on Quality Assurance** continues to produce publications that are of value to chemists in analytical laboratories; e.g. Revision of the IUPAC/ISO/AOAC protocol for proficiency testing; Harmonised guidelines for single-laboratory validation of methods of analysis; and Terminology for soil sampling. The WPQA will make a major presentation at the GA on "Metrological Traceability of Results in Chemical Measurement."
- (d) The Solubility and Solution Equilibrium Data sub-committee (SSED) has a very active program of projects that embrace the critical evaluation of solubility data related to (a) mobility of metals in the environment, (b) industrial processes, (c) human health. The outputs appear as papers in the Journal of Physical and Chemical Reference Data or as

book volumes and are thence transferred to the NIST-IUPAC Solubility Database: http://srdata.nist.gov/solubility/. A significant new project is a 25-Chapter book volume on "Solubility for Industry". Another project is concerned with Chemical speciation of environmentally significant heavy metals with inorganic ligands.

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

Chemistry-related industry is served by the active program of critical evaluations of solubility data and of solution equilibrium data, and by the continuance of data evaluation and compilation for the IUPAC Stability Constant Database. The current projects on pH (*Comparable pH measurements by metrological traceability.*) and metrological traceability (*Metrological Traceability of Results in Chemical Measurement*) are highly relevant to industry. The SSED were joint organisers of the 11th International Symposium on solubility phenomena (Aviero, 2004) at which there was significant emphasis on industrial issues and involvement of industrial chemists (*PAC*, 77(3), 2005).

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

Analytical Chemistry in Developing countries

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

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

Building bridges with other organisations.

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

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

Better Communication.

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

The Division has been pro-active in recommendations for improved IUPAC representation at conferences. It considers that there is scope for enhanced involvement of IUPAC representatives at IUPAC-sponsored conferences. This could be aided if conference organisers were required to discuss the nomination of an IUPAC representative with the relevant Division ahead of submitting the AIS. It is all too easy for Conference programs to be 'finalised' ahead of representative appointment, or without reference to IUPAC requirements.

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

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

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

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

III. Challenges and Solutions

The principal challenges to the ACD are typical of many IUPAC Divisions:

- The breadth of its portfolio.
- The generation of members' collective responsibility for
 - the goals of the Division
 - the needs of countries not represented
 - the long-range goals of IUPAC
- Maintaining momentum through the biennium and with the change of biennia.

Strategy adopted by the ACD to address these challenges:

- Identification of a manageable number of priorities for the biennium.
- Formation of Teams, each with collective responsibility for one priority area.
- Effort focused on the needs of developing countries and on links with other agencies.
- Use of mini-symposia to bring in external expertise.
- Maintaining active communication between members, e.g. through the newsletter, Teamwork.

IV. CURRENT PROJECTS

*Interdivisional projects

1999-044-2-500 - Terminology for the description of peak asymmetry in chromatography

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

2000-003-1-500 - <u>lonic strength corrections for stability constants</u>

2000-004-2-500 - IUPAC stability constants database - completion of data collection up to 2000+

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

2001-063-1-500 - Revision of terminology of separation science

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

2002-002-2-500 - Recent advances in electroanalytical techniques: characterization, classification and terminology

2002-003-2-500 - <u>Performance evaluation criteria for preparation and measurement of macro and microfabricated ion-selective electrodes</u>

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 - <u>Terminology</u>, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry

2003-037-1-500 - Optical biosensors and bioprobes; Series on Nomenclature, Symbols, and Units in Spectrochemical Analysis

2003-056-2-500 - Standard definitions of terms relating to mass spectrometry*

2004-005-2-500 - Comparable pH measurements by metrological traceability*

2004-016-2-500 - Guidelines for potentiometric measurements in suspensions

2004-017-1-500 - Standardization of analytical approaches and analytical capacity-building in Africa*

2004-041-1-500 - Uncertainty estimation and figures of merit for multivariate calibration

INTERDIVISIONAL WORKING PARTY ON HARMONIZATION OF QUALITY ASSURANCE

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

2003-004-1-500 - Interdisciplinary harmonised approach to metrological traceability of chemical measurement results

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

2001-052-1-500 - Solubility of volatile and gaseous fluorides in all solvents

2002-025-1-500 - <u>Solubility data of compounds relevant to mobility of metals in the environment.</u> Inorganic actinide compounds

2002-031-1-500 - <u>Solubility data of compounds relevant to mobility of metals in the environment.</u>
Alkaline earth metal carbonates

2002-032-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates

2002-033-1-500 - <u>Solubility data related to oceanic salt systems</u>. Part I - Binary systems containing sodium, potassium, and ammonium sulfate

2002-034-1-500 - Solubility data related to oceanic salt systems. Part II - magnesium chloride-water and calcium chloride-water and their mixtures

2002-035-1-500 - Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis

2002-036-1-500 - Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates

2002-037-1-500 - Solubility data of compounds relevant to human health. Solubility of haloganated aromatic hydrocarbons

2002-038-1-500 - Solubility data of compounds relevant to human health. Antibiotics: peptide antibiotics and macrocyclic lactone antibiotics

2002-042-1-500 - Solubility data related to industrial processes. Lead sulfate

2002-043-1-500 - Solubility data related to industrial processes. Carbon dioxide and the lower alkanes at pressures above 2 bar: methane to butane

2002-044-1-500 - <u>Solubility data related to industrial processes</u>. <u>Carbon dioxide in aqueous non-electrolyte solutions</u>

2002-045-1-500 - Solubility data related to industrial processes. Solids and liquids in supercritical carbon dioxide

2002-050-1-500 - Solubility data related to industrial processes. Acetonitrile: ternary and other multicomponent systems

2003-018-1-500 - Mutual solubility of hydrocarbons and water (update of SDS Vol 37 & 38)

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

OTHER INTERDIVISIONAL PROJECT

2003-011-3-600 - A critical compendium of pesticide physical chemistry data

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

2004-021-1-300 - Reference methods, standards and applications of photoluminescence

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

PROJECTS NEAR COMPLETION / IN PRESS

510/31/95 - Nomenclature for X-ray emission spectroscopy

550/64/97 - Non-selective sensors arrays ("Electronic Nose", "Electronic Tongue") chemical analysis: classification and characterization

2001-055-1-500 - Critical evaluation of stability constants of metal complexes of complexones for biomedical and environmental applications

2001-038-2-500 - Recommendations for NMR measurements of high pK values and equilibrium constants in strongly basic solutions

2001-009-1-500 - Revision in the international harmonised protocol for the proficiency testing of (chemical) analytical laboratories

PUBLISHED REPORTS (2004-2005)

523/2/89 - <u>Determination of trace elements bound to soil and sediment fractions</u>. <u>Pure Appl. Chem.</u> 76(2), 415-442, 2004

550/47/89 - Electrochemical detection in flowing media: Classification and recommendation. *Pure Appl. Chem.* 76(6), 1119-1138, 2004

510/35/97 - Guidelines for calibration in analytical chemistry. Part 2: multicomponent calibration. *Pure Appl. Chem.* 76(6), 1215-1225, 2004

550/62/97 - Electroanalysis with piezo-electric devices. *Pure Appl. Chem.* 76(6), 1139-1160, 2004 1999-050-1-500 - Chemical speciation of environmentally significant heavy metals and inorganic ligands. Part I Mercury. *Pure Appl. Chem.*, 77(4), 739-800, 2005. Chemical speciation of Hg(II) with environmental inorganic ligands. *Australian J.Chem.*, 57, 1-8 (2004)

2000-033-1-500 - Assessment of uncertainty associated with soil sampling in agricultural, seminatural, urban and contaminated environments (SOILSAMP). *Pure Appl. Chem.* 77(5), 827-841, 2005

2001-021-1-500 - Analytical electromigration techniques. Pure Appl. Chem. 76(2), 443-451, 2004.

2001-025-1-500 - <u>Critical evaluation of the state of the art of the analysis of light elements in thin films</u>. <u>Pure Appl. Chem. 76(6), 1161-1213, 2004</u>

2001-075-1-500 - Compilation of k0 and related data for NAA in the form of electronic database. *Pure Appl. Chem.* 76(10), 1921-1925, 2004

2001-085-1-500 - <u>IA and IIA azoles, cyanates, cyanides and thiocyanates. *J. Phys. Chem. Ref. Data* 2004, **33**, No. 1, 1-176.</u>

IUPAC REPRESENTATION AT CONFERENCES

Inaugural Conference for the Southern and Eastern Africa Network of Analytical Chemists (SEANAC), 7-10 July 2003, Gaborone, Botswana.

Colloquium Spectroscopicum Internationale 33rd Colloquium Spectroscopicum Internationale, 2003,7-12 September 2003, Granada, Spain.

Solubility Phenomena 11th International Symposium on Solubility Phenomena, Including Related Equilibrium Processes (11th ISSP), 25-29 July 2004, Aveiro, Portugal.

Trace Elements in Food, 2nd International Symposium on Trace Elements in Food (TEF 2),7-8 October 2004, Brussels, Belgium.

Analytical Forum 2004, July 2004, Warsaw, Poland.

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

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



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

January 2004 – June 2005

Kenneth D. Racke

1. HIGHLIGHTS

1.1 Terms of Reference

Through its internationally recognized membership and project teams, the Division of Chemistry and the Environment (DCE) will provide unbiased and timely authoritative reviews on the behavior of chemical compounds in food and the environment. The DCE will undertake both fundamental and applied evaluations that contribute to solving environmental problems and enhancing the quality of food on a global scale (revised May-2004).

1.2 Organization

The Division Committee is currently comprised of 10 TM's, 7 AM's, and 6 NR's. The 7th AM was a new position added during 2004 to accommodate a closer working relationship with IOCD. A new Division President assumed responsibilities during 2004. Several of the newly elected members for the 2004-2005 biennium are from outside the IUPAC family and have brought fresh perspectives. The work of the Division Committee is assisted by the efforts of several subcommittees, which help identify new priority project areas, stimulate proposals and recruit potential project leaders, and facilitate external communication encompassing the broad areas of environmental and food chemistry:

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

Unfortunately Dr. Dysseler has been hospitalised with a serious illness for a significant portion of this reporting period.

1.3 Projects

Projects sponsored by the DCE generally fall into three broad categories. First, state-of-the-art **authoritative reviews** of a particular area of environmental chemistry are developed and published in book form. To this end, the Division has a long-standing working partnership with Wiley Press. Second, **technical evaluations** focus on critical assessment and development of specific recommendations for an area of environmental chemistry so as to assist and influence research and

public policy. Primary areas of emphasis include definitions, methodologies, and regulations. Third, **outreach** activities help move IUPAC project outcomes outside the small circle of specialists and into the broader scientific and regulatory arena, with a strong emphasis on technology transfer to developing countries. These outreach activities include both regional workshops and international congresses that maintain a high level of IUPAC involvement and serve to highlight ongoing and completed IUPAC projects.

During the period of this report the Division completed 8 projects and terminated 1 moribund project. From a total of 13 submitted project proposals, 7 new projects have been accepted and funded by the Division, including 3 with interdivisional participation. This brings the total number of active projects to 22 as of June 2005 (see section 5).

1.4 Collaboration

The Division has maintained historically strong collaboration with a number of external bodies including several Codex committees, FAO, International Standard Organization (ISO), Intergovernmental Forum on Chemical Safety (IFCS), and ICSU Scientific Committee on Problems of the Environment (SCOPE). The Division has recently moved to increase collaboration with the WHO International Program on Chemical Safety (IPCS), Association of Official Analytical Chemists International (AOAC), International Organization for Chemistry in Development (IOCD), and International Union of Soil Sciences (IUSS). Within IUPAC, DCE has recently cultivated increased collaboration with the Analytical Chemistry Division (V), and as a result two interdivisional projects have recently been initiated.

2. PROJECT ACTIVITIES

Examples of some of the project activities of DCE during the reporting period are provided below in relation to several of the long-range goals established by IUPAC. This is only a sampling, but should provide insight into the project areas of greatest involvement for the Division.

- 2.1 IUPAC will provide leadership as a worldwide scientific organization that objectively addresses global issues involving the chemical sciences.
- Impact of Transgenic Crops on the Use of Agrochemicals and the Environment (2001-24-2-600). This topic area is of the utmost interest with respect to current scientific, regulatory, political and public perception issues surrounding transgenic crops and provides an opportunity for IUPAC to take important leadership roles in promoting the importance of chemistry in molecular biology.
- 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.

- International Workshop "Fats, Oils and Oilseeds Analysis and Production" Tunis, Tunisia, December 2004 (2002-011-2-600). Organized by IUPAC and AOCS in cooperation with the Tunisian Office National de l'Huile (ONH), the American Soybean Association (ASA), and the International Olive Oil Council (IOOC). This workshop continued a series supported by IUPAC, the last in Brasil in 2000. The analytical sessions provided support for the oil refining/oil processing sessions. Tunisian oil experts were included in the program and served as a focus for developing nations to obtain information critical to upgrading their food processing systems.
- International Workshop "Crop protection chemistry in Latin America", San Jose, Costa Rica, February 2005 (2003-013-1-600) Organized by IUPAC in cooperation with the Costa Rica Ministry of Agriculture, the University of Costa Rica, and the agrochemical industry association CropLife Latin America. This workshop continued a series supported by IUPAC-DCE, the last in Korea in 2003. Major topics included pesticide environmental fate and impacts, analysis and monitoring of residues, risk assessment, and regulation. It served as a focus for regional efforts to improve their research and regulatory systems in these areas.
- XI International IUPAC Symposium on Mycotoxins and Phycotoxins, Maryland, USA, May 2004. This symposium was only the latest in a long-standing series that has become the premiere forum for exchange of research results and methodologies related to these important naturally occurring toxins. The traditional strength of IUPAC as related to the chemistry aspects of these biotoxins has been an important factor in the success of this series. The next symposium is now being planned for Istanbul, Turkey in 2007.
- "Environmental Chemistry & Green Chemistry" Symposium at 40th IUPAC Chemistry Congress, Beijing, August 2005. The Division has taken leadership in organising this session, along with Professor Xiaoba Xu (China). DCE will provide 6 of the 10 plenary speakers giving overview lectures on environmental research of international significance.
- 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.
- 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.
- Glossary of Atmospheric Chemistry (2003-030-1-600) and Glossary of Pesticide Chemistry (2004-002-1-600). These two projects are approaching completion and are providing authoritative updates of existing IUPAC recommended definitions. Both printed and internet-based versions are envisioned. Collaboration with WHO-IPCS and OECD is being pursued to enable the broadest possible acceptance of the revised IUPAC recommendations.
- Terminology and Measurement Techniques of Starch Components (2004-022-3-400). This recently approved project will provide internationally needed guidance on the terminology for these very important food components of the complex carbohydrate class. Starches present a

- number of difficult issues relating to both terminology and methods for determination which are of importance to nutrition, food quality and international trade.
- Wiley-IUPAC book series "Analytical and Physical- Chemistry of Environmental Systems" Professor Nicola Sensi provides the impetus at the Divisional level for the continuing publication of this series of multi-chapter critical-reviews (Series Editors, J. Buffle and H. Van Leeuwen). No. 9 in the series "Physicochemical Kinetics and Transport at Chemical-Biological Membranes" was published in 2004. Two current projects are producing volumes No. 10 and 11: "Biophysico-Chemistry of Fractal Structures and Processes in Environmental Systems" (2003-014-2-600) and "Environmental Colloids: Behaviour, Structure & Characterisation" (2004-015-1-600). A related project is producing another book to be published by Wiley but not in the above series: "Biophysico-chemical process of heavy metals and metalloids in soil environments" (2004-003-2-600). The highest academic standards are being maintained in these books through the careful selection of the chapter authors and thorough review and editing procedures. This ensures the credibility of IUPAC remains in these areas of environemental physico-biological chemistry.
- 2.3 IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.
- Development of Simplified Methods for Ecological Risk Assessment of Pesticides (2004-011-1-600). This 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. A project team consisting of leading government, industry, and academic modellers and risk assessment experts has been assembled to make rapid progress.
- Standardization of Analytical Approaches and Analytical Capacity-Building in Africa (2004-017-1-500). See above.
- Regional Pesticide Chemistry Workshops. During the past 15 years DCE has sponsored a series of regional workshops focused on broadening the adoption of harmonized, international approaches to pesticide research and regulation in developing countries. 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 IUPAC-University of Costa Rica Workshop on Crop Protection Chemistry in Latin America (2003-013-1-600) was held in San Jose during February 2005 and had a similar impact on the Central American and Andean regions.
- Regional Workshops on Fats, Oils, Oilseeds Analysis and Production The first such IUPAC workshop on this topic occurred in Brazil during 2000 (1999-042-1-600). The second workshop, in what hopefully will become a standing series, was held in Tunis, Tunisia during December 2004 (2002-011-2-600) and was targeted at the important vegetable oil-exporting region of North Africa.

3. FUTURE OPPORTUNITIES AND DIRECTION

To remain effective and maintain relevance, the Division will need to pay attention to both current strengths and weaknesses of the IUPAC approach, and seek a way forward that takes advantage of

the opportunities while avoiding looming threats. The Division Committee recently took the first steps toward development of a long-range Division activities plan in alignment with the IUPAC long-range goals.

One immediate outcome of the long-range planning exercise involves a move to reinvigorate the area of food chemistry. Through past mergers of Commissions with divergent interests (oils and fats standardized methods vs. food-borne mycotoxin chemistry) and subsequent disbandment of the hybridized Food Chemistry Commission, the current level of expertise for food chemistry available to IUPAC has been depleted and food chemistry-related project activities have been reduced. A new sub-committee has organized a half-day workshop in Beijing to reexamine the IUPAC approach to food chemistry and chart a new direction which brings to bear the traditional strengths of the Union with contemporary issues and problems related to food chemistry.

4. **PUBLICATIONS (January-2004 to June-2005)**

- Anklam, E.; Stroka, J. "Collaborative Trial Tests for Method Validation: Lessons to be Learned." *Chem. Int.*, (**2004**) 26:7-9.
- Cantrill, R.; Dysseler, P. "Report on the IUPAC-AOCS Workshop on Fats, Oils, and Oilseeds Analysis and Production." *Chem. Int.* (2005) 27 (in press).
- Carazo, E.; Racke, K.D. (eds.) *Proceedings of the IUPAC-UCR-MAG Internat Workshop on Crop Protection Chemistry in Latin America*. University of Costa Rica, San Jose, (2005) 217 pages.
- Hamilton, D.J.; Ambrus, A.; Dieterle, R.; Felsot, A.; Harris, C.; Petersen, P.; Racke, K.; Wong, S., Gonzalez, R.; Tanaka, K.; Earl, M.; Roberts, G.; Bhula, R. "Pesticide Residues in Food: Acute Dietary Exposure." *Pest Manag. Sci.* (2004), 60:311-339.
- Koester, W.; Van Leeuwen, H. (eds.) *Physicochemical Kinetics and Transport at Chemical-Biological Membranes*, Series on Analytical and Physical Chemistry of Environmental Systems, Vol. 9, John Wiley & Sons, New York (**2004**) 576 pages
- Racke, K.D. "Pesticide Science Harmonization of Data Requirements and Evaluation. Report on Workshop" *Chem. Int.* (**2004**) 26:18-20.
- Slanina, S.; Zhang, Y. "Aerosols: Connection between Regional Climate Change and Air Quality." *Pure Appl. Chem.* (**2004**) 76:1241-1253.
- Zhang, Y.; Zhu, X.; Slanina, S.; Shao, M.; Zeng, L.; Hu, M.; Bergin, M.; Salmon, L. "Aerosol Pollution in Some Chinese Cities." *Pure Appl. Chem.* (2004) 76:1227-1239.

5. ACTIVE PROJECTS (as of June-2005)

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

IUPAC Division VII. Chemistry and Human Health

Council Report: 2003-2005

I. Executive Summary

The merger of the former Medicinal Chemistry and Clinical Chemistry/Toxicology Sections into the Division of Chemistry and Human Health (VII) has proven to be an effective way for the IUPAC to oversee and allocate funding to each of these areas while using a condensed administrative infrastructure. To promote the core of expertise required to support the technical diversity afforded by these areas, Division VII, in turn, maintains three, standing Subcommittees led by appointed Chairpersons who are recognized internationally within each of their fields. These Subcommittees (and their respective Chairpersons) are: (i) Medicinal Chemistry and Drug Development (MC; C. Robin Ganellin); (ii) Nomenclature, Properties and Units in Laboratory Medicine (C-NPU; Urban Forsum); and, (iii) Toxicology and Risk Assessment (TOX; John Duffus). A fourth subcommittee, also led by an appointed Chairperson (Tom Perun), has additionally been organized to deal with the IUPAC nomination and election processes for the Division. While a few members of each Subcommittee also sit on the Division Committee, the majority of the technical Subcommittee members are drawn as volunteers from each of these fields, respectively. The Election Committee has representation from all three technical areas.

The Subcommittees hold independent meetings on a regular basis and each Chairperson provides an update about their activities by either personally attending or forwarding a written report to the Division meetings which, in turn, are held twice each year. This focus of expertise coupled with the broader perspectives afforded during the Division meetings, has proven to be an effective way to encourage and initiate the evaluation of new IUPAC Project submissions, as well as to provide for assessments of ongoing projects and their subsequent impact. Final approval of new projects and additional tracking of ongoing projects, occur at the Divisional level wherein an equitable balance across all activities and the Division VII's IUPAC-allocated funds is sought among all three Subcommittees. Presently, Division VII is carrying 24 projects and has 16 projects undergoing review. It can be additionally noted that these same demarcations of expertise are also used advantageously when projects reach completion wherein final reports, recommendations or other publications then typically require review and/or extensive editing. In this regard, each Chairperson ultimately assumes final responsibility for assuring the quality of products derived from their particular area of expertise.

A representative highlight from each of Division VII's three technical areas follows. One of the most exciting developments within the MC Subcommittee is the recent formation of the 'IUPAC-Richter Prize in Medicinal Chemistry.' Funded by a generous donation from Richter Pharmaceuticals, Ltd. (Budapest, Hungary), this program will recognize one scientist every two years whose work has made a significant contribution to medicinal chemistry within the context of drug discovery and development. Awardees will receive

a \$10,000.00 cash prize at an IUPAC-associated scientific meeting wherein they will be expected to deliver a lecture about their work. Funding has been allocated for five of such awards across ten years. A noteworthy development within the clinical arena is that the C-NPU database (http://dior.imt.liu.se/cnpu) has been upgraded with codes for the most common properties associated with clinical chemistry using mass concentrations along with identifiers for clinical molecular biology, transfusion medicine and immunoheamatology. The database is published on the IFCC homepage (Scientific Division) and on the IUPAC homepage (Division VII) with a link to the server Dior. Both the IFCC and IUPAC are owners of the property (intellectual content and the physical database). Finally, a noteworthy development for the TOX Subcommittee is the nearly completed second edition of the popular text entitled 'Fundamental Toxicology for Chemists.' All existing chapters have been revised and a number of new chapters have been added including 'Pharmaceutical Toxicology,' 'Toxicology in the Clinical Laboratory,' and 'Pathways and Behavior of Chemicals in the Environment.' The new edition will soon be published by the Royal Society of Chemistry.

II. Activities Organized by the Six Goals of the IUPAC Strategic Plan

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

Division VII's organization into three subcommittees allows this objective, as well as all of the other strategic objectives, to be focused within the specific contexts of Clinical Chemistry, Medicinal Chemistry and Toxicological Chemistry. Each Subcommittee brings together a group of experts from around the globe to discuss items relevant to their area. For example, through such discussions, the Medicinal Chemistry group has determined that the global harmonization of patent laws impacting upon the pharmaceutical industry would benefit from a broad consideration of several issues. Toward that end, a project proposal has been drafted to objectively address these issues by starting with a general survey that will be administered globally to a variety of scientists, practitioners and administrators for whom patents are an important aspect of their work. Already approved at the Division level, it is anticipated that a final version of this project proposal will be delivered to the Secretariat during third-quarter 2005.

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

All three of Division VII's Subcommittees remain extremely active in producing glossaries and recommendations for standardization of terms within their respective areas. A quick scan down the list of completed, ongoing and proposed projects indicates our numerous activities in this area (see Section IV. Tabular Material).

Another type of tool that Division VII has effectively deployed is that of the Internet accessible database. The C-NPU database has already been described in the highlights of the Executive Summary (Section I). Similarly, but this time in conjunction with the IUPHAR and the latter's initial funding supplied by the ICSU, Division VII is

constructing an Internet database that will contain human drug metabolism data and will, in turn, be made available to users across the globe via a non-profit basis. With an emphasis on the chemical structures for both the parent drug or xenobiotic and the various metabolic biotransformation products, the Human Drug Metabolism Database (hDMdb) will be extremely useful to both the medicinal and toxicological chemistry arenas. The importance of such projects within the chemical community is only just now beginning to be fully appreciated. For example, statements quoted in a <u>C&E News</u> (June 28, 2004 pages 37-41) article that highlighted an international conference dedicated to 'Charting Chemical Space: Finding New Tools To Explore Biology' indicate that one of the 'grand challenges' elaborated by these well-recognized scientists was an outright appeal for the production of open databases having chemical structures connected to biological properties.

3. Assist the chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement in the quality of life.

Moving forward from one of its earlier publications ('Medicinal Chemistry in the Development of Societies: Biodiversity and Natural Products,' <u>Eur. J. Med. Chem.</u>, **32**, 2000, pages 1121-1125) which specifically addresses the critical role that the pharmaceutical industry can play in developing nations, Division VII is now undertaking follow-up projects that intend to bring workshops on this topic to such countries. Our initial program will target the pharmaceutical industry in India which has heretofore been able to establish strengths in process (scale-up) chemistry but not in the earlier stages of drug discovery and invention, despite their long history with natural product-based remedies and herbal medicines. This undertaking may also be applicable to China and many other Eastern countries. Even less developed nations are being targeted in a somewhat different manner (see Strategic Goal 4.)

4. Foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.

The aforementioned hDMdb project is also applicable to this goal. For example, during a poster presentation about this project at the recent International Society for the Study of Xenobiotics (ISSX) meeting (Vancouver, September, 2004), its 'free-access-for-all' principle was applauded by several scientists from less developed nations who happened to have become engaged in a broader discourse with scientists from some advanced countries who wanted to know if the database might be able to be commercialized so as to generate funding that could move its development along at a faster pace (but with the inherent principle then falling into place that the db would thus be made available only to those who could afford to purchase it).

Continuing from Strategic Goal 3, we have determined that the best follow-up to our earlier publications for countries which are in the very early stages of development in that they completely lack any type of sophisticated chemical industry infrastructure, needs to be approached at a more fundamental level, i.e. by educational programs directed through their budding academic institutions rather than at the industrial level. Division VII's

ongoing projects on basic clinical/medicinal/toxicological chemistry education within the Latin America region represents an initiative along these lines. Also in this regard and similar to all of the other Divisions, Division VII repeatedly votes in favor of IUPAC sponsorship of meetings and conferences applicable to our area whenever they are to be organized or hosted by less developed nations and wherein the caliber of the related chemical technologies is to be held in the highest regard. During the period of this report, Division VII has favorably reacted to about two of such requests for IUPAC sponsorship each quarter.

Finally, along this same theme it can be noted that several members of the MC Subcommittee participated without remuneration in the Brazilian 'XI Summer School in Medicinal Chemistry' (held February 14-18 in Rio de Janeiro) by delivering several lectures to an enthusiastic group of graduated students who attended from various South American countries.

5. Utilize the IUPAC's 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.

Ongoing chemical education initiatives pertinent to human health have been described above for audiences in industry (Strategic Goal 3) and academia (Strategic Goal 4). For the public at large, one additional initiative deserves mention. As a follow-up to our prior, somewhat technical article ('Natural and Non-natural Substances Related to Human Health,' PAC, 74, 2002, pages 1957-1985) Division VII produced a summary version which compares the attributes of synthesized drug versus natural sources for chemical compounds in laypersons terms. Subsequent to publication of the latter in CI, this has now been picked-up within the lay press with translations being effected by other countries as evidenced by the entries noted on the Web-based, Eureka Alert Service.

6. Broaden national membership base and seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender and age.

One of the new project criteria that Division VII has laid in place from the onset during the Subcommittee meetings and then further reinforces at the Division level, is that the proposed project participants list reflects the exact spirit conveyed by this final IUPAC strategic goal. That these participants might then become future members in various IUPAC bodies provides a grass-roots technical approach toward accomplishing this end. Exemplifying this scenario is the fact that the current President of Division VII first became involved with the IUPAC via an invitation to participate on a project about ten years ago and has gradually become more and more active. The same philosophy has been applied to the Subcommittee charged with the Division VII-related nomination and election processes, although in this case there is the possibility that a new member might become immediately involved at a higher administrative level within the IUPAC infrastructure.

In terms of seeking younger members (also applicable to Strategic Goal 5.), Division VII had the pleasant experience of hosting a 'Young Observer' during the Ottawa meeting. To further support this program, Division VII subsequently encouraged this individual to seek IUPAC sponsorship for a symposium that he was trying to set-up in his country. This has all occurred favorably and a full set of proceeding papers covering the symposium's cutting-edge chemistry in the area of nuclear delivery and functional modification by small molecules was recently published in <u>PAC</u>. It is hoped that through such mentoring, this young and rising investigator will gradually become more and more active within the IUPAC as well. Finally, as a US-based scientist, the Division VII President has also become involved with the US National Academy of Sciences IUPAC Relations Committee wherein young observers from the US are selected and mentored. From this relationship, Division VII is scheduled to assist in mentoring two of such young observers during the Beijing meetings.

III. Other Information

After favorable and supportive discussions in Bled, Division VII is beginning to move forward with its plan to raise money to enhance its various activities and meetings associated with its IUPAC endeavors. The fund-raising plan is as follows:

- 1. Subcommittee member/team proposes a fund-raising effort on behalf of his/her/their subcommittee activities and/or project(s).
- 2. Subcommittee Chairperson submits summary to the Division about how funds are to be sought and specifies how the money will be spent in a non-profit manner to enhance the Subcommittee's activities and/or to further support its ongoing projects.
- 3. Division provides approval for Subcommittee to initiate fund-raising effort and forwards the summary to the Secretariat.
- 4. Incoming money is deposited directly into general IUPAC account(s) via Secretariat.
- 5. Secretariat sets-up a "Fund Project" using its Project System mechanism specifying the Subcommittee Chairperson as the Project Leader who can then spend the money via the same expense submission process used for any other projects. No "cuts" will be excised by either the Secretariat or the Division, i.e. 100% of the funds that are raised will be returned to the Subcommittee.

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

Likewise, Division VII is in the process of adopting a more formal 'project tracking system' for our projects in a format that would go out to all Project Leaders on a regularly scheduled basis, e.g. just prior to our DC meetings or at least on an annual basis. Based upon the form already being used by Division V, the Division VII form requests the following information:

- 1. IUPAC Project # and Title:
- 2. Project Leader:
- 3. E-Mail, Telephone # and FAX#:
- 4. Project Start Date:

Amount budgeted:

Recorded Completion Date:

5. Estimate Completion Percentage:

Amount Spent:

Anticipated Completion Date:

What Will Be Delivered First:

6. List of changes in the Project Team's membership (provide complete contact information for any new members):

IV. Tabular Material (2003-2005)

Publications

- 1. R. Dybkaer. Units For Quantities Of Dimension One. <u>Metrologia</u> **41**, 69-73 (2004).
- 2. R. Dybkaer. An Ontology On Property For Physical, Chemical And Biological Systems. APPMIS Supplement 117, **112** (2004).
- 3. P.S. de Araujo, B. Zingales, P. Alia-Ramos, et al. Properties And Units In The Clinical Laboratory Sciences Part XVIII. Properties And Units In Clinical Molecular Biology. <u>PAC</u>, **76**, 1799-1807 (2004).
- 4. M. Nordberg, J.H. Duffus and D.M. Templeton. Glossary of Terms used in Toxicokinetics. <u>PAC</u>, **76**, 1033-1082 (2004).
- 5. M. Nordberg. Glossary of Terms Used in Toxicokinetics. <u>Chemistry International</u>, **26**, No 5, 21 (2004).
- 6. M. Nordberg, Explanatory Dictionary of Concepts in Toxicokinetics. <u>Chemistry International</u>, **26**, No 4, 23-24 (2004).
- 7. D.M. Templeton. Mechanisms of Immunosensitization to Metals. <u>PAC</u>, **76**, 1255-1268 (2004).
- 8. R. Klein, M. Schwenk, R. Heinrich-Ramm, D.M. Templeton. Diagnostic Relevance of the Lymphocyte Transformation Test for Sensitization to Beryllium and Other Metals. <u>PAC</u>, **76**, 1269-1281 (2004).
- 9. J. Duffus, et al. Exposure Assessment and Decision Rules in compliance Testing for Implementation of Exposure Limits. Published.
- 10. Natural and Unnatural Substances Related to Human Health initially published in <u>PAC</u> with follow-up summary in <u>CI</u> by T. Perun and P. Erhardt, and which then prompted several lay press publications during this report period.
- 11. D.M. Templeton et al. Properties and Unites for Transfusion Medicine and Immunohaematology. Published.

Current Projects (all project numbers end in -700)

1999-047-1-	Immunochemistry of Metal Sensitization.
2000-009-1-	Drug Metabolism Terms.
2000-010-1-	Human Drug Metabolism Database.
2000-014-1-	Recommendations for the Use of Nanotechnology in Clinical
	Laboratories.
2001-048-2-	Research and Training in Medicinal Chemistry in India, Pakistan and Sri
	Lanka.
2001-049-2-	Glossary of Terms Used in Process Chemistry/Manufacturing of Active
	Pharmaceutical Ingredients, and Pharmaceutics.
2001-050-2-	Chemical, Pharmacological Aspects of Natural Products with Medicinal
	and Nutritive Value.
2001-053-2-	Fundamental Toxicology for Chemists.
2001-058-1-	Concepts and Structure for Requests in Clinical Laboratories.
2001-066-1-	Global Use of the C-NPU Concept System for Properties in Toxicology.
2001-067-1-	Properties and Units for Function Examinations.
2001-068-1-	Properties and Units in Medical Molecular Biology.
2001-070-1-	Properties and Units for Urinary Calculi.
2002-001-1-	Compendium of Terms Associated With Drug Discovery and
	Development.
2002-051-1-	Analogue-Based Drug Discovery.
2003-001-2-	Explanatory Dictionary of Concepts in Toxicokinetics.
2003-028-1-	Glossary for Chemists of Terms Used in Toxicology: Revision and
	Updating.
2003-044-1-	Glossary of Terms Used in Combinatorial Chemistry.
2003-059-1-	Quantifying the Effects of Compound Combinations.
2004-019-3-	Glossary of Terms Used in Biomolecular Screening.
2004-023-1-	Internationally Agreed Terminology for Observations in Scientific
	Communication.
2004-025-1-	Compendium of Targets of the Top 100 Commercially Important Drugs.
2004-028-1-	Practical Studies for Medicinal Chemistry: An Integrating Approach for
	Developing Countries.
2004-045-01	Training of School children on Pesticides and Health

Projects Undergoing IUPAC Review

- 2001-069-1- C-NPU Concepts and Traceability of Measurements.
- 2003-016-1- Integrating Environmental Exposure Pathways for Medicinal Products.

Projects Undergoing Divisional Discussion

1. Bioinformatics: Prototype Analysis Of Molecular Biomarkers Of Diseases.

- 2. Prototype Analysis Of Glossary Terms To Establish Biological Context By Text Data-Mining.
- 3. IUPAC Survey And Discussion Group On Present Trends In Patenting Drug-Related Technologies.
- 4. Nutraceuticals Derived From Plant Sources Of South America.
- 5. Nutraceuticals Derived From Marine Sources.
- 6. Prediction Of Storage Stability Of Drugs And Compound Libraries.
- 7. Introduction Of The NPU-Database Into The Russian System.
- 8. Revision Of The Silver Book.
- 9. Extension Of The SCNPU-System To Imaging.
- 10. Problems Of Metrology Dealing With Uncertainty.
- 11. Educational Material / ToxLearn.
- 12. Joint Project Clinical And Medicinal Chemistry: Validated Targets of Individual Drugs and Analogues.
- 13. Kids In Life Science.
- 14. Properties And Units In CD Markers.

IUPAC DIVISION (VIII) OF CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION

Report to IUPAC Bureau and Council, August 2005

I. Highlights

- *I.1* **IUPAC International Chemical Identifier (InChI).** Version 1 released; enthusiastic response and widespread implementation in chemical databases (item II.3.1)
- 1.2 Organic Preferred Names. Final revision of the new Blue Book, including recommendations for selecting Preferred IUPAC Names (PINs), following ICTNS and public review (item II.3.2)
- **I.3 Revised Red Book.** Scheduled for publication in August 2005 (item II.3.3).
- **I.4 Fullerenes.** "Numbering of Fullerenes" published (item II.3.5).
- **I.5 Graphical representation standards for chemical structures.** Guidelines for graphical representation of configuration undergoing final revision, as the first component of this project (item II.3.8).

II. Report of activities 2004-2005

- II.1 Context. The work of the Division of Chemical Nomenclature and Structure Representation is concerned entirely with standards for the transmission of chemical information, and as such addresses the following long-range IUPAC goals:
 - b) IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion.
 - d) IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.
- II.2 Constitution of the Division. Division VIII consists of a Division Committee (sixteen members from eight nations and nine National Representatives) and an Advisory Subcommittee (44 people from 18 nations). The Joint IUPAC-IUBMB Commission on Biochemical Nomenclature (nine members from seven nations) reports to the Division Committee. Division members have access to a Web Discussion Board, on which minutes of meetings and current draft recommendations are posted for comment.

II.3 Current projects

II.3.1 IUPAC International Chemical Identifier (InChI).

A further test version of the software was distributed in July 2004, and comments were accommodated in a final test version issued in February 2005. To allow trademark copyright and licensing issues to be resolved, the name of the Identifier was changed to International Chemical Identifier (InChI) [formerly IUPAC-NIST Chemical Identifier (INChI)]. Version 1 was

finally released in April 2005: see www.iupac.org/inchi and an announcement in *Chemistry World*:

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

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

- P. Murray-Rust, H. S. Rzepa and Y. Zhang, "Googling for INChIs; A remarkable method of chemical searching": http://lists.w3.org/Archives/Public/public-swls-ws/2004Oct/att-0019/index.html
- S.J. Coles, N.E. Day, P. Murray-Rust, H.S. Rzepa and Y. Zhang, "Enhancement of the chemical semantic web through the use of InChI identifiers," *Org. Biomol. Chem.*, 2005, **3**(10), 1832-1834: http://pubs.rsc.org/ej/OB/2005/b502828k.pdf
- M.D. Prasanna, J. Vondrasek, A. Wlodawer and T.N. Bhat, "Application of InChI to Curate, Index, and Query 3-D Structures," *Proteins: Structure, Function, and Bioinformatics*, 2005, **60**, 1-4

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

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

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

- NIST 150,000 structures
- NIH/NCBI/PubChem project 800,000+ structures
- ISI 2+ million structures
- NCI Database 23 million+ structures
- EPA-DSSToX Database 1450 structures
- KEGG database 9584 structures
- UCSF ZINC 3.3 million structures
- Chemical Entities of Biological Interest (ChEBI) database of the European Bioinformatics Institute 5000 structures
- BRENDA database (University of Cologne) 36,000 structures

Other InChI developments include:

- Integration by ACD/Labs into their chemical structure drawing program, ChemSketch.
- Discussions on adoption by the new *Nature Chemical Biology*
- Discussions on use in the new *Beilstein Journal of Organic Chemistry*.

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

- to promote the use of the Identifier throughout the chemical information community
- to extend its applicability to include polymeric structures
- to explore the need for other extensions, including the ability to handle Markush structures, and to include information on other attributes such as phases and excited states

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

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

II.3.2 Organic Preferred IUPAC Names (PINs)

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

II.3.3 Revision of "Nomenclature of Inorganic Chemistry"

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

II.3.4 Rotaxanes

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

II.3.5 Fullerene nomenclature Part II

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

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

II.3.6 Extension of rules for stereodescriptors to include coordination numbers 7-12

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

II.3.7 Nomenclature of cyclic peptides

The document is undergoing revision following ICTNS and public review.

II.3.8 Graphical representation standards for chemical structures

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

Macromolecular Nomenclature Projects

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

II.3.10 Terminology and nomenclature of macromolecules with cyclic structures

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

II.3.11 Terminology and structure-based nomenclature of dendritic and hyperbranched polymers

This is almost ready for expert review.

II.3.12 Nomenclature for chemically modified polymers

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

II.3.13 Source-based nomenclature of single-strand organic polymers

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

II.3.14 Nomenclature of macromolecular rotaxanes

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

II.4 Joint IUPAC-IUBMB Commission on Biochemical Nomenclature (JCBN) Joint activities of the two Unions are channelled through this Joint Commission. Its main activities are:

II.4.1 Maintenance and updating of the Enzyme List

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

II.4.2 Maintenance and development of specialised naming systems for natural products

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

II.4.3 Advice for biochemists on names for specific compounds of biochemical importance

II.4.3.1 Synonyms databases.

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

II.4.3.2 Phosphorus compounds

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

II.4.3.2 Small molecules glossary

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

III. Project Development

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

IV. Division VIII Publications

Since January 2004, the following publications have appeared:

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

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

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

- IV.2 Numbering of Fullerenes, Pure Appl. Chem, 2005, 77, 801-923: http://www.iupac.org/publications/pac/2005/7705/7705x0843.html
- IV.3 "International chemical identifier goes online", Chem. World, 2005, 6, 7:
 http://www.rsc.org/chemistryworld/Issues/2005/June/this_month/International_chemical_identifier.asp

Alan McNaught 16 June 2005

IUPAC Committee on Printed and Electronic Publications

Report to Council, 2003-2004

CPEP met in Ottawa, Canada, in 2003 and in London, UK, on 26-27 June, 2004. The two-day annual meeting is currently structured so that project business and strategic electronic publishing issues are discussed on one day and operational issues, such as reviewing reports on IUPAC publications, are dealt with on the alternate day. On its first (reporting) day, the London meeting was attended by both the Secretary General and by Dr Wendy Warr, the latter in her capacity as ICSTI representative. Other invited attendees were Dr Steve Heller (Div. VIII representative) and Prof. Robert Lancashire (leader of a Data Standards group). Between annual meetings, the committee members have communicated regularly with each other, and the Secretariat, mainly by Email.

CPEP is currently responsible for four projects and for the publications of IUPAC.

1999-046-2-024 - <u>Data exchange standard for electron paramagnetic resonance data types (incl. ESR EMR etc.)</u>
2002-020-2-024 - <u>Data exchange standard for near infrared spectra and general spectroscopic calibration data types</u>
2002-022-1-024 - <u>Standard XML data dictionaries for chemistry</u>
2002-055-3-024 - <u>XML-based IUPAC standard for experimental and critically evaluated thermodynamic property data storage and capture</u>

Data Exchange Standards: The projects under this heading are organized by a Subcommittee of CPEP (coordinated by Tony Davies, Secretary of CPEP, and reported by him) and constitute a series of projects with the purpose of providing a common framework for electronic data exchange. Collaborative work with ASTM International is proceeding on the new Analytical Information Mark-up Language, AnIML, which will be a series of XML standards.

Standard XML Data Dictionaries:

These projects (under the guidance of Steve Stein and Michael Frenkel, both associated with NIST) are intended to provide interoperability solutions for interpretation and use of chemical data, a critical objective for data use across the board.

INChI (International Chemical Identifier): This is a project of Div. VIII, about which CPEP has an intimate concern and which maintains an interest in its very successful progress.

Colour Books: The standard XML data dictionaries for chemistry are important projects intended to facilitate electronic intercommunication. As such, they will complement (and update) the IUPAC Gold and Green Books (respectively, "Compendium of Chemical Terminology", 1997, and "Quantities, Units and Symbols in Physical Chemistry", 1993). Work on the Gold Book has proceeded apace, but the contents of the Green Book (which is out of print) had not been provided by the author so that progress was halted.

The Purple Book ("Compendium of Macromolecular Nomenclature", 1991) is also out of print while updates to the Red Book ("Nomenclature of Inorganic Chemistry", 2000) and Blue Book ("A Guide to IUPAC Nomenclature of Organic Compounds", 1994) were reported in 2004 to be in review status. The Orange Book ("Compendium of Analytical Nomenclature", 1997) was made available online in August, 2002. The Silver Book ("Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences", 1995) and White Book ("IUBMB Biochemical Nomenclature", 1992) were reported to be available. A Website for the latter is maintained by Dr Gerry Moss at http://www.chem.qmul.ac.uk/iupac/bibliog/white.html; there has been some discussion with Dr Moss (as yet fruitless) regarding the transfer of this site to the IUPAC Webserver.

Pure and Applied Chemistry (PAC)

The publication process for PAC has been much facilitated by the successful review and implementation of recommendations on electronic submission and control systems. Problems still remain with regard to ensuring that plenary speakers at IUPAC Congresses meet their obligation to publish their contributions in PAC.

The Editorial Advisory Board (EAB), in its earlier form, had been abolished and James Bull, in his capacity as Scientific Editor, has drafted proposals for the re-establishment of the EAB, in a revised format.

Pricing for PAC was proposed as follows: Standard USD1500; Electronic USD900; Individual USD99; Single Copies UD150; and Single Articles USD25. The last price was set so as to make it more expensive to generate (in effect) a Single Copy by purchase of the set of Single Articles!

The important task of generating Web access to back numbers was being efficiently organized by Bohumir Valter, a Committee member (back to 1965 at the time of the London meeting.)

Chemistry International (CI)

The much improved format and content of CI has been noted, and Fabienne Meyers (as Editor) congratulated on the progress. The Institutional Subscription price was set as USD99.

Web Access (http://www.iupac.org)

Web access to IUPAC information is of increasing importance for members, subscribers and interested persons. Considerable effort is being expended in improving access, in terms of organization, linking, and provision of material. The hosting and services have recently undergone formal review and a series of recommendations for improvement will be implemented by the secretariat. The important assistance of Bohumir Valter is gratefully acknowledged.

Membership of outside bodies:

ICSTI and IUPAP: Wendy Warr; CODATA: Tony Davies; ICSU: John Jost.

Two projects were submitted in the name of IUPAC to CODATA for funding at the 2004 CODATA GA and rejected. The submissions were not known to the Secretariat or the Secretary General and were not presented by the IUPAC representative to the meeting who was forced to admit that he had no knowledge of the submissions. We have good arguments for receiving additional CODATA funding for our projects but a substantial improvement in the way we approach such applications would be helpful.

CPEP Membership

Chairmanship of CPEP transferred to Leslie Glasser (Australia) in 2004.

Leslie Glasser Chair, CPEP 8th July, 2005

Report to Council and Bureau: CHEMRAWN Committee 2004-2005

I. Highlights

Since the CHEMRAWN conferences began in 1978, fourteen events have been held addressing important aspects of the global theme: **CHEM**ical **Research Applied to World Needs**. The most recent conference, *CHEMRAWN XV: Chemistry for Water* took place in Paris on June 21-23, 2004. A meeting of the CHEMRAWN committee was held jointly with that conference. The minutes of the meeting are available on http://www.iupac.org/standing/chemrawn.html

<u>Current activities</u>: Members and associates of the committee have been engaged in the following activities:

- CHEMRAWN XII: African Food Security and Natural Resource Management; the New Scientific Frontiers, A workshop on Soil Fertility and African Food Supplies was held on August 7, 2004 at the International Congress on Chemistry in Africa (ICCE), in Arusha, Tanzania. A report of the workshop and plans for CHEMRAWN XII was published in a cover article in "Chemistry International" (1).
- CHEMRAWN XIII: Chemistry for Clean Energy. At its meeting in Paris the committee heard a proposal to reschedule the conference to a new venue, in China in 2006.
- CHEMRAWN XIV: Toward Environmentally Benign Products and Processes. The Future Actions Committee has met regularly and has used funds from CHEMRAWN XIV to support international workshops, exchanges of personnel and contributions to green chemistry programs.
- CHEMRAWN XV: Chemistry for Water. The conference was held successfully on June 21-23, 2004 in Paris at the Maison de la Chimie. The meeting was described in detail in Chemical and Engineering News (2) and in Chemistry International (3).
- Solving the Problem of Arsenic Contamination in the Water in Bangladesh, CHEMRAWN representatives reported at CHEMRAWN XV on their visit to Bangladesh to plan a workshop addressing the problem.
- CHEMRAWN XVI: Innovation and the Chemical Industry, was held on 9 August, 2003 in Ottawa during the IUPAC Congress and General Assembly. The conference was described in a cover article in Chemistry International (4).
- *CHEMRAWN XVII: Greenhouse Gas Mitigation Strategies*. The organizing committee has proposed that the conference be held in Canada in 2007.

• Frontiers of Chemical Science: Research and Education in the Middle East, The CHEMRAWN and CCE committees were represented among the organizers of this conference held in Malta in December 2003 (5). The committee helped to obtain UNESCO funding for that conference and committee members are assisting with organization of the Malta II conference scheduled for late 2005.

II. Support for the Six IUPAC Goals

<u>Strategic Planning</u>. The CHEMRAWN committee continues to focus upon strategic objectives, in concert with IUPAC's six overall goals, as follows.

Address global issues:

Each CHEMRAWN conference focuses on a major issue. Specific examples are: chemistry as a tool for sustainable development; food security; mitigation of greenhouse gases; sources of cleaner energy; pollution prevention through the redesign of chemical processes; and adequacy of supply of pure water and sanitation.

Advance research through scientific discussion:

The findings and recommendations arising from each conference usually include instances where advances in research have made significant contributions and where further work is warranted. CHEMRAWN XIV, for example, highlighted the advances being made in Green Chemistry and proposed areas for further research. CHEMRAWN XV described numerous research advances relevant to purification of water. CHEMRAWN XVI outlined how innovation takes place productively in the chemical industry.

Assist industry toward sustainable development, wealth creation, and improvement of the quality of life.

Starting with CHEMRAWN I: Future Sources of Organic Raw Materials, CHEMRAWN conferences on advanced materials, ocean resources, health, atmosphere, sustainable development, greener manufacturing processes, innovation in industry, and chemistry and water have all focused on the needs of industry and have been attended or anticipated to be attended and supported by major chemical firms. This has continued through the most recent conference, CHEMRAWN XV: Chemistry for Water.

Foster communication among chemists and organizations with special emphasis on needs in developing countries.

Virtually all CHEMRAWN conferences have emphasized issues of major import to the developing world, most recently through (1) a workshop on soil fertility and food supplies in Africa and (2) our project dealing with the problem of arsenic contamination of groundwater in Bangladesh.

Enhance education and the appreciation of chemistry globally.

One of the most challenging conferences to develop and hold was focused on educational issues (CHEMRAWN X); especially the education of industrial chemists who will work for "trans-national" companies. The committee seeks to include an education component in all future conferences.

Increase the diversity in IUPAC bodies.

The CHEMRAWN Committee works continually to include underrepresented minorities in its membership and also to organize its conferences with diverse partners worldwide.

III. Other Substantive Issues.

- A. The Committee continues to be engaged by strategic issues of
 - 1) Obtaining funding of major conferences and finding less costly ways to carry out our mission.
 - 2) Increasing the impact of conferences, workshops and studies through practical and actionable recommendations by the Future Actions Committee, many of which can be implemented by the Committee or individuals and organizations which it can directly influence.
 - 3) Formulating activities that complement the organization of traditional CHEMRAWN conferences. This includes fostering scientific exchanges and small workshops, carrying out studies, and drafting position papers.
 - 4) Reaching out to cooperate with other IUPAC Committees and Divisions as well as with international organizations such as the International Council for Science (ICSU).
 - 5) Obtaining adequate publicity and recognition for the results of CHEMRAWN conferences, which will be essential in securing the resources necessary for future activities.

- B. Members of the Council and Bureau can help support the work of the CHEMRAWN Committee by
 - Recommending individuals to serve on the Committee or act as "friends" in organizing conferences or carrying out a CHEMRAWN study or workshop.
 - Calling upon the Committee to provide a "Future Actions Committee" for one of your conferences where major issues are discussed and a set of findings and recommendations should be developed and disseminated and
 - Urging the Committee to address a particular issue with a conference or workshop where there is broad interest throughout the chemical community.

C. At the request of the IUPAC Vice-President, the CHEMRAWN committee chair is compiling an in-depth summary of CHEMRAWN conferences and their efficacy in addressing world problems. The analysis will be available at the 43rd IUPAC General Assembly in Beijing.

IV. Tabular material

Titular members

John M. Malin USA Chair Jerzy A. Kopytowski Poland Secretary Fedor A. Kuznetsov Associate Chair Russia Kew-Ho Lee Korea Norma S. Nudelman Argentina Swaminathan Sivaram India Alan Smith UK Gary van Loon Canada

Associate Members

Stanley Langer
Venelin G. Marinov
Nthabiseng A. Ogude
Yukihiko Suematsu
Ayhan Ulubelen

UK
Bulgaria
South Africa
Japan
Turkey

Recent Publications

(1) I. Onyido, "Exploring Solutions to Africa's Food Crisis," *Chemistry International*, 2005, 27 (3), 8-10

- (2) M. Freemantle, "Chemistry for Water", *Chemical and Engineering News*, July 19, 2004, p. 25-30.
- (3) A. Smith, "Chemistry for Water CHEMRAWN XV Conference," *Chemistry International*, 2004, 26 (5)
- (4) J.A. Kopytowski, "Innovation in the Chemical Industry," *Chemistry International*, 2004, 26 (5)
- (5) J. M. Malin, "Frontiers of Chemical Science Research and Education in the Middle East," *Chemistry International*, 2004 26, (3)

Current and Recent Projects

2001-086-1-021 – CHEMRAWN XII – Chemistry, Sustainable Agriculture and Human Well Being in Sub-Saharan Africa

2001-087-1-021 – CHEMRAWN XIII – Chemistry for Cleaner Energy

2003-003-1-021 – CHEMRAWN XVI – Innovation in the Chemical Industry: the Way from Pure to Applied Chemistry

2003-050-1-021 – Solving the Problem of Arsenic Contamination in Water in Bangladesh

List of CHEMRAWN Conferences

- I. Toronto, Canada (1978). Future Sources of Organic Raw Materials
- II. Manila, Philippines (1982) Chemistry and World Food Supplies: The New Frontiers
- III. The Hague, the Netherlands (1984) Resources Material Conversion
- IV. Keystone, Colorado, USA (1985) Modern Chemistry and Chemical Technology Applied to the Ocean and its Resources
- V. Heidleberg, Germany (1986) Current and Future Contributions of Chemistry to Health
- VI. Tokyo, Japan (1987) Advanced Materials for Innovations in Energy, Transportation, and Communications
- VII. Baltimore, Maryland, USA (1991) The Chemistry of the Atmosphere: Its Impact on Global Change
- VIII. Moscow, Russia (1992) Chemistry and Sustainable Development

- IX. Seoul, Korea (1996) Advanced Materials and Sustainable Development
- X. Budapest, Hungary; Washington, DC, USA; Honolulu, Hawaii; and Brisbane, Australia (1999-2000) The Globalization of Chemical Education Preparing Chemical Scientists and Engineers for Transnational Industries
- XI. Montevideo, Uruguay (1998) Latin American Symposium on Environmental Analytical Chemistry
- XIV. Boulder, Colorado, USA (2001) Toward Environmentally Benign Processes and Products
- XV. Paris, France (2004) Chemistry for Water
- XVI. Ottowa, Canada (2003) Innovation and the Chemical Industry

John M. Malin, Chair CHEMRAWN Committee

I. Summary and Highlights

Following the 2003 General Assembly in Ottawa, COCI entered a new phase of its development with significant changes in membership and a new funding model. In addition to the 2004 Annual COCI meeting held in Brussels held in May, two strategy meetings have been held (Farnham, UK, Feb 2004, Oxford, April 2005) to map out the future direction and priorities for COCI. These strategy meetings were attended largely by the titular members. The main outcomes:

- Establishment of a project structure with the titular members each responsible for a project area. These include:
 - Company Associates program
 - Trade Associations program
 - o Safety Training Program and workshops
 - o Public Appreciation of Chemistry(contribution to CCE program)
 - o Liaison with NAO's and national chemical societies
 - o IUPAC inter-divisional activities
 - o Non- and inter-governmental (NGO/IGO) liaison
- Definition of a model for project working and appointment of Aldo Alles as overall project coordinator
- Establishment of objectives for the COCI projects.
- Review of strategic priorities in conjunction with COCI terms of reference and IUPAC's strategic goals

Selected outcomes are listed in Section II, taken in concert with the strategic priorities of IUPAC. The full details are available in the minutes for the meetings described, and these are posted on the COCI page of the IUPAC website. Visual aids presented at the meetings are also included in these minutes. Highlights include:

- Continuing success of the IUPAC-UNESCO-UNIDO Safety Training Program into 2005 with seven former trainee Fellows attending a workshop session scheduled for the IUPAC Congress in Beijing. A workshop is being planned in Africa for 2006.
- Increased impetus behind the Company Associates (CA) program, with a prime focus on recruitment. A universal format for recruitment has been mapped out, and clarification of accountabilities of NAO's and COCI has resulted. A new brochure explaining the IUPAC CA program has been prepared and widely distributed. Two digests of projects aimed at highlighting those of particular interest to industry have been produced and it is anticipated that these will be produced twice yearly. A positive development is that conference sponsors in several countries have been offered a one year CA membership gratis, again to encourage recruitment.
- The DIDAC program has now entered its rollout and assessment phase and it was thus considered appropriate to transfer the leadership of this project to CCE. Written material, transparencies and CD-ROMs have been prepared in several languages.

- The NGO/IGO liaison project has continued to develop links with funding authorities and it is pleasing to note that UNESCO continues to support the Safety Training Program.
- In order to enhance interaction with the IUPAC Divisions, each has been approached to nominate a representative to COCI. It is anticipated that the COCI meeting at Beijing will be attended by the Divisional representatives.
- The Trade Association Project continues to develop and links with the International Council of Chemical Associations (ICCA) are being explored, in particular with regard to the Safety Training Project and the public image of chemistry.
- The Public Appreciation of Chemistry project has been concerned largely
 with contributing to, and supporting the Value of Chemistry project
 (Przybylowicz), the Propagation of Chemistry project (UK Resolution,
 Ottawa 2003) and the WCLM. Aspects of all three programs have now
 coalesced.

II. COCI contributions to IUPAC's strategic goals

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

1. Strategy Meetings (Farnham, UK, Feb, 2004 and Oxford, UK, April 2005)

- A key objective for these meetings was to identify the unique role of COCI (and IUPAC) over and above national societies. It is essential to avoid unproductive duplication. With respect to COCI, many national chemical societies have highly successful industrial divisions which offer members a locally customised range of benefits.
- We concluded that our emphasis should be upon projects which share best practice globally and build upon, customise and disseminate the work of the national organisations in the following prime areas:
 - o Capacity building (e.g. safety training)
 - o Public perception of chemistry
 - Authoritative NGO role of IUPAC forum for public and political debates
 - o Reputation and trust

Our focus for these topics should include economic development as well as societal and environmental factors.

2. Trade Associations program

- Liaison and cooperation with Trade Associations has been recognised as a key
 priority for COCI. Its program is anchored by Colin Humphris of CEFIC. The
 appropriate global conduit for COCI for the chemical industries is the
 International Council of Chemical Associations (ICCA). We have recognized that
 the potential value in the relationship with the industry representative bodies
 comes through the global science perspectives of IUPAC and its reputation for
 scientific excellence.
- We are seeking support for existing projects (Safety Training Program and DIDAC; see below) from the ICCA, which through its support for Sustainable Development, has a keen commitment to capacity building.
- We are initiating a dialogue for shaping new projects relating to public
 perceptions of science where we can seek alignment between the industry's global
 concerns with those of chemistry as a whole.
- It has been suggested that IUPAC could play a greater proactive role as an NGO in brokering multi-partite debates on topics of public interest. Such events promoted by a trade association can be perceived to be biased by self interest and can thus preclude attendance by certain groups (e.g. politicians). The independence and the formidable reputation of IUPAC for scientific probity could ensure wider participation.

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

The chemical industry values IUPAC's work on standards very highly. COCI will emphasise this work in its reports to CA's and as part of its recruitment efforts. Many

IUPAC-sponsored scientific conferences are highly appreciated by staff in the chemical industries, as evidenced by the level of attendance at many events.

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

1. COCI Company Associates Program

- Policy requires that recruitment of CA's is an NAO function whereas it is COCI's role to communicate benefits to the CA membership. In short, it is COCI's job to provide a focus for CA members and to influence IUPAC activities to provide benefits to the CA's, whilst representing CA issues to the various IUPAC bodies. In practice, the situation is not effective in that it appears that the majority of NAO's are passive with regard to CA recruitment. In the first instance, COCI members are approaching their local NAO to establish a cooperative mechanism for recruitment in cases where no procedure exists. The revamped brochure mentioned in Section I above also explains the benefits of CA membership and is being used to promote recruitment drives.
- An initiative organised by the Secretariat is offering one year's free CA membership to companies which have sponsored certain IUPAC conferences.
- Akira Ishitani (Japan) leads the CA program. Japan has by far the largest number of CA's and a very successful meeting of Japanese CA representatives was held in July 2004.

2. Trade Associations Program

• A common point of interest between the Trade Associations and COCI is the area of Reputation and Trust. This is a potential future topic for pursuance.

3. Liaison with IUPAC Divisions

- Alan Smith acts as the Divisions Coordinator for COCI. In this role, he is
 vetting projects in other divisions for particular relevance to the chemical
 industry. A twice-yearly digest is being produced consisting of abstracts of
 existing and new IUPAC projects of particular relevance to the industry, and
 dispatched as a booklet to CA's. A first contribution has been distributed and a
 second has been prepared.
- Each IUPAC Division has been invited to nominate a representative to COCI with a purpose of improving understanding between the commercial and academic aspects of IUPAC's activities.
- d) IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.

1. Safety Training Program and Workshops

As indicated in Section I, capacity building in developing countries is a
cornerstone of COCI's future ambition. The IUPAC-UNESCO-UNIDO Safety
Training Program (and associated Workshops), led by Mark Cesa, is COCI's
flagship program. This continues to thrive and has elicited significant interest
from potential trainees from developing countries. Success of the Safety

Training Program into 2005 continues with seven former trainee Fellows attending a workshop session scheduled for the IUPAC Congress in Beijing. A workshop is being planned in Africa for 2006.

2. Teaching Materials

 There has been significant recent progress with the production and dissemination of DIDAC teaching materials. The material is of particular utility in support of teaching chemistry in developing countries – see II e 1 below.

3. Responsible Care

- The Responsible Care program, originating in Canada, has been successfully
 customised in many countries. As a part of its capacity building initiatives,
 COCI, led by Bernard West and Colin Humphris, is investigating the
 feasibility of establishing training programs and workshops targeted at
 developing countries and emerging economies.
- e) IUPAC will utilise its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry

1. DIDAC

- The development of DIDAC as a project with the objective of producing chemistry teaching materials was initiated by Agfa Gevaert. IUPAC's formal involvement was initiated by \$4000 seed funding by COCI. Alex Pokrovsky has been instrumental throughout in gaining funding and commitment from UNESCO A meeting was held with Agfa in February 2004 at which the DIDAC project was officially transferred to UNESCO.
- COCI, through its members and its links with UNESCO, has been the prime
 driving force within IUPAC of the development of the DIDAC teaching
 materials and their customisation and distribution. Monographs, CD-ROMs,
 transparencies and posters have been translated into several languages, with
 notable recent progress in China and Japan.
- The focus for DIDAC activities is now moving from production of materials to its use in teaching. Accordingly, it is considered that IUPAC's future interest in DIDAC is now more appropriately pursued within CCE. The transition has been organised with the CCE chairman, Peter Atkins. COCI involvement will continue, particularly with regard to fund raising.

2. Public Appreciation of Chemistry (PAC)

- The public appreciation of chemistry has been recognised as one of the key elements of COCI's strategy. One of COCI's objectives here is to represent industry concerns and viewpoints within the wider IUPAC ambit.
- In the IUPAC community at large, there is a massive amount of excellent PAC material available and consequently much duplication and dissipation of effort. In this light, it has been agreed that the leadership of PAC activities should rest with CCE, with COCI as a contributor with particular emphasis upon the industry aspects and concerns.

- The formal contributions of COCI to this project have been limited, and include its support of the Value of Chemistry project and, in conjunction with CCE, the project in support of the UK resolution at Ottawa relating to the propagation of chemistry.
- Personal contributions of COCI members to this effort in a national context are at a significant level. One objective is to pool material and to make this publicly available via the COCI web-page.

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

National Representative (NR) Co-ordination

- The COCI membership is notably diverse with regard to geography and its national representatives make a major contribution to this. Nevertheless, there are a number of appropriate countries which are not represented and with whom we have very limited contact. The committee is deficient with regard to gender and age balance and furthermore is lacking in members who are currently employed in the chemical industries.
- The leader of COCI's National Representatives program, Jonas Unger, recognises the imbalance and has formulated optimal criteria for future NR's. A program to increase awareness of COCI's strategy and objectives amongst the national societies is a future objective.

IV Major Challenges facing COCI

1. CA recruitment

- As indicated in paragraph II c1 above, CA recruitment suffers from diffusely-shared accountabilities amongst the IUPAC community. It is also clear that the role of the NAO in recruitment has not been fully communicated, accepted or legitimised in many cases.
- COCI clearly has a major role to play in CA recruitment and is energised so to do. Notwithstanding, a more widely supported CA program would be a major mechanism to interact with chemistry's largest constituent body namely chemists working in industry.
- At the 2004 Bureau meeting in Bled, it was proposed that the Executive should establish a task team to streamline the CA recruitment process. In particular, the ownership of the program by the NAO's is a critical success factor.

2. Public Appreciation of Chemistry

• It is clear in very many countries that the image of chemistry in the public eye is at best misunderstood and more often is distinctly negative. The responsibility for restitution of the good name of chemistry falls upon all who espouse the profession. It is proposed that this topic be addressed by IUPAC with greater urgency and more resource than hitherto.

3. Funding Model for COCI

- Michael Booth has been appointed Treasurer of COCI with responsibility for expenditure accounts, budgets, forward planning and funding mechanisms.
- Given the geographic diversity of COCI's membership, the biennial grant is totally consumed to cover committee meetings. COCI does not receive a grant to fund its own projects. In the past, profits from conferences have alleviated the situation but these funds have now been exhausted
- A request was made at the 2004 Bureau that COCI be granted a project budget in line with other Divisions and Standing Committees. Without this facility, COCI will be unable, for example, to run its Safety Training Program which requires committing to trainees and participating companies well in advance.
- One of COCI's objectives is to attract funds from the industry to support IUPAC initiatives and projects. In this context, the provision and communication of the benefits to industry of IUPAC's work is crucial. Whereas we recognise that in today's industrial climate, cash donations are scarce, we have been successful in receiving benefits-in-kind and significant living expenses for STP trainees during their period with the host company.

In conclusion, we believe that COCI has made good progress over the past biennium with regard to adaptation to its changed status. A distinct strategy, with associated

priorities, has been agreed and adopted. Clear accountabilities and processes are in place and projects and programs have realistic objectives. In addition to the challenges mentioned above, a key goal for the next biennium will be to engage more members who continue to be active in the chemical industry, and particularly those from developing countries.

David A. Evans 27.06.05

REPORT

of the

COMMITTEE ON CHEMISTRY EDUCATION

2004-2005

I HIGHLIGHTS

The principal activities of CCE centre on its two major subcommittees, PUC and CED:

1. Report of the subcommittee on Public Understanding of Chemistry (PUC)

Chairman: Peter Mahaffy

- (a) Public Understanding of Science: Identifying IUPAC's Niche. Members of the Project team have prepared a report after meeting for three days in May, 2005 in Edmonton to review IUPAC's role, survey the literature, and prepare this report. The purpose of the Beijing workshop will be to consider recommendations to the Bureau on roles for IUPAC in promoting public understanding of science. The final stage of this project will take place at and following the 19th ICCE in Seoul in August 2006, where a special symposium on the Public Understanding of Chemistry will take place.
- (b) Young Ambassadors for Chemistry (YAC). The YAC initiative was launched in Taipei, followed by implementation in the second proposed site, Buenos Aires. The objective of YAC is to enhance the public understanding of chemistry through teacher and school audiences in target locations of regions in transition. YAC is a partnership between IUPAC and Science Across the World (SAW), building on a previously successful collaboration to organize a global poster competition. Additional partners for YAC include Glaxo-Smith-Kline, the British Council, and for Taiwan the National Taiwan Normal University, The Chinese Chemical Society, and the National Science Council. The Taipei launch was covered in the March-April, 2005 issue of Chemistry International. Organization of activities for the third and fourth sites, in Russia and South Africa, are under way.
- (c) PUC symposium The Flow of Ideas (2003 Ottawa IUPAC Congress): Follow up. Canadian Chemical News (ACCN), the national news magazine of the Chemical Institute of Canada (CIC), has followed up this symposium and solicited from symposia speakers; CIC is building on the momentum to create sustained activities at annual national conferences. The Chemical Heritage Foundation in Philadelphia has inquired about outcomes from this symposium, in conjunction with a proposal to study public attitudes toward,

and understanding of, chemistry.

(d) Standards for colours in electrostatic potential maps. A new IUPAC project to address the need for systematisation is being considered. Peter Mahaffy convened an informal meeting of possible participants at the 2005 Gordon Research Conference on Visualization in Science & Education, July 3-7, 2005, Oxford UK.

2. Report of the subcommittee on Chemistry Education for Development (CED)

Chairman: Ram Lamba

- (a) e-Quiz Project: promoting Chemical Education in India. In Istanbul the CCE approved USD2k as seed money and encouraged the applications to come back with a revised proposal with various technical solutions to points that had been raised. The revised project aims to develop assessment tools, a test bank in several Indian languages, motivation of high school students to improve their chemistry knowledge and continue studies in this area, conceptual understanding, teacher training through the outcomes of their students in the e-quiz, web-based interaction among students and teachers, newer practices in certain regions of India through hands-on Chemistry (such as micro-scale and the use of low-cost equipment), and benchmarks and standards at high school level. The intention is to extend the program to SE Asia.
- **(b) Micro-scale Chemistry** The Micro-scale UNESCO-IUPAC Global Program has been continued during this period.

Consultant: John Bradley

Two-day introductory workshops have been conducted with the aim of introducing the concept to senior educators. Since the last report in Ottawa, these workshops have taken place (chronologically) in:

Azerbaidjan, Russian Federation (Bashkhortostan, Tatarstan), Cote d'Ivoire, Comoros, Djibouti, Equatorial Guinea, Zimbabwe, Angola, Norway, Sweden, Finland, Turkey, Malawi, Zambia, Mauritania, Congo (DRC), Bangladesh, Maldives, Thailand and Pakistan

The large pilot project for 22 African countries has been completed and a final report submitted to UNESCO and GIFCA. As part of the preparations for the completion of the report, a number of evaluation workshops were also held. These took place in

Dakar (Senegal), Johannesburg (S Africa), and Windhoek

(Namibia).

The final report preparation took place in Johannesburg. The report, which is being evaluated by the donors, includes recommendations for expansion of the project to support wider implementation in some of the countries involved.

The translation of the micro-scale chemistry worksheets into languages other than English has always been part of the program of dissemination. This continues, whilst at the same time the existing English and French versions are now accessible free to all on the UNESCO website (www.unesco.org/science/bes). Most of this program has been funded by UNESCO, using extra-budgetary funds from a number of different sources. There remains a list of countries which have requested introductory workshops and we hope to organize visits in the months ahead.

(c) Flying Chemist Program (FCP) The FCP is a major new initiative of the CCE. The aim is to provide emerging countries means to improve the teaching and learning of chemistry at primary, secondary, and tertiary levels. The FCP will provide a country with the expertise needed to strengthen chemistry education and to assist them in its development. The program is preferably to be implemented for the development of economically disadvantaged countries. The host country will provide local costs (board and lodging), and CCE (in collaboration with the Project Committee) will provide the air fare. It is expected that visits will in due course be developed in collaboration with UNESCO, but their participation is not essential (except to broaden the activity). It is anticipated that visits will be considered only if invitations are received from a National Society, a Ministry of Education or Technology, or another comparable substantial organization.

Possible scenarios for the FCP are:

- 1. To assist in the development of curricula.
- 2. To help develop or recommend new tools of assessment.
- 3. To help recommend implementation of hand-on experiences at all levels of chemistry education.
- 4. To assist in the establishment of partnerships among universities, industries, and governments.
- 5. To help develop different approaches to the teaching of chemistry.
- 6. To develop successful international conferences to achieve expert advice on a particular aspect of chemistry education.
- 7. To help develop and implement teacher training and preparation programs.
- 8. To help identify and approach sources of funding.
- 9. To assist in other matters of chemistry education.

The Executive Committee of the FCP will consist of the Chairman and the chairmen of the two Subcommittees, with the chairman of CED as Convenor and Project Leader.

Under this program:

- (i) India The first implementation of this program is to India, to implement improvements to chemistry education. This project is in collaboration with the DAV College Managing Society, New Delhi (DAV Managing Society manages an educational network comprising over 500 schools spread throughout India). The chairman of CCE and the chairman of the CED visited Delhi in July, 2005.
- (ii) Peru The Association of Chemistry Educators of Peru has been sent the criteria for the FCP program.
- (iii) Sri Lanka In response to the effects of the 2004 tsunami and in collaboration with the RSC, which has committed substantial funds in support, and its local branch in Sri Lanka, plans are moving forward other to proceed with a conference and workshops to develop and improve chemistry education in Sri Lanka. The chairmen of CCE and CED visited Sri Lanka for one day after their visit to India in July in order to see and discuss first-hand the needs of the country. The meetings are planned for 2006.
- (iv) Iran A request is expected to come officially from Iran through the CCE chairman.
- (d) Flying Scientist Program (FSP) The idea for this program is to extend FCP to all science-based subjects and to collaborate with other Unions and make use of ICSU and possibly UNESCO resources.
- (e) **Medicinal Chemistry** It is proposed to hold a symposium in Korea 2006 in connection with ICCE-19.
- (f) The 2nd International Conference "Chemistry Education and Sustainable Development (Moscow, October 2004). The report on this conference has been recently published in CI. The chairman of CCE attended and presented a paper.
- **3. Other significant activities** A significant collaboration has been established between CCE and OPCW [the Organization for the Prohibition of Chemical Weapons] in response to the request to the CCE that it should examine the educational aspects of chemical weapons mentioned in the IUPAC Report [PAC]. A meeting, jointly funded by IUPAC and OPCW took place in Oxford, July 9—13 2005 with a view to taking this matter forward and preparing a report for consideration by

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the States Signatories of the Convention later in the year. The meeting is scheduled to take place after the deadline for this report to Council and will be included in the oral report.

II ACHIEVEMENT OF GOALS OF THE STRATEGIC PLAN

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

The role of the CCE is to encourage good practice in chemical education worldwide and to promote the public appreciation of chemistry. It continues to play a central role in providing assistance to developing countries and countries in transition, particularly through its. Collaboration with UNESCO and the propagation of its microscale kits (see the CED report), and is organizing symposia to propagate chemistry to the general public (see PUS report). The CCE is encouraging the development of curricula that have regional relevance. In particular, it has established a 'Flying Chemists Program' (FCP) where the expertise of the committee is offered to governments and other substantial organizations with the aim of developing their provision of chemical education.

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

The CCE regards research in chemical education as an intellectually valid domain of original investigation, and intends to continue to encourage its acceptance, for instance, by examining the origins of misconceptions and the role of animations.

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

The chairmen of CCE and COCI have become representatives on each others' committee and have been fully involved in matters of mutual concern. Although the chairman of COCI was unable to attend the off-year meeting of CCE (in Istanbul), the chairman of CCE was able to attend the off-year meeting of COCI in Oxford and is fully informed about that committee's activities. The CCE recognizes that the education of chemists is the prime source of talent and hence profit for the chemical industry.

(d) IUPAC will foster communication among individual chemists and scientific (with special emphasis on the needs of chemists in developing countries.

As has been pointed out previously, the CCE has a huge membership, with a large number of NRs from developing countries. As in the Ottawa meeting, we shall include

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symposia at which NRs present summaries of what each of their countries need, and the CCE will continue of build a program of relevant projects. The FCP is a particularly relevant example of our involvement with developing countries.

(e) IUPAC will utilize its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.

This goal lies at the heart of the CCE, and all the activities of the CCE are directed towards its achievement.

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

The chairman of the CCE seeks to involve a wide range of its members in its activities and planning. In the course of his travels he has encouraged a number of countries to consider membership.

III FUTHER SUBSTANTIVE INFORMATION

This part of the report consists of summaries relating to the structure of the CCE, its subcommittees, and its projects.

1. Composition and structure The membership of the CCE is shown in Table 1. We have developed the structure of the committee following our off-year meeting in Istanbul in the course of the ICCE in August 2004. See Table 2.We have aimed at a global distribution of members. In addition, we have established three working groups: See Table 3.

This biennium sees the retirement of its Chairman (PWA) and its Secretary (EMP). It is proposed that the Chairmanship for the next biennium be taken by Peter Mahaffy, who will in due course reallocate responsibilities. The President has been offered the names of Eva Akesson (Sweden) and Choon Do (Korea) as replacement Titular Members. The Chairman is *ex officio* a member of COCI, and reciprocally. The CCE has had close and valuable relations with COCI and has developed themes of mutual interest.

- **2. Project advisory subcommittee** We have established a protocol for dealing speedily with applications:
 - 1. Project proposal received by Secretariat.
 - 2. Project Coordinator receives proposal from Secretariat (FM).
 - 3. If FM is uncertain whether the Project is of interest to CCE, FM consults Project Coordinator.

- 4. FM distributes the proposal to all Project Group members and comments are to be returned to her; this first round of review by all members should take 1 week.
- 5. FM will collate all comments and send that to the Project Coordinator who will than formulate a decision.
- 6. If comments diverge, the Project Coordinator can ask for a second round of comments; to initiate such a round, all the comments initially collected will be circulated to all members of the Project Group for additional comments.
- 7. The Project Coordinator will report to FM (a) to support or not to support; (b) suggestions for external referees, (c) the level of CCE financial support.

Current projects are listed in Table 4.

- **3. ICCE program** As its flagship activity, the CCE is responsible for the sequence of ICCEs. A highly successful ICCE-18 was held in Istanbul in 2004, with a large and gratifying number of attendees from the Middle East. The next ICCE (ICCE-19, in August 2006) will be held in Seoul. Because there is now a more vigorous interest in the program, the CCE has established the following criteria on which to base its selection:
 - **1.** The availability, style, quality, and location of lecture rooms.
 - 2. The availability, style, quality, and location of dining rooms.
 - **3.** The availability, style, quality, and location of laboratories, technology resources, and access to the internet.
 - **4.** The number and level of expertise of the conference committee involved in the management of the conference.
 - **5.** Financial resources to host the conference
 - **6.** Accommodation availability and costs
 - **7.** International access to host city by air travel and availability of competitive airfares.
 - **8.** An assessment of the ability of the conference to attract teachers and other interested parties from the region and their ability to attend.
 - **9.** A (non-binding!) assessment of the weather conditions at the planned meeting time.
 - **10.** Opportunities for excursions and entertainment.

The CCE intends to make its selections helped by advice from its Conference coordinator., whose role also includes informing members of the CCE about other conferences with an educational content.

Peter Atkins Chairman, CCE June, 2005

Table 1 Committee membership

Titular Members	
Prof. Peter W. Atkins	1998-2005
Prof. M. Elisa M. Pestana	1996-2005
Prof. Warren Beasley	2004-2007
Prof. Masato Ito	2004-2007
Prof. Ram S. Lamba	2002-2005
Prof. Peter G. Mahaffy	2002-2005
Dr. Lida Schoen	2002-2005
Prof. Natalia P. Tarasova	2004-2007

Associate Members	From Division	
Prof. Christopher M. A. Brett	Physical and Biophysical Chemistry	2002-2005
Prof. Leonard Interrante	Inorganic Chemistry	2004-2005
Prof. Maria F. da Silva	Organic and Biomolecular Chemistry	2004-2005
Prof. Jung-II Jin	Polymer	1998-2005
Prof. Roger M. Smith	Analytical Chemistry	2004-2005
Prof. Nicola Senesi	Chemistry and the Environment	2002-2005
Dr. Mukund S. Chorghade	Chemistry and Human Health	2002-2005
Prof. Herbert D. Kaesz	Chemical Nomenclature and Structural Representation	2002-2005

National Representatives	Country	
Prof. Hector Santiago Odetti	Argentina	2004-2005
Dr. Mauro Mocerino	Australia	2004-2005
Dr. San Hoa Thang	Australia	2004-2005
Prof. Ludo Brandt	Belgium	2004-2005
Prof. Alvaro Chrispino	Brazil	2002-2005
Prof. Borislav V. Toshev	Bulgaria	2002-2005
Prof. Qiankun Zhuang	China/Beijing	2000-2005
Mei-Hung Chiu	China/Taipei	2002-2005
Dr. Helena Klímová	Czech Republic	2002-2005
Prof. Amen Farouk Mohamed Fahmy	Egypt	2000-2005
Dr. Ahmed S. Shoukry	Egypt	2004-2005
Prof. Matti E. Näsäkkälä	Finland	1994-2005
Prof. Françoise Rouquérol	France	2000-2005
Prof. Terence N. Mitchell	2004-2005	Germany
Prof. Miklos Riedel	Hungary	2004-2005
Prof. A. K. Bakhshi	India	2004-2005

Prof. Uday Maitra	India	2004-2005
Prof. Peter E. Childs	Ireland	2004-2005
Dr. Mordechai Livneh	Israel	2002-2005
Prof. Paolo E. Todesco	Italy	2004-2005
Prof. Choon H. Do	Korea	2000-2005
Dr. Maryam Al-Wateed	Kuwait	2002-2005
Prof. Józef J. Ziólkowski	Poland	2000-2005
Dr. Eva Akesson	Sweden	2002-2005
Prof. Hale Bayram	Turkey	2002-2005
Dr. Anthony D. Ashmore	United Kingdom	1992-2005
Prof. Morton Z. Hoffman	USA	2004-2005
Prof. John D. Bradley	South Africa*	

^{*} Ex-Officio; Consultant for Microscale Project/Program

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Subcommittee on Chemistry Education for Development (CED)
Prof. Ram S. Lamba (Chairman)
Dr. Eva Akesson
Dr. Anthony D. Ashmore
Prof. Warren Beasley
Prof. John D. Bradley
Dr. Mukund S. Chorghade
Prof. M. Elisa M. Pestana
Prof. Natalia P. Tarasova
Prof. Chung-Yuan Mou

Subcommittee on Public Understanding of Chemistry (PUC)		
Prof. Peter G. Mahaffy (Chairman)		
Dr. Anthony D. Ashmore		
Dr. D. Balasubramanian		
Prof. Robert B. Bucat		
Prof. Choon H. Do		
Prof. Masato Ito		
Dr. Lida Schoen		
Prof. Joseph Schwarcz		

Table 2 Officers

Office	Holder	Country
Chairman	Peter Atkins	UK
Chairmen of the CED Subcommittee and PUS Subcommittee	Ram Lamba Peter Mahaffy	Puerto Rico Canada
Secretary	Elisa Maia	Portugal
Project Coordinator	Choon Do	Korea
Divisional Coordinator	Eva Akesson	Sweden
Conference Coordinator	Warren Beasley	Australia
Treasurer	vacant	-

Table 3 Subcommittees and working parties

Task	Members	Countries
Project management	Choon Do	Korea
	Eva Akesson	Sweden
	Tony Ashmore	UK
	Hale Beyram	Turkey
Educaitonal aspects of	Natalia Tarasova	Russia
chemical weapons	Jun-II Jin	Korea
	Elisa Maia	Portugal
Networking and	Warren Beasley	Australia
developing DIDAC		

Table 4 Projects in progress

Number	Title
2001-003-5-050 -	Organisation of Clearing House for the translation, publication, and dissemination of the IUPAC-sources materials and ideas in chemical education in Russia and CIS
2001-016-1-050	IUPAC chemical nomenclature for chemistry teachers at secondary schools
2001-046-1-050	Introduction of small scale chemistry experiments - teacher training
2002-010-1-050	Toward a core organic chemistry curriculum for Latin American universities*
2002-021-2-050	A feasibility study of the scope and limitation of machine translations as a means of disseminating useful reading material for chemical education to be used on the internet
2003-055-1-050	Young Ambassadors for Chemistry (YAC)
2004-047-1-050	Public understanding of science: identifying IUPAC's niche
2005-004-1-050	Flying chemists program - 2005 visit to India
2000-020-2-200 *	Collecting, testing and dissemination of experiments in solid state and materials chemistry
2003-022-1-020*	Chemistry's contributions to humanity - A feasibility study
2004-037-1-400*	Design of polymer education material for French speaking countries
2004-045-1-700*	Training of school children on pesticides and health
2004-048-1-020*	A joint OPCW - IUPAC project on education and outreach regarding chemical weapons

^{*} Interdivisional project

Report of the Project Committee to IUPAC Council

Submitted by **Gus Somsen**, PC Chairman 20 June 2005

The Project Committee (PC) is tasked with two programs:

1. the project-driven system

The PC reviews and evaluates requests for interdivisional/interdisciplinary projects, for large proposals (meaning requesting approximately more than 10% of the Division/Standing Committee project budget), or for proposals supported by a Standing Committee that has no budget for projects.

2. the financial support for conferences

The PC assumes the responsibility for reviewing and recommending funding of proposals for Conferences in New Directions in Chemistry and Scientifically Emerging Regions. This program is essentially the merging of the 2 older programs, namely the earlier program developed after the 1999 Council to financially support conferences in developing and economically disadvantaged countries, and the 'New Directions conferences' which resulted in the financial support of the first 2 Workshops on Advanced Materials.

Project-Driven System

Since its establishment in April 1999, the PC has been involved in two kinds of activities:

- 1. Reviewing of proposals and making decisions on funding as defined in the terms of reference of the committee.
- 2. Taking part in the discussions on the development and the implementation of the project review process.

These activities have reached a steady state where by the review and funding decisions of proposals are performed routinely and on a timely basis. The overall review process continues to benefit from smooth interactions between the PC, and the Division Presidents and the Chairmen of the Standing Committees. The PC relies on the expert opinion of these bodies for making the final funding decision. Such essential communication has been facilitated by the usage of an explicit document suggesting questions to be addressed by Officers of Divisions and Standing Committees when recommending a proposal to the Project Committee.

Since the 2003 meeting, only minor adjustments have been introduced in the review procedure and corresponding documentations. One practical change has been to initiate a prompt outside review concurrent to the internal evaluation if it is perceived that the proposal does not present major concerns or deficiencies.

The projects that received financial support by the PC since the last report to Council dated 9 June 2003 and since the beginning of the current biennium are listed in the annex.

As of today, and out of its 2004-2005 budget of USD 110 000, the PC made commitments for a total USD 106 300, covering 11 projects. Out of these 11 approved projects, 5 were interdivisional projects summing to USD 19 800, and 6 were for larger projects with a PC commitment summing to USD 86 500.

Comparison with previous biennia

	\$ PC budget	\$ PC
	_	spending
2000-01		152 500
2002-03	250 000	170 000
2004-05	110 000	106 300*

as of 21 May 2005

Financial Support for Conferences

As a result of a Bureau decision in 2002, the PC now also assumes responsibility for the review of, and recommending funding for, proposals for Conferences in New Directions in Chemistry and Conferences in Scientifically Emerging Regions.

In 2003, and to adjust to the transition, the application form and guidelines have been reconciled to support both programs. After a year, the PC at its meeting in Bled (Oct 2004) reviewed the documentation once again, putting at use the experience acquired during the evaluation of the most recently submitted applications. In some specific instances, the wording on the application form, the guidelines for completion, the policy guidelines, and the website, needed some tuning. In Bled, the Chairman also assembled with the Division Presidents and Standing Committee Chairmen to stress the role of their bodies in the reviewing process. At its meeting in Bled, the PC also considered the misunderstanding around 'sponsorship' and 'financial support'. Although it might appear that for many people outside IUPAC, 'sponsorship' implies financial support, this is not the case within the IUPAC organization. The traditional 'IUPAC sponsor' label should be preserved unchanged.

A review of the forms and guidelines was completed early Jan 2005, which led to a documentation that clearly reflects the policy guidelines. The documents - FSC New Directions in Chemistry and FSC Scientifically Emerging Regions are presented as two separate documents with the corresponding guidelines integrated in the forms.

Originally, the Conference Policy Development Committee proposed, and the Bureau approved, a program that stimulates Divisions and Operational Standing Committees through proactive efforts. This aspect was highlighted at the DP meeting in Bled.

For the 2004-2005 biennium, the funding available for this program is USD 65 000. The PC reached his commitments limit in April 2005. Yet, concurrently, as the program is becoming more widely known, it is expected that more applications will be submitted.

The PC plans to improve its evaluation procedure and to implement a review cycle to overcome the problem of having to turn down applications because of shortage of budget. The guidelines for applications shall be unchanged, but the PC will discuss in Beijing the evaluation procedure by considering the following points:

- 1. Applications should be submitted preferably one year prior to the start of the conference to allow for careful evaluation.
- 2. To reinforce/enforce the role and involvement of the Divisions and Committees, applicants should address themselves directly to the appropriate Division President or Committee Chairman as explained in the guidelines. Applications that do not follow this rule should be sent back to the submitter with an indication of how to handle them.
- 3. Conferences requesting funding under the program for Scientifically Emerging Regions should be held in these regions, or, exceptionally, in their direct vicinity.
- 4. Partial/incomplete applications (mostly missing budget information) will not be distributed to the PC for evaluation, with the intent of 'gaining' time. Only completed applications including a full review and recommendation from the supporting Division or Standing Committee will be considered.
- 5. A review cycle of 4 or 6 months will be considered instead of the current practice that is to review the applications when they are filed. For such a period a proportional part of the total budget will be available. In principle, this procedure opens the possibility to set up a ranking of the applications which makes the procedure more competitive.

Annex

Projects that received financial support by the PC between <u>9 June 2003</u> (date of the previous report to the Council) and 31 December 2003.

The dollars amount granted by the PC is highlighted as bold; for projects that are interdivisional, that amount is bold and underlined. In the period of 9 June – 31 Dec 2003, the total amount granted by the PC was USD 71500:

XML-based IUPAC standard for experimental and critically evaluated thermodynamic property data storage and capture

2002-055-3-024M. Frenkel CPEP

Date of application Date of decision Amount granted (requested) 9/2/2003 10000 (10000)

Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry

2003-015-2-500 M.L. Bonardi Div V

Date of application Date of decision Amount granted (requested)

3/28/2003 9/5/2003 **16000** (21000) + Div V: 5000

Selected free radicals and critical intermediates: Thermodynamic properties from theory and experiment

2003-024-1-100 B. Ruscic Div I

Date of application Date of decision Amount granted (requested)

7/25/2003 10/16/2003 **17000** (22000) + Div I: 5000

A critical compendium of pesticide physical chemistry data

2003-011-3-600 D. Wauchope and D. Shaw Div VI and V

Date of application Date of decision Amount granted (requested)

10/8/2003 11/11/2003 **7000** (15000) + Div VI: 4000 + Div V: 4000

Classification, terminology and nomenclature of borophosphates

2003-034-1-200 M. Kizilyalli Div II and VIII

Date of application Date of decision Amount granted (requested) 12/29/2003 16000 (22000)

Solving in the problem of arsenic contamination in water in Bangladesh

2003-050-1-021 S. Ahuja and J. Malin CHEMRAWN

Date of application Date of decision Amount granted (requested)

10/28/2003 12/30/2003 **5500** (5000)

Projects that received financial support by the PC since 1 January 2004. The total amount granted by the PC as of 21 May 2005 is USD 106300:

Graphical representation standards for chemical structure diagrams

2003-045-3-800 B. Town Div VIII

Date of application Date of decision Amount granted (requested)

10/14/2003 3/18/2004 **24000** + Div VIII: 11000 (35000)

Young ambassadors for chemistry

2003-055-1-050 L. Schoen CCE

Date of application Date of decision Amount granted (requested)

11/17/2003 5/25/2004 **12000** + CCE: 4000 (16000)

Reference methods, standards and applications of photoluminescence

2004-021-1-300 E. San Roman and F. Brouwer Div III, I and V

Date of application Date of decision Amount granted (requested)

4/21/2004 7/30/2004 **4000** + Div III: 5000 + Div I: 2500 + Div V: 2500 (14000)

Standardization of analytical approaches and analytical capacity-building in Africa

2004-017-1-500 W. R. Benson Div V and VI

Date of application Date of decision Amount granted (requested)

3/19/2004 8/17/2004 **3000** + Div V: 5000 + Div VI: 2000 (10000)

Categorizing hydrogen bonding and other intermolecular interactions

2004-026-2-100 E. Arunan Div I

Date of application Date of decision Amount granted (requested) 7000 + Div I: 7000 (17000)

Establishing recommended data on thermodynamic properties of hydration for selected organic solutes

2004-036-1-100 V. Majer Div I

Date of application Date of decision Amount granted (requested) 9/29/2004 12/29/2004 13000 + Div I: 2000 (14000)

Comparable pH measurements by metrological traceability (revised title)

2004-005-2-500 M.F. Camoes Div V

Date of application Date of decision Amount granted (requested)

8/10/2004 1/4/2005 <u>2300</u> + Div V: 4000 + Div I: 1000 + Div VI: 1000 (8300)

IUPAC-NIST Chemical Identifier (INChl) promotion and extension

2004-039-1-800 A. McNaught Div VIII

Date of application Date of decision Amount granted (requested) 1/1/2004 1/19/2005 10000 + Div VIII: 5000 (15000)

A database of water transitions from experiment and theory

2004-035-1-100 J. Tennyson Div I

Date of application Date of decision Amount granted (requested) 10/1/2004 1/19/2005 20500 + Div I: 4000 (24500)

Design of polymer education material for french speaking countries

2004-037-1-400 G. Froyer Div IV and CCE

Date of application Date of decision Amount granted (requested)

10/19/2004 3/29/2005 **3500** + Div IV: 0 + CCE: 1500 (5000)

Terminology and measurement techniques of starch components

2004-022-3-400 M. Fitzgerald Div IV. VI. and VII

Date of application Date of decision Amount granted (requested)

12/1/2005 5/13/2005 <u>7000</u> + Div IV: 0 + Div VI:0 + Div VII: 0 (7000)

Conferences that received financial support by the PC

- Approved during the first year of the program, between $\underline{1 \text{ Jan} 31 \text{ Dec } 2003}$ (events listed in the order of granting date)
 Between 1 Jan 31 Dec 2003, the total amount granted was USD 36100
 - CHEMRAWN Consultation Forum Innovation in the Chemical Industry: the Way from Pure to Applied Chemistry [New Directions, Chremrawn]
 Ottawa (GA/IUPAC Congress2003), August 2003 > USD 3100
 - Biophysical Complexity [New Directions, div I] Southampton, UK, April 2003 > USD 4000
 - Chemical Thermodynamics, 18th IUPAC Conference on (ICCT 18) [Emerging Region, div I]
 China; Aug 2004 > USD 10000
 - Physical Chemistry of Bio-Interfaces [New Directions, div I]
 Australia, May 2004 > USD 5000
 - Chemistry Conference in Africa (ICCA 9) [Emerging Region]
 Tanzania, Aug 2004 >USD 4000
 - UNESCO Introductory Course & Conference on Macromolecules Polymers in Medicine, Nanotechnology and Degradation [Emerging Region & New Directions, div IV] South Africa, Apr 2004 > USD 10000
- Approved since 1 January 2004 (up to 21 May 2005) The total amount granted as of 21 May 2005 = USD 70760.
 - DNA Supramolecular Assemblies [New Directions, div VII]
 France, May 2004 > USD 5000
 - Environmental Significance of Mineral-Organic Component-Microorganism Interactions in Terrestrial Systems [New Directions, div VI] China, Sep 2004 > USD 3060
 - Chemical Education and Sustainable Development [Emerging Region, CCE] Russia, Nov 2004 >USD 5000
 - UNESCO School & IUPAC Conference on Macromolecules Biopolymer [Emerging Region, IV]
 Mauritius, June 2005 > USD 10000
 - Nanotechnology: Science and Application (NanoTech Insight '05) [Emerging Region & New Directions, div I & II]
 Egypt (Luxor), Feb 2005 > USD 7000
 - Solution Chemistry, (ICSC-29) [New Directions, div I & V]
 Slovenia (Portoroz), Aug 2005 > USD 4200
 - Chemical Thermodynamics (RCCT-2005) [Emerging Region, div I] Russia (Moscow), June 2005 > USD 5000
 - Analytical Chemistry and Chemical Analysis [Emerging Region, div V] Ukraine (Kiev), Sep 2005 > USD 5000

- Enhancing Students' Interest in Learning Science, European Science Education Research Association (ESERA) [New Directions, CCE] Spain(Barcelona), Aug 2005 > USD 5000
- Remediation of Groundwater Contamination by Arsenic [Emerging Region, Chemrawn]
 Bangladesh (Dhaka), Dec 2005 > USD 5000
- Advanced Materials (WAM III) focusing on Nanostructured Advanced Materials, IUPAC New Direction in Chemistry [New Directions, div II]
 South Africa (Stellenbosch), Sep 2005 > USD 10000 (note 1)
- Nuclear Analytical Methods in the Life Sciences (NAMLS-8) [Emerging Region, div V]
 Brazil (Rio de Janeiro), April 2005 > USD 4000
- Molecular Mobility and Order in Polymer Systems [Emerging Region, div IV] Russia (Saint-Petersburg), June 2005 >USD 2500

Evaluation Committee Report

The objectives of the committee are, in a few words, to check on the retrospective evaluation of projects under the relatively new project-driven system. Conference evaluation is also seen to come under this objective.

(a) Project evaluation: methodology.

As set out in the minutes of the 2004 EvC meeting, the first step is for the Secretariat to compile a list of measures for each completed project (e.g. citation data), to be sent to the EvC Chair and thence to the appropriate DP with a request for the appropriate information. In actuality, the requested information was not made available to the current EvC.

As it became apparent that the information could not be obtained in time for the Beijing meeting, the EvC Chair sent the following request to the DP of Divisions I-VII:

For two projects which have been completed within the last three years:

- Name of project
- Original milestones as listed in the application
- Milestones as actually achieved (papers, reports, etc.)
- Original criteria listed for retrospective evaluation
- Achievement of those criteria, or at least as much information as available at present.

(Division VIII was felt to be too new for meaningful data to be available and so was excluded from this request. Also it was felt that receiving evaluation information for only two projects per Division was better than requesting much more detailed information but receiving none.) Reminders were sent to DPs before the due date.

Replies were received from Divisions I, V and VI. These are given in the Appendix.

(b) Conference evaluation: methodology.

As set out in the minutes of the 2004 EvC meeting, the first step is for the Secretariat to compile annually the information for all approved conferences for review by the EvC. This information will include the forms, AIS and FIS submitted, and the reviews provided. It will also include citation data for those conferences published in *PAC*. The EvC would then proceed to an appropriate form of evaluation.

In actuality, the requested information was not made available to the current EvC.

(c) Conclusions

It is apparent, for the projects from the Divisions which replied, that these projects are fulfilling their original goals (or the spirit of these goals), as stated in the original project applications.

No comments can be made about other projects, including those from other Divisions, and there is not enough information from the whole gamut of projects to make any generic conclusions.

The overall conclusion is that the present retrospective evaluation system cannot work until a reliable mechanism for collecting the necessary data can be achieved.

(d) Recommendations of Evaluation Committee Chair

- That an *ad hoc* committee be set up to recommend a mechanism for an effective retrospective project evaluation procedure to be implemented, and that conferences can be evaluated.
- This committee could comprise a former DP, a person nominated by the NAOs making the largest IUPAC financial contributions (the top rung of the levy scale), and a person nominated by the Bureau from other NAOs. (The NAOs provide funding for IUPAC projects; the former DP could provide expertise in project administration.)
- Set up a system in the Secretariat so that the information needed for preliminary and subsequent evaluation is automatically flagged to the EvC Chair and to the DPs.
- That information be requested at the following intervals: (a) 6 months after the termination date originally given in the Project Submission form, (b) at the date nominated by the DP at which the project is effectively completed (e.g. submission of last report to P&AC), and (c) at a later period nominated by the DP appropriate for the retrospective evaluation stated in the original project application.
- The work required to supply the requested information is only a tiny fraction of that required to complete the project.
- The following quote from the VP's critical assessment is noted: "Discussions should begin in an attempt to achieve a consensus as to how any future increases in Division/Standing Committee project funding might be tied to success within the project system"
- One might have a simple evaluation score based on information provided for retrospective evaluation of a Division's projects (say, with a score for each project of 0–4, on a scale of project not completed through to project completed and exceeding evaluation criteria as stated on original application).
- "Project not completed" include not completed in a timely manner (obviously, unexpected minor delays would not be a problem: for example, completion of a 3-year project in 3 ½ years is certainly within the spirit of timely completion).
- That this information be part of the data sent to Council.

Appendix: responses received from Division Presidents

Division I

Ron D. Weir 22 June 2005

Original Milestones: Work on data collection is being carried out, with data assessment, recommendation and estimation of uncertainties to follow. A meeting of the Task Members to discuss the recommended values and their uncertainties, and prepare these for publication, will be arranged when the preliminary results for these series of compounds have been prepared.

1. Milestones actually achieved:

A. Seven papers in the series "Vapour-Liquid Critical Properties of Elements and Compounds" were published in the *Journal of Chemical & Engineering Data*: Part 1. An introductory survey, **40**, 345-350 (1995); Part 2. Normal alkanes, **40**, 531-546 (1995); Part 3. Aromatic Hydrocarbons, **40**, 547-558 (1995); Part 4. Aliphatic Alkanols, **40**, 1025-1036 (1995); Part 5. Branched Alkanes and Cycloalkanes, **41**, 365-372 (1996); Part 6. Unsaturated Aliphatic Hydrocarbons, **41**, 645-656 (1996); Part 7. Oxygen Compounds other than Alkanols and Cycloalkanols, **46**, 457-479 (2001); Part 8. Organic Sulfur, Silicon and Tin Compounds **46**(3) 480-485 (2001).

- B. The following papers are in the final stages of publication.
- (i). Part 9 **Nitrogen compounds:** reviews from 8 referees have been received and the report will be finalized for publication in *Journal of Chemical & Engineering Data* for June 2005.
- (ii). Part 10 **Halogen compounds:** manuscript ready to be sent to IUPAC reviewers in June 2005.
- (iii). Part 11 **Miscellaneous compounds** is 95 % complete and is awaiting the publication of parts 9 and 10.
- 3. Original criteria listed for retrospective evaluation:

The following is quoted from the project application form. The success of this project can only be determined by the use which is made of the recommended values as, for example, by the number of citations which the publications receive after 5 years.

4. Achievement of those criteria:

The citation numbers for each of the journal Parts in paragraph 2 A above are as follows. The numbers are cumulative to 20 Jun 05.

Part 1 – 19; Part 2 – 83; Part 3 – 28; Part 4 – 22; Part 5 – 27; Part 6 – 20; Part 7 – 102; Part 8 – 37.

Title: New Edition of Experimental Thermodynamics Vol II (120/16/97)

1. Original Milestones: The original milestone defined a single large volume. This was revised into two separate volumes of manageable sizes. The original target date of publication of 2000 had to be revised due to changes in publishers. First the original agreement that IUPAC would publish the volumes changed and the subsequent arrangement between IUPAC and Blackwell's collapsed. Arrangements were finally concluded successfully that Elsevier would publish the two volumes.

2. Milestones actually achieved:

Experimental Thermodynamics: Volume VI. Measurement of the Thermodynamic Properties of Single Phases. Editors: A.R.H. Goodwin, K.N. Marsh, W.A.Wakeham. Elsevier: Amsterdam. 2003. 558pp. cloth: ISBN 0-444-50931-3.

Experimental Thermodynamics: Volume VII. Measurement of the Thermodynamic Properties of Multiple Phases. Editors: Th. DeLoos, R.D. Weir. Elsevier: Amsterdam. Late 2005. About 450 pp. cloth: ISBN 0-444-51977-7.

- 3. Original criteria listed for retrospective evaluation: The success of this project can be determined by the use that is made of the books. The number of citations that the publications receive after 5 years is one measure of the success.
- 4. Achievement of those criteria: It is too soon to know the number of citations. Volume VII is slated to appear late in 2005.

Division V

1. Name of project:

IUPAC 2000-033-1-500 Assessment of uncertainty associated with soil sampling in agricultural, semi-natural, urban, and contaminated environments (SOILSAMP)

This is a large international project to which IUPAC was invited to participate. The mode of participation was that IUPAC representative (A. Fajgelj) was invited to be a member of the international Advisory Expert Board of SOILSAMP project. Project itself was fully funded by the Italian Environment Protection Agency (APAT), including IUPAC part (reimbursement of the second payment is pending from APAT).

2. Original milestones as listed in the application

[From EvC Chair:] Extensive information given in various attachments. In brief: Selection of sampling areas and procedures; Definition of the nomenclature to be used; Determination of reference distribution of trace elements in the soil; Intercomparison between soil sampling devices; Analysis by INAA; Data evaluation; Guidelines and recommendations; Workshop

3. Milestones as actually achieved (papers, reports, etc.)

Meetings organized in schedule, IUPAC reports submitted in time. Numerous publications have been produced within the frame of the project, but there was no reason for IUPAC to be involved in all of them.

4. Original criteria listed for retrospective evaluation

This project is not a classical IUPAC project and was also not requested/approved in a standard way.

5. Achievement of those criteria, or at least as much information as you have at present.

There are numerous measurable criteria:

- 1. The sampling site in northern Italy, selected and characterized within this project, has become the testing site for evaluation of measurement uncertainty associated with sampling equipment.
- 2. Terminology article has been published
- 3. Report in the International Conference on Biological and Environmental Reference Materials BERM 9 was presented in Berlin 2003.
- 4. There were numerous other publications resulting from SOILSAMP where IUPAC was not directly involved

Division VI

Project No: 1999-017-1-600

Title: Regulatory limits for pesticide residues in waters

Original Milestones:

- Preliminary workplan and assignments (3Q/1999)
- Draft report and preliminary recommendations (4Q/2000)
- Final recommendations and report publication (3Q/2001)

Proposed Evaluation Criteria:

- A measure of success would be the degree of adoption of the findings by national regulatory agencies and international advisory bodies, but this is unlikely to happen in the short term.
- Another measure of success would be to evaluate the number of literature citations to the published report as summarized in a scientific citation index. This would be most appropriate about 3-4 years post-project completion

Actual Project Outcomes

- "Regulatory limits for pesticide residues in water", IUPAC Technical Report, *Pure Appl. Chem.* 75(8), 1123-1155, 2003.
- "Evaluation and standards for pesticide residues in water", *Proceedings of the IUPAC-KSPS International Workshop on Pesticides*, 13-16 October 2003, Seoul, South Korea, pages 70-75.
- "Regulatory limits for pesticide residues in water", *ILSI-ICMR-ITRC International Symposium on Risk Assessment of Pesticide Residues in Water and Food*, 28-29 October 2003, New Delhi, India.

"Establishment and interpretation of limits for pesticide residues in water", *Proceedings of the IUPAC-UCR-MAG International Workshop on Crop Protection Chemistry in Latin America*, 14-17 February 2005, San Jose, Costa Rica, supplement pages 1-7.

Project No: 2000-016-1-600

Title: Environmental implications of endocrine active substances: Present state-of-the-art and future research needs

Original Milestones:

- June 2000 SAC (Scientific Advisory Committee) meeting to initiate the project
- August 2000 Each topic contributors' meeting
- June 2001 SAC meeting for evaluating and confirming the progress
- November 2002 SAC meeting to evaluate draft reports
- November/December 2002 Workshop
- March 2003 SAC meeting to complete the project, and to prepare for publishing the report

Proposed Evaluation Criteria:

- Submission of a questionnaire to academic societies, and other interested sectors.
- Checking No. of citation in academic journals.

Actual Project Outcomes

- The International SCOPE/IUPAC Symposium on Endocrine Active Substances, Yokohama, Japan, 17-21 November 2002.
- Environmental Implications of Endocrine Active Substances, Conference Report, *Chem. Int.* 25(2) 2003.
- Special Topic Issue on the Implications of Endocrine Active Substances for Humans and Wildlife, *Pure Appl. Chem.* 75(11-12), 1617-2615, 2003.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

INTERDIVISIONAL COMMITTEE ON TERMINOLOGY, NOMENCLATURE AND SYMBOLS (ICTNS)

REPORT TO IUPAC COUNCIL, 2005

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

- 1.0 Technical Reports and Recommendations; total accepted or under review: 48.
 - 1.1 Technical Reports reviewed and published in Pure and Applied Chemistry: 19 (list attached)
 - 1.2 Recommendations reviewed and published in Pure and Applied Chemistry: 7 (list attached)
 - 1.3 Recommendations reviewed and published elsewhere: 1 (*Nomenclature of Inorganic Chemistry*, in press RSC).
 - 1.4 Recommendations accepted for publication elsewhere: 2 Revisions of the VIM (*International Vocabulary of Metrology*) and Supplement 1 of the GUM (*Guide to Uncertainty in Measurement*) for BIPM-ISO.
 - 1.5 Technical Reports accepted as of 2005-06-20: 3
 - 1.6 Recommendations accepted as of 2005-06-20: 0
 - 1.7 Technical Reports under review as of 2005-06 20: 11
 - 1.8 Recommendations under review as of 2005-06-20: 5

2.0 New duties for Chairman and Secretary of ICTNS

The holders of these positions are now also Editors, Technical Reports and Recommendations, for *Pure and Applied Chemistry*. The Chairman is a member of the Editorial Advisory Board for PAC.

3.0 Revision of *IUPAC Handbook*

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

4.0 Interactions with the International Scientific Community

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

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

Appendix: Technical Reports and Recommendations published in *Pure and Applied Chemistry* 2003 through June 2005

Technical Reports

Critical evaluation of stability constants for alpha-hydroxycarboxylic acid complexes with protons and metal ions and the accompanying enthalpy changes. Part II. Aliphatic 2-hydroxycarboxylic acids,

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Pure Appl. Chem. 75(5), 631-681, 2003

J. Lintelmann, A. Katayama, N. Kurihara, L. Shore, and A. Wenzel

Critical review of analytical applications of Mössbauer spectroscopy illustrated by mineralogical and geological examples,

Pure Appl. Chem. 75(6), 801-858, 2003

E. Kuzmann, S. Nagy, and A. Vértes

Atomic weights of the elements. Review 2000,

Pure Appl. Chem. 75(6), 683-799, 2003

J. R. de Laeter, J. K. Böhlke, P. De Bièvre, H. Hidaka, H. S. Peiser, K. J. R. Rosman, and P. D. P. Taylor

Significance of impurities in the safety evaluation of crop protection products,

Pure Appl. Chem. 75(7), 937-973, 2003

A. Ambrus, D. J. Hamilton, H. A. Kuiper, and K. D. Racke

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T. Imasaka, D. S. Moore, and T. Vo-Dinh

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D. J. Hamilton, ?. Ambrus, R. M. Dieterle, A. S. Felsot, C. A. Harris, P. T. Holland, A.

Katayama, N. Kurihara, J. Linders, J. Unsworth, and S.-S. Wong

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S. Beuermann

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R. D. Loss

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H. Egli, M. Dassenakis, H. Garelick, R. van Grieken, W. J. G. M. Peijnenburg, L.

Klasinc, W. Kördel, N. Priest, T. Tavares

Appendix: Technical Reports and Recommendations published in *Pure and Applied Chemistry* 2003 through June 2005

Properties and units in the clinical laboratory sciences. XIX. Properties and units for transfusion medicine and immunohematology,

Pure Appl. Chem. 75(10), 1477-1600, 2003

K. Varming, U. Forsum, I. Bruunshuus, and H. Olesen

On the claims for discovery of elements 110, 111, 112, 114, 116, and 118,

Pure Appl. Chem. 75(10), 1601-1611, 2003

P. J. Karol, H. Nakahara, B. W. Petley, and E. Vogt

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Appendix: Technical Reports and Recommendations published in *Pure and Applied Chemistry* 2003 through June 2005

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Pure Appl. Chem. 76(6), 1269-1281, 2004

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E. C. Robert, R. Bruessau, J. Dubois, B. Jacques, N. Meijerink, T. Q. Nguyen, D. E. Niehaus, and W. A. Tobisch

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S. Hatscher, H. Schilder, H. Lueken, and W. Urland

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Appendix: Technical Reports and Recommendations published in *Pure and Applied Chemistry* 2003 through June 2005

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J. Y. Shin, J. Y. Park, C. Liu, J. He, and S. C. Kim

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M. Terazima, N. Hirota, S. E. Braslavsky, A. Mandelis, S. E. Bialkowski, G. J. Diebold,

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P. de Zorzi, S. Barbizzi, M. Belli, G. Ciceri, A. Fajgelj, D. Moore, U. Sansone, and M.

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Numbering of fullerenes, *Pure Appl. Chem.* 77(5), 843-923, 2005 F. Cozzi, W. H. Powell, and C. Thilgen

International Union of Pure and Applied Chemistry Vice President's Critical Assessment, 2005

Bryan R. Henry

ABSTRACT: The focus of this year's critical assessment is a review, assessment and analysis of our project system. The report is based on information obtained from interactions with members of various Divisions and Standing Committees, and attempts to provide an overview and to identify best practices. A series of Table provides data on a number of project related parameters from 1998 to the present. The report presents a set of observations and challenges, and concludes with five summary recommendations directed to project generation, monitoring, and funding, and to project activity in the Operational and Advisory Standing Committees. A final recommendation deals with increasing the profile of IUPAC.

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1. INTRODUCTION

IUPAC is a worldwide organization that has an impressive track record in enabling the language of chemistry to be understood globally. It acts as an authoritative nongovernmental agency to provide standards for chemical nomenclature and terminology, and sponsors numerous conferences on a wide range of chemical themes. While these activities are well known and respected by the international scientific community, the IUPAC project system is perhaps less appreciated. This project system lies at the very heart of IUPAC activities. It involves the volunteer efforts of close to 1000 scientists worldwide. It is nurtured, monitored, and organized by IUPAC's eight scientific Divisions and three operating Standing Committees. Oversight is provided by the IUPAC Bureau and by advisory Standing Committees such as the Project Committee, the Evaluation Committee, and the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS). The range of projects covers the whole gamut of chemistry from chemical education, critically evaluated databases, and precise and reliable atomic weights, to the political arenas of chemical disarmament, sustainable development, meeting the needs of developing countries, the requirements of chemical industry, and a plethora of other areas.

The project system in its current form is a relatively new development in the history of IUPAC. Our organization, which was formed in 1919, operated for most of its existence on the basis of a commission system. It is not my purpose here to review that system, but rather to briefly summarize our passage from the commission system to our current project mode of operation. The transition was passed by the Bureau in 1998 and approved by Council in August 1999. While the vote in Council was overwhelmingly in favor, the topic was hotly debated with doubts expressed both by some Divisions and some National Adhering Organizations (NAO)s. The principal concern seemed to be that the fundamental focus of IUPAC operations would change. Reassurance was offered that any money saved by eliminating commissions would be devoted to scientific work. The project system was fully phased in within the 2002–2003 biennium.

The successful operation of the project system has been a clear priority for IUPAC. The transition was given strong support by the Bureau and by President Jortner in 1999. In his detailed and exhaustive 2001 Vice President's Critical Assessment (VPCA), President Steyn reviewed the new system and identified the challenges that would need to be faced for its successful implementation. In particular, he noted that the generation of new projects with broad international appeal would require "proactive efforts at all levels within the Union". In his 2003 VPCA, President Sydnes noted that although some observers believed that restructuring to the project system appeared to be beneficial, analysis of the full effects would require more time. However, he did point out a need to broaden the geographic participation in project Task Groups, and suggested that both improved visibility of IUPAC activities and improved communication within IUPAC would be helpful in this regard.

Two years have passed, and perhaps now is a good time to assess how our new system is functioning. This will be the principal topic of this VPCA. The preliminary answer is

that the system is functioning very well, perhaps even better than expected. However, as with any new system, there may be opportunities to improve performance by making incremental changes and attempting to benefit from best practices. One difficulty we have as a large and diverse organization is that we have a tendency to solve our problems in isolation. Joint meetings of Division Presidents and Standing Committee Chairs can serve to share best practices, but those meetings are rather infrequent and often rushed. In this report, I will attempt to provide an overview and to hone in on what is working well. I will address a number of project-related questions. Are there any problems involving project generation? Are project approval mechanisms working efficiently? How can we effectively control the length of time to complete projects? What steps are in place to monitor and improve the quality of projects? Are project dissemination methods functioning effectively? Do the Evaluation Committee and ICTNS have the best tools and resources to function effectively in the new system? Should changes in project funding allocations to Divisions and Standing Committees be determined on the basis of their success within the project system?

While the project system will provide the focus in what follows, other issues deserve some attention. We need to continue to seek ways to improve the involvement of industry in IUPAC activities. There may be opportunities for IUPAC to expand its impact through changes in its relationships with other organizations such as the International Council for Science (ICSU), the World Trade Organization (WTO), the United Nations Industrial Development Organization (UNIDO), the United Nations Educational, Scientific and Cultural Organization (UNESCO), and the International Atomic Energy Agency (IAEA). For example, could IUPAC do more to help developing nations overcome non-tariff barriers that affect their market access?

2. METHODOLOGY

The philosophy in preparing this report was to listen and learn from the members, Officers and Chairs of the Divisions and Committees. In that way, the suggestions for change and improvement come from those directly involved in the project system. Prior to the Bureau meeting in Bled in October 2004, I was fortunate to be able to attend the off-year meetings of the Inorganic Chemistry Division (II), the Polymer Division (IV), the Analytical Chemistry Division (V), the Chemistry and Human Health Division (VII), and the Chemical Nomenclature and Structure Representation Division (VIII). Scheduling did not permit me to attend the remaining Divisional off-year meetings. Meetings with Tom Tidwell (Division Past President) and David Black (former Division Vice President) provided feedback on the Organic and Biomolecular Division (III). In addition, I met with the Chairs of the Committee on Chemistry and Industry (COCI), the Committee on Chemistry Education (CCE), and CHEMRAWN (CHEMical Research Applied to World Needs), and with representatives of the Royal Society for Chemistry (RSC) and the American Chemical Society (ACS). These were all useful meetings, and I learned a great deal. I would like to thank all of the individuals involved for their kindness and hospitality. Reports of the meetings were written and circulated to the IUPAC Officers and to the Division Presidents and Committee Chairs. These reports provide the basis for this document.

One side effect of these meetings was an improvement in communications between the Officers and Secretariat on the one hand, and the Divisions/Committees on the other. As President Sydnes has so clearly pointed out in his VPCA, communication within IUPAC is an important priority. In many instances, these interactions represented the first time that an officer had attended such a meeting. In most cases, there was a valuable exchange. I hope to be able to attend the off-year meetings of the Physical and Biophysical Chemistry Division (I), Division III, and the Chemistry and Environment Division (VI) in 2006, if only to complete my education. The 2004 Bureau meeting in Bled provided the opportunity to meet with all of the Division Presidents and Committee Chairs that were present. Subsequent to Bled, I was able to enjoy an afternoon with the Chair of ICTNS. As Vice President, I am a member of the Project Committee and thus have ongoing access to their activities.

3. DIVISION SUMMARIES

The following summaries reflect what I learned from the interactions described in the previous section. More detail is provided for those Divisions where I had the privilege of attending their meetings. It should be recognized that what is given here is my own perspective, and is nothing more than a snapshot in time. All of these Divisions are actively involved in strategic planning and are constantly evolving. The dedication and hard work of the Division Officers and the Division Committees represent a core strength for IUPAC.

Physical and Biochemistry Division (I): Overall, the project system seems to be working well, and the current officers support the new system. There has been a slight reduction in the number of projects approved, but the dollar value of the projects has increased. The Division has established an Advisory Committee consisting of 61 distinguished international scientists and engineers. One role of this committee has been in the assessment of project proposals and in generating new projects. A result has been the reduction in approval time for new projects. Once per year, a written report is expected from the Task Group Chair (TGC). The Division President and Vice President are both active in the monitoring process. ICTNS works well for their projects. The atmospheric kinetic database is currently stored on a Web site associated with Cambridge University. It is also mirrored on the server that hosts the IUPAC Web site. Although this arrangement has worked well, the Division would like to look at streamlining the current method of recording the number of hits.

Inorganic Chemistry Division (II): This Division has one of the two Commissions remaining within IUPAC (the Commission on Isotopic Abundance and Atomic Weights). Thus, in part, they have encountered some difficulties in the transition to the project system. There is no shortage of important projects meeting high scientific standards in the area related to their Commission. However, concentration in this area has resulted in decreased activities in their other two areas, materials and molecular. Generation of projects and increased activities in these latter areas are current Divisional strategic goals. In particular, they have set up a subcommittee in the molecular area to nurture and build

this aspect of their activities. The Division is moving toward some form of block funding for the Commission, but the Commission will continue to access the project system in the usual competitive fashion. The Division has a successful monitoring system whereby each project is assigned an active individual monitor. Currently, they are devising a common reporting form, which will be used by task groups to respond every six months through their monitors.

Organic and Biomolecular Chemistry Division (III): The current executive believes there are no inherent problems with the project system. However, they did experience some transitional difficulties. On passage to the project system, the authority to generate projects passed to the various Division Committees. Within Division III, their subcommittees have this responsibility. One Titular Member (TM) on each subcommittee is responsible for the organization of project generation. While this process was successful for some subcommittees, others experienced difficulties. However, all of the subcommittees now appear to be operating successfully. They perceive a need to get completed projects reviewed and evaluated.

One area of interest is documentation of the effects of herbal medicine. The aim would be to help people in areas of the world where international medicine is not always affordable. The Division is willing to look at improvements in project monitoring.

Polymer Division (IV): This Division seems to be thriving under the project system. They make extensive use of feasibility studies to generate projects. Typically, these studies are done by e-mail over a two-year period and are funded from the operating funds of the Division. A feasibility study goes back to the relevant subcommittee, which suggests any needed changes and assigns a priority. A given subcommittee will have six or more projects running and several ongoing feasibility studies. New projects also come from IUPAC-sponsored macromolecular conferences. Overall, the Division has no problem with project generation. Their problem is lack of funds to support existing projects. Currently, they impose a ceiling of \$2000 per year per project in order to spread the funds around.

The Division is involved in several interdivisional projects, which they believe work very well, with one of the participating Divisions taking the lead. It is common for one person to work on several projects. The Division operates a taxing system to generate funds for face-to-face meetings that serve as breeding grounds for new projects. Projects are monitored, and project completion does not appear to be a major problem in that relatively few projects are classified as dormant. However, the Division sees benefits in a common, more regulated monitoring system. For some of their projects, citation numbers are particularly impressive. The Division has beneficial interactions with industry, and some of their projects have direct industry involvement. The Division makes use of their relatively high number of IUPAC-sponsored conferences to introduce additional participants into macromolecular projects. At the introduction of the new system, there was some strong opposition among veteran members of the Division. However, the current accepted view appears to be that the change has been a positive one and has introduced more flexibility.

Analytical Chemistry Division (V): The Analytical Chemistry Division has handled the move to the project system very efficiently. The Division Committee takes on the responsibility for generating projects, and the Division President serves as the project coordinator. In generating projects, they use young observers, both as a source of projects, and in an attempt to introduce new blood. They also use conferences and the corresponding IUPAC representatives in generating projects. They hold workshops at their Division meeting and at the General Assembly, and one goal of such workshops is project generation.

They have procedures for active guidance in bringing a project to a stage where it can compete for funding. This nurturing process clearly benefits the quality of the resultant projects. An example proposal is posted online, and they make extensive use of *Chemistry International (CI)* to advertise existing projects. In fact, communication within this Division is very good. They publish a Divisional newsletter. A project reporting form is required every six months. This monitoring system works very well. The officers carry out an in-depth review of all projects at their officers meeting, which precedes the Divisional meeting. Projects are also reviewed at the Divisional meeting. For most projects, one Task Group meeting is adequate. Under the project system, the average duration to carry out a given scientific investigation has decreased. They find ICTNS to be very helpful, particularly with regard to Gold Book entries. They believe that interdivisional cooperation is working well. An important issue for the Division is that IUPAC maintains access to the computer capability to maintain their project-generated databases such as the Stability Constants Database. The Division believes that the project system is more flexible, and they have no desire to return to commissions.

Chemistry and the Environment Division (VI): There have been some difficulties in moving from the commission-based system to the project system. There is a perceived need to find new areas of strength as some traditional areas of strength are experiencing difficulties in generating new projects. However, in some areas, there are plenty of projects, and the Division usually spends all of its project money. (Note: In fact, this process of evolution was one of the reasons the project system was introduced. Under the project system, areas that do not generate projects do not consume resources, whereas within the commission system it was difficult to eliminate a commission due to lack of activity.) The Division believes that they could carry out more projects if they had more money. In fact, they have been successful in obtaining additional IUPAC funds to support projects beyond their budget. They are not using feasibility studies or scoping exercises for project generation.

Questions are sent out to all project leaders to assist in project monitoring. However, some members of the Division believe that monitoring is not always functioning as well as it should. They are also concerned about effective peer reviews of completed projects. Typically, projects are completed within two to three years. Division VI has been involved in collaborations with outside organizations associated with ICSU. In particular, they have had a very successful interaction on endocrine disruptors with the ICSU Scientific Committee on Problems of the Environment (SCOPE). They would like to see

expanded cooperation with other organizations. They believe that subcommittees function most effectively with face-to-face meetings.

Chemistry and Human Health Division (VII): They have a small Division Committee with two of the members from industry. They operate with three diverse subcommittees, but still believe that they have been very successful within the project system ("The project system is great"). The subcommittees attempt to meet at technical meetings which they would normally attend. The subcommittees generate the projects, with few projects coming from outside. Each project has an active mentor who is a member of a subcommittee or a Division Committee member. The Division uses the project system to actively recruit new blood. The subcommittees identify a technical need and go out and find new people with that expertise. They try to understand where their field is moving in the future and who they want to serve. In their words, they are "attempting to solve tomorrow's problems today". One of their strategic directions is to get less-developed nations more involved.

Most projects take two to three years. The Division believes that they could carry out more projects if they had more money. They were successful in obtaining additional IUPAC funds to support projects beyond their budget. They are looking into ways to raise funds beyond IUPAC to support their projects and meetings. One issue that is particularly important in the health field is that technical investigations can have political consequences. For example, the Division believes that patents in the health field should not prevent the development of that field.

Chemical Nomenclature and Structure Representation Division (VIII): This is the newest Division. It was established in 2002 in an attempt to bring all nomenclature-related activities within one Division. They use scoping exercises (feasibility studies) to generate new projects and to bring new people on board. There are several active projects with many waiting to be done. Several projects are interdivisional, particularly with Division IV. Progress on projects is generally very good although delays do occur. The difficulty is neither a lack of money nor a shortage of projects, but rather a need for scientists with the time, expertise, and inclination to help. There is a critical need to get more people involved in the nomenclature activities of IUPAC. One beneficial aspect of the project system is that it is easier to keep people working in the nomenclature area beyond 12 years by involving them in a number of projects. In fact, given the time it takes someone to be productive in nomenclature activities, the Division believes that it might be reasonable to extend time limits for the Divisional Committee beyond 12 years.

They have had some recent success in bringing younger people to serve on new projects and onto their Division Committee. Industry is actively involved in Divisional activities. They use both their Advisory Committee and National Representatives as a source of new people to work on nomenclature related projects. The Division uses a Web Board to facilitate communication between the Division Committee, Task Groups, and the Advisory Committee. One issue for them is an improvement in IUPAC computer resources in order to facilitate storage and access to Division VIII databases, and to support their Web Board.

4. OPERATIONAL STANDING COMMITTEES

The use of the project system is a more recent development for these committees, and so it is still too early to make definitive judgments. What follows is very much a progress report.

Committee on Chemistry and Industry (COCI): COCI has developed a project team that will monitor COCI projects and will vet all IUPAC projects for potential COCI interest. COCI is keen that projects be time-limited, demand-led, and meet IUPAC's strategic directions. Regarding the public perception of chemistry, COCI activity is a component of the CCE initiative in that it attempts to provide an industrial viewpoint.

COCI is particularly interested in the public appreciation of chemistry. They would also like to see a broadening of industrial interest in IUPAC to include areas like the pharmaceutical industries. A key issue here is the role of IUPAC as a nongovernmental organization (NGO) in its actions to bring rational discussion to chemical issues. They believe that the Company Associates (CA) program could be used to greater effect, and they have drafted a revised approach to industry regarding the CA program.

Committee on Chemistry Education (CCE): A system is in place for project review, evaluation, and recommendation. There is a need for joint projects with Divisions where there is an educational component. DIDAC will now be part of CCE, working jointly with COCI. In development projects, while CCE will do all that is possible to help project leaders achieve collaboration with local NGOs to get products distributed, CCE does not have the resources to distribute material. Continued partnership with UNESCO is very important to CCE, as is any initiative to help young people appreciate chemistry.

CCE can work effectively within the project system and believes it to be more flexible and adaptable. However, for many CCE activities, face-to-face meetings are needed in the sense that they can be more efficient than electronic communication. The existence of a separate project budget for CCE has been helpful.

CHEMRAWN Committee: They want to draw up a set of rules for future organizers of CHEMRAWN conferences to provide guidance for conference funding and interactions with IUPAC. CHEMRAWN wants to follow up on our work on chemical weapons, as well as extending the work they have done concerned with arsenic in drinking water in Bangladesh. They are very involved in chemical sciences and education in the Middle East with the Malta II conference.

Recently, the Chair of CHEMRAWN drafted a report that essentially summarizes the first 16 CHEMRAWN conferences. In many cases, these conferences produced a set of recommendations. Actions based on these recommendations are often followed up by a Future Actions Committee (FAC). Notable successes involved CHEMRAWNs II, IV, and XIV where the FACs sent copies of recommendations to a number of governmental personnel, including all members of the U.S. Congress and Senate. In other cases, the

conferences led to significant science. For example, CHEMRAWN VII launched a series of studies of atmospheric modeling.

This report is the beginning of an attempt to help CHEMRAWN publicize its contributions. It is a very important report and it needs to be given wide publicity and a high priority. More information will be gathered, and hopefully in some cases, it will be possible to demonstrate why the world has become a better place because of a given CHEMRAWN conference.

FACs have been most successful when there have been funds available to finance their activities. For example, these funds can come from the conference making a profit. If the FAC has one or more focused initiatives growing out of a CHEMRAWN conference, they could be encouraged to use the project system to accomplish their goals.

5. PROJECT-RELATED ADVISORY STANDING COMMITTEES

I have included a few comments here in recognition of the extent to which these three committees are involved in the project system. The Evaluation Committee is still in its early days, as the opportunity to evaluate completed projects under the new system is just beginning. ICTNS has extensively revised its operations in response to the new system, and it is timely to examine its activities over the last two years.

Project Committee: The description of the activities of the Project Committee can be found in the terms of reference in the current *IUPAC Handbook* and in the Chair's (Prof. Gus Somsen) recent report to the Bureau in Bled. In summary, this committee makes funding decisions on projects that are interdisciplinary in nature or where the funds requested are beyond the Division/Standing Committee budget. They also review applications for financial support for conferences in scientifically emerging regions, and for financial support for conferences on new directions in chemistry.

The committee operates efficiently, and funding decisions are reached in a timely fashion. Critical factors in making decisions are the expert analyses provided by Divisions and Standing Committees. The Project Committee did not spend the project part of its biennial allocation in either of its first two biennia (2000–2001 and 2002–2003). However, they are on track to completely use their current 2004–2005 budget of \$110,000. It also appears that the 2004–2005 conference budget of \$65,000 will be fully utilized.

The committee is in the process of considering a change in their procedures for awarding financial support for conferences. They are discussing a system whereby they consider applications two or three times per year. Such an approach would permit a ranking of the relevant conferences and make the procedure more competitive.

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS): ICTNS exists primarily to provide quality control for IUPAC recommendations on nomenclature, terminology, symbols, and units, and to act as a means of liaising with

other Unions and cognate bodies in these areas. Under the previous regime (as IDCNS), this was done in part by asking IDCNS members (primarily the Chairman and the Secretary) to review all documents submitted for publication, and to propose additional reviewers if it was felt that this was necessary. The composition and terms of reference for the committee can be found on pp. 66 and 67 of the current *IUPAC Handbook*. The current version of ICTNS was established in 2002 and since 2003 has successfully cleared a backlog of reports and recommendations.

ICTNS deals with both Technical Reports and Recommendations.

Technical Reports (TRs): TRs go first to the Division, which ensures that the science is correct and that the report is written according to the Guidelines for Drafting Technical Reports and Recommendations. This may or may not involve external reviews. The Division President approves the TR and sends it to the Secretariat who forwards it to ICTNS. They check the compatibility of the document with IUPAC recommendations on terminology, nomenclature, and symbols. The manuscript is then forwarded to the Production Editor, for publication in *Pure and Applied Chemistry (PAC)*.

ICTNS guidelines for technical reports as outlined in the *IUPAC Handbook* are not always followed, which causes delays and frustration. Divisions differ in the degree to which they carry out scientific review. A solution would be for Divisions to both thoroughly review the science and to keep potential authors informed as to the need to follow the guidelines. The latter could become a routine part of the project monitoring process. Alternatively, there is the possibility that ICTNS could simply refuse to accept TRs that don't follow the guidelines. The current ICTNS committee does not believe that their role should be to act as copy editors.

Recommendations: These can be divided into two types. The first type deals primarily with non-nomenclature items such as terminology and glossaries. The second type involves recommendations on nomenclature. For the first type, the Recommendation document is sent initially to ICTNS to check conformity with ICTNS guidelines. After ICTNS approval, the document is submitted through the Secretariat to the Division President who arranges for the Secretariat to submit it to a panel of 15 experts. After the Division President's approval, the Secretariat posts the title, synopsis, and full text on the IUPAC Web site as a Provisional Recommendation. At this point, the Recommendation begins a period of public review (5 months). At the completion of the expert review, the Recommendation is returned to ICTNS. ICTNS attempts to complete their review at least one month before the end of the public review period.

As with TRs, problems can occur when Recommendations do not take account of existing IUPAC definitions. Provisional Recommendations are posted when the Division President approves. This step can take place before the expert reviews are received. If a Provisional Recommendation subsequently proves to be incorrect, it can create problems in that it is not always easy to remove it expeditiously. The procedure could be changed such that the document could be posted as a Provisional Recommendation only after the

completion of expert review. However, such a change would require attention to timing as an extension of the overall time for approval would be undesirable.

The second type of Recommendation involves nomenclature. The procedures are the same as for non-nomenclature Recommendations, except that the report is vetted by Division VIII before it is sent to the 15 experts. ICTNS believes that this procedure is working well and that the resultant reports are consistently of high quality.

Perhaps it would be timely to reconsider the role of ICTNS in the review of nomenclature recommendations in light of the creation of a Division devoted entirely to nomenclature. In a sense, Division VIII produces the rules and ICTNS applies them. In that light, ICTNS can act as a valuable additional source of expert input. However, the identification of 15 expert reviewers outside of Division VIII could be problematic. In addition, it is worth reconsidering whether terms of reference (v) and (vi) on p. 67 of the current *IUPAC Handbook* should be the sole responsibility of ICTNS or whether Division VIII should play a defined role. There is also a need to find better mechanisms to obtain meaningful outside reviews of the Red Book (*Nomenclature of Inorganic Chemistry*) and the Blue Book (*Nomenclature of Organic Chemistry*).

Evaluation Committee: The beginnings of this group can be traced back to 1999. The Evaluation Committee developed a set of Guidelines for project evaluation which was based on test evaluations of selected projects. They published a document entitled "Advice to Task Group Chairmen". They have made a list of projects completed in 2002–2003. Since the first projects within the new system have only recently been completed, the Evaluation Committee has just begun to function fully. There was a particular concern about the length of time to complete projects, and whether projects were meeting their originally stated completion deadlines. Obtaining the necessary data to provide meaningful evaluation has proven to be problematic. The evaluation of conferences is just beginning. Some of these issues will be dealt with in the next section.

6. TABULAR OVERVIEW OF THE CURRENT PROJECT SYSTEM

Tables I–VI contain a summary of the status of the total number of IUPAC projects over the last five years as of 17 January 2005. The best comparisons occur from biennium to biennium, and since the project system was fully operational in the 2002–2003 biennium, it is still far too early to trace trends in any quantitative sense. Nevertheless, some qualitative observations can be made that indicate areas to watch in the future.

Tables I–IV focus on the number of projects. There was clearly a decrease in the number of projects as we moved from the old commission-based system in 1998–1999 through the transitional years 2000–2001 to the project-based system in 2002–2003. However, the last column of Table I indicates a resurgence. Perhaps the most hopeful sign in Table II is the marked decrease in the number of abandoned projects from January 2002 onward. The abandoned projects in the years 2000, 2001, and 2002 were primarily projects initiated under the commission system, and not projects that had been reviewed and

evaluated under the new system. This process of "cleaning house" helped to launch the new system with a minimum of inherited problems.

The tracking of projects has improved dramatically, and hopefully this will allow Divisions and Committees to focus not only on project generation but also on project completion. The newly approved projects in Table III are a reflection of how quickly the Divisions and Committees adapted to the new system and reflect the comments given previously in Sections 3 and 4. Table IV indicates little change in the number of submitted proposals when 2000–2001 is compared to 2002–2003.

Table I Current projects.

	IUPAC Handbook 1998–1999	IUPAC Handbook 2000–2001 (as of 1 Jan 2000)	IUPAC Handbook 2002–2003 (as of 15 Feb 2002)*	IUPAC Handbook 2004–2005 (as of 31 Dec 2003)
CTC/CCE	9	9	Nr	7
Other STCs	9	14	5	10
Div I	51	40	10	14
Div II	22	22	8	10
Div III	21 + 4 biotech	22	6	14
Div IV	33	30	11	22
Div V	111	88	25	23 + 17 SDS
Div VI	52	40	12	15
Div VII	28	17	9	17
Div VIII			8	10
TOTAL	340	282	94	143**

^{*}Starting with that compilation, only the projects approved in the new system were accounted for.

^{**}The sum of 142 does not include all the solubility data series. 143 accounts for one "umbrella" project for the "solubility data series".

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Table II Completed projects.

	IUPAC	IUPAC	IUPAC	From the Web
	Handbook	Handbook	Handbook	Completed
	2000–2001	2002–2003	2004–2005	since Jan 2004
	Completed in	Completed in	Completed in	
	1998–1999*	2000–2001	2002–2003	
CTC/CCE	1	1	1	2
Other		6	4	2
STCs				
Div I	11 (3)	10 (6)	3	1 (1)
Div II	6	9	2	0
Div III	5 (5)	5 (1)	4	3
Div IV	5 (1)	6 (1)	12	3
Div V	18 (14)	23 (17)	17	8 (2)
Div VI	13 (6)	17 (3)	11 (1)	3 (1)
Div VII	4 (8)	7 (2)	3 (1)	2
Div VIII			1	0
TOTAL	63 (37)	84 (31)	58 (2)	24 (4)

^{*}These numbers reflect projects completed (or abandoned) since the previous compilation of current projects published in the 1998–1999 *IUPAC Handbook*.

Table III Newly approved projects.

	Approved in 2000–2001	Approved in 2002–2003	Approved in 2004
CTC/CCE	2	6	1
Other STCs	3	6	5
Div I	7	8	3
Div II	6	3	2
Div III	5	9	1
Div IV	12	18	4
Div V	12	11	2
Div VI	10	9	9
Div VII	4	14	7
Div VIII	3	5	1
TOTAL	64	89	35

Note: The numbers reflect the tabulations presented online under http://www.iupac.org/projects/new_projects.html, and summed by biennia.

Table IV Number of proposals submitted per year.

2000	37
2001	87*
2002	65
2003	63
2004	48

^{*}Includes a few "old projects" reintroduced into the system.

Table V Current and "overdue" projects as of 18 Jan 2005.

	Total current projects	Current project "overdue"	Overdue + 6 months*
CTC/CCE	6	3	2
Other STCs	14	2	1
Div I	18	9	7
Div II	11	7	6
Div III	14	10	7
Div IV	26	13	8
Div V	37	29	16
Div VI	19	7	5
Div VII	22	13	8
Div VIII	12	7	4
TOTAL	179	100	64

^{*}Current projects where the originally intended date of completion was 30 June 2004 or later.

Table V indicates an area of some concern. We are a volunteer organization, and we depend on talented and committed scientists from all over the world to carry out IUPAC projects. One of our very real strengths is the willingness of scientists to take time from their hectic schedules to work on IUPAC projects. These tasks are inevitably taken on with the best of intentions, but other pressures frequently cause delays. In Table V, a comparison of columns 2 and 4 shows that an average of 36 % of projects are overdue by more than six months (the range is 7 to 54 %). A mitigating circumstance is that completion dates on the project submission forms are usually overoptimistic. Moreover, delays in the approval process can cause hold ups. However, even in light of these considerations, the numbers in column 4 are higher than they should be. In three cases, the ratio of significantly delayed projects exceeds 40 %. Another possible reason for these delays is the reduction of face-to-face meetings of Task Groups in lieu of more frequent use of e-mail correspondence. The requirement to face your peers and present

progress on a project is one of the best inducements to meet deadlines. One possible way to alleviate the delays is improvement in project monitoring.

In many ways, the most interesting of these tables is Table VI. There are small differences between the number of projects in round brackets in Table VI and the corresponding number of newly approved projects in Table III. The Table III numbers come from the Web and do not include projects that are extensions of existing projects. In addition, Web pages are at times created for projects early in a new year where the project was approved in the previous year. Table VI represents the core data that are maintained systematically during the submission, review, and final accounting of the allocated funds, for each project. They include projects that are classified as dormant. Thus, the project numbers in Table VI are often slightly larger than those in Table III.

The comparison that stands out for Table VI is the change in the total funds devoted to IUPAC projects as we moved from the transition years of 2000–2001 to the first years of the project mode in 2002–2003. The dollars made available to projects changed from \$376,350 to \$622,472, which represents an increase of 65 %. Based on the figures for 2004, we appear to be maintaining this level of funding for the 2004–2005 biennium. Thus, the promise that any savings from the shift to the project mode would be passed on to scientific endeavors appears to have been kept! The net result has been an increase in the average grant per project, although that change has been far from uniform from Division to Division.

It is worth noting here that the system has considerable flexibility. Divisions or Committees that have suitable reviewed projects ready to be funded, but that have run out of project funds, can apply to the Secretary General and Treasurer for additional funds from their reserve for a given biennium. In 2002–2003, all but one of the Divisions and all of the Standing Committees did just that. A total of 12 additional projects were funded.

A version of Table VII also appeared in President Sydnes' VPCA. In all, 57 countries are represented. The Table specifically notes those countries with Task Group Members (TGMs) that are Associated National Adhering Organizations (ANAOs) or that are not an NAO or an ANAO (noted as a nonmember, NM). In general, the countries that have members on Division/Executive Committees or governing bodies like the Bureau or Executive Committee have the most TGMs. However, the distribution is impressive and emphasizes the global nature of IUPAC.

It is a continuing goal of IUPAC to increase the geographic representation on Task Groups. Division V uses IUPAC conferences to generate new projects and to attract new scientists into IUPAC projects. Division VII actively recruits new TGMs to expand the scientific scope of their project portfolio. These sorts of activities should be encouraged and adopted more widely. The recent formation of the Union Advisory Committee (UAC) could be used to make scientists more aware of IUPAC project activities, and thus serve to increase participation by a wider range of countries.

Table VI Dollar values of projects granted in year X*.

	2000	2001	SUM 2000 + 2001	2002	2003	SUM 2002 + 2003	2004
CTC/CCE*		6000 (1)	6000 (1) [6000]	37000 (5)	6000 (1)	43000 (6) [7167]	16000 (1)
All other STCs above	5000 (1)	20000 (3)	25000 (4) [6250]	22000 (4)	55600 (7)	77600 (11) [7055]	21000 (4)
Div I	15500 (3)	70800 (7)	86300 (10) [8630]	30000 (4)	61300 (7)	91300 (11) [8300]	54100 (5)
Div II	14500 (3)	16600 (3)	31100 (6) [5183]	4800 (1)	40000 (4)	44800 (5) [8960]	14800 (1)
Div III	16700 (2)	7000 (3)	23700 (5) [4740]	16500 (5)	28600 (6)	45100 (11) [4500]	14000 (1)
Div IV	34000 (9)	4500 (2)	38500 (11) [3500]	24500 (10)	19000 (6)	43500 (16) [2719]	31250 (9)
Div V	24000 (5)	21730 (17)	45730 (22) [2079]	22900 (4)	41450 (11)	64350 (15) [4290]	19100 (3)
Div VI	65000 (10)	0 (0)	65000 (10) [6500]	28802 (5)	76000 (5)	104802 (10) [10480]	58400 (9)
Div VII	12500 (2)	7000 (2)	19500 (4) [4875]	48000 (13)	11500 (2)	59500 (15) [3967]	29200 (7)
Div VIII	23000 (1)	12520 (2)	35520 (3) [11840]	29500 (5)	19020 (3)	48520 (8) [6065]	43000 (4)
TOTAL	210200 (36) [5839]	166150 (40) [4154]	376350 (76) [4952]	264002 (56) [4714]	358470 (52) [6894]	622472 (108) [5764]	300850 (44) [6838]

^{*}The values represent the total dollar commitment summed on the leading Division from all sources.

^{**}The notation is in the form of dollars (corresponding # projects) [\$ average per project].

Table VII Task Group membership by NAO (as of 14 February 2005).

United States190United Kingdom101Germany82Japan54France44Australia36Russia32
United Kingdom 101 Germany 82 Japan 54 France 44 Australia 36
Germany 82 Japan 54 France 44 Australia 36
Japan54France44Australia36
France 44 Australia 36
Australia 36
Russia 32
Canada 27
Czech Republic 26
Netherlands 25
Belgium 24
Switzerland 23
India 21
Italy 20
Sweden 17
Poland 16
Brazil 14
China/Beijing 13
Argentina 12
Portugal 12
Spain 12
Israel 11
Korea 11
Hungary 10
Denmark 9
South Africa 9
Austria 8
New Zealand 8
Turkey 7
Bangladesh 6
Finland 6
Mexico (ANAO) 6
Bulgaria 4
Chile 4
Kenya (ANAO) 3
Malaysia (ANAO) 3
Ireland 4 Kenya (ANAO) 3 Malaysia (ANAO) 3 Nigeria (NM) 3 Norway 3
Norway 3

NAO	TGM
Slovakia	3
Botswana (NM)	2
Costa Rica (NM)	2
Croatia	3 2 2 2 2 2 2 2 2 2 2 2
Egypt	2
Pakistan	2
Singapore (NM)	2
Slovenia	2
Thailand (ANAO)	2
Uruguay (ANAO)	2
Venezuela (NM)	2
Armenia (NM)	1
Ethiopia (NM)	1
Greece	1
Hong Kong	
(ANAO)	1
Jamaica (NM)	1
Philippines	
(ANAO)	1
Kuwait	0
Puerto Rico	0
Serbia &	
Montenegro	0
China/Taipei	0

Note: NM corresponds to a nonmember.

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7. OTHER ISSUES

While the project system occupies the principal focus of this VPCA, there are a number of other issues that deserve mention. For most of these, either an observation or a suggestion that the topic merits further discussion will be found in the following section of this document. Here, I will simply mention the issues and indicate why they are of interest or concern.

President Sydnes fully addressed the need for improved communication in his VPCA. As I visited the various Divisions and Committees in the process of gathering data for this report, it is clear that we have a ways to go in improving communications within the IUPAC family. In an organization as large, diverse, and complex as ours, full understanding and communication will be a constant challenge, and we must continually search for improvements. In particular, as I have alluded to previously, there appears to be a lack of full awareness of the activities of the Divisions and Standing Committees on one hand, and the Officers and Secretariat on the other. The difficulty is certainly not one of ill feeling or mistrust, but simply a lack of understanding as to how the various bodies function.

One of the principal reasons for the formation of IUPAC in 1919 was to meet the international needs of chemical industry. Over the years, industry has been closely associated with IUPAC activities, and has contributed a great deal to IUPAC's success. However, at least in the last decade, industry has been less involved. There are some bright spots, for example, within Divisions IV, VII, and VIII. However, in my view, there is ample room for improvement. President Hayes identified this area as a priority in his 1999 VPCA. Recently, Dr. David Evans, the current chair of COCI, and his COCI colleagues have introduced a number of new initiatives to attempt to address this problem. We can offer industry a voice through exploiting our status as a respected and independent NGO. In this way, we can assist in bringing rational scientific viewpoints to issues that are often judged on emotional grounds without any basis in science. Increased involvement of industry has the potential to provide leadership and guidance as IUPAC searches for instances where we can contribute and make a difference. These issues need not be limited to scientific areas such as our work on chlorine and endocrine disruptors. For example, is there a role for IUPAC in assisting industry with the internationalization of initiatives like "Responsible Care"?

Is there any prospect of including pharmaceutical and small chemical process industries within IUPAC? Can we work more closely with trade associations? Can closer ties with industry help us improve our communication and continuing contacts with CAs? How can we increase the number of CAs and use them to help us to serve the needs of chemical industry?

We need to work at increasing the profile of IUPAC. While our name is certainly recognizable, often there is little recognition of our activities outside of traditional areas such as nomenclature. Hopefully, the formation of the UAC will assist in promoting IUPAC within NAOs. However, we can and should investigate other opportunities. For

example, the Thieme-IUPAC prize awarded by Division III is currently the only prize of this type. Prizes such as this can offer industry an opportunity to achieve wider recognition and can help IUPAC increase its profile. The Samsung-IUPAC fund is another valuable initiative along similar lines.

We have traditionally developed relationships with other organizations such as ICSU and UNESCO. Those relationships require ongoing attention if we are to continue to achieve meaningful goals in a global environment. In the past, such partnerships have helped us contribute to issues of global concern such as chemical weapons, the contamination of drinking water, and overcoming non-tariff barriers to trade in developing countries. I think we could do a better job of publicizing our involvement in these kinds of activities. The earlier discussion of CHEMRAWN initiatives is a step in that direction. Moreover, perhaps we need to look more broadly at developing partnerships with other organizations like UNIDO, IAEA, and the WTO. In this way, we could significantly increase our involvement in fields that are vital to the improvement of our world.

8. OBSERVATIONS, CHALLENGES, AND TOPICS FOR DISCUSSION

For the project system, the following points, for the most part, comprise a set of observations and suggestions that are based primarily on best practices from the current procedures used by Divisions and Committees. The other suggestions follow largely from Section 7 on other issues. They are meant to provide guidance for our discussions as we continue our quest to improve the profile, impact, and universality of IUPAC.

Project System:

- 1. Feasibility studies appear to work well in generating projects for those Divisions that have used them. Other Divisions might want to consider such an approach, especially if they are experiencing difficulties in generating projects in particular areas.
- 2. IUPAC conferences can be valuable in generating projects, as can workshops at Division meetings.
- 3. Publicity can be useful in generating new projects. In particular, each project has its own Web page, and it helps if the approved project Web pages are kept up to date. General descriptions of projects are requested by the editor for *CI*, and these articles can also provide valuable publicity.
- 4. The use of subcommittees and/or project coordinators to foster and to nurture prospective proposals works well. Divisions should be encouraged to adopt such approaches, especially with task groups involved with IUPAC projects for the first time.
- 5. Some Divisions have experienced difficulties in obtaining timely and useful project peer reviews. We need to initiate discussions to address this issue.

- 6. Face-to-face meetings of technical subcommittees can often be accomplished at little cost to IUPAC through attendance at a relevant scientific meeting where professional considerations dictate attendance. One model that has seen limited use is for the participants to have the expenses for an extra day covered from the Division Committee's budget. Divisions might want to actively consider such opportunities in their planning. Moreover, despite the undoubted efficiency and cost effectiveness of electronic interactions, IUPAC should recognize that face-to-face meetings are sometimes essential to deal with aspects of project generation, monitoring, and completion.
- 7. Monitoring needs some attention. There are considerable differences among Divisions, and more uniformity would be helpful. For example, differences in monitoring procedures can make interdivisional projects more difficult. One system that seems to work well is a standard project reporting form that is filled in and filed with the Division President or his/her delegate every six months.
- 8. Project monitoring can be used effectively to make TGCs aware of standard accounting procedures as well as ICTNS guidelines for Technical Reports and Recommendations.
- 9. Project completion is a problem especially in some Divisions (see Table V). Hopefully, a more systematic approach to monitoring will help produce improvements. In general, projects should be completed within a two- to three-year time span.
- 10. Science in general increasingly requires a multidisciplinary approach to solve today's problems. Within IUPAC, we should encourage interdivisional projects, including interdivisional projects that involve CCE and COCI.
- 11. The central computer capability of IUPAC and its Web site are issues that are important to the project system, as well as to other areas such as IUPAC's profile, publicity, and accessibility. Access to central computer facilities, and the nature and function of those facilities, is currently under active review. The resolution of perceived difficulties and improvements should be a matter of high priority.
- 12. The Operational Standing Committees should continue to explore opportunities to use the project system. In particular, CHEMRAWN should use the project system where appropriate to fund activities of FACs. The current CHEMRAWN initiative to document measures taken as a result of past CHEMRAWN conferences should be encouraged and given a high priority.
- 13. The level of project funding is not a specific indication of a project's significance. There are important projects with zero funding, and they should still be tracked in the usual fashion.

- 14. It may be possible to improve timing issues with regard to ICTNS operations particularly with regard to the posting of Provisional Recommendations. It would be helpful for a small committee consisting of the ICTNS Chair, a Division President, an Officer, and a member of the Secretariat to attempt to find a solution to the current perceived problems.
- 15. The Project Committee should be encouraged and supported in its current initiative to move to competitive procedures in awarding financial support for conferences.
- 16. The terms of reference of ICTNS should be reconsidered in light of the creation of Division VIII.
- 17. The Evaluation Committee was envisioned as a valuable component of the project system. We must find a method whereby they can obtain expeditiously the data that they need to carry out their job.
- 18. We should continue to strive to increase the geographic representation on Task Groups through a number of strategies including those used by Divisions V and VII.
- 19. The increase in project funding has been used very well by the Divisions and Committees. A system that allows applications for additional project funds after budgets are used up has proven to be flexible and useful, and should continue, at least until current reserves are expended. Most of the Divisions and Committees have indicated that they can use additional project funds. Given this scenario, I believe that it would be helpful to begin discussions to achieve a consensus as to how future increases in Division/Committee project funding can be tied to success within the project system.

Additional Priorities:

- 1a. The visits to the off-year meetings of Divisions and visits with Committee Chairs were an essential part of gathering data for this VPCA. In addition, as noted previously, I believe they played a valuable role in increasing communication and understanding between the Divisions/Committees and the Officers/Secretariat. In my view, such interactions should continue but perhaps on a reduced scale.
- 2a. The very worthwhile initiatives of COCI in attempting to broaden and strengthen interactions between IUPAC and industry should be encouraged and given a high priority. We very much need industry involvement to help guide our priorities. Only then will we be able to contribute significantly to industry needs. In this regard, as COCI has recognized, we need to be much more aggressive in promoting our CA program. The CA program is a source of income, but I believe it is even more valuable as a tool to increase the involvement of industry in IUPAC activities.

- 3a. One mutually beneficial way in which industry and IUPAC can interact is through the endowment and awarding of prizes for prominent scientists, especially those directly involved in IUPAC work. I believe we can do much more in this area, and I believe there is a positive role to be played by Officers, Division Presidents, and Committee Chairs. Such prizes can serve to provide wider recognition for an industry and to enhance the profile of IUPAC.
- 4a. Interactions with multidisciplinary, multifaceted organizations like ICSU and UNESCO can be a challenge. Nevertheless, if IUPAC is to play a significant role in helping solve the major problems of a global society, we need to find a way to successfully interact with such organizations. I believe we need to increase our efforts to achieve productive partnerships. Moreover, we should look beyond our traditional partners to others such as the WTO, UNIDO, etc.
- 5a. As mentioned in Section 7, IUPAC has had some success in contributing to issues of global concern. I believe that we should aggressively seek opportunities to expand our activities in these areas. Moreover, we should seek better ways to publicize these efforts within the international scientific community.

9. SUMMARY RECOMMENDATIONS

In the following project related recommendations, reference to "Divisions" can also include Operational Standing Committees if appropriate. Bracketed numbers refer to the observations in Section 9.

- 1. If Divisions want an increase in the quantity and/or quality of new projects, they should consider employing strategies that include feasibility studies, workshops, publicity, nurturing mechanisms, and face-to-face meetings of subcommittees (1, 2, 3, 4 and 6).
- 2. It would be helpful if projects were monitored with a standard instrument (see 7), and the process used to encourage timely project completion as well as compliance with ICTNS guidelines (8 and 9).
- 3. The Operational Standing Committees should continue their full integration into the project system. In particular, CHEMRAWN should consider using the project system to fund activities of their FAC's (12).
- 4. The Advisory Standing Committees should continue to revise their procedures to adapt to the project system. In particular, an ad hoc committee should examine timing and terms of reference for ICTNS, and discussions should ensue regarding provision of data for the Evaluation Committee (14, 15, 16, 17 and 18).

Item 11: Report of the Vice President: Critical Assessment of IUPAC

- 5. Discussions should begin in an attempt to achieve a consensus as to how any future increases in Division/Standing Committee project funding might be tied to success within the project system (19).
- 6. IUPAC needs to give high priority to increasing its profile. In particular, efforts should continue to increase participation in the Company Associates program, and to attract further endowment of industrially sponsored IUPAC prizes (2a and 3a). We need to continue to achieve productive partnerships with a variety of other organizations, and to increase publicity for our own global activities (4a and 5a).

10. LIST OF ACRONYMS

ACS American Chemical Society

ANAO Associated National Adhering Organization

CA Company Associate

CCE Committee on Chemistry Education

CHEMRAWN CHEMical Research Applied to World Needs

CI Chemistry International

COCI Committee on Chemistry and Industry

FAC Future Actions Committee

IAEA International Atomic Energy Agency ICSU International Council for Science

ICTNS Interdivisional Committee on Terminology, Nomenclature and Symbols

NAO National Adhering Organization NGO Non-Governmental Organization

NM Non-Member

PAC Pure and Applied Chemistry
RSC Royal Society for Chemistry

STC Standing Committee

SCOPE Scientific Committee on Problems of the Environment

TGC Task Group Chair
TGM Task Group Member
TM Titular Member
TR Technical Report

UAC Union Advisory Committee

UNESCO United Nations Educational, Scientific and Cultural Organization

UNIDO United Nations Industrial Development Organization

VPCA Vice President's Critical Assessment

WTO World Trade Organization

Introduction

The governance of IUPAC has been discussed for more than a decade, but the topic was brought thoroughly into focus in 2001 by a proposal to restructure the Union and replace the Bureau and the Executive Committee with a new governing body. In September 2002, the Bureau authorized the formation of a committee, coined the Governance Structure Committee (GSC), to analyze the current governance structure and operations and to propose alternative structures, as outlined in the following charge:

- 1. Analyze the strengths and weaknesses of the current structure and operation of the Bureau, including its Executive Committee.
- 2. Develop proposals for alternative structures and analyze their potential strengths and weaknesses. Consider any impact on the functioning of other IUPAC bodies, including the Council, and any financial impact. Consult widely within IUPAC to obtain additional suggestions, also on improving communication between the Bureau and the Divisions and Committees of IUPAC.
- 3. Provide a preliminary report to the Executive Committee and to all National Adhering Organizations by April 2003. Request comments and additional suggestions for structural changes that can be considered for inclusion in the final report. Provide options and recommendations to the Bureau and Council in August 2003.

The committee produced a thorough report, which concluded that the current Bureau governance structure did not meet the needs of the Union and should be substantially altered. The committee recommended that the Council adopt a new governance structure and modify operations of some existing bodies, based on the following proposals:

- Abolish the Bureau and Executive Committee.
- Establish an Executive Board [EB], consisting of the five IUPAC Officers plus four other members, all elected by Council that would assume all the responsibilities and authorities now given to both the Bureau and Executive Committee.
- Establish a Union Policy Committee [UPC], with one member appointed by each NAO, to work closely with the Executive Board and to advise the EB on matters of IUPAC policy.
- Provide for an annual meeting between the EB and the Division Presidents plus the Chairmen of the Operational Committees.
- Extend the length of the Council meeting by one-half day to permit time for more meaningful discussion of issues by Delegates.

Ottawa Discussion and Decision

The GSC report and the recommendations outlined above were thoroughly discussed at the Council meeting in Ottawa in August 2003. The discussion can briefly be summarized as follows:

An important feature of the proposals is that the UPC will give each member country a direct role to play in the governance of the Union. Currently, the National Adhering Organizations (NAOs) have a limited opportunity to influence Union policy since the Council meets only every two years. Furthermore, the Council delegates are often new to IUPAC and unfamiliar with the issues before the Council meeting. There is an opportunity in this proposal for greater continuity of membership. The members of the UPC would become familiar with the issues facing IUPAC during the biennium since they would see material provided to the Executive Board on important matters and would be asked to provide comments on the policy aspects of issues being considered.

Further to this issue it was pointed out that replacement of the Bureau and Executive Committee by a single body, called the Executive Board, eliminates a source of confusion in the governance of the Union. In the current structure it is sometimes unclear if a particular decision can be made by the Executive Committee or if it should be left to the Bureau. Creation of the UPC would give the member countries a greater and more effective voice in IUPAC than is provided by the current Elected Members of the Bureau. In practice, some NAOs never, or very rarely, have an elected Member of the Bureau. The comment was made that it will be important that the NAOs name UPC members who are in a position to provide policy guidance and can solicit broad input from members of the chemical community in their home country.

The concern was expressed that the meeting of the UPC during the General Assembly would duplicate the discussion of items on the Council Agenda. The suggestion was made that this could be avoided by having the group meet after the Council meeting. It was then proposed that the agenda of the UPC should be devoted to future issues rather than the items on the agenda of the Council. It was felt that in this way the UPC could make significant contributions to set the agenda for the work of the Executive Board for the coming biennium.

Although many delegates expressed support for the GSC proposals, a fair number preferred a stepwise approach where the first step would be establishment of the Union Policy Committee and the second step could be replacement of the Bureau and the Executive Committee with a new governing body, called the Executive Board by GSC. Ultimately this position was supported by Council. However, there was dissatisfaction with the name Union Policy Committee, and a proposal to change the name to the Union Advisory Committee (UAC) was put forward and approved by Council.

Thus, the Council decided to establish a Union Advisory Committee [UAC] as an *ad hoc* committee and directed the Executive Committee to formalize UAC with respect to its composition, terms of office, and terms of reference.

UAC – Establishment and Activity

The decisions made by Council were implemented quickly. The Composition and Terms of Office were approved as follows:

- (i) The Union Advisory Committee is an ad hoc committee with one Member chosen by each National Adhering Organization.
- (ii) The period of service of a Member shall be two years (initially for the period 1 January 2004 to 31 December 2005) subject to reappointment.

(iii) The President shall serve as chairman of the Committee.

Furthermore, the Terms of Reference, also approved by the Executive Committee, have the following wording:

- (i) To provide advice to the Executive Committee on Union policy matters as requested, e.g., on the governance of the Union.
- (ii) To bring to the attention of the Executive Committee matters of importance to be considered by the Officers, the Executive Committee, or other IUPAC bodies.
- (iii)To serve as a principal two-way communication link between the Executive Committee and each National Adhering Organization, as well as the chemical community in the member country.
- (iv) To meet at a General Assembly on the call of the Chairman but otherwise to conduct business primarily by e-mail, phone, and postal communication.

Appointment of members to the UAC was solicited from all the NAOs, and by January 1st 2005, almost all of the 45 member countries had appointed their members. The members have been kept informed by e-mail of matters being considered by the Executive Committee, and several significant matters have been referred to the committee for comments, assessment, and feedback. Collectively the response from the committee members has not been as expected, but on the other hand it is encouraging to observe 1) that the reply frequency has been more than twice of that achieved regularly when comments are solicited from the NAOs, and 2) that this frequency is increasing. It is therefore reasonable to believe that when the UAC has been in function for a longer period of time, the communication between the IUPAC governance and the NAOs will have improved.

Among the proposals sent to the UAC for comments and feedback was the proposal to establish an Executive Board, consisting of the five IUPAC Officers plus four other members, all elected by Council, which would assume all the responsibilities and authorities now given to both the Bureau and Executive Committee. While the majority of the answers from the UAC members were in favour of going ahead with the change, only eleven responses were received. The Executive Committee believes that on such an important issue we require an overwhelming majority; thus, the EC decided to postpone the decision to the General Assembly in Torino in 2007. This conclusion was arrived at for two reasons:

- (1) When the UAC has been in operation for two more years, its position within IUPAC will be stronger. Quite a few members of the committee have been members for less than one year and have thus had little opportunity to interact. However, they are senior scientists, who will be able and willing to provide sound advice, and to communicate when needed to and from the NAO and its appropriate committees and staff. Furthermore, the UAC meeting in Beijing will help develop personal interactions and relationships. This will conceivably increase the committee's engagement and activity to a considerable extent, and that will be important when/if the Bureau and the Executive Committee are going to be replaced by an Executive Board.
- (2) Establishment of an Executive Board to replace the Bureau and the Executive Committee requires the revision of a number of Statutes and Bylaws. In fact, the consequences of such a change will not become completely clear before such a revision

has been carried out, particularly since the current version of the Statues and Bylaws dates back to 1975 and contains inconsistencies and ambiguities that have crept into various sections in the intervening years. It therefore makes sense to revise the Statutes and Bylaws and present a version, at the General Assembly in Torino in 2007, which is based on the assumption that an Executive Board is introduced in place of the Bureau and the Executive Committee. With such a timetable it will be possible to consult thoroughly with the UAC as well as the NAOs in the process, which in this way will become both interactive and transparent.

On this basis we are bringing before the Council the following motion:

Council authorizes the President to appoint a small working party, under the chairmanship of the Secretary General, to draft the revised Statutes and Bylaws necessary to implement the replacement of the Bureau and Executive Committee with an Executive Board. A final decision on whether to accept the revised Statutes and Bylaws and to create an Executive Board would then be made at the next Council meeting at Torino in 2007.

If the motion to draft fails, the proposal to replace the Bureau and Executive Committee with an Executive Board will lapse.

Item 13.1: Biennial Report of Treasurer

Treasurer's Review

I am happy to report that the financial situation of IUPAC is still in line with our plans and at the present time well in balance with the Budget the Bureau and Council voted on at Ottawa in August 2003. As you will see from the Finance Committee report, the reserves are adequate and our earlier losses due to the turmoil in the finance markets have been made up. The Financial Committee has made the right moves in the investments area and our reserves secure operations for the next biennium.

That is the good news.

Unfortunately we had to take actions against some National Adhering Organizations who had not paid their National Subscriptions for more than two years. Fairness and our rules were clearly applied; in one instance we received payment of part of the dues in arrears.

If we look to the future and anticipate the changes in the next years, some concerns have to be outlined. The worldwide economy continues to turbulent, some of our National Adhering Organizations are facing financial bottlenecks, and governments are actually overspending to accelerate the economy, consequently creating large debt. Practically all our direct and indirect sources for funds have seriously decreased spending and have cost cutting actions in place. Not-for-profit organizations like ours are competing in this increasingly difficult market for financial support. Talking to industry and industry-related organizations, we have had to face tough questions about validating our spending and our returns. Our Strategic Plan is to some extent an answer to the changed economic and political environment. A good part is dedicated to a better understanding of our future with our internal and external constituents. We do not have the means to finance all our ideas but will need to continue to concentrate and focus on topics we feel are our strengths.

We have learned to cope with the uncertainty in the economy. It seems that our billing of the National Subscription in local currency has reduced some of the trouble our National Adherent Organization had in the past. The rather weak USD helped as well. I should point out that because of government regulations some of our NAOs must be billed in USD.

In the past Biennium we were able to fund all approved projects. A survey of the projects shows that, with a few exceptions, the spending discipline is good.

The Table that follows this report summarizes the financial results for IUPAC for 2002, 2003, and 2004 as contained in the audited Financial Statements. The discussion below reviews and comments on some significant aspects of the Union's finances.

Income

Membership Dues from National Adhering Organization

Council at Ottawa approved the billing of National Subscriptions in national currencies. As expected this change has had only a small effect on the Union's income. The expenses for the Ottawa General Assembly included the cost for the transportation and subsistence expenses of one delegate to the Council from each NAO.

As mentioned above action was taken to sanction those NAOs more than two years in arrears in their National Subscriptions. As of 31 December 2004 the total of these arrears was USD 46 392. In April 2005Brazil paid USD 24 477 with a promise that the balance of its arrears would be paid by 1 July. Chile and Argentina have not paid their arrears as of 20 June and very unfortunately the Council now has to decide on sanctions. In all cases we have tried to convince the National Adhering Organization that a payment avoids serious consequences.

Item 13.1: Biennial Report of Treasurer

National Subscriptions are the main source of our income. Therefore we have to observe a normal payment cycle in the name of fairness. We recognize and are thankful that most of the National Adhering Organizations pay on time.

Publications and other income sources

Pure and Applied Chemistry: Due to a modestly higher subscription rate for 2004 and a lower than expected decline in the number of subscribers, publications revenue increased in 2004. Certain one time income also contributed to the increase. However, the long-term trend of slowly declining subscriptions is likely to continue, so an increase in the subscription rate for 2006 will be necessary to maintain the revenue. Please note that the revue from publications is partly offset by expenses associated with publications included in the Program Expenses line of the Table.

Income from Investments: Our long-term accounts have recovered their losses from previous years. A greater portion of our investment income is interest than in the past due to the shift of our portfolio from equities to bonds.

Grants: IUPAC organized a workshop on Chemical Weapons in Bergen, Norway, in 2002 and received substantial grants from foundations, government agencies and industry to support the worshop. In 2003 we received a major contribution from the Samsung Chemical Company. The income from this grant will be used to support awards to excellent researchers and students in polymer science and to support the educational programs of the IUPAC Polymer Division. The fund will be an endowment type fund that will assure annual awards for the future in this field. These two items explain the unusually large amount shown for the Grants and contributions line item in 2002and 2003 vs. 2004.

Expenses

As is usual, expenses for 2004 were lower than for the previous year due to the expense of the General Assembly in 2003. Expenses were lower than operating income in 2004 and 2005 appears to be on track to end the biennium in balance.

Summary and Conclusions

It is important to recall that it is not the purpose of IUPAC to accumulate reserves, however, the income from the reserves allows the Union to support a more extensive program than it could based on operating income alone. The strong reserves also allow the Union to accept short-term losses, such as will no doubt occur in some years due to the payment of National Subscriptions in national currencies. In general the Union's reserves give it flexibility and scope for activity.

Acknowledgements

The work of the Treasurer was only possible thanks to the great cooperation and help of the Executive Director and the Finance Committee.

Audited Financial Statements 2002-2004

	2002	2003	2004
Support			
Grants and contributions	130,575	184,767	83,478
National Subscriptions	690,161	713,735	726,650
Affiliate Membership Program	74,731	82,461	71,650
Total Support	895,467	980,963	881,778
Other Revenues			
Publications	765,569	770,572	838,462
Investment income	(119,133)	720,148	523,793
Other	18,347	25,709	3,050
Total Other Revenues	664,783	1,516,429	1,365,305
Total Support and Other Revenues	1,560,250	2,497,392	2,247,083
Expenses			
Program	845,425	1,198,304	919,768
Management and general	639,853	610,756	765,954
Total expenses	1,485,278	1,809,060	1,685,722
Increase (Decrease) in net assets	74,972	688,332	561,361
Net assets, beginning of year	4,222,468	4,297,440	4,985,772
Net assets , end of year	4,297,440	4,985,772	5,547,133

13.2 Report of the Finance Committee (FC)

The FC has the following responsibilities within IUPAC:

- (i) To advise the President and the Executive Committee on financial matters.
- (ii) To make financial recommendations for decision by the President and/or the Executive Committee.
- (iii) To review the IUPAC securities at least annually and to make such changes as appear appropriate.
- (iv) The Finance Committee shall not have executive functions except with respect to dealings in securities. The Finance Committee shall have executive authority with respect to selection, purchases, and sales of securities held by IUPAC, provided that the Treasurer concurs with the decisions of the Finance Committee.

In the context of these responsibilities, the FC reviews the financial operations of IUPAC against approved budgets, reviews proposed budgets and sources of income and makes recommendations regarding these matters to the Executive Committee, Bureau and Council. The FC has management responsibility for the long term account of the Union insuring that sufficient funds are available to support its work not only in the current year, but for the foreseeable future. This report consists of three parts: (1) a status report on the long term account, (2) the Long Term Policy Statement, and (3) the Funds Policy Statement. The latter two statements describe policies that govern the investments and use of the long term account of the union.

Long Term Account

The value of the USD value of the IUPAC long-term portfolio and its growth over the last 6 years is shown in Figure 1. The portfolio consists of 65% bond and 35% equity investments and the investments are roughly 40% in European-based companies and 60% in U.S.-based companies. The bond portfolio consists of 23% Euro-denominated bonds.

The FC has actively managed this account conservatively. Decisions taken by the FC during the past 6 years to shift its portfolio from equities into bonds and to invest a significant portion of its portfolio in Euro-denominated bonds is responsible for the good performance of the portfolio.

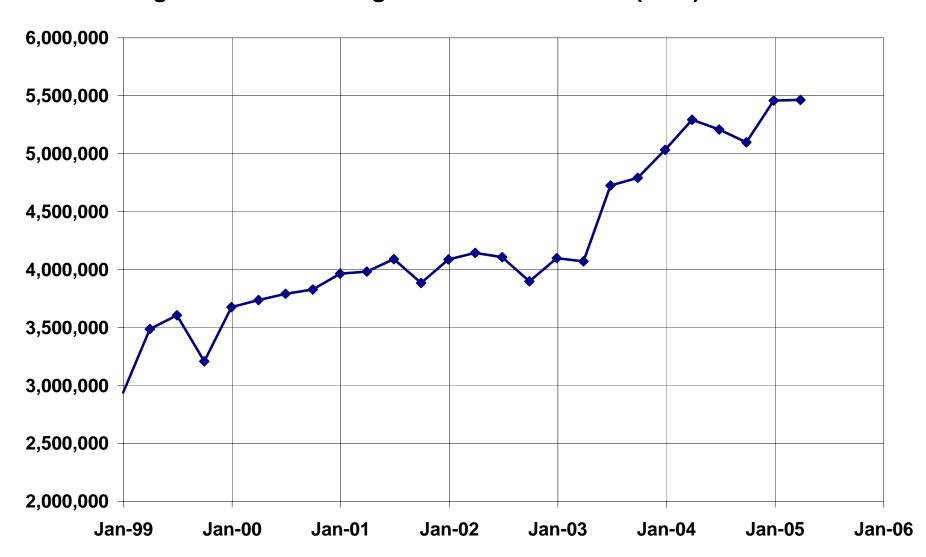
The overall performance of the portfolio is considered excellent and has outperformed the market in most years. This account insures that the Union has sufficient resources to support its programs into the foreseeable future.

Investment and Fund Policy Statements

The Investment Policy and Fund Policy statements are attached for information.

This was the last meeting for Ed Przybylowicz, who has been a member of the committee for 12 years and will complete his term at the end of 2005. Luzius Senti has agreed and been appointed for 2 years as chairman of the FC.

Figure 1: IUPAC Long Term Portfolio Value (USD) - 6 Years



Investment Policy Updates

Each year at its annual meeting, the Finance Committee reviews the policy statements governing its investments and fund allocations. The Finance Committee action is either approval or modification of the attached policies.

The Investment Policy statement that follows has been updated with last year's performance data to show how the investments are performing relative to the established guidelines. This review can result in either an endorsement of the present policy, or a revision of the guidelines. Once the policy is approved by the Finance Committee, it is then reviewed at the spring meeting of the Executive Committee meeting and later in the year with the Bureau for information and input.

The Fund Policy is a statement of how the total long-range portfolio is segmented relative to its intended purposes. This statement has evolved over the past four years to its present definitions and guidelines. It is presented here as a statement that has been reviewed and approved by the Executive Committee at its April 2005 meeting.



International Union of Pure and Applied Chemistry

INVESTMENT POLICY STATEMENT

1.0 PURPOSE

The purpose of this document is to identify a set of investment objectives and constraints, asset allocation parameters, performance measurement benchmarks, and guidelines for the International Union of Pure and Applied Chemistry (IUPAC) long term investments. The investment policy statement is intended to assure the Officers, Executive Committee and Bureau of IUPAC that reserve assets are being invested in accordance with the best long-term interests of IUPAC, given the following considerations:

- IUPAC's risk tolerance, or its willingness to withstand substantial losses due to adverse market conditions.
- IUPAC's need to obtain real, or inflation-adjusted, growth in its asset base.
- IUPAC's requirement for current income to support IUPAC programs and activities.
- IUPAC's liquidity requirements, or its need to maintain adequate cash balances to accommodate share withdrawals from the long term portfolio when needed.

2.0 INVESTMENT OBJECTIVES AND CONSTRAINTS

2.1 Objectives

The primary objective of having reserve funds is provide continuity in the programs set out in the IUPAC Strategic Plan regardless of short term financial discontinuities and disruptions. With this objective, the reserve funds must (1) provide protection for biennial operating expenses, (2) provide for periodic, planned extraordinary expenses (such as moving the Secretariat), (3) provide for extraordinary expenses in connection with General Assembly and Congress meetings held in regions of the world which would increase the normal expenses, and (4) support endowed programs of the organization. It is expected that under normal circumstances, the National Subscriptions plus other annual sources of operating income will cover normal operating expenses.

To meet these objectives the reserve funds of IUPAC must earn an annual real, or inflation adjusted (OECD), total return of 4.5%. It is recognized that the real return objective may not be achieved during each year, however, the fund will be structured to enhance the probability of earning an annualized real return of 4.5% over the long term.

The risk tolerance of the organization should be viewed as moderate. Volatility in the fund's returns can be tolerated provided that there are reasonable expectations that the fund will achieve its desired return over the long term. The reserve portfolio will not be structured to incur unnecessary risk. On an overall portfolio basis, risk shall be controlled through the use of more than one asset class as well as a regional distribution of investments throughout the world, consistent with the investment objectives.



2.2 Constraints

The liquidity requirements of the reserve funds are minimal. At least 2% of the fund shall be available on short notice (30 days) for conversion into liquid assets without significant penalty.

Since IUPAC's 501 (c)(3) tax-exempt status extends to the reserve funds, tax considerations are not a constraint in the management of this fund.

3.0 ASSET CLASSES AND ALLOCATION

In order to minimize the total risk of the reserve funds, three asset classes will be utilized in order to derive the benefits of diversification. Accordingly, the investment portfolio will be managed as a balanced fund consisting of mutual funds, bonds, and cash equivalents.

Asset allocation will be structured to achieve the primary objective of an inflation-adjusted annualized return of 4.5% over a full market cycle. Based on historic performance over the twenty-five year period from 1975-1999, a low-risk portfolio providing this level of return would be comprised of 25% large-company equities (average annual real return of 13.2%) and 75% fixed income instruments having an average annual real return of 5.4%. This assumes an historic average inflation rate of 3%.

As a guideline, the Finance Committee will review and adjust the ratio of equity-to-fixed income on an annual basis or more frequently if necessary, to provide the expected return. The equity percentage in the portfolio is expected to vary from 20 to 40% of the portfolio.

The balance between stocks and bonds will be determined by prevailing capital market conditions and the relative valuations between asset classes.

4.0 PERFORMANCE MEASUREMENT

4.1 Total Return

The primary objective of the fund is to achieve an annualized total return, in real terms, of 4.5% over the long term. In terms of relative performance, the objective will be to outperform a benchmark portfolio. The return on each asset class will be that of its respective market index (i.e. MSCI-North America, MSCI-Europe, Lehman Brothers Aggregate Index, etc.). Analysis of the actual return of the reserve fund as compared to the benchmark portfolio will determine if adjustments need to be made to the portfolio. While this analysis will be done on a quarterly basis, adjustments to the portfolio shall be made on an annual basis after review and discussion of the portfolio performance at the Finance Committee meeting early in the year.

5.0 REPORTING

The Chairman of the Finance Committee and the Treasurer will report on the performance of the reserve funds at each meeting of the Executive Committee and as appropriate at the Bureau and Council meetings.



Year 2004 Performance

For the year 2004, the long-term portfolio showed the following performance in comparison with the relevant indices.

	Percent of Total Assets	Annual TotalReturn	Annual Weighted Return
	(Ave. during Yr.)		-
Asset Class			
Equities	37%	7.3%	2.7%
Bonds	62%	9.9%	6.1%
Cash Equivalents	1%	2.0%	0.1%
Total	100%		8.9%
MSCI-North America	25%	9.4%	2.4%
MSCI-Europe	13%	17.9%	2.3%
DJ Corp Bond Index	62%	7.3%	4.5%
Total	100%		9.2%

- MSCI is the Morgan Stanley Capital Index that is reported country by country as well as by region. The DJ Corp Bond Index is the 10-year Dow Jones Corporate Bond Index total return change reported annually.
- Annual Weighted Return is the Percent of Total Assets (Average during the Year) in a given Asset Class multiplied by the Annual Total Return.

It is interesting to note that the IUPAC Total portfolio performed close to the value predicted by the indices (8.9% vs. 9.2%). The equity portion of the IUPAC portfolio under-performed the combined indices for Europe and North America whereas the IUPAC bonds performed substantially better than the Dow Jones Bond Index.



International Union of Pure and Applied Chemistry

Fund Policy Statements

1. PURPOSE

Biennium Operating Reserve Fund This fund shall contain an amount of money equal to the currently approved biennium budget minus the operating funds for the publications. It is the prime financial protection for the Union in the event of a severe worldwide economic downturn.

General Assembly Special Fund This fund is to be used to supplement the expense of holding General Assembly meetings in locations where the costs are considerably more expensive than the norm. General Assembly meetings such as the recently held one in Brisbane, Australia and the upcoming 2005 General Assembly in Beijing, China will draw on this fund.

<u>IUPAC Endowment Fund</u> This will be treated as an "endowment fund", that is, only the interest earned on the principal in this fund will be used for special projects of a broad nature that enhance the stature of the Union. For example, the recently established IUPAC Prize for Young Chemists will be supported by the proceeds from this fund. Other projects approved by the Executive Committee and the Finance Committee may be supported by this fund..

Special Funds IUPAC encourages individuals and organizations to participate in its mission. While in most cases this takes the form of collaboration and participation in IUPAC projects, it can also be financial aid to various IUPAC activities. Such financial aid can directly support specific IUPAC projects, or it can be set up as a special fund that is used to accomplish certain goals over a period of time or in perpetuity. Special Funds may also consist of those royalty streams from books published by a Division or commission that have an ongoing activity to update the publication.

2. Investment of Funds

The aggregate of these funds is managed as a single long term portfolio according the IUPAC Investment Policy and the guidelines contained therein.

3. Allocations to Funds

<u>Biennium Operating Reserve Fund</u> This fund shall contain an amount equal to the total approved budget for the next biennium.

<u>General Assembly Special Fund</u> The level of this fund shall be set by the Finance Committee at its annual meeting. The maximum held in this fund is \$250,000 USD. (At the present time, 1 March 2002, it totals \$150,000 since \$100,000 was approved to be used to support the higher expenses of the 2001 General Assembly in Brisbane, Australia

<u>Special Funds</u> Any funds which are set up as Special Funds shall have the amounts designated according to agreements with the Division controlling these funds. These funds will appear as separate line items in the accounting documents of the organization.



<u>IUPAC Endowment Fund</u> The level of this fund shall be the residual long-term portfolio after allocations for the Biennium Operating Reserve Fund, General Assembly Special Fund and any Special Funds are subtracted.

4. Disbursement Guidelines from Funds

Disbursement of funds from these accounts must be approved by the Finance Committee, or the Treasurer and Chairman acting on behalf of the Finance Committee.

As needed funds from the Biennium Operating Reserve Fund and General Assembly Special Fund may be approved for disbursement, decreasing these funds until new levels are established at the annual Finance Committee meeting.

Disbursement of Special Funds shall follow the following guidelines:

- 1. The goals for which such a special fund is established must be consistent with and support the IUPAC mission and goals.
- 2. The purposes of the fund should be defined and the body or group within IUPAC that is responsible for administering the funds should be specifically identified (i.e. is it a Division Committee, the President of IUPAC etc.).
- 3. The fund should be categorized as either an endowment (i.e. only the interest on the money will be used to fund projects) or a consumable fund (i.e. a fund in which both the interest and some principal will be used until the fund is exhausted).
- 4. The money in the fund shall be invested in the long-term IUPAC investment portfolio and shall earn the prevailing interest based on the portfolio of fixed income instruments in the IUPAC portfolio such as bonds and fixed income funds. In recent years this has provided an annual return in the range of 5 to 6%.

The disbursement from these special funds will be under the control of the responsible group subject to all the guidelines contained in this policy and the accepted IUPAC practices for reimbursed expenditures such as travel and subsistence.

The IUPAC Endowment Fund will maintain its principal and the funds available for disbursement will not exceed the annual yield on this fund at the fixed interest rate (bonds and fixed funds). Currently that is 6.0%.

Financial Statements

December 31, 2003 and 2002

(With Independent Auditors' Report Thereon)

BATCHELOR, TILLERY & ROBERTS, LLP

CERTIFIED PUBLIC ACCOUNTANTS
POST OFFICE BOX 18068
RALEIGH, NORTH CAROLINA 27619

RONALD A. BATCHELOR ANN H. TILLERY FRANKLIN T. ROBERTS WM. JAMES BLACK, JR. 3105 GLENWOOD AVENUE, SUITE 301 RALEIGH, NORTH CAROLINA 27612 TELEPHONE (919) 787-8212 FACSIMILE (919) 783-6724

Independent Auditors' Report

The Executive Committee
International Union of Pure and Applied Chemistry:

We have audited the accompanying statements of financial position of the International Union of Pure and Applied Chemistry ("IUPAC") as of December 31, 2003 and 2002, and the related statements of activities, cash flows, and functional expenses for the years then ended. These financial statements are the responsibility of IUPAC's management. Our responsibility is to express an opinion on these financial statements based on our audits.

We conducted our audits in accordance with auditing standards generally accepted in the United States of America. Those standards require that we plan and perform the audit to obtain reasonable assurance about whether the financial statements are free of material misstatement. An audit includes examining, on a test basis, evidence supporting the amounts and disclosures in the financial statements. An audit also includes assessing the accounting principles used and significant estimates made by management, as well as evaluating the overall financial statement presentation. We believe that our audits provide a reasonable basis for our opinion.

In our opinion, the financial statements referred to above present fairly, in all material respects, the financial position of the International Union of Pure and Applied Chemistry as of December 31, 2003 and 2002, and the changes in its net assets and its cash flows for the years then ended in conformity with accounting principles generally accepted in the United States of America.

Batchelor, Tillery & Robert, LLP

March 19, 2004

Statements of Financial Position

December 31, 2003 and 2002

	2003	<u>2002</u>
<u>Assets</u>		
Current assets:		
Cash and cash equivalents	\$ 517,660	811,018
Subscriptions receivable (net of allowance for doubtful		
accounts of \$46,000 in 2003 and \$40,000 in 2002)	28,975	49,558
Other receivables	9,211	7,381
Inventories	14,000	20,720
Prepaid expenses and other assets	<u>16,156</u>	9,871
Total current assets	586,002	898,548
Furniture, fixtures, and equipment, net	38,776	43,776
Investments, at market value	5,036,153	4,158,757
,		
	\$ <u>5,660,931</u>	<u>5,101,081</u>
<u>Liabilities and Net Assets</u>		
Current liabilities:		
Accounts payable and accrued expenses	104,100	75,894
Unearned subscriptions	571,059	727,747
Total current liabilities	675,159	803,641
Commitments		
Net assets:		
Unrestricted	4,851,185	4,275,781
Temporarily restricted	3,928	16,000
Permanently restricted	130,659	5,659
Total net assets	4,985,772	4,297,440
	\$ <u>5,660,931</u>	<u>5,101,081</u>

Statements of Activities

	2003				
		Temporarily	Permanently	ý	2002
	Unrestricted	restricted	restricted	<u>Total</u>	<u>Total</u>
Support:					
Grants and contributions	\$ 59,767	_	125,000	184,767	130,575
National subscriptions and service charges	713,735	-	-	713,735	690,161
Affiliate membership program	82,461	-	-	82,461	74,731
Net assets released from restrictions	16,000	(<u>16,000</u>)			
Total support	871,963	(16,000)	125,000	980,963	895,467
Other revenue:					
Publications	770,572	_	-	770,572	765,569
Investment income (loss), net	716,220	3,928	-	720,148	(119,133)
Other	25,709			25,709	18,347
Total other revenue	1,512,501	3,928		<u>1,516,429</u>	664,783
Total support and other revenue	2,384,464	(12,072)	125,000	2,497,392	1,560,250
Expenses:					
Program and publications	1,198,304	-	-	1,198,304	845,425
Management and general	610,756			610,756	639,853
Total expenses	1,809,060			1,809,060	1,485,278
Increase (decrease) in net assets	575,404	(12,072)	125,000	688,332	74,972
Net assets, beginning of year	4,275,781	16,000	5,659	4,297,440	4,222,468
Net assets, end of year	\$ <u>4,851,185</u>	3,928	130,659	4,985,772	4,297,440

Statements of Activities, Continued

	2002			
		Temporarily	Permanently	I
	<u>Unrestricted</u>	restricted	restricted	<u>Total</u>
Support:				
Grants and contributions	\$ 114,575	16,000	_	130,575
National subscriptions and service charges	690,161	-	_	690,161
Affiliate membership program	74,731	-	-	74,731
Net assets released from restrictions	5,000	<u>(5,000)</u>		
Total support	884,467	11,000		895,467
Other revenue:				
Publications	765,569	-	-	765,569
Investment (loss) income, net	(119,133)	-	-	(119,133)
Other	18,347			18,347
Total other revenue	664,783			664,783
Total support and other revenue	1,549,250	11,000		1,560,250
Expenses:				
Program and publications	845,425	-	-	845,425
Management and general	639,853			639,853
Total expenses	1,485,278			1,485,278
Increase in net assets	63,972	11,000	-	74,972
Net assets, beginning of year	4,211,809	5,000	<u>5,659</u>	4,222,468
Net assets, end of year	\$ <u>4,275,781</u>	<u>16,000</u>	<u>5,659</u>	<u>4,297,440</u>

Statements of Cash Flows

	<u>2003</u>	<u>2002</u>
Cash flows from operating activities:		
Increase in net assets	\$ 688,332	74,972
Adjustments to reconcile increase in net assets		
to net cash provided by operating activities:		
Depreciation and amortization	15,912	16,611
Bad debt expense	5,659	27,693
Realized losses on investments	4,934	27,037
Unrealized (gains) losses on investments	(548,319)	249,043
Loss on disposal	-	2,924
Changes in operating assets and liabilities:		
Subscriptions receivable	14,924	(55,801)
Other receivables	(1,830)	20,383
Inventories	6,720	8,862
Prepaid expenses and other assets	(6,285)	1,734
Accounts payable and accrued expenses	28,206	866
Unearned subscriptions	(<u>156,688</u>)	<u>151,350</u>
Net cash provided by operating activities	51,565	<u>525,674</u>
Cash flows from investing activities:		
Purchases of furniture, fixtures, and equipment	(10,912)	(8,780)
Proceeds from sale of equipment	-	300
Proceeds from sales of investments	485,276	136,830
Purchases of investments	(<u>819,287</u>)	(<u>439,762</u>)
Net cash used in investing activities	(344,923)	(<u>311,412</u>)
Net (decrease) increase in cash and cash equivalents	(293,358)	214,262
Cash and cash equivalents, beginning of year	<u>811,018</u>	<u>596,756</u>
Cash and cash equivalents, end of year	\$ <u>517,660</u>	<u>811,018</u>

Statements of Functional Expenses

		2003		
	Program and	Management		2002
	publications	and general	<u>Total</u>	<u>Total</u>
Administrative costs	\$ 174,404	8,716	183,120	73,360
Audit and accounting	-	30,213	30,213	32,719
Bad debt expense	-	5,659	5,659	27,692
Contracted services	402,475	58,158	460,633	388,630
Contributions	30,200	-	30,200	25,352
Depreciation and amortization	-	15,912	15,912	16,611
Insurance	-	1,936	1,936	2,512
Prizes and awards	-	-	-	480
Maintenance	-	738	738	300
Office supplies and expenses	-	33,298	33,298	34,008
Payroll taxes and benefits	-	46,518	46,518	40,222
Postage	4,495	16,616	21,111	27,924
Printing and publications	28,454	13,572	42,026	53,787
Building operations	-	17,775	17,775	17,775
Salaries	-	282,439	282,439	265,209
Travel and subsistence	533,147	61,000	594,147	459,766
Utilities	-	17,686	17,686	14,118
Miscellaneous	25,129	520	25,649	4,813
	\$ <u>1,198,304</u>	<u>610,756</u>	<u>1,809,060</u>	<u>1,485,278</u>

Statements of Functional Expenses, Continued

	2002		
	Program and	Management	
	<u>publications</u>	and general	<u>Total</u>
Administrative costs	\$ 64,305	9,055	73,360
Audit and accounting	-	32,719	32,719
Bad debts expense	-	27,692	27,692
Contracted services	349,612	39,018	388,630
Contributions	25,352	-	25,352
Depreciation and amortization	-	16,611	16,611
Insurance	-	2,512	2,512
Prizes and awards	-	480	480
Maintenance	-	300	300
Office supplies and expenses	-	34,008	34,008
Payroll taxes and benefits	-	40,222	40,222
Postage	4,671	23,253	27,924
Printing and publications	19,111	34,676	53,787
Building operations	-	17,775	17,775
Salaries	-	265,209	265,209
Travel and subsistence	381,686	78,080	459,766
Utilities	-	14,118	14,118
Miscellaneous	688	4,125	4,813
	\$ <u>845,425</u>	639,853	1,485,278

Notes to Financial Statements

December 31, 2003 and 2002

(1) Nature of Organization and Significant Accounting Policies

The International Union of Pure and Applied Chemistry (IUPAC), founded in 1919, is a voluntary nongovernmental, nonprofit association of forty-four national adhering organizations representing the chemists of their countries. Additionally, there are twenty associate national adhering organizations, thirty-three associated organizations, and more than one hundred ten company associates.

The objectives of IUPAC are to promote continuing cooperation among the chemists of the member countries, to study topics of international importance to pure and applied chemistry which need standardization or codification, to cooperate with other international organizations which deal with topics of a chemical nature, and to contribute to the advancement of pure and applied chemistry in all its aspects.

The significant accounting policies of IUPAC are as follows:

Support, Revenues, and Expenses

IUPAC derives its revenues primarily from national subscriptions, publication income, and investment income. Support, revenues, and expenses are recorded on the accrual basis, and revenue received for future subscriptions is deferred until the applicable year.

Contributions received are measured at their fair values and are reported as an increase in net assets. IUPAC reports contributions of cash and other assets as restricted support if they are received with donor stipulations that limit the use of the donated assets or if they are designated as support for future periods. When a donor restriction expires, that is, when a stipulated time restriction ends or purpose restriction is accomplished, temporarily restricted net assets are reclassified to unrestricted net assets and reported in the statement of activities as net assets released from restrictions. Donor restricted contributions whose restrictions are met in the same reporting period are reported as unrestricted support.

Cash and Cash Equivalents

Cash and cash equivalents include commercial checking and money market accounts. At year-end and throughout the year, IUPAC had on deposit with a financial institution amounts in excess of FDIC insurance limits. IUPAC has not experienced any losses in such accounts and believes it is not exposed to any significant credit risk on cash and cash equivalents.

Allowance for Doubtful Accounts

An allowance is provided for uncollectible receivables equal to the losses that are estimated to be incurred in the collection of all receivables. The allowance is based on historical collection experience combined with a review of the current status of the existing receivables.

Notes to Financial Statements, Continued

December 31, 2003 and 2002

(1) Nature of Organization and Significant Accounting Policies, Continued

Inventories

Inventories, consisting of various publications, are stated at the lower of cost or market, with cost determined on the weighted-average method.

Investments

Investments in marketable securities are stated at fair market value. Investment income (including gains and losses on investments, interest, and dividends) is included in the statement of activities as a change in unrestricted net assets, except for earnings on permanently restricted net assets which are reported as temporarily restricted.

Furniture, Fixtures, and Equipment

Furniture, fixtures, and equipment are recorded at cost. Depreciation is provided over the estimated useful lives of the assets using the straight-line method.

Income Taxes

IUPAC is exempt from federal and state income taxes under Section 501(c)(3) of the Internal Revenue Code and applicable state statutes.

Use of Estimates

The preparation of financial statements in conformity with accounting principles generally accepted in the United States of America requires management to make estimates and assumptions that affect the reported amounts of assets and liabilities and disclosure of contingent assets and liabilities at the date of the financial statements and the reported amounts of revenues and expenses during the reporting period. Accordingly, actual results could differ from those estimates.

Reclassifications

Certain reclassifications have been made in the 2002 financial statements to conform with the 2003 presentation. Such reclassifications have no impact on change in net assets or net assets.

Notes to Financial Statements, Continued

December 31, 2003 and 2002

(2) Furniture, Fixtures, and Equipment

Furniture, fixtures, and equipment consist of the following:	<u>2003</u>	<u>2002</u>
Equipment	\$ 56,102	52,772
Furniture and fixtures	48,877	41,294
Leasehold improvements	16,097	16,097
•	121,076	110,163
Less accumulated depreciation and amortization	<u>(82,300</u>)	<u>(66,387</u>)
	\$ 38,776	43,776

(3) Investments

IUPAC's investments are held by Merrill Lynch. The following table presents the fair market value of those investments (investments that represent five percent or more of net assets are separately identified):

	200	<u>2002</u>	
	Number of	Fair	Fair
	shares/par	<u>value</u>	<u>value</u>
Corporate bonds (4.25% - 8.0%), with			
various maturities through May 2015	\$ <u>2,431,000</u>	\$ <u>2,804,842</u>	<u>2,416,314</u>
Equity securities:			
Defined Asset Fund, S&P Midcap Trust	247,549	395,262	292,257
MLIIF European Value Portfolio, Class A2	9,730	336,755	251,130
Defined Asset Fund, S&P 500 Trust 2	147,320	295,185	230,135
MLIIF UA Basic Value Portfolio, Class A2	6,797	269,977	-
Other	-	934,132	968,921
Total equity securities		2,231,311	1,742,443
		\$ <u>5,036,153</u>	4,158,757

The carrying amount of investments totaled \$4,517,887 and \$4,133,818 as of December 31, 2003 and 2002, respectively.

Notes to Financial Statements, Continued

December 31, 2003 and 2002

(3) Investments, Continued

Investment income (loss), net, consists of the following:

	<u>2003</u>	<u>2002</u>
Dividends and interest	\$ 176,763	156,947
Realized losses	(4,934)	(27,037)
Unrealized gains (losses)	<u>548,319</u>	(<u>249,043</u>)
	\$ 720,148	(119,133)

(4) Leases

IUPAC leases its facilities under an operating lease, which began in March 1997. This lease has a term of ten years with options to extend the term of the lease for successive one-year periods not to exceed ten additional years. Building operating expenses totaled \$23,699 and \$22,788 in 2003 and 2002, respectively.

Future estimated minimum rental expenses are as follows:

Year ending December 31,	
2004	\$ 23,375
2005	23,375
2006	23,375
2007	_5,844
	\$ 75,969

IUPAC subleased a portion of its facilities under an agreement which became effective October 1, 1997, for a term of five years and three months. Rental income under this sublease was \$1,723 and \$10,340 for 2003 and 2002, respectively. The sublease was terminated in February 2003.

(5) Net Assets

Temporarily restricted net assets of \$3,646 as of December 31, 2003 consist of interest earned on the Samsung General Chemicals Endowment Fund. Temporarily restricted net assets of \$16,000 as of December 31, 2002 consist of an Army Reserve grant restricted for travel and subsistence for attendees at the 42nd IUPAC General Assembly held in Ottawa, Canada in August 2003.

Notes to Financial Statements, Continued

December 31, 2003 and 2002

(5) Net Assets, Continued

Permanently restricted net assets consist of the Paulo Fransozini Endowment Fund totaling \$5,659 and the Samsung General Chemicals Endowment Fund totaling \$125,000. Income earned by the Paulo Fransozini Endowment Fund is restricted for awards to science students to attend particular IUPAC meetings. Income earned by the Samsung General Chemicals Endowment Fund is restricted for awards to students and researchers in the field of polymer science and support of educational projects of the IUPAC Macromolecular Division. Such income is recorded as temporarily restricted when earned.

(6) Concentrations of Credit and Market Risk

Financial instruments that potentially expose IUPAC to concentrations of credit and market risk consist primarily of cash equivalents, investments, and subscriptions receivable. Cash equivalents and investments are held by Merrill Lynch and Wachovia Bank, N.A., and no single investment exceeds ten percent of total investments. Subscriptions receivable are amounts due from national adhering organizations. Management provides for probable uncollectible amounts through a provision for bad debt expense and an adjustment to a valuation allowance based on its assessment of the current status of individual accounts.

Beginning in 2004, national adhering organizations were billed their annual national subscriptions in their national foreign currency. As a result, IUPAC has assumed the risk of changes in the foreign currency rates in relation to the United States dollar on these billings. IUPAC has made purchases of certain foreign currency-denominated investments in an effort to reduce the risk of foreign currency exchange losses on these billings when collected.

Financial Statements

December 31, 2004 and 2003

(With Independent Auditors' Report Thereon)

BATCHELOR, TILLERY & ROBERTS, LLP

CERTIFIED PUBLIC ACCOUNTANTS
POST OFFICE BOX 18068
RALEIGH, NORTH CAROLINA 27619

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Independent Auditors' Report

The Executive Committee
International Union of Pure and Applied Chemistry:

We have audited the accompanying statements of financial position of the International Union of Pure and Applied Chemistry ("IUPAC") as of December 31, 2004 and 2003, and the related statements of activities, cash flows, and functional expenses for the years then ended. These financial statements are the responsibility of IUPAC's management. Our responsibility is to express an opinion on these financial statements based on our audits.

We conducted our audits in accordance with auditing standards generally accepted in the United States of America. Those standards require that we plan and perform the audit to obtain reasonable assurance about whether the financial statements are free of material misstatement. An audit includes consideration of internal control over financial reporting as a basis for designing audit procedures that are appropriate in the circumstances, but not for the purpose of expressing an opinion on the effectiveness of IUPAC's internal control over financial reporting. Accordingly, we express no such opinion. An audit also includes examining, on a test basis, evidence supporting the amounts and disclosures in the financial statements, assessing the accounting principles used and significant estimates made by management, as well as evaluating the overall financial statement presentation. We believe that our audits provide a reasonable basis for our opinion.

In our opinion, the financial statements referred to above present fairly, in all material respects, the financial position of IUPAC as of December 31, 2004 and 2003, and the changes in its net assets and its cash flows for the years then ended in conformity with accounting principles generally accepted in the United States of America.

Batcheln, Jillery & Roberts, LLP

June 2, 2005

Statements of Financial Position

December 31, 2004 and 2003

Assets

<u>/ Alberta</u>	2004	2003
	<u> 2004</u>	2005
Current assets:		
Cash and cash equivalents	\$ 757,058	517,660
Subscriptions receivable (net of allowance for doubtful		
accounts of \$48,000 in 2004 and \$46,000 in 2003)	124,365	28,975
Other receivables	14,219	9,211
Inventories	11,500	14,000
Prepaid expenses and other assets	30,381	16,156
Total current assets	937,523	586,002
Furniture, fixtures, and equipment, net	25,495	38,776
Investments, at market value	5,336,526	5,036,153
	\$ 6,299,544	5,660,931
Liabilities and Net Assets		
Current liabilities:		
Accounts payable and accrued expenses	61,001	104,100
Unearned subscriptions	691,410	571,059
Total current liabilities	752,411	675,159
Commitments		
Net assets:		
Unrestricted	5,341,213	4,851,185
Temporarily restricted	75,261	3,928
Permanently restricted	130,659	130,659
Total net assets	5,547,133	<u>4,985,772</u>
	\$ 6,299,544	5,660,931

Statements of Activities

Year ended December 31, 2004, with comparative totals for 2003

	2004				
	Unrestricted	Temporarily restricted	Permanently restricted	Total	2003 <u>Total</u>
Support:					
Grants and contributions	\$ 11,530	71,948	-	83,478	184,767
National subscriptions and service charges	726,650	-	-	726,650	713,735
Affiliate membership program	71,650	-	-	71,650	82,461
Net assets released from restrictions	7,600	(7,600)			
Total support	817,430	64,348		881,778	980,963
Other revenue:					
Publications	838,462	-	_	838,462	770,572
Investment income, net	516,808	6,985	-	523,793	721,206
Other	3,050			3,050	25,709
Total other revenue	1,358,320	6,985		1,365,305	1,517,487
Total support and other revenue	2,175,750	71,333		2,247,083	2,498,450
Expenses:					
Program and publications	919,768	-	-	919,768	1,198,304
Management and general	765,954			765,954	611,814
Total expenses	1,685,722			1,685,722	1,810,118
Increase in net assets	490,028	71,333	-	561,361	688,332
Net assets, beginning of year	4,851,185	3,928	130,659	4,985,772	4,297,440
Net assets, end of year	\$ 5,341,213	75,261	130,659	5,547,133	4,985,772

(Continued)

Statements of Activities, Continued

Year ended December 31, 2003

	2003				
			Temporarily	Permanently	
	U	nrestricted	restricted	restricted	<u>Total</u>
Support:					
Grants and contributions	\$	59,767	-	125,000	184,767
National subscriptions and service charges		713,735	-	-	713,735
Affiliate membership program		82,461	-	-	82,461
Net assets released from restrictions	_	16,000	<u>(16,000</u>)		
Total support	_	871,963	(16,000)	125,000	980,963
Other revenue:					
Publications		770,572	-	-	770,572
Investment income, net		717,278	3,928	-	721,206
Other	_	25,709			25,709
Total other revenue	<u>1</u>	,513,559	3,928		1,517,487
Total support and other revenue	2	2,385,522	(12,072)	125,000	<u>2,498,450</u>
Expenses:					
Program and publications	1	,198,304	-	-	1,198,304
Management and general	_	611,814			611,814
Total expenses	<u>1</u>	,810,118			1,810,118
Increase (decrease) in net assets		575,404	(12,072)	125,000	688,332
Net assets, beginning of year	<u>4</u>	1,275,781	16,000	5,659	4,297,440
Net assets, end of year	\$ <u>4</u>	<u>1,851,185</u>	3,928	130,659	4,985,772

Statements of Cash Flows

Years ended December 31, 2004 and 2003

	2004	2003
Cash flows from operating activities:		
Increase in net assets	\$ 561,361	688,332
Adjustments to reconcile increase in net assets to		
net cash provided by operating activities:		
Depreciation and amortization	14,124	15,912
Bad debt expense	2,128	5,659
Realized losses on investments	71,745	4,934
Unrealized gains on investments	(353,738)	(548, 319)
Changes in operating assets and liabilities:		
Subscriptions receivable	(97,518)	14,924
Other receivables	(5,008)	(1,830)
Inventories	2,500	6,720
Prepaid expenses and accrued expenses	(14,225)	(6,285)
Accounts payable and accrued expenses	(43,098)	28,206
Unearned subscriptions	120,351	<u>(156,688</u>)
Net cash provided by operating activities	258,622	51,565
Cash flows from investing activities:		
Purchases of furniture, fixtures and equipment	(842)	(10,912)
Proceeds from sales of investments	726,603	485,276
Purchases of investments	<u>(744,985)</u>	<u>(819,287)</u>
Net cash used in investing activities	(19,224)	(344,923)
Net increase (decrease) in cash and cash equivalents	239,398	(293,358)
Cash and cash equivalents, beginning of year	517,660	811,018
Cash and cash equivalents, end of year	\$ 757,058	517,660

Statements of Functional Expenses

Year ended December 31, 2004, with comparative totals for 2003

		2004		
	Program and	l Management		2003
	publications	and general	Total	Total
Administrative costs	\$ 114,897	12,699	127,596	183,120
Audit and accounting	-	25,694	25,694	30,213
Bad debt	-	2,128	2,128	5,659
Contracted services	338,310	20,145	358,455	460,633
Contributions	25,202	-	25,202	30,200
Depreciation and amortization	-	14,124	14,124	15,912
Insurance	-	1,273	1,273	1,936
Maintenance	-	821	821	738
Office supplies and expenses	-	32,449	32,449	33,298
Payroll taxes and benefits	-	57,078	57,078	46,518
Postage	18,700	18,883	37,583	21,111
Printing and publications	79,924	89,005	168,929	42,026
Building operations	-	17,775	17,775	17,775
Salaries	-	323,207	323,207	282,439
Travel and subsistence	342,335	134,127	476,462	594,147
Utilities	-	15,164	15,164	17,686
Miscellaneous	400	1,382	1,782	26,707
	\$ 919,768	765,954	1,685,722	<u>1,810,118</u>

Statements of Functional Expenses, Continued

Year ended December 31, 2003

		rogram and oublications	Management and general	Total
	ł	<u>numications</u>	and general	<u> 10141</u>
Administrative costs	\$	174,404	8,716	183,120
Audit and accounting		-	30,213	30,213
Bad debt		-	5,659	5,659
Contracted services		402,475	58,158	460,633
Contributions		30,200	-	30,200
Depreciation and amortization		-	15,912	15,912
Insurance		-	1,936	1,936
Maintenance		-	738	738
Office supplies and expenses		-	33,298	33,298
Payroll taxes and benefits		-	46,518	46,518
Postage		4,495	16,616	21,111
Printing and publications		28,454	13,572	42,026
Building operations		-	17,775	17,775
Salaries		-	282,439	282,439
Travel and subsistence		533,147	61,000	594,147
Utilities		-	17,686	17,686
Miscellaneous	•	25,129	1,578	26,707
	\$	1,198,304	611,814	<u>1,810,118</u>

Notes to Financial Statements

December 31, 2004 and 2003

(1) Nature of Organization and Significant Accounting Policies

The International Union of Pure and Applied Chemistry (IUPAC), founded in 1919, is a voluntary nongovernmental, nonprofit association of forty-five national adhering organizations representing the chemists of their countries. Additionally, there are twenty associate national adhering organizations, thirty-three associated organizations, and more than one hundred ten company associates.

The objectives of IUPAC are to promote continuing cooperation among the chemists of the member countries, to study topics of international importance to pure and applied chemistry which need standardization or codification, to cooperate with other international organizations which deal with topics of a chemical nature, and to contribute to the advancement of pure and applied chemistry in all its aspects.

The significant accounting policies of IUPAC are as follows:

Support, Revenues, and Expenses

IUPAC derives its revenues primarily from national subscriptions, publication income, and investment income. Support, revenues, and expenses are recorded on the accrual basis, and revenue received for future subscriptions is deferred until the applicable year.

Contributions received are measured at their fair values and are reported as an increase in net assets. IUPAC reports contributions of cash and other assets as restricted support if they are received with donor stipulations that limit the use of the donated assets or if they are designated as support for future periods. When a donor restriction expires, that is, when a stipulated time restriction ends or purpose restriction is accomplished, temporarily restricted net assets are reclassified to unrestricted net assets and reported in the statement of activities as net assets released from restrictions. Donor restricted contributions whose restrictions are met in the same reporting period are reported as unrestricted support.

Cash and Cash Equivalents

Cash and cash equivalents include commercial checking and money market accounts. At year-end and throughout the year, IUPAC had on deposit with a financial institution amounts in excess of FDIC insurance limits. IUPAC has not experienced any losses in such accounts and believes it is not exposed to any significant credit risk on cash and cash equivalents.

Allowance for Doubtful Accounts

An allowance is provided for uncollectible receivables equal to the losses that are estimated to be incurred in the collection of all receivables. The allowance is based on historical collection experience combined with a review of the current status of the existing receivables.

Notes to Financial Statements, Continued

December 31, 2004 and 2003

(1) Nature of Organization and Significant Accounting Policies, Continued

<u>Inventories</u>

Inventories, consisting of various publications, are stated at the lower of cost or market, with cost determined on the weighted-average method.

Investments

Investments in marketable securities are stated at fair market value. Investment income (including gains and losses on investments, interest, and dividends) is included in the statement of activities as a change in unrestricted net assets, except for earnings on permanently restricted net assets which are reported as temporarily restricted.

Furniture, Fixtures, and Equipment

Furniture, fixtures, and equipment are recorded at cost. Depreciation is provided over the estimated useful lives of the assets using the straight-line method.

Income Taxes

IUPAC is exempt from federal and state income taxes under Section 501(c)(3) of the Internal Revenue Code and applicable state statutes.

Use of Estimates

The preparation of financial statements in conformity with accounting principles generally accepted in the United States of America requires management to make estimates and assumptions that affect the reported amounts of assets and liabilities and disclosure of contingent assets and liabilities at the date of the financial statements and the reported amounts of revenues and expenses during the reporting period. Accordingly, actual results could differ from those estimates.

Reclassifications

Certain reclassifications have been made in the 2003 financial statements to conform with the 2004 presentation. Such reclassifications have no impact on change in net assets or net assets.

Notes to Financial Statements, Continued

December 31, 2004 and 2003

(2) Furniture, Fixtures, and Equipment

Furniture, fixtures, and equipment consist of the following:

	2004	2003
Equipment	\$ 56,944	56,102
Furniture and fixtures	48,877	48,877
Leasehold improvements	16,097	16,097
·	121,918	121,076
Less accumulated depreciation and amortization	(96,423)	(82,300)
	\$ 25,495	38,776

(3) Investments

IUPAC's investments are held by Merrill Lynch. The following table presents the fair market value of those investments (investments that represent five percent or more of net assets are separately identified):

	_	2004			2003
		Number of shares/par		Fair <u>value</u>	Fair value
Corporate bonds (4.25% - 7.38%), with various maturities through June 2033	\$	2,731,000	\$	3,207,801	2,804,842
Equity securities:					
Defined Asset Fund, S&P Midcap Trust		187,505	\$	345,347	395,262
MLIIF European Value Portfolio, Class A2		9,730		404,963	336,755
MLIIF UA Basic Portfolio, Class A2		6,797		293,630	269,977
Other		-		1,084,785	1,229,317
Total equity securities				<u>2,128,725</u>	2,231,311
			\$	5,336,526	5,036,153

The cost of investments totaled \$4,426,183 and \$4,517,887 as of December 31, 2004 and 2003, respectively.

Notes to Financial Statements, Continued

December 31, 2004 and 2003

(3) Investments, Continued

Investment income, net, consists of the following:

	2004	2003
Dividends and interest Realized losses	\$ 241,800 (71,745) 353,738	177,821 (4,934) 548,319
Unrealized gains	\$ <u>523,793</u>	<u>721,206</u>

(4) Leases

IUPAC leases its facilities under an operating lease, which began in March 1997. This lease has a term of ten years with options to extend the term of the lease for successive one-year periods not to exceed ten additional years. Building operating expenses totaled \$21,253 and \$23,699 in 2004 and 2003, respectively.

Future estimated minimum rental expenses are as follows:

Year ending December 31,

2005 2006 2007	\$ 22,575 22,575 6,844
	\$ 51,994

IUPAC subleased a portion of its facilities through February 2003. Rental income under this sublease was \$0 and \$1,723 for 2004 and 2003, respectively.

(5) Net Assets

Temporarily restricted net assets of \$78,481 as of December 31, 2004 consist of interest earned on the Samsung General Chemicals Endowment Fund and various grants not fully expended as of December 31, 2004. Temporarily restricted net assets of \$3,646 as of December 31, 2003 consist of an Army Reserve grant restricted for travel and subsistence for attendees at the 42nd IUPAC General Assembly held in Ottawa, Canada in August 2003.

Notes to Financial Statements, Continued

December 31, 2004 and 2003

(5) Net Assets, Continued

Permanently restricted net assets consist of the Paulo Fransozini Endowment Fund totaling \$5,659 and the Samsung General Chemicals Endowment Fund totaling \$125,000. Income earned by the Paulo Fransozini Endowment Fund is restricted for awards to science students to attend particular IUPAC meetings. Income earned by the Samsung General Chemicals Endowment Fund is restricted for awards to students and researchers in the field of polymer science and support of educational projects of the IUPAC Macromolecular Division. Such income is recorded as temporarily restricted when earned.

(6) Concentrations of Credit and Market Risk

Financial instruments that potentially expose IUPAC to concentrations of credit and market risk consist primarily of cash equivalents, investments, and subscriptions receivable. Cash equivalents and investments are held by Merrill Lynch and Wachovia Bank, N.A., and no single investment exceeds ten percent of total investments. Subscriptions receivable are amounts due from national adhering organizations. Management provides for probable uncollectible amounts through a provision for bad debt expense and an adjustment to a valuation allowance based on its assessment of the current status of individual accounts.

Beginning in 2004, national adhering organizations were billed their annual national subscriptions in their national foreign currency. As a result, IUPAC has assumed the risk of changes in the foreign currency rates in relation to the United States dollar on these billings. IUPAC has made purchases of certain foreign currency-denominated investments in an effort to reduce the risk of foreign currency exchange losses on these billings when collected.

Item 13.4: Recommendation on Appointment of Auditors for 2005 and 2006

Bureau has recommended to Council the appointment of Batchelor, Tillery & Roberts, LLP, of Raleigh, North Carolina, USA as IUPAC Auditors for 2005 and 2006. Council is asked to approve this recommendation.

Item 14.1: Proposed Budget for 2006-7

Item 14.2: National Subscriptions for 2006-7

Budget Proposal and National Subscription 2006-2007

As you have seen in the Treasurer's Review and the Report of the Finance Committee, the financial situation of IUPAC is still strong. However there are serious potential problems. Publication income continues be under pressure from the long-term decline in institutional subscriptions while some NAOs continue to have difficulty in paying their National Subscriptions. The following pages contain the proposed budget, the proposed Division and Standing Committee allocations, and the calculated National Subscriptions based on the proposed budget. The National Subscriptions are shown in national currencies according to the method approved at Ottawa by Council. National Subscriptions were calculated in USD using the standard formula relating chemical turnover and National Subscription; these were converted to national currencies using the exchange rates for the first quarter of 2005. Certain NAOs have requested billing in USD due to foreign exchange control regulations in effect in their countries.

The format of the budget is the same as that used at Brisbane and Ottawa. This format emphasizes the sources of the Union's funds and the uses of those funds. The categories used should be self-explanatory. The category Division Operations is 25 % of the total Division allocations for the previous biennium and 30 % for the current biennium, while the category Projects (Commitments) is 75 % and 70 % of the Division allocations for the two biennia respectively, plus the Division Reserve and the Project Reserve. The Project Reserve is used by the Project Committee to fund projects that are too large for a Division to fund while the Division Reserve is used by the Treasurer and Secretary General to fund projects when the Division has committed its Project Budget.

Due to the moderate OECD inflation of <3% we are proposing an increase of only 1 % per annum for the total National Subscription. The subscriptions of individual NAOs will depend on changes in the chemical turnover since the last Council. As in the past, the chemical turnover values have been taken from latest CEFIC and UNIDO figures.

We think that with the new way of operation IUPAC shows a positive attitude to change. For sustainability of our operations, we are asking for your support, commitment and enthusiasm. IUPAC has the intention to give to all its members a great value for money. It is therefore important that we can count on your financial support and help.

Significant changes from the 2004-5 budget are described below.

- 1. *National Subscriptions*: Total National Subscription has been increased by 1 % each year.
- 2. *Division Budgets*: These have been held constant except for those of Division IV, which has been increased by USD 5000, and Division II, which has been increased by USD 2000. The increase in Division Operations expense and the Decrease in Projects are due to the change in the proportion of the total Division Budgets allocated to these categories as noted above.
- 3. *General Assembly*: The budget includes USD 80 000 to fund the support for Council delegates approved by the Bureau in 2003.
- 4. *Administrative*: An allowance for Foreign Exchange differences of USD 60 000 has been included to take into account the billing of National Subscriptions in

Item 14.1: Proposed Budget for 2006-7

Item 14.2: National Subscriptions for 2006-7

national currencies. The Secretariat component in the Administrative category is unchanged from the 2004-5 budget. The Secretariat will be at its authorized staffing level for the coming biennium.

- 5. *General*: The General category includes Governance expense, the *IUPAC Handbook*, the cost of *CI* for Fellows and Members, as well the cost of the IUPAC Prize and cost of IUPAC representatives to other organizations. The budgets for *CI* for Fellows and Members have been increased to account for the increase in the number of Members and Fellows. Governance Expense has been increased to account for greater travel by the officers. The budget for the *Handbook* has been decreased by USD 40 000 in line with the recommendation of the Finance Committee and the Executive Committee to no longer publish a *Handbook* and instead publish the list of members of IUPAC bodies in *CI* and rely on the web for the other information in the Handbook.
- 6. *AMP*: & *CI*: The increased cost of *CI* is due to both the change to full color and the greater number of complimentary copies provided to IUPAC sponsored conferences for distribution to conference participants.
- 7. *Publications*: Revenue from *PAC* is expected to increase due to an increase in the subscription rate for institutional subscriptions. Costs for Printing & Editing are expected to increase due to increased costs from the printer. The net result is a slight increase in budgeted income for Publications.
- 8. *Projects*: The Project Reserve has been set at USD 110 000; the Divisional Reserve is USD 97 400
- 9. *Dividends & Interest*: This item has increased due to the greater proportion of the Union's portfolio invested in fixed income securities rather than in equities.

Sources and Uses Analysis of 2006-7 Budget

	Budget 2004-5	Budget 2006-7	Change Increase/ (Decrease)
National Subscriptions	\$1,420.3	\$1,448.8	\$28.5
Dividends & Interest	\$260.0	\$368.0	\$108.0
Other Income	\$28.9	\$40.0	\$11.1
Publications	\$873.5	\$890.0	\$16.5
Total Income	\$ <u>2,582.7</u>	\$2,746.8	\$ <u>164.1</u>
AMP and CI	\$41.5	\$119.0	\$77.5
Administrative	\$930.0	\$914.0	(\$16.0)
General	\$364.5	\$433.0	\$68.5
General Assembly	\$320.0	\$350.0	\$30.0
Advisory Standing Committees	\$121.5	\$121.5	\$0.0
Operating Standing Committees (Operations)	\$67.6	\$67.6	\$0.0
Division Operations	\$121.8	\$148.3	\$26.5
Projects (Commitments)	\$615.8	\$593.4	(\$22.4)
Total Expense	\$ <u>2,582.7</u>	\$2,746.8	\$ <u>164.1</u>
Net Income/(Expense)	\$ <u>0.0</u>	\$ <u>0.0</u>	(<u>\$0.0</u>)

Division Allocations	Budget 2006-7	Projects 2006-7	Operations 2006-7
I Physical	65.3	45.7	19.6
II Inorganic	53.2	35.8	17.4
III Organic	60.4	42.3	18.1
IV Macromolecular	52.5	33.3	19.3
V Analytical	56.6	39.6	17.0
VI Chemistry & the Environment	68.0	47.6	20.4
VII Chemistry & Human Health	58.3	40.8	17.5
VIII Chemical Nomenclature and Structure Representation	80.0	56.0	24.0
Divisional Reserve	97.4	97.4	-
Total Divisions	591.7	438.5	153.2
Project Reserve		110.0	
Standing Committee Allocations Executive	35.3		35.3
Bureau	40.5	-	40.5
CHEMRAWN	29.3	_	29.3
CPEP	16.4		16.4
CCE	38.3	20.0	18.3
COCI	40.0	20.0	20.0
FC	13.3	-	13.3
Evaluation Committee	8.0	_	8.0
ICTNS	8.0	_	8.0
Total Standing Committees	229.1	40.0	189.1

IUPAC NATIONAL SUBSCRIPTIONS FOR 2006-7

NAO	Currency	2005	2006	2007
Argentina	ARS	13.0	11.0	12.0
Australia	AUD	17.7	12.7	12.9
Austria	EUR	5.5	4.5	4.5
Bangladesh	USD	1.0	1.0	1.0
Belgium	EUR	19.4	17.3	17.4
Brazil	BRL	86.0	62.4	62.9
Bulgaria	BGN	2.9	2.2	2.2
Canada	CAD	24.0	20.9	21.1
Chile	CLP	2,800.0	2,700.0	2,700.0
China/Beijing	CNY	335.0	368.0	372.0
China/Taipei	TWD	530.0	516.0	523.0
Croatia	USD	1.0	1.0	1.0
Czech Republic	CZK	120.0	90.0	90.0
Denmark	DKK	45.0	41.0	41.0
Egypt	EGP	23.0	23.0	24.0
Finland	EUR	5.4	4.5	4.5
France	EUR	35.1	28.8	29.1
Germany	EUR	49.7	39.7	40.1
Greece	EUR	3.5	2.7	2.7
Hungary	HUF	860.0	730.0	750.0
India	USD	945.0	20.0	20.0
Ireland	EUR	12.5	13.5	13.7
Israel	ILS	24.0	20.0	20.0
Italy	EUR	30.1	24.0	24.2
Japan	JPY	8,550.0	7,230.0	7,310.0
Korea, Republic	KRW	28,000.0	23,300.0	23,500.0
Kuwait	KWD	0.3	0.3	0.3
Netherlands	EUR	18.1	15.1	15.3
New Zealand	NZD	7.8	5.9	6.0
Norway	NOK	35.0	33.0	33.0
Pakistan	PKR	180.0	180.0	180.0
Poland	PLN	27.0	22.0	22.0
Portugal	EUR	4.8	3.6	3.6
Puerto Rico	USD	16.4	16.0	16.1
Russia	USD	10.4	9.2	9.2
Serbia & Monter	USD	1.0	1.0	1.0
Slovakia	SKK	110.0	120.0	120.0
Slovenia	SIT	730.0	680.0	700.0
South Africa	ZAR	67.0	47.0 16.5	47.0
Spain Sweden	EUR	20.4	16.5	16.6
Sweden	SEK	80.0	71.0	72.0
Switzerland	CHF	23.5	26.4	26.6
Turkey	TRL	15,000,000.0	14,600,000.0	14,800,000.0
UK	GBP	18.0	15.0	15.0
USA	USD	112.3	112.0	113.1

Item 15 NAOs in Arrears

Three NAOs are seriously in arrears, Argentina, Brazil, and Chile. Argentina has not paid their National subscription for 2001, 2002, 2003, and 2004; Chile has made a partial payment for 2002 and has not paid the National Subscriptions for 2003 and 2004. Brazil recently paid the National Subscriptions for 2002 and 2003 and is still in arrears for 2004. Egypt has made a partial payment of the 2003 National Subscription and has not paid for 2004. Pakistan and Portugal have not paid their 2004 National Subscriptions and have been informed that they will not be allowed to vote at Council at Beijing if payment is not received before 1 August 2005. Both Egypt and Portugal expect to be able to pay their arrears with the start of the new fiscal year in July.

The Executive Committee has sanctioned Argentina, Brazil, and Chile by preventing any of the members of Committees from these NAOs receiving IUPAC support to attend meetings or to be considered for election or appointment to any IUPAC Committee until the amounts in arrears have been paid. The Chairman of the Brazilian Chemistry Committee for IUPAC has informed the Treasurer that efforts are being made to obtain the necessary funds from non-governmental sources. There has also been correspondence on this subject with other interested groups and individuals in Brazil. The NAO for Argentina has informed the Secretariat that they expect to be able to pay the National Subscriptions in arrears by 1 July but payment has not been received as of 27 June. The Chilean NAO has informed us that there is an as yet unknown problem with the government agency responsible for payment of the National Subscription. They have not been able to resolve this problem

The EC has recommended to Bureau and Council at Beijing that all those NAOs still in arrears for 2003 and earlier by the end of 2005 be suspended from NAO status until payment in full is received. The Finance Committee supported this recommendation at its meeting in February.

Motion: Council approves the suspension of NAO status for those NAOs who have not paid their 2003 and earlier National Subscriptions by 31 December 2005 until such time as the 2003 and earlier National Subscriptions are paid.

Item 16: Applications for National Adhering Organization Status

The Caribbean Academy of Sciences (CAS) – Jamaica Chapter has requested approval of its application for National Adhering Organization status. A letter from Professor Tara P. Dasgupta, and a copy of the Statutes and Bylaws of the CAS, in which are a brief description of the goals of the National Academy and its significant activities, follow this page.

Motion: Council approves National Adhering Organization status for the Caribbean Academy of Sciences – Jamaica Chapter.

The Jordanian Chemical Society has requested approval of its application for National Adhering Organization status. A letter from the President of the Jordanian Chemical Society, Prof. Sultan T. Abu-Orabi, and a copy of the Statutes and Bylaws of the JCS, in which are a brief description of the goals of the JCS and its significant activities, follow this page.

Motion: Council approves National Adhering Organization status for the Jordanian Chemical Society.

The National Academy of Sciences of Ukraine has requested approval of its application for National Adhering Organization status. A letter from Academician-Secretary of the Chemistry Division of the National Academy of Sciences of Ukraine, Academician V. Goncharuk, and a copy of the Statutes and Bylaws of the National Academy of Sciences, in which are a brief description of the goals of the National Academy and its significant activities, follow this page.

Motion: Council approves National Adhering Organization status for the National Academy of Sciences of Ukraine.



Caribbean Academy of Sciences Jamaica Chapter 23rd June 2005

Dr John W. Jost, Executive Director, IUPAC Secretariat P.O. Box 13757 Research Triangle Park, NC 27709-3757, U.S.A.

Re: Application for National Adhering Organisation membership from Jamaica

Dear Dr. Jost,

Jamaica wishes to become a formal Member of the Union and the organisation best able to represent Jamaican Chemists is the Caribbean Academy of Sciences (CAS) – Jamaica Chapter. Although CAS was first established in Trinidad and Tobago, the Jamaica Chapter has over 100 members of which Chemists make up the largest number. The Chapter is very active and holds meetings every month.

The University of the West Indies (UWI) is a regional institution and has campuses in Jamaica, Barbados and Trinidad and Tobago. Chemistry is taught at the three campuses and the Mona Campus currently has about 20 academic staff and 40 postgraduate students. The Department has a strong foundation for carrying out high level research and produces about 30 research papers in international journals per year. It has a strong outreach and consultative programme that supports both the public and private sectors.

There is a vibrant student Chemical Society at Mona where I have been operating an IUPAC Affiliation programme for the last 15 years. There are 30 affiliate members in Jamaica and all belong to the Chemical Society of the UWI, Mona Campus. All undergraduate and graduate chemistry students are encouraged to participate in the various activities of the Chemical Society.

I think that the time has come for Jamaica to be more involved in the various activities of IUPAC and participate in the decision making processes of the Union. I would appreciate it if you would consider our application to be a formal member of the Union.

Sincerely yours,

(Professor Tara P. Dasgupta)

Jana P. Sare

IUPAC Affiliate Membership Coordinator

And Professor of Inorganic Chemistry.

CONSTITUTION Of The CARIBBEAN ACADEMY OF SCIENCES

ARTICLE I – NAME

The name of the Academy shall be The Caribbean Academy of Sciences, hereafter called CAS.

ARTICLE II – OBJECTIVES

CAS shall be a non-profit, non-political, and non-governmental body which shall not discriminate on the basis of ethnicity, clays, gender or religious persuasion and whose objectives shall be:

- 1 To provide a forum for the consideration of ideas and issues related to science and technology.
- 2 To serve as a source of advice to governments and non-governmental organizations on scientific and technological matters.
- 3 To facilitate cooperation in scientific and technological research with special reference to the Caribbean region.
- 4 To recognize outstanding performance or achievement in science and technology.
- 5 To undertake or facilitate the publication and collation of the results of scientific research.
- 6 To promote public awareness and appreciation of the importance and potential of science and technology in the Caribbean region.
- 7 To promote ethical conduct in all matters relating to science and technology.
- 8 To maintain contact with similar bodies abroad.
- 9 To do all such other things which the Council may deem necessary to fulfil its objectives.

ARTICLE III – STRUCTURE

- 1 The Academy shall consist of a Council, an Executive Committee, Chapters and the Membership.
- 2 The Executive Committee will comprise the President, who shall be a Fellow, the Foreign Secretary, who is the Immediate Past President, Secretary, Treasurer, Public Relations Officer and the Chairpersons of each Chapter. If the Immediate Past President declines to serve as Foreign Secretary, the position will be filled in accordance with Article V. The candidate for this post must be a Fellow.
- 3 The Council will comprise the Executive Committee, one member nominated by each Chapter and one Ordinary Member elected at the Annual General Meeting
- 4 Chapters may be formed in regional territories by application of Members to the Council. Council shall, from time to time, determine what minimum number of Members shall comprise a Chapter and accordingly shall have full power to merge, sub-divide, dissolve and modify Chapters. Chapters shall be subject to the rules and bye-laws of the Academy.

ARTICLE IV - MEMBERSHIP

The membership shall comprise the following categories: Ordinary Member, Associate Member, Junior Member, Fellow and Honorary Member.

IV. 1 - ORDINARY MEMBERS

- 1 Any citizen or resident of the Caribbean region who has produced and published scientific work of a high standard is eligible to be an Ordinary Member.
- 2 Nomination to membership shall be in writing to the Secretary at least four weeks before the Annual General Meeting Each nomination shall be signed by two persons who are either Ordinary members or fellows of CAS in good financial standing and must be accompanied by a curriculum vitae of the nominee.
- 3 The Secretary shall forward the nominations to the Membership Committee which shall forward recommendations to the Annual General Meeting.
- 4 The Annual General Meeting shall vote on the nominations. Election to membership shall require a simple majority of the members present.

IV. II -ASSOCIATE MEMBERS

- 1 (a) Any citizen or resident of the Caribbean region who is not otherwise qualified for Ordinary Membership but whose work is deemed valuable to the purposes of CAS is eligible to be an Associate Member.
- (b) Any non-citizen or non-resident of the Caribbean region, who has produced and published scientific work of a high standard shall be eligible for election as an Associate Member.

CONSTITUTION OF CAS 1/3

- (c) Any institution or body duly constituted in the Caribbean region and whose work is deemed valuable to the purposes of the Academy shall be eligible for election as an Associate Member and shall be entitled to send a representative to the Annual General Meeting.
- 2. Nomination and election of Associate Members to the Academy will conform to the same rules as those established for Ordinary Members. In the case of an application under IV. II 1(c) the institution or body will be required to submit its aims, objectives and constitution.
- 3 Associate Members shall have no voting rights.

JUNIOR MEMBERS

- 1. Any citizen or resident of the Caribbean region whose activities are deserving of association with the work of CAS is eligible to be a. Junior Member.
- 2. Nomination and election of Junior Members to CAS will conform to the same rules as those established for Ordinary Members.
- 3. Junior Members shall have no voting rights.

IV. IV - FELLOWS

- 1. Any citizen or resident of the Caribbean region who has made a significant contribution to the field of science and technology is eligible to become a Fellow.
- 2. Nomination to Fellowship shall be in writing to the Secretary by September 30 of each calendar year. A nomination shall be signed by two persons being either Ordinary Members or Fellows of the Academy in good financial standing and must be accompanied by a curriculum vitae.
- 3. The Secretary shall forward the nominations by October 15, to the Fellowship Committee.
- 4. The Fellowship Committee shall consider the nominations received and come to a decision which shall be final.
- 5. The President will inform the relevant parties of the decision of the Fellowship Committee and within one month of the decision and will announce at the Annual General Meeting the names of new admission to Fellowship. The term of new Fellows will commence at the Annual General Meeting.
- 6. No more than two Fellows may be admitted in any Annual General Meeting.
- 7. Fellows shall have full voting rights.

IV. V -HONORARY FELLOWS

- 1. Any person whose merit is internationally recognized and who has made a significant contribution to the progress of science and technology or to human welfare is eligible to be an Honorary Fellow.
- 2. Election of Honorary Fellows shall be determined by Council.
- 3. Honorary Fellows shall have no voting rights.

ARTICLE V - ELECTION OF THE EXECUTIVE COMMITTEE

- 1. Where a vacant post in the Executive Committee exists or will exist in the current calendar year due to the expiration of term, resignation, abandonment or removal from office or howsoever such post may be vacated, the Chairperson of the Election Committee will invite nominations from Ordinary Members and Fellows in good financial standing ("voting members") at least four months prior to the start of the next Annual General Meeting.
- 2. The return date for nominations will be set by the Election Committee and marked on all nomination ballots distributed. This date must not extend beyond a day which is less than two months prior to the start of the next Annual General Meeting.
- 3. A voting member may nominate one person who is an Ordinary Member or Fellow in good financial standing for each position for which nominations are invited by having each such nomination seconded by a voting member and returning the completed nomination ballot to the Election Committee by the return date.
- 4. A list of candidates for each vacant post ("the election ballot") shall be compiled by the Election Committee from the nominations returned as in clause 3 above and distributed to all voting members at least six weeks prior to the start: of the Annual General Meeting of that year.
- 5. A voting member will cast their vote by indicating their candidate of choice for each post from among the candidates listed on the election ballot and returning the said ballot to the Election Committee at least two weeks prior to the start of the Annual General Meeting.
- 6. Election ballots shall be opened and counted by the Chairperson of the Election Committee or his nominee at the Annual General Meeting and the results announced.
- 7. If there is no nomination for any Executive position, the incumbent will remain in office and the election process repeated in 6 months. In this case the ballot will be opened in the presence of the Executive Committee.

 CONSTITUTION OF CAS

 2/3

8. The Executive will be elected biennially. Any member of the Executive shall not hold the same office for more than two consecutive terms. A person who is Immediate Past President shall not be re-elected to the Executive Committee before a period of two terms.

ARTICLE VI - COMMITTEES

- 1. The Executive shall appoint Committees as deemed necessary to assist in the functioning of CAS.
- 2. There shall be a Membership Committee comprising five members elected by Council with the President or his nominee as Chair. The term of office shall be at the discretion of Council.
- 3. There shall be a Fellowship Committee comprising five Fellows nominated by the President and five Ordinary Members elected at the Annual General Meeting. The President shall chair this Committee. The term of office shall be at the discretion of the Council.
- 4. There shall be an Election Committee set up by Council comprising three persons who may or may not be members of CAS. Council will name the Chairperson and specify its term of office.

ARTICLE VII - DUTIES OF MEMBERS AND POWERS OF COUNCIL AND THE EXECUTIVE

- 1. Council shall be the highest policy-making authority of CAS and as such its responsibilities shall include, inter alia, (a) Duties specified in relevant Articles above
- 2. (b) Approving the Strategic and Work Plan
- 3. (c) All such lawful things as may be conducive to fulfilling the mission of CAS and promoting and carrying out its objectives
- 4. The Executive is charged with the responsibility of implementing the decisions of the Council.
- 5. The President shall preside at all meetings of CAS. In his/her absence, the Immediate Past President shall preside.
- 6. The Secretary shall be the custodian of the records and papers of CAS, shall keep a record of the proceedings of CAS and make a report in writing on the year's activity.
- 7. The Treasurer shall receive dues of the members, administer all funds which must be lodged in an approved financial institution, keep a record of the receipts and expenditure of CAS and present a financial statement at the Annual General Meeting of CAS.
- 8. The Foreign Secretary shall be concerned with international relations and shall work towards the promotion of better relations between CAS and other similar organizations regionally and internationally.
- 9. The *PRO* shall be concerned with public relations and relations with the media and shall work towards the promotion of better understanding between CAS and the communities of the region.

ARTICLE VIII - MEETINGS

- 1. CAS shall hold a meeting to be known as the Annual General Meeting of CAS each year and shall give six months notice of the Meeting. This Meeting shall be announced by a first circular at least six months in advance. A final announcement of the meeting shall be sent out at a suitable time prior to the meeting. The programme and the place and date of the meeting shall be determined by the Executive.
- 2. The Annual General Meeting of CAS shall normally rotate among member territories of the region.
- 3. Special Meetings of CAS may be called by The President or a simple majority of Council.
- 4. At General Meetings of CAS, twenty percent of voting members shall constitute a quorum.

ARTICLE IX -DUES

The dues of Members shall be set by Council. There shall be a registration fee and an Annual Fee. Annual Fees are payable; by April 2.

ARTICLE X - LEGAL RESIDENCE

CAS shall be legally resident in Trinidad and Tobago.

ARTICLE XI - AMENDMENTS

Any proposed amendment to the Constitution will be discussed at the Annual General Meeting. Thereafter, the text of the amendment will be circulated by the Chairperson of the Election Committee to all voting members of CAS who will be asked to signify their approval of disapproval in an accompanying ballot.

The Constitution may be amended by 75% of the members voting 'yes'. If the response is less than 75%, then it may be mended by 75% of the Membership in good standing at an Annual General Meeting of not less than 20 members.

CONSTITUTION OF CAS 3/3

Bylaws of The Jamaica Chapter of The Caribbean Academy of Sciences

Article I – Organisation and Purpose

- 1. Name: The name of this Chapter shall be the Jamaica Chapter of the Caribbean Academy of Sciences.
- 2. The objective of this Chapter shall be:
 - (a) To promote the mission statement of the Caribbean Academy of Sciences through various activities.
 - (b) To foster closer relationships among members of the Academy in Jamaica.
 - (c) To promote and achieve, as far as possible, the Academy's objectives in Jamaica.
 - (d) To arrange a suitable programme of scientific and technological activities annually in Jamaica.

Article II – Membership and Subscriptions

- 1. Membership: The Chapter shall consist of duly elected members of the Academy domiciled/residing in Jamaica as per Article XIX of the Academy. Application for membership shall first be submitted to the Academy.
- 2. Subscription: Members shall pay annually such dues as the Chapter shall determine at the annual meeting by a majority vote. Any member two (2) years in arrears of subscriptions after due notices, shall stand suspended from the Chapters' privileges until such arrears are paid. The Secretary shall notify such members of their delinquency. Should dues not be paid within six (6) months thereafter, the said member will be dropped from the roll. Reinstatement may be sought after payment of dues.

Article III - Officers and Committees

- 1. Officers: The officers of the Chapter shall consist of a Chairperson, Vice Chairperson, Secretary, Treasurer, Assistant Secretary-Treasurer and a Programme Officer.
 - (a) The Chairperson shall preside at all meetings of the Chapter and such other functions customary for the office. The Chairperson shall represent the Chapter at the Academy's Executive Council. He/She shall serve a term of one (1) year, which term shall be renewable by vote but not exceeding two (2) consecutive terms.

- (b) The Vice-Chairperson shall preside at all meetings in the absence of the Chairperson and assist the Chairperson in managing the Chapter's affairs. He/She serves a term of one (1) year, which term shall be renewable by vote but not exceeding two (2) consecutive terms.
- (c) The Secretary shall be responsible for the Chapter's record keeping, all necessary correspondence, issuance of timely minutes. The Secretary shall attend the Executive Council meeting of the Academy. The term of office shall be two (2) years, of which term shall be renewal by vote for an extra term of one (1) year only.
- (d) The Treasurer shall be responsible for the collection of subscriptions and the administration of funds. The term of office shall be two (2) years.
- (e) The Assistant Secretary-Treasurer shall assist the Secretary and the Treasurer and carry out any other duties deemed fit by the Executive Committee from time to time. He/She shall act in the absence of the Secretary or Treasurer. The term of office shall be one (1) year, which term shall be renewable by vote but not exceeding two (2) terms.
- (f) The Programme Officer shall be responsible for developing the annual programme(s) of the chapter which shall be discussed, amended and/or passed for action by majority vote at a general meeting. The Programme Officer shall be responsible for the planning and execution of all programmes approved by the Chapter using all appropriate means-media etc. The term of office shall be one (1) year, which terms shall be renewable by vote for an additional year.
- 2. Election of Officers: Nomination of officers shall be made one (1) month prior to the annual general meeting/extra ordinary meeting called by signature of two-thirds membership. Officers shall be elected by a majority vote of members present and voting at the annual general meeting or an extra-ordinary meeting. Any member of the chapter may propose nominees for any of the offices.
- 3. Committees: There shall be three committees (i) the Executive Committee, (ii) the Nominating Committee and (iii) Public Affairs and Programming Committee.
 - (a) Executive Committee The officers of the chapter shall constitute the Executive Committee, which Committee shall have the authority to designate place and date of the annual meeting and to fill vacancies occurring in the offices between annual meetings or extra-ordinary meetings
 - (b) Nominating Committee The Committee together with one-member-atlarge duly elected shall function as the nominating Committee, which Committee shall receive nominations and present at the annual general meeting a list of nominees for the offices to be filled. The member-atlarge shall Chair this Committee.

- (c) Public Affairs and Programming Committee This Committee shall consists of the Chairperson, Secretary-Treasurer, Programme Officer and one other member elected by the membership. This Committee shall be responsible for programming and public affairs or science and technology issues. This Committee shall be chaired by the Programme Officer.
- 4. Executive Report The following officers shall submit annual reports for approval Chairperson and Treasurer.

Article IV - Meetings

- 1. Meetings: There shall be an annual general meeting. A joint general meeting with the Academy may be held when deemed necessary.
- 2. Quorum: Two thirds of the membership shall constitute a quorum for General and Committee Meetings.

Article V - Amendments

- 1. These bylaws may be amended by a three-fourths majority of the members present and voting at any quorate annual meeting.
- 2. Notice of amendment Notice of proposed amendments shall be sent to all members at least six (6) weeks prior to such meeting by the secretary.

Absent members may vote by mailing their signed ballots to be received by the Secretary at least one (1) week before the annual meeting.

Amendment for Academy's Constitution

Academy - Article XIX - Amendment - Chapters

- 1. Any regional grouping of at least ten (10) members, if so desired, may establish a Chapter in a particular territory to foster the aims/objectives of the Academy without incurring any activities deemed inimical to the Academy.
- 2. The said Chapter shall develop bylaws to be approved by the Academy.

JORDANIAN CHEMICAL SOCIETY P.O. BOX 13070 Amman 11942 JORDAN



الجمعية الكيميائية الأردنية ص.ب:13070 عمان 11942 الأردن

الرقم : JCS 17 التاريخ: 1 / 4 / 2005

No. : JCS 17 Date: 1 / 4 / 2005

Prof. Leiv K. Sydnes
President of IUPAC
University of Bergen
Department of Chemistry
Allegaten 41
N-5007 Bergen,
Norway

Dear Prof. Leiv Sydnes

I am pleased to inform you that Jordan is interested in applying for the International Union of Pure and Applies Chemistry (IUPAC) as National Adhering Organization (NAO), presented by the Jordanian Chemical Society (JCS).

Please find enclosed a copy of the Statutes, Bylaws of the JCS, in which you will find a brief description of the goals of the JCS and its significant activities.

The Jordanian Chemical Society was established in 1976 with 30 members, and the number has increased to reach now to about 300 members.

Looking forward for receiving your positive response

Sincerely yours

Prof.Sultan T. Abu-Orabi

Tafila Technical University/President

Tafila P.O. Box 179 Jordan

Jordanian Chemical Society/President

Arab Union of Chemists/President

Tafila Jordan

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JORDAN CHEMICAL SOCIETY

ARTICLE OF ASSOCIATION

(BYELAW AND THE FINANCIAL SYSTEM)

Amended for the year 1988

FIRST CHAPTER

NAME, HEAD OFFICE & OBJECTIVE

Article (1)

The name of the society based upon this system will be the Jordanian Chemical Society

Article (2)

The Society Registered Office will be in Amman, and it has the right to open branches inside the Kingdom, based upon the existence of the chemicals and according to the decision of the board of directors and putting into considerations, the articles stated in the Third Chapter of this system.

Article (3)

THE SOCIETY OBJECTIVES

- 1- Strengthening the relationship among the Jordanian Chemists themselves and among their Arab Chemist colleagues.
- 2- Strengthening the relationship among the chemists, institutions and the scientific associations.
- 3- Introduce the role of the chemistry in all fields of the community development
- 4- Upgrade the chemists affairs and promote their scientific and practical level and organize the necessary programs.
- 5- Contribute in supporting the scientific research in the different chemical fields
- 6- Contribute in developing the chemical education programs for the different educational levels.
- 7- Propose the scientific and technical consultations in the field of Chemistry Science
- 8- Propagate the Jordanian Chemists activities and performances in the different news media.
- 9- Communicate with the Arab and International Chemistry organizations, institutions and societies in order to attain the above stated objectives.
- 10- Perform any other activities that promote the chemistry and chemists affairs and serve specially the Jordan community and the Arab community in general

The society achieves these objectives through the following methods:

- 1- Calls for an educational and scientific conferences, seminars ,lectures, exhibitions and the scientific visits as well as the training courses.
- 2- Issue the periodical publications and pamphlets related to the chemistry science and it's application which serve the society objectives.
- 3- Cooperate with the local, Arabic and International universities and institutes.
- 4- Cooperate with the local, Arab and international chemistry industry associations.
- 5- Perform activities aimed to teach the chemistry in the different educational stages.
- 6- Perform social and sport activities.

Article (4):

This society has no political, faction, sectarian or tribal activities and it is not ready to receive supports or donations from any factions or political coalition entities.

SECOND CHAPTER

MEMBERSHIP

Article (5)

Operative membership

- A- The pre- requisite for the operative membership applicant is:
 - A-1 Must have a bachelor degree or equivalent in the chemistry or any of it's branches as a minimum from any accredited universities and institutes.
 - A-2 Must enjoy his complete civil rights and did not commit a crime against the honor and dignity.
 - A-3 Must submit an application to affiliate to the society according to the authorized form and must be approved by the board of directors.
- B- Non Jordanian Chemists membership residing in Jordan whom they meet the above mentioned conditions will be accepted after get the approval of the board of directors.
- C- In case of approving the membership, he must pay the affiliation fees and pay the established annual subscription (or part of it), and submit an evidences of his scientific qualifications stipulated in Paragraph (A) of this article.
- D- In case of rejecting the affiliation application, the applicant has the right to get the reasons of refusal from the board of directors.

E- The operative member will be committed upon acceptance with the society article of association and its objectives.

Article (6):

SUBSIDIARY MEMBERSHIP

- 1- The subsidiary membership is a right to whom he got a chemistry qualification less than it is stipulated in article (A-1) from article (5).
- 2- The subsidiary membership is a right to whom he got a bachelor degree or equivalent as a minimum in any of the other branches of science.
- 3- The membership conditions stipulated in (A-2),(A-3),C,D and E from article (5) applies on the subsidiary membership.
- 4- The subsidiary membership has the right participate in all society activities.
- 5- The subsidiary membership has no right for nomination, election or voting on the board of directors decisions.
- 6- The fees for the subsidiary membership fifty percent of the operative membership, while the subscription fees will be equal the ones for the operative membership.
- 7- In case the affiliation application is rejected for the subsidiary membership, the board of director is not committed to give justifications.

Article (7)

HONOR MEMBERSHIP

Honor membership is granted to whom he presented a magnificent services to the society helps in achieving it's objectives with the board of directors uncontestation, in condition that the general assembly approve it in it's first meeting.

Article (8)

LOOSING THE MEMBERSHIP

The member losses his membership in the following cases:

- A- The signed written resignation from the date of it's acceptance by the board of directors.
- B- Delay in paying his subscriptions for one year in condition that he must be notified in writing for the due in subscription one month prior to the expiration of this period.
- C- Dismiss from membership according to the stipulations of article (9).
- D- Death

Article (9)

MEMBERSHIP DISMISSAL

The member who breaches the society regulations and the decisions of the general assembly is dismissed through a decision by the board of directors putting into consideration the stipulations of article (11).

Breeching the society regulations will be in the following cases:

- A- Breeching what is stated in Article (4) of this system.
- B- Insulting the reputation of the society.
- C- Proofing that there is an instigations on raising problems and spread discrimination among the society members.

Article (10)

Membership is resumed to whom he was dismissed based upon article (9) via a decision issued from the general assembly and according to the following:

- A- The membership is resumed to whom he was dismissed based upon item (A) from article (9) by renewing the affiliation fees.
- B- The membership is resumed to whom he was dismissed based upon item (B) from article (9) by paying the affiliation fees and the unpaid from the date of dismissal. Subscription.
- C- The dismissed member has the right to claim in righting from the board of directors to claim to list the subject of his membership on the general assembly agenda and the board of directors must commit to that.
- D- In case the general assembly refuses to resume the membership, so, he has the right to appeal his application in the next general assembly meeting, and the decision of the general assembly in this time is final and irrevocable.

Article (11)

STOPPING THE MEMBERSHIP AND RESUMPTION

- A- The board of directors has the right to stop the membership of whom he breeches the society regulations and rules for any period deems necessary but not to exceed more than one year and after notifying the member in writing for one time.
- B- It is possible to stop the membership of whom he applied in writing for a specific period of time and he will be exempted during it from paying the subscriptions and his request must be justified with reasons approved by the board of directors.

C- The membership is returned back to whom his membership was stopped according to the two items (A), (B) of this article in case that the period of stopping the membership is over and the reasons are finished.

THIRD CHAPTER

OPEN BRANCHES TO THE SOCIETY

Article (12)

- A- It is conditioned to open a branch for the society in any area in the Kingdom that there must be at least twenty chemists qualified for the operative membership.
- B- Must be at least ten chemists in that area whom they spent at least one year in their operative membership
- C- A written application to open a branch for the society is submitted to the board of directors signed by twenty chemists have the operative membership capacity whom they are available in that area intended to open a branch in it.
- D- An election will be made in the concerned area after the approval of the board of directors on the request to elect the chief of the branch committee and elect four chemists to the membership of the seat committee under the supervision of the society board of directors —main offices— and the right of nomination and election will be limited to chemists whom they are residing in that area or work permanently in that area.
- E- The branch committee is composed from the following:
 - 1-Chief of the committee
 - 2- Deputy chief of the committee
 - 3- Secretary general and finance
 - Two members
- F- Election will be conducted via the secret voting and according to the method of election to the main offices board of directors.
- G- The duration period of the branch committee will synchronized with the duration period for the main offices board of directors.
- H- The operative members in the branches will participate in the elections of the main offices board of directors
- I- It is not permitted for any operative member to nominee himself to the main office board of directors and to the membership of a committee of any branch at the same time.

Article (13)

A- the branch will be affiliated to the main offices in all it's activities and the board of directors in the main offices must be notified and got their approval on the activities intended to be

- conducted and the branches must submit a periodical reports about it's activities to the board of directors/main offices.
- B- The main offices of the society will provide morale and financial support (if possible) to the branch programs and activities.
- C- The board of directors /main offices will invite representatives from the branch committees to attend the main office board of directors meetings in the capacity of controller as needed.

Article (14)

The society article of association items are binding to the branches, committees and members and the branches are managed according to the methods of managing the society by the board of directors/main office.

Article (15)

Any branches will be liquidated by the approval of the general assembly landslide majority and based upon a recommendation from the board of directors stating the justifications for that.

FORTH CHAPTER

Associations that represents the Society

Article (16)

A- General Assembly

The general assembly consists from all operative members and the subsidiary members, honor members and president emeritus have the tight in the capacity of controllers.

Article (17)

- A- The general assembly convened it's ordinary meetings one every time in condition that the time of the meeting will be during the month of February from each year in condition that the members must be notified for that one month prior to the meeting date.
- B- The general assembly convened in an extraordinary meeting upon necessary by invitation from the board of directors in condition that the members must be notified at least two weeks prior to the date of the meeting.
- C- Each member of the general assembly members whom his membership was accepted at least before six months has the right to submit an application to the general assembly for an extraordinary meeting if he got the approval of two third of the general assembly members.

Article (18)

- A- The meeting of the general assembly will be considered legally if attended by the majority of members (half +1)
- B- If the quorum of the general assembly meeting was not complete, it will be deferred to another date after two weeks from the date of the first meeting and the second meeting will be considered legally regardless of number of attendees unless the liquidation of the board of directors, so, this case required to have the general assembly landslide majority.

Article (19)

The general assembly has the right to dissolve the board of directors if the general assembly members agreed by the landslide majority in a meeting conducted for this purpose, in condition that the general assembly ask the board of directors to determine a meeting date during one month to elect a new board of directors, and the duration of the elected board of directors until the legal expiration date of the previous board of directors,

B- BOARD OF DIRECTORS

Article (20)

- A- The board of directors consists of seven members elected by the general assembly though the secret voting taking into consideration the text of article (34) and by the attendance of a representative from the concerned official authorities, in condition that these authorities must be notified before two weeks from the date of the meeting.
- B- The duration of the board of directors will be for two years from the date of it's election putting into considerations what is stated in article (19).
- C- In case one or more members of the board of directors **refrained** but do not exceed more than three members, he /they will be replaced with the candidate /candidates whom they got more votes among the candidates whom they did not win in the membership of the board of directors (reserve members), putting into consideration the texts of articles (35) & (36).
- D- In case of equalization of the reserved members votes, the board of directors and by the attendance of these members draw by lot among them to select the placement members and whom delayed to attend the draw by lot after he is being notified will be considered refrained.
- E- The board of directors considered resigned if four or more of it's members submit their resignations.

F- In case of resignation of the board of directors before it's duration period is over, the chief of board of directors will invite to an extraordinary meeting to the general assembly to elect a new board of directors during g a period do not exceed more than one month from the resignation date of the board of directors, and the resigned board of directors will continue it's mission until the date of the extraordinary meeting is convened putting into consideration what is stated in article (19).

FIFTH CHAPTER

NOMINATION AND ELECTION

Article (21)

Each operative member whose membership exceeds at least three months has the right to practice his right to elect the board of directors/or/branch committees in condition that he had paid his subscription fees until the date of the election.

Article (22)

Each operative member whose membership more than one year at least to nominate himself to the membership of the board of directors in condition that he had paid his subscription fees until the date of the election.

Article (23)

It is not permitted to the operative to nominate himself for more than three consecutive periods if he won the membership of the board of director during these consecutive periods.

Article (24)

The board of directors announced about the general assembly meeting date that the election will be conducted in it before one month, and that announcement must be published at least in one local newspaper and forward the invitation letters to the members according to the suitable methods.

Article (25)

Board of directors will announce for the opening of the nomination date to the new board of directors membership one month prior to it's date means with the date of the general assembly.

Article (26)

Nomination date is closed one week prior to the date of the election and the board of directors determine the closing hour on that date.

Article (27)

Nomination request to be submitted in writing from the operative members whom they meet the conditions stipulated in the article of association and handled to the chief of the society or the secretary general or their representatives, and if the nomination request send though the mail, it must be through the registered mail.

Article (28)

If the number of nominees less than the required number to establish the board of directors, the nomination date will continue opened until the starting date of the general assembly meeting.

Article (29)

Nominees' name will be posted on the bulletin board of the society /main offices or the branch as applicable.

Article (30)

Board of directors will form a triplicity auditing committee, includes to members from the board of directors and one non nominated member from the general assembly, it's mission is to check the nominee's requests and their ability and verify it's applicability to this system.

Article (31)

In case any of the nominees requests is refused, the auditing committee will notify him as quickly as possible and he ahs the right to object before the general assembly in it's first meeting and she has the right to confirm the rejection or accepted it by the landslide majority.

Article (32)

Before conducting the election, the general assembly establish an election committee from the non-nominated general assembly members to supervise the progress of the election and sorting the votes and announce the result.

Article (33)

Contestations in the capacity of any nominated member or elections will be in writing before conducting the election, and the general assembly has the right to accept the contestation or refuse it by the landslide majority.

Article (34)

The president of the board of directors will take over by the one who got the highest number of votes during the elections, whereas the elected board of directors will select a vide president, secretary, cashier and the members.

Article (35)

In case of an equalization in number of votes among two nominees or more whom they got the highest or less number of votes, the lection process will be repeated among them in the same meeting to determine the winner, unless one of them draws for the benefit of the other one.

Article (36)

In case the position of the president became vacant for any reason, his deputy will replace him and his decisions will be valid until the date of conducting a first general assembly following that.

Article (37)

In case the position of the president became vacant for any reason, the board of directors will elect one among their members to replace him while the vacant position will be tasked to one of the reserved members according to what is stipulated in the two paragraph D, E from article (20).

SIXTH CHAPTER

BOARD OF DIRECTORS (MISSIONS AND WORK PROCEDURES)

Article (38)

The board of directors binds to conduct it's meetings weekly or as needed to follow up and implement the society activities, in condition that the board of directors must conduct it's meetings as minimum one time every month, and if it is difficult to conduct the board of directors meeting during three months, it the right of each member in the general assembly to call for an extraordinary meeting to the general assembly to discuss this subject and put into considerations the text of paragraph (B) from article (19).

Article (39)

Board of directors members binds to attend the board of directors meetings and whom he got absent of these meetings for more than three consecutive times or six non consecutive times with an accepted justification, he will receive a final warning in writing and if this occurred he will be dismissed from the board of directors membership.

Article (40)

Board of directors will document its minutes of meetings in a special registration and a copy of the minutes of meeting will be posted on the bulletin board for the information of the general assembly.

Article (41)

Board of directors will takes it's decisions by the consent of the majority it's attendees members whom their attendance will complete the legal quorum and the voice of the president will be the casting voice in case of vote equalization.

Article (42)

The board of directors will submit an annual report about the society activities, programs, and works to the general assembly in it's ordinary meeting or any extraordinary meeting on the agenda.

Article (43)

THE MISSION OF THE PRESIDENT

- 1- Supervise on all society activities
- 2- Chairing the board of directors and general assembly sessions and send the invitations to it's meetings.
- 3- Represents the society before the official and international entities and departments as well as before the judicial authorities.
- 4- The president has the right to task any of board of director members in writing to perform any mission related to the activity of the society in condition that must be documented in the board of directors minutes of meeting.

Article (44)

THE MISSIONS OF THE PRESIDENT DEPUTY

- 1- Assist the president in fulfilling his mission
- 2- Take over the responsibilities tasked to him by the president and/or the board of directors and he represents him during his absent.

Article (45)

THE MISSION OF THE SECRETARY GENERAL

- A- Write down the board of directors as well as the general assembly's minutes of meetings and keep the records and supervise it's organization and prepare the agenda for the board of directors sessions.
- B- Dispatch the letters, messages and perform communications based upon the quest of the board of directors.

Article (46)

THE MISSIONS OF THE CASHIER

- 1- Full supervision on all the society financial issues in cooperation with the president
- 2- Sign on all financial documents with the president
- 3- Keep the financial documents and transactions inside the society center.
- 4- Prepare the financial and annual reports.

CHAPTER SEVEN

SOCIETY PRESIDENT EMERITUS

Article (47)

THE PRESIDENT EMERITUS

The board of directors after election will recommend and elect a society president emeritus from the Jordanian VIP's whom their background, positions and interests suits the objectives and ambitions of the society and the president emeritus duration for one year and can be renewed according to the decision of the board of directors.

CHAPTER EIGHT

The Committees

Article (48)

The board of directors has the right to form the necessary committees to practice and follow up the society activities. These committees will be responsible before the board of directors about implementing the works tasked to it and submit it's reports to the board of directors.

Article (49)

Each committee consists from number of general assembly members and one or more member of the board of directors but not to exceed more than five members.

Article (50)

The board of directors issues it's directives and instruction related to the organizations of the committee works and it's activities in condition that this will not contradict with any of the society article of association articles.

FINANCIAL SYSTEM

NINTH CHAPTER

FINANCIAL RESOURCES – DEPOSITS AND CONTROL

Article (51)

The society financial resources consist of the following:

- 1- Fees of Affiliation and subscription of the members
 - 1- Donation and contributions from individuals and associations but do not contradict with the test of article (4)
 - 2- Activities income from the society and it's branches
 - 3- Investments

Article (52)

The society funds will be deposited in any bank inside the Kingdom by the approval of the board of directors and draw it by a signature from the society chief and cashier collectively.

Article (53)

- 1- The member pay upon affiliation to the society an amount of five Jordan dinars.
- 2- The annual subscription fees is six Jordan dinars and it can be paid for a half Jordan dinar monthly.

Article (54)

The society general assembly selects annually a chartered accountant in it's annual meeting and putting the best offers submitted.

TENTH CHAPTER

METHODS AND PROCEDURES OF ISSUE

Article (55)

The society funds is disbursed on the activities, and works stipulated in the society internal system articles.

Article (56)

The board of directors will be incharge of spending the society funds according to the annual budget items presented to the board of directors to be approved by the general assembly in it's ordinary or extraordinary meetings and the general assembly has the right to enter any changes deems necessary on the budget before adaptation.

Article (57)

The board of directors has the right to transfer the allotments in any item of the budgets to another item if it sees that necessary in condition that it will not exceed the transferable allotments more than 20% from the allotments of the items transferred to it.

Article (58)

The cashier has the right to spend an amount of thirty Jordan dinars to finalize the urgent benefits of the society without going back to the board of directors, in condition that he must inform the board of directors in it's first meeting.

Article (59)

The society president and it's cashier will sign collectively on all financial transactions related to the society and put into consideration the test of article (56).

ELEVENTH CHAPTER

THE BRANCH FUNDS

Article (60)

Any funds and assets of any of the branches will be affiliated to the Society /main offices

Article (61)

The Society cashier in the main center will be in charge of the branch financial affairs and the board of directors/in the main offices will issue the special instructions for that.

Article (62)

The cashier in cooperation with the secretary general will be incharge in the branch committee to execute these instructions.

Article (63)

The stipulations of chapter ten and twelfth article swill apply on the branches funds.

TWELFTH CHAPTER

Article (64)

The society is dissolved by the consent of 90% of the general assembly during an extraordinary meeting called to it the general assembly in condition that the approval of the official authority must be obtained.

Article (65)

In case, that the society is dissolved, all it's funds and properties will be transferred to the similar scientific societies in condition it must be transferred for the purpose of scientific research and in case any dispute occurred to distribute the society funds, a committee will be formed consists of the society president and the president deputy and the cashier and four members representing the society general assembly to take the necessary actions.



НАЦІОНАЛЬНА АКАДЕМІЯ НАУК УКРАЇНИ

Відділення хімії НАН України

Kyiv-1, Volodymirska Str., 54 tel. 38(044)234-1944, 239-6450

18 May 2005

Dear Dr. John Jost,

Subject: Application for NAO Status Ukraine

We are sending you the requested document (Statutes is attached) in addition to the application letter from the 7th September, 2004 of Academician B.Paton, the President of the National Academy of Sciences of Ukraine (NAS of Ukraine) with official request on admission the NAS of Ukraine to the IUPAC as National Adhering Organization.

We hope that our cooperation will be successfully developed.

With best regards,

Sincerely yours,

Academician V.Goncharuk

Academician-Secretary of the Chemistry

Division of the National Academy of

Sciences of Ukraine

Dr. John W. Jost, Executive Director of IUPAC IUPAC Secretariat PO Box 13757 Research Triangle Park, NC 27709-3757, USA

REGISTERED

by MINISTRY OF JUSTICE OF UKRAINE 11 June 2002 ORDER No 47/5

COORDINATED

With changes and additions July, 18, 2003

APPROVED

by GENERAL MEETING of NATIONAL ACADEMY OF SCIENCES OF UKRAINE 5 APRIL 2002

Changes and additions were approved by the General meeting May, 15, 2003.

STATUTE

of the National Academy of Sciences of Ukraine

I. General Provisions

- 1. The National Academy Sciences of Ukraine (hereafter referred to as "NAS of Ukraine") is the higher state scientific organization of Ukraine, that was founded on the state property and uses the rights of self-governing. The NAS of Ukraine acts under the current legislation of Ukraine and present Statute.
- 2. The goal of activity of the NAS of Ukraine is obtaining of new knowledge and generalization of the existing ones on nature, man and society; creation of scientific fundamentals of scientific and technical, socio-economic and cultural development of the State; training of highly qualified scientific personnel.
- 3. The NAS of Ukraine organizes and performs fundamental and applied researches on important problems of natural, technical and sociohumanitarian sciences, and also coordinates the performing of fundamental investigations at scientific institutions and organizations of Ukraine irrespective of ownership forms. The Interagency Council on coordination of fundamental research in Ukraine is acting at the NAS of Ukraine.
- 4. The status of the NAS of Ukraine as the State institution is based on all-round support of its activity from the State side, on perpetual and free assignment of State property to it for use (without right on changing of ownership form), on granting lands to it for use in perpetuity according to land-laws of Ukraine, determination in the State budget of Ukraine, as a separate line, funds for ensuring its activity.
 - The NAS of Ukraine by accomplishing the authority on management of objects of property complex of the National Academy of Sciences of Ukraine ensures realization of rights of State as the object's proprietor, which are linked with their effective use and control within limits determined by legislative of Ukraine with aim of satisfaction of state and public needs.
- 5. The NAS of Ukraine annually reports to the Cabinet of Ministers of Ukraine about results of its scientific and scientific-and-technological activities and the use of the means allocated to it from the State budget.
- 6. The governmental management of scientific and scientific-and-technological activity of the NAS of Ukraine is carried out according to the current legislation of Ukraine and it doesn't violate the freedom of scientific work and self-government of the NAS of Ukraine in the solution of questions of activities covered by the present Statute.
- 7. The self-government of the NAS of Ukraine consists in:
 - 1) independent determining of research area, of its structure, solution of scientific organizational, economic, personnel questions, realization of the international scientific contacts;
 - 2) electivity and collective nature of management bodies, realization of the functions of the superior body by General meeting of the NAS of Ukraine.
- 8. The NAS of Ukraine unites the members of the NAS of Ukraine the Full Members (Academicians), the Corresponding Members and the Foreign Members, who are elected by the General meeting of the NAS of Ukraine, and the researchers of the NAS of Ukraine.
- 9. Under the jurisdiction of the NAS of Ukraine there are institutions, organizations, enterprises (hereafter referred to as "institutions", which are considered under the jurisdiction of the NAS of Ukraine) according to the list, which shall be approved by the Cabinet of Ministers of Ukraine on presentation of the NAS of Ukraine.

10. The NAS of Ukraine is a legal entity, it has accounts in institutions of the Treasury of Ukraine, the round seal with the picture of the State Emblem of Ukraine, another seals and stamps needed for carrying out office work.

The NAS of Ukraine is the legal successor of the Academy of Sciences of Ukraine. The President of the NAS of Ukraine represents the NAS of Ukraine as the legal entity.

Legal address of the NAS of Ukraine is 01601, Kyiv-30, 54 Volodymyrska St.,

II. The main objectives of the National Academy of Sciences of Ukraine

- 11. The main objectives of the NAS of Ukraine are:
 - 1) organization, carrying out and coordination of researches on fundamental and applied problems of natural, technical and sociohumanitarian sciences;
 - 2) fulfillment on a world standards level of fundamental and applied researches on priority directions of science and strengthening of impact of their results on innovation development of economics, education and culture in Ukraine;
 - 3) participation in formation of state policy in field of scientific and scientific-and-technical activities;
 - 4) preparation of scientific assessments and prognosis of social and political, socioeconomic and cultural progress of State, its economic position, development of appropriate propositions and recommendations on these matters;
 - 5) assistance in progress and integration of science, education and manufacturing in Ukraine;
 - 6) joining up of scientists of the NAS of Ukraine, institutions of higher education and other scientific institutions into scientific councils, committees, commissions and other advisory-consultative bodies of the NAS of Ukraine;
 - 7) training of highly qualified scientific personnel, intake of gifted youth, reveal and support of talented researchers, encouragement of creative growth of young scientists, ensure the heredity of generations of scientists;
 - 8) assistance in integration of native intellectual potential into world scientific space;
 - 9) protection of rights of members of the NAS of Ukraine and its institutions stuff.
- 12. The NAS of Ukraine for implementation of its objectives:
 - 1) specifies the priority directions of fundamental and applied researches in the field of natural, technical and sociohumanitarian sciences and corresponding basic lines of investigation for scientific institutions of the NAS of Ukraine;
 - 2) establishes the scientific councils, committees, commissions and other advisory-consultative bodies of the NAS of Ukraine on the most important problems in the field of natural, technical and sociohumanitarian sciences;
 - 3) convenes scientific sessions, congresses, conferences, etc.;
 - 4) carries out training of scientific personnel, takes actions on raising the level of scientific stuff's skill, provides conditions for creative and productive work of scientists;
 - 5) carries out publishing activities;

- 6) carries on propaganda of achievements of science and engineering, promotes the scientific knowledge dissemination;
- 7) stores manuscripts of scientists and cultural workers, archival materials of the institutions of the NAS of Ukraine and another materials, which have scientific, cultural and historical value;
- 8) carries out on an unprofitable basis an exchange of printing publications and other types of information with institutions and funds in Ukraine and abroad.
- 9) establishes and awards the honorary titles of the NAS of Ukraine, and also the prizes for the prominent scientific works, the grants for young scientists and students;
- 10) carries out an international scientific and scientific-and-technological cooperation, enters into an agreements with foreign scientific centers, takes part in a work of international scientific organizations, including with the rights of national member;
- 11) determines its structure including creation, reorganization and liquidation the research institutes and other institutions of the NAS of Ukraine;
- 12) realizes the authorities on management of objects of property complex of the NAS of Ukraine, which are provided by the present Statute and current legislation.

III. Structure and Membership of the National Academy of Sciences of Ukraine

- 13. The NAS of Ukraine has in its structure the Presidium of the NAS of Ukraine, the Sections, the Divisions of science branches, the Regional Scientific Centers, and also institutions of the NAS of Ukraine, specified by article 9 of the present Statute.
- 14. Main unit of the structure of the NAS of Ukraine is research institutes and equated to them other scientific institutions (observatories, botanical gardens, reserves, libraries, etc.). Scientific institutions of the NAS of Ukraine are the legal entities. They act under their own Statutes, which are developed in accordance with the present Statute and the "Main principles of organization and activity of a research institute of the NAS of Ukraine", and are subject to approval and registration in the Presidium of the NAS of Ukraine.

The directors of the research institutes and equated to them other scientific institutions are elected on competitive base by the appropriate Divisions and are approved by the Presidium of the NAS of Ukraine according to the order established by the NAS of Ukraine.

Other institutions attributed to the jurisdiction of the NAS of Ukraine act under statutes and regulations, which are subject to approval and registration in the Presidium of the NAS of Ukraine, and also in the order established by the current legislation in institutions of local governing. A procedure of filling the post of director for these institutions is established by the Presidium of the NAS of Ukraine in accordance with the current legislation.

- 15. The Section of the NAS of Ukraine is collective coordinating body of the NAS of Ukraine that unites the appropriate Divisions of Sciences and separate institutions of the NAS of Ukraine for solving of major pantoacademic scientific and scientific-and-technological problems of interdisciplinary character.
- 16. The Division of the NAS of Ukraine unites in accordance with the appropriate fields and directions of the sciences the Members of the NAS of Ukraine, the scientific institutions of the NAS of Ukraine and all scientists of the institutions of the NAS of Ukraine, which are belonging to the Division.

The Division of the NAS of Ukraine is established with aim to specify the priority directions and themes of fundamental and applied researches and to carry out their overall discussion, to prepare expert conclusions on the appropriate branch of a science, to organize researches on these directions and to estimate their results, to coordinate fundamental researches on the appropriate branch of a science.

17. The Sections and the Divisions of the NAS of Ukraine carry out their activities in accordance with appropriate Regulations that shall be approved by the Presidium of the NAS of Ukraine.

The quantity of the Sections and the Divisions and their titles are determined by the General meeting of the NAS of Ukraine.

18. The Regional Scientific Centers of the NAS of Ukraine are established with aim to raise in Ukraine the role of science in the development and realization of the effective regional policy, which is oriented on joining of the State and regional interests.

Creation and liquidation of the Regional Scientific Centers of the NAS of Ukraine are accomplished by the General meeting of the NAS of Ukraine.

The Regional Scientific Centers of the NAS of Ukraine act under Statutes (Regulations), which shall be approved by the Presidium of the NAS of Ukraine.

19. The Membership of the NAS of Ukraine comprises the Full Members, the Corresponding Members and the Foreign Members of the NAS of Ukraine.

The scientists, who have made the large contribution to the development of the appropriate directions of a science, are elected the Full Members of the NAS of Ukraine.

The scientists, who have enriched a science by outstanding achievements, are elected the Corresponding Members of the NAS of Ukraine.

As the Full Members and the Corresponding Members of the NAS of Ukraine, the citizens of Ukraine could be elected.

As the Foreign Members of the NAS of Ukraine are elected the scientists – the citizens of another countries, who's scientific works have been obtained the recognition of international scientific community and which powerfully promoted the development of the international scientific communications of the NAS of Ukraine.

The Members of the NAS of Ukraine are elected for life.

The Members of the NAS of Ukraine are joined into the appropriate Divisions of the NAS of Ukraine.

IV. General meeting of the National Academy of Sciences of Ukraine

- 20. The superior body of the NAS of Ukraine is the General meeting that consists of the Full Members and the Corresponding Members of the NAS of Ukraine. The Foreign Members, the directors of the scientific institutions and representatives of the scientific community could take part in the General meeting with advisory votes.
- 21. The Full Members and the Corresponding Members of the NAS of Ukraine enjoy the right of deciding vote at the General meeting, except the cases when the present Statute stipulated another thing.
- 22. The General meeting of the NAS of Ukraine:

- 1) takes part in formation of public policy in area of scientific and scientific-and-technical activities, specifies the main directions of the scientific work of the NAS of Ukraine;
- 2) solves questions of organization of scientific activity and internal life of the NAS of Ukraine;
- 3) hears the reports of scientific and scientific-organizational character;
- 4) elects the Full Members, the Corresponding Members and the Foreign Members of the NAS of Ukraine according to the order stipulated by the present Statute;
- 5) elects the President, the Vice-Presidents, the Chief Scientific Secretary of the NAS of Ukraine, elects or approves the members of Presidium of the NAS of Ukraine according to the order stipulated by the present Statute;
- 6) considers a question on the budget of the NAS of Ukraine;
- 7) considers and approves reports on activities of the NAS of Ukraine;
- 8) approves the Statute of the NAS of Ukraine, produces changes and additions into it;
- 9) works out other questions that in accordance with Statute are attributed to the competence of the General meeting of the NAS of Ukraine.
- 23. Regularly scheduled sessions of the General meeting of the NAS of Ukraine are convoked not less often than once a year.
 - The extraordinary sessions of the General Meeting are convoked on decision of the Presidium of the NAS of Ukraine or at the written requirement not less than one-third of the total number of the Full Members and the Corresponding Members of the NAS of Ukraine.
- 24. The General meeting of the NAS of Ukraine has the right to approve the decisions if at its session present not less than half of the total number of the Full Members and the Corresponding Members of the NAS of Ukraine, except for cases when the present Statute provides other.
 - The decisions at the General meeting of the NAS of Ukraine are accepted by open voting by the simple majority of votes of the present Full Members and Corresponding Members of the NAS of Ukraine, except for cases when according to the present Statute or to the decision of the General meeting the other order is provided.
 - The Presidium of the NAS of Ukraine has the right with the special decision to exclude from the numerical strength those the Full Members and the Corresponding Members of the NAS of Ukraine, whose state of health or other circumstances not to allow them to take part in the General meeting and in voting.
- 25. The General meeting of the NAS of Ukraine may by secret voting by the simple majority of votes of total number of the Full Members and the Corresponding Members of the NAS of Ukraine to stop before the appointed time powers of the separate members of the Presidium of the NAS of Ukraine or the Presidium as a whole, and to elect the new members or Presidium as a whole in the order determined by the present Statute.

V. Procedure of Election of the Full Members (Academicians), the Corresponding Members and the Foreign Members of the National Academy of Sciences of Ukraine

26. Elections of the Full Members and the Corresponding Members of the NAS of Ukraine shall be carried out not less often than once per three years and are called by the Presidium of the NAS of Ukraine

- 27. The announcement of the Presidium of the NAS of Ukraine of holding of election of the Full Members and the Corresponding Members of the NAS of Ukraine (titles of specialities, quantity of vacancies and their distribution) is published in press not later than three months before holding of election.
 - Revising of the titles of specialities, quantity of vacancies and their distribution between Divisions after publication of the announcement is not allowed.
- 28. The right to propose candidates in the Full Members and the Corresponding Members of the NAS of Ukraine is given to the scientific councils of the scientific institutions and institutions of higher education, to the State and public organizations, to the Full Members and the Corresponding Members of the NAS of Ukraine. The appropriate materials and grounds are sent to the NAS of Ukraine within one month from the date of the publication.
 - The register of nominated and registered candidates in the Full Members and the Corresponding Members of the NAS of Ukraine shall be published in press not later than one month before the date of election holding.
- 29. Elections of the Academicians and the Corresponding Members shall be carried out into two stages at the general meetings of the Divisions, and then at the General meeting of the NAS of Ukraine. The General meeting of the NAS of Ukraine elects the Full Members and the Corresponding Members of the NAS of Ukraine from candidates have been elected by the general meetings of the Divisions within the limits of the announced vacancies.
- 30. Elections and election campaign shall be carried out on democratic basis, in conditions of complete knowledge of a scientific community. The necessary conditions for overall discussion of the candidates shall be ensured at the General meeting of the NAS of Ukraine and at general meetings of the Divisions.
- 31. Elections of candidates in the Full Members of the NAS of Ukraine at general meetings of the Divisions shall be carried out by secret voting of the Full Members of the NAS of Ukraine of the appropriate Division, and candidates in the Corresponding Members of the NAS of Ukraine shall be carried out by secret voting of the Full Members and the Corresponding Members of the NAS of Ukraine of the appropriate Division. The elections shall be considered valid in case of presence at meeting not less 2/3 of the total number correspondingly of the Full Members or of the Full Members and the Corresponding Members of the NAS of Ukraine, which are the members of Division.
- 32. The persons, who have received not less 2/3 of votes of Members of the NAS of Ukraine of appropriate Division, taking part in voting, shall be declared elected as candidates in the Members of the NAS of Ukraine.
- 33. Elections of the Full Members of the NAS of Ukraine shall be carried out by the General meeting of the NAS of Ukraine by secret voting of the Full Members of the NAS of Ukraine, and of the Corresponding Members of the NAS of Ukraine by secret voting of the Full Members and the Corresponding Members of the NAS of Ukraine. The elections shall be considered valid in case of presence at meeting not less 2/3 of the total number correspondingly of the Full Members or of the Full Members and the Corresponding Members of the NAS of Ukraine.
- 34. The persons, who have received not less 2/3 of votes of the Members of the NAS of Ukraine, taking part in voting, shall be declared elected as the Full Members and the Corresponding Members of the NAS of Ukraine.
 - Election results are published in press.

35. Candidates in the Foreign Members of the NAS of Ukraine shall be proposed by general meetings of the Divisions on vacancies opened by the Presidium, and shall be elected by the General meeting of the NAS of Ukraine. The Full Members and the Corresponding Members of the NAS of Ukraine take part in elections of the Foreign Members of the NAS of Ukraine. The elections shall be considered valid in case of presence at meeting not less 2/3 of the total number of the Full Members and the Corresponding Members of the NAS of Ukraine. The persons, who have received not less 2/3 of votes of the Members of the NAS of Ukraine, taking part in voting, shall be declared elected.

Under the decision, correspondingly of general meetings of the Division and the General meeting of the NAS of Ukraine at nomination of candidates and at elections in the Foreign Members the open voting could be used.

VI. The duties and rights of the Full Members (Academicians), the Corresponding Members of the National Academy of Sciences of Ukraine

36. The principal duty of the Full Members and the Corresponding Members of the NAS of Ukraine consists in enrichment of science with new achievements and discoveries by carrying out personally the research studies, in organization of collective development of problems and of scientific head of works.

The Members of the NAS of Ukraine should take an active part in fulfillment of tasks entrusted to the NAS of Ukraine.

The Members of the NAS of Ukraine actively assist in applying of the science achievements to production and in their use in socio-economic and cultural development, carry out work aiming on scientific staff training and on raising the level of scientific personnel's skill. They should execute orders of the Presidium of the NAS of Ukraine and the appropriate Division.

37. Each Full Member and the Corresponding Member of the NAS of Ukraine is a member of one of Divisions of the NAS of Ukraine correspondingly to his speciality.

Transfer from one Division to another occurs at own member's wish and on decisions of general meetings of the both Divisions of the NAS of Ukraine.

The Full Members and the Corresponding Members of the NAS of Ukraine, who belong to some Division could on the agreement of general meeting of another Division take part in its work with right of the advisory vote.

- 38. Every year the Member of the NAS of Ukraine submits report on his activity to an appropriate Division of the NAS of Ukraine.
- 39. The Members of the NAS of Ukraine have preferential rights on providing them with conditions for carry out researches at institutions of the NAS of Ukraine.
- 40. The Full Members and the Corresponding Members of the NAS of Ukraine after coming of age 65 years may at their own wish and on decision of the Presidium of the NAS of Ukraine be appointed counselors of a board of directors of the appropriate scientific institution of the NAS of Ukraine.

VII. The Presidium of the National Academy of Sciences of Ukraine

41. The Presidium of the NAS of Ukraine carries out the management of work of NAS in the period between sessions of the General meeting.

The Presidium is elected by the General meeting of the NAS of Ukraine for a term of five years and consisting of the President, the Vice-Presidents, the Chief Scientific Secretary, the Academicians - Secretaries of Divisions, the Chairmen of Regional Scientific Centers, and also of other Members of Presidium in amount, which is determined by the General meeting of the NAS of Ukraine.

42. The President, the Vice-Presidents and the Chief Scientific Secretary shall be elected by the General meeting of the NAS of Ukraine from among the Full Members of the NAS of Ukraine by secret voting by the simple majority of votes.

The Vice-Presidents and the Chief Scientific Secretary shall be elected at the suggestion of the President of the NAS of Ukraine.

The Academicians - Secretaries of the Divisions shall be elected by the general meetings of the Divisions of the NAS of Ukraine from among the Full Members of the NAS of Ukraine and approved by the General meeting of the NAS of Ukraine by secret voting by the simple majority of votes.

Other members of the Presidium of the NAS of Ukraine shall be elected by the General meeting of the NAS of Ukraine from among the Full Members of the NAS of Ukraine by secret voting by the simple majority of votes.

The Presidium of the NAS of Ukraine could have the councilors with the right of an advisory vote.

- 43. The President of the NAS of Ukraine organizes the work of the NAS of Ukraine, he is the head of the Presidium and the Bureau of the Presidium of the NAS of Ukraine, leads the working and solution of manpower policy problems, realizes the contacts of the NAS of Ukraine with the government bodies, represents the NAS of Ukraine in the government bodies, state institutions, public and others organizations.
- 44. Distribution of duties between the members of the Presidium of the NAS of Ukraine is established by the Presidium of the NAS of Ukraine
- 45. The Presidium of the NAS of Ukraine in accordance with established procedure:
 - 1) convokes sessions of the General meetings of the NAS of Ukraine;
 - 2) approves the quantity and list of vacancies of the Full Members, the Corresponding Members and the Foreign Members of the NAS of Ukraine and nominates elections of the Members of the NAS of Ukraine;
 - 3) represents for discussion and approval of the General meeting of the NAS of Ukraine of the programs, forecasts and reports on activities of the NAS of Ukraine and its institutions;
 - 4) prepares for consideration by the General meeting of the NAS of Ukraine a question of the budget of the NAS of Ukraine and its implementation;
 - 5) organizes the coordination of scientific investigations in the field of natural, technical and sociohumanitarian sciences;
 - 6) establishes the scientific councils, committees, commissions and other deliberative-consultative bodies of the NAS of Ukraine on the most important problems in the field of natural, technical and sociohumanitarian sciences, hears the reports on their activities;
 - 7) promotes use of results of research works in the national economy, culture, in social sphere;
 - 8) organizes scientific contacts with branch academies of sciences and other scientific institutions in the country and abroad, establishes the international scientific and scientific technical communications, concludes the appropriate agreements and contracts;

- 9) approves Regulations for the Section of the NAS of Ukraine, the Division of the NAS of Ukraine and the "Main principles of organization and activity of a research institute of the NAS of Ukraine";
- 10) creates, reorganizes and liquidates the institutions of the NAS of Ukraine", approves the priority directions of their scientific activities, determines their tasks and belonging to the structure of the NAS of Ukraine;
- 11) organizes an execution of governmental attestation of scientific institutions of the NAS of Ukraine and complex inspections of their activities;
- 12) approves the decisions of the general meetings of the Divisions of the NAS of Ukraine on election of directors of scientific institutions of the NAS of Ukraine;
- 13) maintains records of objects of property complex of the NAS of Ukraine, carries out their administration and control of efficiency of their use and safety, in particular:
 - assigns property of the NAS of Ukraine to institutions, which are under its jurisdiction;
 - determines in accordance with current legislation of Ukraine and Statute's tasks of the NAS of Ukraine the limits of property management, including ones from the side of institutions on which balance it is taken into account;
 - carries out property redistribution between institutions of the NAS of Ukraine;
 - authorizes the transmission of rights of user on property, on objects of intellectual property etc. as contributions at establishment and operation of subjects of entrepreneurial activity and another organizations, stands as a founder of enterprises with mixed ownership form;
 - stands as a lessor of integrated property complexes and immovables, that have been transferred to the NAS of Ukraine in perpetual use by the State;
 - authorizes the institutions, which are under the jurisdiction of the NAS of Ukraine, for the conclusion of contracts of rent of property, including immovable which is taken into account on balances of their organizations;
 - authorizes for write-off of property which is on balances of institutions of the NAS of Ukraine;
 - makes a decision on accommodation of institutions of the NAS of Ukraine in administrative houses and uninhabited premises of the organizations, which are under the jurisdiction of the NAS of Ukraine, and determines the size of payment for using these houses and premises.
- 14) makes suggestions as for the transfer of objects of property complex of the NAS of Ukraine to management sphere of other bodies, authorized to operate the state property, in the municipal property, and also concerning the transfer of objects of the municipal property to a State ownership, and their attribution to property complex of the NAS of Ukraine:
- 15) carries out other authorities concerning management of objects of the property complex of the NAS of Ukraine, stipulated by the current legislation;
- 16) determines according to the legislation the order of use of objects of the intellectual property which are created in institutions of the NAS of Ukraine;

- 17) approves and registers statutes (regulations) of institutions of the NAS of Ukraine, carries out the control over their observance and makes of the decisions in case of infringement of requirements of statutes (regulations);
- 18) concludes and breaks off contracts with heads of corresponding institutions and contracts assignments with the authorized persons;
- 19) secures in institutions of the NAS of Ukraine preservation of the State secret;
- 20) establishes and awards honorary titles of the NAS of Ukraine, the premium after the name of known scientists of Ukraine, the grant and the premium to the young scientists and students of higher educational institutions of Ukraine for the best scientific works and other awards of the NAS of Ukraine;
- 21) organizes publishing activities of the NAS of Ukraine;
- 22) solves the primary tasks of social development.
- 46. The Presidium of the NAS of Ukraine makes a decision on distribution of budgetary funds, which main manager is the NAS of Ukraine, allocates base budgetary financing between the Sections, the Divisions and institutions of the NAS of Ukraine, supervises correctness of use of means in institutions of the NAS of Ukraine.
- 47. The Presidium of the NAS of Ukraine carries out the control over observance of the Statute of the NAS of Ukraine.
- 48. The Bureau of Presidium of the NAS of Ukraine composed of the President, the Vice-Presidents and the Chief Scientific Secretary of the NAS of Ukraine is created for consideration and the operative solution of separate questions of activity of the NAS of Ukraine.
 - The competence of the Bureau of Presidium of the NAS of Ukraine as body of management is determined by the Presidium of the NAS of Ukraine.
- 49. The Presidium of the NAS of Ukraine has the permanent apparatus, which provides realization of decisions of the Presidium of the NAS of Ukraine.
 - The apparatus of the Presidium of the NAS of Ukraine operates on the basis of the regulations authorized by the Presidium of the NAS of Ukraine. The general management of activity of the apparatus of the Presidium of the NAS of Ukraine is carried out by the Chief Scientific Secretary of the NAS of Ukraine, and on separate questions the members of the Presidium of the NAS of Ukraine according to distribution of duties.

VIII. The financial and economic basis of activity of the National Academy of Sciences of Ukraine

- 50. The economic basis of activity of the NAS of Ukraine is formed by key assets, circulating assets and fictitious assets, including:
 - 1) charges from the basic fund of the State budget of Ukraine which are directed on maintenance of authorized activity of the NAS of Ukraine and are determined annually in the State budget of Ukraine by separate line;
 - 2) the State property, which without payment has been transferred (and it is transferred) by the State for perpetual using for maintenance of authorized activity of the NAS of Ukraine and is on balance of its institutions;
 - 3) the means received from use of objects of property complex of the NAS of Ukraine;

4) the property and means that the NAS of Ukraine and its institutions receive as a result of scientific and technical, information and foreign trade activities, charitable payments and donations of physical and legal persons (including from abroad), gifts and on other bases which have been not forbidden by the current legislation of Ukraine.

The property (property rights or property obligations) given to the NAS of Ukraine or to its institutions in the form of charitable payments, gifts, donations or under the will, is used on conditions which are determined by the corresponding act (agreement) and the legislation of Ukraine.

- 51. The subject of law to dispose of objects of a property complex of institutions that are under jurisdiction of the NAS of Ukraine, is the Presidium of the NAS of Ukraine.
 - The order of possession, using and disposal of the property and means of the NAS of Ukraine shall be approved by the Presidium of the NAS of Ukraine.
- 52. The funds of basic researches, of scientific and technical and social development, of currency receipts, of innovative, of charitable, of insurance and funds of other assignment may be created in the NAS of Ukraine on presentation of institutions of the NAS of Ukraine and to the decision of the General meeting of the NAS of Ukraine.
 - The order of their creation and use shall be determined by separate regulations about these funds and other statutory acts of the NAS of Ukraine.
- 53. Institutions of the NAS of Ukraine have the right according with the current legislation of Ukraine to realize at the internal and external markets devices, the equipment, materials and other high technology production, rights on objects of the intellectual property and other property rights; to carry out foreign-economic relations; to make scientific and scientific-and-technical expert examination; to render scientific-and-technical services, to carry out advertising actions, to act as participants and founders of subjects of enterprise activity in accordance with established in the NAS of Ukraine order.

IX. The order of acceptance and making changes and additions to the Statute of the National Academy of Sciences of Ukraine

54. The Statute of the NAS of Ukraine, changes and additions to it shall be approved by the decision of the General meeting of the NAS of Ukraine accepted by not less 2/3 votes of the total number of the Full Members and the Corresponding Members of the NAS of Ukraine, with preliminary discussion by institutions of the NAS of Ukraine and scientific community, and shall be registered by the Ministry of Justice of Ukraine.

Item 17: Proposals Formally Received from National Adhering Organizations

No proposals were received from National Adhering Organizations.

Item 18.1: New Division Rules

The former Secretary General, Dr. Becker, initiated a program to revise the then existing Division rules to bring them into conformance with the Statutes and Bylaws of the Union and the current structure of the Divisions. Council at Ottawa approved new rules for Divisions IV and V.

Council is asked to approve the new Division Rules for Division I, II, III, and VIII as shown on the following pages.

8 April 2005

Physical & Biophysical Chemistry Division

DIVISION RULES

- 1. The mission of the Physical & Biophysical Chemistry Division is to promote pure and applied physical and biophysical chemistry. Terms of Reference are attached.
- 2. Under the Statutes, Bylaws, and policies of the Union, the Division is managed by its Division Committee. S10 and B4.1 and their subsections are particularly relevant. The Division Committee is responsible for initiating and managing scientific projects, symposia and other activities within its area of responsibility and for cooperating with other Divisions and Standing Committees in initiating and managing interdisciplinary projects, symposia and other activities.
- 3. In accord with B4.103, the composition of the Division Committee is as follows:
 - (a) No more than 10 Titular Members (including all Officers as defined below)
 - (b) No more than six Associate Members
 - (c) No more than six National Representatives
- 4. (a) Titular Members of the Division Committee are nominated and elected for a term of four years by the electorate defined in B4.103 and Bureau decisions pursuant to B4.103. Candidates for titular membership are nominated by the Nominating Committee described below.
 - (b) Associate Members may be elected by the Division Committee for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.
 - (c) National Representatives may be elected by the Division Committee on nomination by National Adhering Organizations for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.
 - (d) Interim appointments to fill vacancies on the Division Committee occurring between meetings may be made by the Division President, after consultation with the other Division Officers, for a term ending at the end of the year in which the next General Assembly is held. Interim appointments are subject to approval by the Bureau or Executive Committee.
- 5. Candidates for Titular Member of the Division Committee are named by a Nominating Committee, prescribed by IUPAC policy and procedures defined by the Bureau, as follows:
 - (a) The nominating committee consists of five members [subject to an exception by the Bureau], with no more than two members from the existing Division Committee and the other three chosen from outside IUPAC on the basis of the breadth of their expertise. The Division President will not be a member of the Nominating Committee.
 - (b) The Nominating Committee is appointed by the Division President with the concurrence of the IUPAC Executive Committee.

- (c) Categories of vacancies may be established by the Division Committee if desired to
 ensure diversity in subject matter, geographic distribution, or other characteristics.
 More than one nominee for each vacancy is desirable but not required.
- 6. Elections shall be conducted by e-mail under procedures defined by the IUPAC Secretariat.
- 7. The Officers of the Division are as follows:
 - (a) The President is the administrative head of the Division, presides at meetings of the Division Committee, and is an *ex officio* a member of all bodies of the Division. The President serves as a member of the Bureau and is the principal representative of the Division within and outside the Union.
 - (b) The Vice President (President-elect) acts for the President in his absence and assists the President as requested. The Vice President shall assume the office of Division President in the event of the President being unable to perform the functions of that office, without prejudice to the forthcoming period of office as President, subject to the terms of B4.103.
 - (c) The Secretary assists the President in carrying out the business of the Division and maintains the records of the Division.
 - (d) The immediate Past President assists the President as requested.
- 8. With the advice of the President of the Union, Officers of the Division are elected by the Division Committee, subject to final approval by the Council. The Officers together form an Executive Committee to act for the Division Committee between meetings. Subject to limitations in B4.103, the terms of office are as follows:
 - (a) The President, President-elect and Past President each serve a term of two [four] years, not subject to reelection, unless approved by the Bureau, and providing the term of office does not exceed four years.
 - (b) The Secretary serves a term of four years and is eligible for reelection to a second term of four years.
- 9. (a) The Division Committee may establish and the Division President may appoint subsidiary bodies, such as subcommittees, working parties and advisory groups, which will all have the status of Division subcommittees, as described in S10.6. The terms of reference or charge to each group, as well as its lifetime, shall be established by the Division Committee. Task groups will be formed to carry out specific projects under general IUPAC policies for the conduct of projects.
 - (b) The Division Committee may propose to the Bureau the establishment of Commissions, with terms of reference and lifetimes, under the provisions of B4.301.
 - (c) The Division Committee and Division President will exercise responsibility and oversight over all bodies created under parts (a) and (b).
- 10. These Rules may be amended by the Division Committee, subject to approval by the Council.

Terms of Reference

The Objectives of the Physical and Biophysical Chemistry Division are

- (i) to organize and promote the international collaboration between scientists in physical chemistry and related fields in order to address problems and formulate recommendations on nomenclature, symbols, units, terminology and conventions in physical and biophysical chemistry, disseminate the recommendations, encourage their translation as well as monitor their acceptance by the chemical community;
- (ii) to establish and stimulate the use of methodologies, standards and reference materials in physical and biophysical chemistry;
- (iii) to encourage the compilation and documentation of critically evaluated physical chemical data;
- (iv) to recognize new developments in physical and biophysical chemistry and its fields of applications; and
- (v) to promote future oriented activities important for the contribution of physical and biophysical chemistry to science and technology and to the needs of the world community.

Inorganic Chemistry Division (II)

DIVISION RULES

- 1. The Inorganic Chemistry Division's responsibilities are to promote, advance, and manage IUPAC activities in the broad field of Inorganic Chemistry, pure and applied. The work covers areas from elements and their properties, through molecules and compounds, to complex solid-state materials.
- 2. The Division is managed by its Division Committee under the Statutes, Bylaws, and policies of the Union; *cf.* S10 and B4.1 and their subsections. The Division Committee initiates and manages scientific projects, conferences, and other activities in Inorganic Chemistry and cooperates with other Divisions and Standing Committees in interdisciplinary programs.
- 3. In accord with B4.103, the composition of the Division Committee is as follows:
 - (a) No more than 10 Titular Members (including all Officers as defined below)
 - (b) No more than six Associate Members
 - (c) No more than six National Representatives
- 4. (a) Titular Members of the Division Committee are nominated and elected for a term of four years by an electorate defined by Bureau decisions pursuant to B4.103. Candidates for titular membership are nominated by the Nominating Committee described below.
 - (b) Associate Members may be elected by the Division Committee for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.
 - (c) National Representatives may be elected by the Division Committee on nomination by National Adhering Organizations for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.
 - (d) Interim appointments to fill vacancies on the Division Committee occurring between meetings may be made by the Division President, after consultation with the other Division Officers, for a term ending at the end of the year in which the next General Assembly is held. Interim appointments are subject to approval by the Bureau or Executive Committee.
- 5. Candidates for Titular Member of the Division Committee are named by a Nominating Committee, prescribed by IUPAC policy and procedures defined by the Bureau, as follows:
 - (a) The nominating committee consists of five members (subject to an exception by the Bureau), with no more than two members from the existing Division Committee and the other three members chosen from outside IUPAC on the basis of the breadth of their expertise. The Division President will not be a member of the Nominating Committee.

- (b) The Nominating Committee is appointed by the Division President with the concurrence of the IUPAC Executive Committee.
- (c) Categories of vacancies may be established by the Division Committee if desired to ensure diversity in subject-matter expertise, geographic distribution, or other characteristics. More than one nominee for each vacancy is desirable but not required.
- 6. Elections are conducted by electronic mail following procedures defined by the IUPAC Secretariat.
- 7. The Officers of the Division are as follows:
 - (a) The President is the administrative head of the Division, chairs meetings of the Division Committee, and is an *ex officio* member of all bodies of the Division. The President serves as a member of the Bureau and is the principal representative of the Division within and outside the Union.
 - (b) The Vice President (President-elect) acts for the President in his absence and assists the President as requested. The Vice President shall assume the office of Division President in the event of the President being unable to perform the functions of that office, without prejudice to the forthcoming period of office as President, subject to the terms of B4.103.
 - (c) The Secretary assists the President in carrying out the business of the Division and maintains the records of the Division.
 - (d) The immediate Past President assists the President as requested.
- 8. As specified in B4.104, Officers of the Division are elected by the Division Committee from among its existing and (subject to confirmation) new Titular Members, subject to final approval by the Council. The Officers together form an Executive Committee to act for the Division Committee between meetings. Subject to limitations in B4.103, the terms of office are as follows:
 - (a) The President, and Vice-President each serve a term of four years, not subject to reelection.
 - (b) The Past President serves a term of two years not subject to reelection.
 - (c) The Secretary serves a term of four years and is eligible for reelection to a second term of four years.
- 9. (a) The Division Committee may establish and the Division President may appoint subsidiary bodies, such as subcommittees, working parties and advisory groups, which all may have the status of Division subcommittees as described in S10.6. The terms of reference or charge to each group, as well as its lifetime, shall be established by the Division Committee. Task groups will be formed to carry out specific projects under general IUPAC policies for the conduct of projects.
 - (b) The Division Committee may recommend to the Council through the Bureau the creation of Commissions to study topics of international scientific or technical significance requiring

- agreement, standardization, or codification, under the provisions of B4.301. The creation, continuation, membership, and activities of Commissions of the Division are governed by the subsections of B4.3.
- (c) The Division Committee and Division President exercise responsibility and oversight over all bodies created under parts (a) and (b).
- 10. These Rules may be amended by the Division Committee, subject to approval by the Council.

Division III: Organic and Biomolecular Chemistry

DIVISION RULES

- 1. The mission of the Division is to promote pure and applied organic and biomolecular chemistry. Terms of Reference are attached.
- 2. Under the Statutes, Bylaws, and policies of the Union, the Division is managed by its Division Committee. S10 and B4.1 and their subsections are particularly relevant. The Division Committee is responsible for initiating and managing scientific projects, symposia and other activities within its area of responsibility and for cooperating with other Divisions and Standing Committees in initiating and managing interdisciplinary projects, symposia and other activities.
- 3. In accord with B4.103, the composition of the Division Committee is as follows:
 - (a) No more than 10 Titular Members (including all Officers as defined below)
 - (b) No more than six Associate Members
 - (c) No more than six National Representatives
- 4. (a) Titular Members of the Division Committee are nominated and elected for a term of two years by the electorate defined in B4.103 and Bureau decisions pursuant to B4.103. Candidates for titular membership are nominated by the Nominating Committee described below.
 - (b) Associate Members may be elected by the Division Committee for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.
 - (c) National Representatives may be elected by the Division Committee on nomination by National Adhering Organizations for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.
 - (d) Interim appointments to fill vacancies on the Division Committee occurring between meetings may be made by the Division President, after consultation with the other Division Officers, for a term ending at the end of the year in which the next General Assembly is held. Interim appointments are subject to approval by the Bureau or Executive Committee.
- 5. Candidates for Titular Member of the Division Committee are named by a Nominating Committee, prescribed by IUPAC policy and procedures defined by the Bureau, as follows:
 - (a) The nominating committee consists of five members [subject to an exception by the Bureau], with no more than two members from the existing Division Committee and the other three chosen from outside IUPAC on the basis of the breadth of their expertise. The Division President will not be a member of the Nominating Committee.
 - (b) The Nominating Committee is appointed by the Division President with the concurrence of the IUPAC Executive Committee.
 - (c) Categories of vacancies may be established by the Division Committee if desired to ensure diversity in subject matter, geographic distribution, or other characteristics. More than one nominee for each vacancy is desirable but not required.
- 6. Elections shall be conducted by e-mail under procedures defined by the IUPAC Secretariat.
- 7. The Officers of the Division are as follows:

- (a) The President is the administrative head of the Division, presides at meetings of the Division Committee, and is an *ex officio* a member of all bodies of the Division. The President serves as a member of the Bureau and is the principal representative of the Division within and outside the Union.
- (b) The Vice President (President-elect) acts for the President in his/her absence and assists the President as requested. The Vice President shall assume the office of Division President in the event of the President being unable to perform the functions of that office, without prejudice to the forthcoming period of office as President, subject to the terms of B4.103.
- (c) The Secretary assists the President in carrying out the business of the Division and maintains the records of the Division.
- (d) The immediate Past President assists the President as requested.
- 8. With the advice of the President of the Union, Officers of the Division are elected by the Division Committee, subject to final approval by the Council. The Officers together form an Executive Committee to act for the Division Committee between meetings. Subject to limitations in B4.103, the terms of office are as follows:
 - (a) The President, President-elect and Past President each serve a term of two years, not subject to reelection.
 - (b) The Secretary serves a term of two years and is eligible for reelection to two further terms of two years.
- 9. (a) The Division Committee may establish and the Division President may appoint subsidiary bodies, such as subcommittees, working parties and advisory groups, which will all have the status of Division subcommittees, as described in S10.6. The terms of reference or charge to each group, as well as its lifetime, shall be established by the Division Committee. Task groups will be formed to carry out specific projects under general IUPAC policies for the conduct of projects.
 - (b) The Division Committee may propose to the Bureau the establishment of Commissions, with terms of reference and lifetimes, under the provisions of B4.301.
 - (c) The Division Committee and Division President will exercise responsibility and oversight over all bodies created under parts (a) and (b).
- 10. These Rules may be amended by the Division Committee, subject to approval by the Council.

Terms of reference

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

Chemical Nomenclature and Structure Representation Division

DIVISION RULES

- 1. The mission of the Chemical Nomenclature and Structure Representation Division is to maintain and develop standard systems for designating chemical structures, including both conventional nomenclature and computer-based systems. Terms of Reference are attached.
- 2. Under the Statutes, Bylaws, and policies of the Union, the Division is managed by its Division Committee. S10 and B4.1 and their subsections are particularly relevant. The Division Committee is responsible for initiating and managing scientific projects, symposia and other activities within its area of responsibility and for cooperating with other Divisions and Standing Committees in initiating and managing interdisciplinary projects, symposia and other activities.
- 3. In accord with B4.103, the composition of the Division Committee is as follows:
 - (a) No more than 10 Titular Members (including all Officers as defined below)
 - (b) No more than six Associate Members
 - (c) No more than ten National Representatives
- 4. (a) Titular Members of the Division Committee are nominated and elected for a term of four years by the electorate defined in B4.103 and Bureau decisions pursuant to B4.103. Candidates for titular membership are nominated by the Nominating Committee described below.
 - (b) Associate Members may be elected by the Division Committee for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.
 - (c) National Representatives may be elected by the Division Committee on nomination by National Adhering Organizations for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.
 - (d) Interim appointments to fill vacancies on the Division Committee occurring between meetings may be made by the Division President, after consultation with the other Division Officers, for a term ending at the end of the year in which the next General Assembly is held. Interim appointments are subject to approval by the Bureau or Executive Committee.
- 5. Candidates for Titular Member of the Division Committee are named by a Nominating Committee, prescribed by IUPAC policy and procedures defined by the Bureau, as follows:
 - (a) The nominating committee consists of five members [subject to an exception by the Bureau], with no more than two members from the existing Division Committee and the other three chosen from outside IUPAC on the basis of the breadth of their expertise. The Division President will not be a member of the Nominating Committee.

- (b) The Nominating Committee is appointed by the Division President with the concurrence of the IUPAC Executive Committee.
- (c) Categories of vacancies may be established by the Division Committee if desired to ensure diversity in subject matter, geographic distribution, or other characteristics. More than one nominee for each vacancy is desirable but not required.
- 6. Elections shall be conducted by e-mail under procedures defined by the IUPAC Secretariat.
- 7. The Officers of the Division are as follows:
 - (a) The President is the administrative head of the Division, presides at meetings of the Division Committee, and is an *ex officio* a member of all bodies of the Division. The President serves as a member of the Bureau and is the principal representative of the Division within and outside the Union.
 - (b) The Vice President (President-elect) acts for the President in his absence and assists the President as requested. The Vice President shall assume the office of Division President in the event of the President being unable to perform the functions of that office, without prejudice to the forthcoming period of office as President, subject to the terms of B4.103.
 - (c) The Secretary assists the President in carrying out the business of the Division and maintains the records of the Division.
 - (d) The immediate Past President assists the President as requested.
- 8. With the advice of the President of the Union, Officers of the Division are elected by the Division Committee, subject to final approval by the Council. The Officers together form an Executive Committee to act for the Division Committee between meetings. Subject to limitations in Bylaw 4.103, the terms of office are as follows:
 - (a) The President and President-elect each serve a term of four years, not subject to reelection; the Past President serves a term of two years, subject to the restriction on total years of service in Bylaw 4.103.
 - (b) The Secretary serves a term of four years and is eligible for reelection to a second term of four years.
- 9. (a) The Division Committee may establish and the Division President may appoint subsidiary bodies, such as subcommittees, working parties and advisory groups, which will all have the status of Division subcommittees, as described in S10.6. The terms of reference or charge to each group, as well as its lifetime, shall be established by the Division Committee. Task groups will be formed to carry out specific projects under general IUPAC policies for the conduct of projects.
 - (b) The Division Committee may propose to the Bureau the establishment of Commissions,

with terms of reference and lifetimes, under the provisions of B4.301.

- (c) The Division Committee and Division President will exercise responsibility and oversight over all bodies created under parts (a) and (b).
- 10. These Rules may be amended by the Division Committee, subject to approval by the Council.

Terms of Reference

The Division is responsible for maintaining and developing standard systems for designating chemical structures, including both conventional nomenclature and computer-based systems. This responsibility is to be fulfilled by:

- 1. Identifying the needs of the user community.
- 2. Generating projects arising from those needs.
- 3. Identifying project leaders and task groups to carry out the work.
- 4. Administering approved projects financially, monitoring their progress, and approving resulting recommendations for review by established IUPAC procedures.
- 5. Identifying new sources of expertise and enabling their involvement in projects.
- 6. As far as possible, ensuring that nomenclature systems projects and the resulting recommendations are compatible with each other, with established IUPAC recommendations, and with computer-based systems for manipulating chemical names and structures.

Item 18.2: Standing Order and Membership of Editorial Advisory Board of *PAC*

Council is asked to approve the Standing Order and Membership of Editorial Advisory Board of *PAC* as shown below.

Pure and Applied Chemistry Editorial Advisory Board

Composition and Terms of Office

- There shall be an Editorial Advisory Board (EAB) for the IUPAC journal *Pure and Applied Chemistry (PAC)*, comprising the Secretary-General (*ex officio*), the President of each Division or his/her nominated representative (*ex officio*), the Chair of the Committee for Printed and Electronic Publications or his/her nominated representative (*ex officio*), the Chair of the Interdivisional Committee for Terminology, Nomenclature and Symbols or his/her nominated representative (*ex officio*), the Scientific Editor (*ex officio*), and up to six invited members.
- The *ex officio* members shall serve for the duration of their IUPAC appointments, subject to confirmation at each General Assembly. Invited members shall be nominated by the President and appointed in consultation with the Executive Committee. Their period of service shall be four years, renewable for a further term of four years.
- The Secretary-General shall Chair any meetings of EAB members, and the Secretariat shall maintain records of such meetings.

Terms of Reference

- The EAB shall monitor scientific and editorial standards of *PAC*, and advise and assist on all aspects of planning, implementation, and evaluation of publication policy and practice.
- The EAB shall respond to requests for critical evaluation of *PAC* activities and initiatives.
- The *ex officio* members of the EAB shall be responsible for reporting back to their respective IUPAC constituencies on relevant *PAC* matters.

Item 20: Plans for 44th General Assembly and 41st Congress (Torino, 2007)

The 44th General Assembly and 41st Congress will be held on 5-11 August 2007 at Torino, Italy. The Theme of all IUPAC Congresses is "Frontiers in Chemistry". This title was chosen not only as a reminder that the subject of an IUPAC Congress is new science at the unexplored frontier of chemistry, but also of the importance of the interaction of chemistry with other disciplines at the frontiers between sciences.

The sub-theme selected for Torino is *Chemistry Protecting Health, Natural Environment and Cultural Heritage*. Therefore, at the Torino Congress we can expect to learn of advances in subjects that are of great interest now, such as nanotechnology, Green or Sustainable Chemistry, Proteomics, the mechanisms of gene expression, progress in drugs for disease treatment, new materials, advances in the use of chemistry for cultural heritage protection and preservation, as well as, topics that are not even thought about now, but will have developed in the intervening two years.

Item 21: Approval of Dates and Sites of 45th General Assembly and 42nd Congress (2009)

The Royal Society of Chemistry has proposed that the 45th General Assembly and 42nd Congress (2009) be held at Glasgow, Scotland. Full details will be presented at Council. Council is asked to approve, or not, the proposal from the Royal Society of Chemistry.

Item 22: Official Language of IUPAC (Statute 5.405)

Statute 5.405 requires Council "to determine every four years, beginning in 1963, the one language in which the official records of the meetings of the Council, Bureau, and Executive Committee shall be kept and published;"

The Bureau proposes that the official language of IUPAC continue to be English.

Item 23: Reauthorization of Commissions.

Bylaw 4.302 states: "At each General Assembly, the Council shall, in the light of the Division or Section President's report and on the recommendation of the Bureau, decide whether or not to continue each Commission." Council is asked to approve the continuation of Commission I.1: Commission on Physicochemical Symbols, Terminology, and Units and Commission II.1: Commission on Isotopic Abundance and Atomic Weights.