

IUPAC

INORGANIC CHEMISTRY DIVISION REPORT

2002-2003 BIENNIUM

I. Highlights and Executive Summary

In this section we focus on issues affecting the present and future productivity of the Division and on the Division's scientific and organizational priorities.

Issues.

The Division has had three elections under the re-organized IUPAC structure and almost four years of working diligently to implement the project system effectively. Significant issues have arisen. Although these concerns are presented as a list, many are inter-connected.

(1) **Generation of projects.** In spite of sustained efforts at brainstorming, participating in project-generation workshops, and giving talks at scientific meetings about IUPAC and describing the opportunities for all to propose IUPAC projects, the Division II experience in initiating projects has been disappointing. All of the Division's projects have been proposed by former members of IUPAC Commissions. As we have become more removed in time from having had active Commissions the number of project submissions has fallen to an extremely low number. The Division is concerned. How can projects be generated? Where will they come from?

(2) **Progress on projects.** It is too early to be certain but there are indications that, as project leaders no longer have peers to face at Commission meetings and report to the Division only by annual e-mail reports, the pace of progress on funded projects is slowing. What can be done to facilitate projects being completed in a timely and exemplary manner – reflecting a quality of science and breadth of vision in accord with the expectations of the Union and the world community?

(3) **People.** The two preceding issues – along with noting that the current nomination and election procedures tend to recruit members to the Division Committee who are eminent and wise but without experience at leading or contributing to IUPAC projects – lead to the question: How can IUPAC locate and develop new volunteers and project participants that are willing to dedicate themselves and their expertise to accomplishing things for the international scientific community through IUPAC?

(4) **Workload** of Division officers. The efforts implied by the above, along with the necessity to respond to numerous requests for input or guidance from project leaders, Division Committee members, the IUPAC executive and the IUPAC Secretariat have become very time-consuming. This Division President, on average, spends 2-3 hours per working day answering (and, at times, generating) IUPAC e-mail. This is not sustainable in a volunteer activity.

(5) **Internal motivation and communication.** There is a huge gap in IUPAC between the executive bodies running the organization and the scientific volunteers carrying out projects. Over and over again one gets the impression that they do not understand each other's perspectives and priorities. If IUPAC is to increase its effectiveness, this is a problem that must be addressed; addressing it is necessary, albeit not sufficient, for making progress on the other issues listed here.

(6) **E-mail communication and the “reward” structure.** The concerns described in 2, 4, and 5 above lead one to wonder if having the organization depend as much as it does on e-mail communication, without face-to-face communication, team-building, and interpersonal relations and rewards, is effective for an international organization that depends upon motivating volunteers.

(7) **Support of the continuing IUPAC efforts in isotopic abundances and atomic weights** and of the core activities of Commission II.1. After much internal examination the Division concluded three years ago, and Council concurred at Brisbane, that IUPAC’s activities in isotopic abundances and atomic weights require a Commission to provide the necessary continuity and expertise in this core undertaking. The Division initially thought that the activities of the Commission could be funded purely by projects. However, our experience during the past two years has been that, in addition to carrying on projects, the Commission has to meet to plan and review activities – at least biennially and perhaps annually. Project funds do not lend themselves to supporting these meetings and the Project Committee, given its charge, does not see support of Commission meetings as part of its task. This leaves the question: How can we fund meetings of Commission II.1?

(8) **Communication with the inorganic chemistry and materials chemistry communities.** It is clear that if IUPAC is to meet the needs of the world chemistry community this Division, like the others, has to find and utilize effective ways to communicate with the international inorganic chemistry community – to speak to them and, just as importantly, to hear from them. The need and goal are clear. The method is not so obvious considering the limitations of both funding and of the time available to devote to this by an already over-burdened group of Division officers.

Priorities and status .

The Inorganic Chemistry Division, reflecting the breadth of inorganic chemistry, is concerned with chemical elements, molecular compounds, and solid materials. As part of the re-organization of the Union and the self-assessment that accompanied that re-organization, the membership, structure, and priorities of the Division Committee reflect and address those disparate elements of inorganic chemistry. In addressing these areas, the Division attempts to ensure appropriate representation of expertise on the Division Committee and oversees its projects using three coordinating groups, one each for elements, molecules, and materials. Priorities and status in each area are as follows.

Elements . This work falls into two areas, both of which are long-standing, highly visible, IUPAC activities, and both of which remain high priorities for the Division.

(a) The **naming of new elements.** The Division has coordinated the interaction of the Union with the IUPAC-IUPAP Joint Working Party charged with vetting the discovery of new elements, and has responsibility for soliciting from the discoverers, and then recommending, a name for new elements whose discovery or synthesis has been confirmed by the IUPAC-IUPAP JWP. This Council will have opportunity to approve the Division’s recommendation that element 110 be named darmstadtium with symbol Ds. In addition the JWP has issued a recent report confirming the discovery of element 111 by the GSI Laboratory in Darmstadt and the Division will shortly begin communicating with the scientific leaders of that effort on a name for element 111. An “IUPAC Periodic Table” reflecting these recommendations, along with all past IUPAC recommendations on its format and the most recent set of IUPAC atomic weights, has been prepared and will be posted prominently on the IUPAC web site.

(b) **Isotopic abundances and atomic weights.** The Division's priority in this area is to support and nurture the activities of Commission II.1 and its subcommittees. Recent accomplishments include changes in the standard atomic weights of the chemical elements zinc, krypton, molybdenum, and dysprosium at Brisbane and a number of accomplishments and publications described in more detail elsewhere in this report.

Molecules. Historically, the bulk of IUPAC's efforts in this central area of inorganic chemistry have been connected with nomenclature. Those efforts have been moved to Division VIII and Division II is attempting, successfully, to contribute to and coordinate with the inorganic nomenclature activities in the Chemical Nomenclature and Structure Representation Division, in part by appointing a Division VIII TM as an AM in Division II. In addition, the Division is making a major effort to recruit outstanding molecular inorganic chemists to the Division Committee and to encourage those members to foster and generate proposals in this area.

Materials. Materials chemistry is an important and growing area of chemistry that involves *all* classical chemical disciplines. The Inorganic Chemistry Division is trying to foster and coordinate the growth and focus of IUPAC efforts in this area by leading the IUPAC Materials Initiative. The first organizational step has been formation of a Materials Chemistry Subcommittee with membership from Divisions I, II, IV, and V, and interest expressed by several other Divisions. The near-term activities of this subcommittee, which meets during the Ottawa General Assembly, are to canvas the international materials community to ascertain interest and ideas for materials chemistry in IUPAC and to develop an expanded portfolio of new projects to add to the half-dozen or so existing IUPAC projects in materials chemistry. The long-term vision is for IUPAC to form a strong new Materials Chemistry Division. In addition to leading the Materials Initiative, Division II coordinates and oversees two prominent series of conferences in the materials area, the Workshops on Advanced Materials and the Conferences on High Temperature Materials Chemistry. The 11th conference in this latter series met very successfully in Tokyo, Japan in May 2003, the first time this conference has been held in Asia.

II. Division Activities 2002-2003 in the Framework of the IUPAC Strategic Plan

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

Three high-priority Division II activities address this strategic goal:

(a) The Division coordinates assessment of whether a new element has been discovered and over-see the process of selecting a suitable name for that new element. Currently this involves the naming of element 110 and initiation of the process to name element 111 following review and publication of the latest report from the IUPAC-IUPAP Joint Working Party.

(b) For several decades, the Commission on Isotopic Abundances and Atomic Weights has met biennially to review the atomic weights of all the chemical elements and biennially has published a revised Table of Standard Atomic Weights, documenting justifications for changes. About every two decades, the Commission publishes a review of the changes and variations that have been recognized in the values and uncertainties of atomic weights on an element-by-element basis. This document was last published in 1985. Thus, in 1999 J. de Laeter agreed to lead a team to prepare and publish "The Atomic Weights Of The Elements: Review 2000." This technical report is in press and will be published in *Pure and Applied Chemistry* in 2003. The report includes an updated Table of Isotopic Compositions of the Elements. The Commission is

active, more or less continuously, in assessing atomic weights as new data are found and in evaluating the effects of isotope abundance variations of elements upon their standard atomic weights and atomic-weight uncertainties.

(c) Division II through the Materials Initiative and associated conferences – the Workshops on Advanced Materials and the High Temperature Materials Chemistry Conferences – is assisting the chemistry community in advancing this key field in cooperation with other disciplines.

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

Many Division II projects address this goal.

(a) Cf. discussion of the activities on the Commission on Isotopic Abundances and Atomic Weights under Goal 1.

(b) Project No. 1999-049-1-200, “Thermodynamic characterization of high-temperature superconductors in the yttrium-barium-copper-oxygen system.”

(c) Project No. 2000-002-2-100, “Standardization of methods for the characterization of inorganic membranes” with Division I.

(d) Project No. 2000-007-1-400, “Glossary of terms relating to polymeric gels and networks, hybrid inorganic polymeric materials and the processing thereof” with Division IV.

(e) Project No. 2000-022-1-200, “Characterization of carbon materials.”

(f) Project No. 2001-015-1, “Standard potentials of radicals” with Division I.

(g) Project No. 2001-019-1, “Guidelines for mass spectrometric isotope ratio measurements.”

(h) Project No. 2001-031-1, “Alignment of nomenclature in areas of overlap between the preferred names for organic nomenclature and the revision of the nomenclature of inorganic chemistry” with Division VIII.

(i) Project No. 2003-006-1-100, “NMR Chemical Shifts: Updated Conventions” with Division I.

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

The Materials Initiative and associated IUPAC conferences, described in the Highlight section and under Goal 1 above, address this goal. This is particularly true of the High Temperature Materials Chemistry conferences which have become the premier international venue for bringing together basic and applied researchers concerned with materials prepared or utilized at high temperatures.

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

Two education projects described under Goal 5 – experiments for solid state and materials chemistry and syllabus suggestions for the teaching of high temperature materials

chemistry – along with the Workshops on Advanced Materials, the most recent of which was held in India, are particularly pertinent to helping chemists in less advanced or developing countries.

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

Three division II activities address this goal:

(a) The Division is preparing and will post on the IUPAC web site an IUPAC Periodic table that consolidates IUPAC recommendations for element names and symbols, atomic weights, and format of the periodic table itself.

(b) Project No. 2000-020-2-200, “Collecting, testing and dissemination of experiments in solid state and materials chemistry.”

(c) Project No. 2000-024-1, “Teaching high temperature materials chemistry at university.”

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.

This has been a guiding principle in the process of soliciting nominations for the Division II Committee.

III. Additional Information

Division II has 14 on-going funded projects, tabulated in the next section of this report. Of these, 5 are joint with other IUPAC Divisions, 4 are under the auspices of the Commission on Isotopic Abundances and Atomic weights, and 6 are part of the Materials Initiative.

Gerd M. Rosenblatt
Berkeley, California
July 2003

RECENT PUBLICATIONS – 2001-2003

W. H. Koppenol, Names for muonium atoms and ions, *Pure Appl. Chem.*, **73**, 377-380, (2001)

P. J. Karol, H. Nakahara, B. W. Petley, and E. Vogt, On the discovery of elements 110 – 112, *Pure Appl. Chem.*, **73**, 959-967 (2001).

W. H. Koppenol, Naming of new elements, *Pure Appl. Chem.*, **74**, 787-791 (2002).

T. B. Coplen, J.K. Böhlke, P. De Bièvre, T. Ding, N.E. Holden, J. A. Hopple, H. R. Krouse, A. Lamberty, H. S. Peiser, K. Révész, S. E. Rieder, K. J. R. Rosman, E. Roth, P. D. P. Taylor, R. D. Vocke, Jr., And Y. K. Xiao, 2002, Isotope-Abundance Variations Of Selected Elements, *Pure Appl. Chem.*, **74**, 1987-2017 (2002).

T. B. Coplen, J. A. Hopple, J. K. Böhlke, H. S. Peiser, S. E. Rieder, H. R. Krouse, K. J. R. Rosman, T. Ding, R. D. Vocke, Jr., K. M. Révész, A. Lamberty, P. Taylor, and P. De Bièvre, Compilation of Minimum and Maximum Isotope Ratios of Selected Elements in Naturally Occurring Terrestrial Materials and Reagents, U.S. Geological Survey Water-Resources Investigations Report 01-4222, 98 pp. (2002).

J. R. De Laeter, J. K. Böhlke, P. De Bièvre, H. Hidaka, H. S. Peiser, K. J. R. Rosman, and P. D. P. Taylor, 2003, The Atomic Weights Of The Elements: Review 2000, *Pure Appl. Chem.*, **75**, 683-799 (2003).

R. Loss, Atomic Weight of the Elements 2001, *Pure Appl. Chem.* (in press, 2003).

CURRENT PROJECTS

Project No: 1999-001-1-200
Submitted by: Connelly
Titled: Nomenclature of inorganic chemistry - Revised 'Red Book' - part I.
Amount Allocated: \$9930

Project No: 1999-043-1-200
Submitted by: de Laeter
Titled: Element by element review of atomic weights to the year 2000
Amount Allocated: \$4000

Project No: 1999-049-1-200
Submitted by: Voronin
Titled: Thermodynamic characterization of high-temperature superconductors in the yttrium-barium-copper-oxygen system
Amount Allocated: \$5000

Project No: 2000-002-2-100
Submitted by: Yi Hua Ma
Titled: Standardization of methods for the characterization of inorganic membranes
Amount Allocated: \$5000 (Div I)
Comments: with Division I

Project No: 2000-007-1-400
Submitted by: Jones
Titled: Glossary of terms relating to polymeric gels and networks, hybrid inorganic polymeric materials and the processing thereof
Amount Allocated: \$9500 (Div IV)
Comments: With Division IV

Project No: 2000-020-2-200
Submitted by: Kizilyalli
Titled: Collecting, testing and dissemination of experiments in solid state and materials chemistry
Amount Allocated: \$8600

Project No: 2000-022-1-200
Submitted by: Boehm
Titled: Characterization of carbon materials
Amount Allocated: \$5500

Project No: 2000-024-1
Submitted by: Balducci
Titled: Teaching high temperature materials chemistry at university
Amount Allocated: \$4800

Project No: 2001-015-1
Submitted by: Stanbury
Titled: Standard potentials of radicals
Amount Allocated: \$15000 (Div I)
Comments: with Division I

Project No: 2001-019-1
Submitted by: Taylor (Walczyk)
Titled: Guidelines for mass spectrometric isotope ratio measurements
Amount Allocated: \$2000

Project No: 2001-031-1
Submitted by: Damhus
Titled: Alignment of nomenclature in areas of overlap between the preferred names for organic nomenclature and the revision of the nomenclature of inorganic chemistry
Amount Allocated: \$7520 (Div VIII funds)
Comments: With Division VIII

Project No: 2001-042-1
Submitted by: Taylor (Ebihara)
Titled: Rev of Isotopic Abund in XT materials
Amount Allocated: \$6000

Project No: 2002-049-2-200
Submitted by: Taylor
Titled: A new comprehensive report on the isotopic compositions of the elements for global users communities (RICE phase I)
Amount Allocated: \$8000
Comments: First meeting to be held August 5, 2003 in Ottawa

Project No: NA
Submitted by: Chatillon, Drowart
Titled: High temperature mass spectrometry: accuracy of the method and influence of the ionization cross- sections
Amount Allocated: NA
Comments: Project held over from pre-project era. Publication undergoing final revision and review

Project No: 2003-006-1-100
Submitted by: Harris/Becker
Titled: NMR Chemical Shifts: Updated Conventions
Amount Allocated: \$2000
Comments: Contribution to Div I project of interest to Div II