

INORGANIC CHEMISTRY DIVISION COMMITTEE OF IUPAC

Minutes of Meeting at Glasgow 31 July and 1 August 2009

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INORGANIC CHEMISTRY DIVISION COMMITTEE OF IUPAC

Minutes of the Meeting at Glasgow, Scotland

July 31 - August 1, 2009

Attendance: Present were *President*, Kazuyuki Tatsumi (Japan); *Vice President*, Robert Loss (Australia); *Past President*, Anthony West (U.K.), *Secretary*, Leonard Interrante (U.S.A.); *Titular Members*: Tyler Coplen (U.S.A.), Tiping Ding (China/Beijing), Javier Garcia-Martinez (Spain), Marku Leskela (Finland), Jan Reedijk (Netherlands), and Myunghyun Pak Suh (Korea); *Associate Members*, Alan Chadwick (U.K.), Milan Drabik (Slovakia), and Norm Holden (U.S.A.), Ken Sakai (Japan); *National Representatives*, Aldo Bologna Alles (Uruguay), Ling-Kang Liu (China/Taiwan), and Lars Öhrström (Sweden), *Young Observers*, Miki Hasegawa (Japan), Torsten Hegmann (Canada), Partha Sarathi Mukerjee (India), Dan Rabinovich (U.S.A.) and Maria Zhaharescu (Romania), *Guests*, Sean Corish (Ireland)(IUPAC Treasurer), Peter Day (U.K.) (Division Project Leader), Herbert Kaesz (U.S.A.).

Apologies were received from *Titular Member* Pavel Karen and *Associate Members*, Sanjay Mathur and Joe Takats, who could not attend.

1 – Introductions and announcements (K. Tatsumi)

The meeting commenced at ca. 1:20 p.m. on Friday, July 31, 2009 due to the (previously announced) late arrival of the Division President in Glasgow this morning. Div. Pres. Tatsumi welcomed the members and guests who introduced themselves and described their professional affiliations and areas of expertise. The arrangements for a dinner this evening at a local Glasgow restaurant were discussed and a group photo was scheduled after the completion of today's meeting.

2 – Presentation and discussion of the Agenda (Tatsumi, Interrante)

The previously distributed Agenda was accepted by President Tatsumi with the addition of reports by representatives from other IUPAC Divisions and Committees.

3 – Approval of Minutes from Division Meeting in Helsinki (Interrante)

Copies of a draft of these minutes were previously distributed by email and are available on the IUPAC Division II web page. These Minutes had been distributed in draft form previously and amended according to corrections and comments received from the Division members. The resulting final version of the Minutes were approved without further change.

4 – Report on the status of the action items from the Helsinki meeting; appointment of a Division member to record a list of action items for this and the next Division meeting (Interrante, Tatsumi)

The action items from the Helsinki meeting were included in the Minutes to that meeting as Appendix 2. Most, but not all, of these items were addressed by the designated individual. Apologies were received from L. Interrante for neglecting to thank Norm Holden for his excellent educational report on the names tungsten/wolfram for element 74

(see the Minutes for the Helsinki Div. II Meeting, page 28 (Appendix 4)). Coplen agreed to note the Action Items for the current meeting, which are included in these Minutes as **Appendix 1**.

5 – Report on the Spring 2009 IUPAC Bureau Meeting (Tatsumi)

The Bureau met in Bratislava, Slovakia on April 18-19 2009. A copy of the minutes of this meeting is available for downloading on the IUPAC website (http://www.iupac.org/web/nt/2009-06-25_87_bureau). Div. Pres. Tatsumi reviewed the main items that were discussed at this meeting, including the following that were of particular relevance to Division II (taken from the Bureau Meeting Minutes, essentially verbatim).

THE INTERNATIONAL YEAR OF CHEMISTRY (IYC)

Prof. Mahaffy (Chair, CCE) reported that the Ethiopian Chemical Society had worked with their UN delegation to have the United Nations proclaim 2011 as the International Year of Chemistry. He noted that the (Bureau) Agenda Book contains various background documents, including the resolution approved by the United Nations. The UN resolution had 35 sponsors. Prof. Mahaffy noted that the UN Resolution had been brought forward under the Sustainable Development agenda.

Prof. Jin reported that he had met with the Secretary General of the United Nations and other members of the United Nations staff in February. He was encouraged by these meetings to invite the UN Secretary General, Mr. Ban-Ki Moon to give a plenary address at the 2011 Congress.

Prof. Henry reported that meetings of IUPAC Officers and ACS officers had been held in August 2008 and March 2009 to discuss the ACS activities that were planned in connection with the IYC. He noted that the ACS had decided to repurpose as many events as possible during 2011 to be part of the celebration of the International Year of Chemistry.

The 46TH GENERAL ASSEMBLY AND 43RD CONGRESS (SAN JUAN, 2011)

Dr. Jost noted that a report had been received from the organizers and that the organization of the Congress and General Assembly appeared to be on course. A number of special events were planned to celebrate the IYC. Prof. Lamba reminded the Division Presidents and Standing Committee Chairs that they should let the organizers know as soon as possible if their Division or Standing Committee would like to organize a session at the Congress. Prof. Tarasova reminded the Bureau that visa applications from some countries for the United States could take many months. The Congress organizers should advise registrants that they should allow six months for the visa application process.

The 47TH GENERAL ASSEMBLY AND 44TH CONGRESS (2013)

Prof. Black reported that one proposal for hosting the 2013 Congress and General Assembly had been received. Dr. Jost noted that this proposal was the same as that made in 2007 and that the facilities proposed had been found suitable in a site visit in 2007. A motion was made and seconded to recommend to Council that the proposal from the Turkish Chemical Society be accepted. The motion was approved unanimously.

The 48TH GENERAL ASSEMBLY AND 45TH CONGRESS (2015)

Prof. Black reported that one proposal for hosting the 2015 Congress and General Assembly had been received from the Korean Chemical Society. Dr. Jost reported that he would do a site visit to review the proposed venues in May. A motion was made and seconded to recommend to Council that the proposal from the Korean Chemical Society be accepted, with the proviso that the proposed venue is found acceptable by the Executive Director. The motion was approved unanimously.

PROJECT FUNDING

Prof. Powell reported that the Committee had reviewed and approved 13 projects that sought funding from the Project Reserve. Commitments to date in this biennium totaled USD 87,900 (80 % of available funds); these have been complemented by supporting commitments of USD 13,000 from the Strategic Opportunities Fund and USD 38,475 from external sources. Three of the Standing Committees and five of the eight Divisions have been beneficiaries of these IUPAC funds, which complemented total Standing Committee/Division commitments of USD 49,500 (a factor of 2.0:1). However, the majority of activity has come from just three Divisions. Prof. Powell noted that the Project Committee also reviewed proposals from Divisions/Standing Committees for financial support of conferences in “scientifically emerging regions” (FSC-SER) and conferences that promote “new directions in chemistry” (FSC-NDC). Across these two categories the biennial budget is USD 65,000. Applications must be made at least 12 months ahead of the conference, and are processed as received. He observed that in the current biennium these two programs are a “missed opportunity”. There have been only four applications, with two being funded (one FSCNDC and one FSC-SER, a total of USD 12,000); one application was declined (FSC-SER) on the basis of ineligibility of the venue as a “scientifically emerging region”, and the other (FSC-NDC) on the basis of being a continuing conference series. In contrast, in the previous biennium a total of 11 conferences were supported financially by IUPAC.

DISCOVERY AND NAMING OF NEW ELEMENTS

Prof. Corish reported that the Joint Working Party had decided to divide its work into two parts; they have first considered the evidence regarding the element of atomic number 112 and will then review claims regarding elements of higher atomic number. This has enabled the naming process for 112 to proceed while the claims for elements of atomic number 113 et seq. are resolved. A first draft of the report on the elements of atomic number 113 and higher has been completed. The report on the element of atomic number 112 was circulated to the laboratories concerned. Their comments were taken into account, and the report was extensively reviewed. It was also reviewed by Division II and ICTNS and approved for publication in *PAC* as a Technical Report. Before publication, the report was submitted for approval by the Executive Committee of IUPAC and the Executive Council of IUPAP. After approval of the report for publication, the Inorganic Chemistry Division will request the group named as the discoverer of the element of atomic number 112 to suggest a name and symbol for the element. A Recommendation will be made available for Public Comment, including an announcement on the IUPAC web site, and will then be brought to the Bureau or Council, whichever meets at the appropriate time, for approval.

The Recommendation will then be published in *PAC*. The Council had previously approved a motion to delegate to the Bureau the approval of a name for element 112 if there is no controversy regarding the assignment of priority of discovery or regarding the proposed name after the public comment period.

SEARCH FOR A NEW EXECUTIVE DIRECTOR

Prof. Black reported that Dr. Jost had announced his intention to retire after August 2010. It is planned to have a replacement selected and hired by early 2010 to allow sufficient time for overlap. An advertisement for the position was placed in *Chemical & Engineering News*, *Chemistry World*, *Science*, the *Chronicle of Higher Education*, and the *Proceedings of the National Academy of Science*. The Selection Committee will review the candidates at a meeting tentatively planned for June.

WEB SITE

The major event regarding the web site continues to be the conversion of the existing site to one based on XML technology. After more than twelve months of operating the new site in "test" mode, there continue to be significant issues. The portions of the site related to the members database and to membership on IUPAC bodies have been converted to accept data generated by the Act databases at the Secretariat. This portion of the new site is largely successful. The portions of the site related to projects and other information continues to need a significant amount of work both by the developers in Prague and Secretariat staff. Communication with the developers has improved somewhat over the past year, but is still a significant barrier to completion of the project. The Committee on Printed and Electronic Publications set up a study group at the 2008 CPEP Meeting in Prague. The Group considered how best to develop the IUPAC Website so as to meet the wishes and needs of both members of IUPAC and of others. The Study Group concluded that a long-term goal for the development of the web site should be the creation of two aspects of the site, one oriented to members and the other oriented to the general public, mainly students and chemists not active in IUPAC. Dr. Jost commented that work on these recommendations would be started only after the current work on the web site described above was completed.

In the discussion of this report by Tatsumi of the Bureau meeting it was decided to delegate a Division member to make input for our Division in connection with events planned for the WCC and the IYC. J. Garcia, who is also the Division II representative on CCE, agreed to serve in this capacity (**Action Item**). Tatsumi noted the issue of visa's for foreign participants in the IUPAC GA/WCC in Puerto Rico and indicated that we would need to make these applications well in advance of the meeting date.

6 - Report from IUPAC Officers - S. Corish, IUPAC Treasurer (and former President of Division II)

Corish expressed the hope that the Division would discuss the IYC during our meeting and plan something in connection with this. He noted that the official opening ceremony will occur in Paris in January of 2010 at the UNESCO Headquarters in Paris, France. Prior

to that a IYC Pre-launch reception will be held at the Pacificchem meeting in Honolulu, Hawaii, USA which will simply highlight the coming celebratory year. The General Assembly in Puerto Rico in August 2011 will be another place in which it will be highlighted. He encouraged us to look at the official website (<http://www.chemistry2011.org/>) for up to date information about the events planned and for ideas ideas and sample activities of earlier projects and an opportunity to become involved at a national or local level.

7 – Report from the nominating committee for the 2009 TM election; list of 2010-11 Division Members (Loss)

Vice-President Loss reported on the results of the 2009 Division II election of TMs for the 2010 - 2013 term. The nominating committee for this election consisted of Prof. Gerhard Erker, Prof. Klaus G. Heumann, Prof. Leonard V. Interrante, Prof. Richard M. Laine, and Nominating Committee Chairman, Prof. Robert D. Loss. Nominations were solicited from the membership of Division II and the NAOs and selected by the Nominations committee so as to form a slate consisting of up to two nominees for each of the four available open positions for TMs. These TM positions were designated according to the three main areas of Division II interests, Atoms, Molecules, and Materials, so as to maintain the current, approximately equal, distribution of Division II TMs among these three areas. In this manner, one slot was designated for candidates in the areas of Atoms (one candidate), one for Molecules (two candidates), one for Materials (two candidates) and one was designated as an open position that could be filled by either a Molecules or Materials candidate (labeled Inorganic/crystalline chemistry). The respective nominees were: Norman Holden (Atoms), Lars Öhrström and Ken Sakai (Molecules), Milan Drábik and Sanjay Mathur (Materials), and Pavel Karen and Ling-Kang Liu (Inorganic/crystalline chemistry). The election was held by the IUPAC Secretariat in early February of 2009 and the elected TMs were Holden, Sakai, Mathur and Karen.

Prior to this election, in November of 2008, Louis Oro, who had been elected TM in 2008 for the term, 2008 -11, resigned from his position as TM, owing to his election as president of EuCheMS, and Jan Reedijk was selected by the Division executive committee, with the approval of the IUPAC Executive Committee, to fill the remainder of Prof. Oro's term, effectively extending Reedijk's term as TM for one year.

Bob Loss will resurrect a nominating committee after a week or so should it be needed to address the changes in Div. II officers required if K. Tatsumi is elected as President of IUPAC (**Action Item**). This did, in fact, occur and a special election was held in September 2009 that resulted in the election of Jan Reedijk as Vice-President, replacing Bob Loss, who succeeded Tatsumi as Division President.

A final list of Division members for the next biennium and their terms of office was obtained from the Secretariat in October 2009 and is attached to these Minutes as **Appendix 2**.

8 - The 2009 edition of the Division newsletter (Loss)

President Loss was congratulated by the members present on his excellent work in preparing the second edition of the Inorganic Division Newsletter, which was completed and distributed to the Division members, the IUPAC Division Presidents, Committee Chairs, Executive Committee and others outside of IUPAC in April of 2009, and is now posted on the Division website (<http://www.iupac.org/web/ins/200>). He was currently collecting input for the next (third) Newsletter, which would be published later this year, and asked the members present to please send their contributions to him by August for inclusion in this Newsletter. He also asked the Division members to distribute the newsletter to their respective communities (**Action Item**).

9- Review of Division budget allocations and expenditures (Tatsumi, Coplen)

It was decided to move this item to the end of Ty Coplen's Project-by-project review of project status.

10- Report from Commission on Isotopic Abundances and Atomic Weights (CIAAW) and its Subcommittees (Coplen, Loss)

Coplen presented some highlights from the CIAAW meeting that was held at the International Atomic Energy Agency in Vienna on July 23-24. This meeting focused in particular on the educational needs of Chemistry students worldwide with its attempt to emphasize the non-constancy (variability) of the atomic weight values of many elements. In connection with this focus the Commission prepared a first draft of a Periodic Table of the Isotopes. This table is designed to help to inform students that chemical elements are made up of stable isotopes and unstable isotopes, while displaying their properties and applications in everyday experiences. A draft report on this meeting is attached to these minutes as **Appendix 3**.

A News Item on a "Summary of the Minutes of the Commission Meeting at IAEA ..." was prepared and transmitted to the Division Secretary for submission to IUPAC for immediate release to the scientific community (**Action Item**). This was done on August 2, 2009, just after our meeting; however, it was later requested by Coplen that this held up be pending publication of the Commission Table of Standard Atomic Weights of the Elements 2009 in PAC near the end of 2009. The thinking was that the PAC report was needed to explain the press release

Loss then presented a report on the meeting of the Subcommittee on Isotopic Atomic Abundances (SIAM), which was held as part of the overall CIAAW meeting in Vienna. The minutes of this meeting are attached as **Appendix 4**. Highlights include:

- The Review of publications of isotope ratio measurements 2003 – 2009 since previous TICE (2001) (TICE = Table of Isotopic Composition of the Elements).
12 elements considered (Ar, Cd, Ge, Pt, La, Lu, Mo, Nd, Ni, Ta, Yb, Zn)

- Recommended that new Best Measurements (column 6) and new Representative Isotopic compositions (Column 9) are to be published for 11 of these in a new TICE 2009.

Progress was made on the Concept and Format, Content and Strategy of the Next TICE table (TICE21 = Table of Isotopic Composition of the Elements for the 21st century))

TICE 2009 Issues

- The large number of newly published data requires a new TICE
- A decision was made to stay with current TICE format of reporting abundances (no ratios)
- Uncertainties in the Representative Isotopic Compositions (column 9) will be reported since ranges in Representative Isotopic Compositions have problems (to be addressed in TICE21)
- Changes made to improved clarity of text associated with describing observed ranges in Isotope Abundances (column 4)

TICE21 Issues – Future SIAM work (IR = isotope ratio) and (GUM = Guide to the expression of Uncertainty in Measurement). For the fifth bullet, insert (IA = Isotopic abundance) and change "National Assessment" to "Natural Assessment"

- Implements a number of the outcomes of RICE1 and RICE2 (e.g., focus on IR, GUM compliant) (RICE = Report on the Isotopic Compositions of the Elements; IR = isotope ratio and GUM = Guide to the expression of Uncertainty in Measurement)
- Major Extension: New electronic data management system (New project based on XML)
- Review of all polyisotopic elements over a 6 year period (24 proposed by 2011)
- Exciting range of user specific outputs
- Many issues to sort including how to handle the Range of IR/IA (will be directed to SNAFU) (The Subcommittee on the Natural Assessment of Fundamental Understanding of Isotopes) (IA = Isotopic Abundance)

11- New Elements: Validation of Claims and Naming – Status of the naming of Element 112 (Corish)

Corish gave a brief summary of the claims for the discovery of new elements beyond element 112 and described the process used to consider these claims and the current status of these claims. Claims for the discovery of a new element are submitted to a joint IUPAC/IUPAP Working Group, who evaluates these claims and establishes a priority among the submitting groups for the proposal of a name and a symbol to the IUPAC Inorganic Chemistry Division. In the case of element 112, this process has reached the stage of joint working group approval of the claim made by the Gesellschaft für Schwerionenforschung (GSI). The GSI team was acknowledged as the discover of the new element, see *Pure Appl. Chem.*, 2009, Vol. 81, No. 7, pp. 1331-1343 and a News Release was issued by IUPAC on July 20, 2009 that noted that "The proposed name, copernicium, and symbol, Cp, will be reviewed by the IUPAC Inorganic Chemistry Division to determine its acceptability, and if it is considered to be necessary, seek its modification."

The proposed symbol, Cp, when announced in an email message that was sent to the Division members prior to this meeting, elicited considerable discussion among the members and a number of objections were raised to this symbol, because of its prior extensive use in inorganic chemistry as the symbol for the cyclopentadiene anion, and also because of its use as the symbol for heat capacity at constant pressure. Lars Öhrström agreed to prepare a report on the proposed name and symbol which he will present after Corish's report.

The WG also considered claims for discovery of 5 other elements beyond 112 and wrote a report on their findings, which is currently in the editing stage (see the section on Naming of New Elements in the excerpts from the minutes of the Bureau Meeting on page 3).

After a brief coffee break, the meeting was reconvened and Lars Öhrström presented a report that he and Norm Holden had prepared on Division II's role in the proposal and decision of names and symbols for new elements. He indicated that the following procedure is to be followed: (1). The discoverer proposes a name and a symbol to IUPAC; (2). IUPAC forwards the proposed name and a symbol to Division. II; (3). Division II votes to accept or reject the name; (4). Division II votes to accept or reject the symbol; (5). The Division president forwards the decisions to IUPAC; (6). IUPAC informs the discoverer. He also noted that, according to the rules set up by IUPAC, *There is no direct communication between Division II and the discoverer and Division II has no role in suggesting alternative names and symbols to the discoverers.*

The following observations summarize the discussions carried out by email since President Tatsumi received the proposal from Professor Hofman of the CSI group in Darmstadt: (1). No members of division II have raised objections to the name Copernicium; (2). Several members of division II have raised objections to the proposed symbol Cp.; (3). No members of division II have expressed support for the proposed symbol Cp.

The objections to the symbol Cp are:

- (a) Its previous use as symbol for element 71 (Lutetium, aka Cassiopeium). Symbols and names cannot be recycled...
- (b) The common use of Cp as the IUPAC approved abbreviation for the cyclopentadienyl ion.

If Division II rejects the symbol Cp the following motivation is suggested:

- The Inorganic Chemistry Division has considered the suggested name of *Copernicium* for element 112 and finds it acceptable.
- The Inorganic Chemistry Division has considered the suggested symbol *Cp* for element 112 and finds it unacceptable.
- There are two major objections to this symbol:

The symbol Cp is already in use as an IUPAC approved (Table VII, item 45, pa 262, Red Book) abbreviation for the ligand cyclopentadienyl in organometallic and inorganic chemistry.

A more serious issue is that the element with atomic number 71, *Lutetium*, until 1949 also went under the IUPAC approved name *Cassiopeium* with symbol Cp. The IUPAC rules for naming elements state that chemical names (and presumably their symbols) previously used for a chemical element and later rejected cannot be reused in the future for another chemical element.

An additional issue is the discoverer's immediate announcement of their choice of name and symbol across the worldwide web well in advance of any opportunity for IUPAC to begin to discuss this issue.

In the future, IUPAC should firmly inform any potential discoverer that any mention of names or symbols should be withheld until IUPAC grants approval. In the past, the policy directed to the Division was that this information is confidential until IUPAC makes a decision. Now this information was spread across the world, before our Division was even informed about the choice that would have to be discussed.

The division views this situation as unacceptable. One consequence is that the information about what may turn out to be an unacceptable choice will exist across the scientific community for months before the correct information is agreed upon. We therefore decided unanimously to accept the name, copernicium, for element 112, but not the proposed symbol, Cp.

Subsequent to our meeting, on August 6, 2009, President Tatsumi communicated our decision regarding the proposed name and symbol for element with atomic number 112 to Prof. Hofman and invited him to propose a new symbol. Hofman then replied, suggesting the alternative symbol Cn, which several of the Division members had previously indicated would be acceptable. It was ultimately decided to approve the use of the symbol Cn for this element.

12- Report from the Subcommittee on Materials Chemistry (West)

Division Past President A. West, who was also the chair of the Subcommittee on Materials Chemistry, reported that an open meeting was held this morning to discuss the future of Materials Chemistry within IUPAC. The discussion centered on the viability of the Subcommittee in the context of the problems that had been experienced over the past several years of its existence, as almost entirely an "inorganic chemistry-focused" entity with minimal participation from members of other IUPAC Divisions. This narrow focus, with a lack of effective participation by other Divisions and its tenuous, low profile, existence within IUPAC, was viewed as inconsistent with the scope and importance of materials chemistry activities worldwide and unsustainable going forward. Therefore, it was felt that a new structure was needed to relace the current "inorganic-centered"

Subcommittee, which would involve the active participation by members of other Divisions representing the broad scope of materials chemistry activities worldwide.

In support of this conclusion, West gave a brief slide presentation which reviewed the history of the Subdivision, starting from its origin in 2000 as a successor of the former Commission 2.4 on High Temperature Materials (Inorganic/Physical Chem) to the present and placed it in the context of the current state of materials chemistry activities worldwide. He noted that ample evidence can be cited to show that MC now ranks alongside Organic, Physical, Macromolecular and Inorganic as a main branch of modern chemistry. In particular, at the World Chemistry Congresses in Beijing, Torino, and at the current Glasgow meeting, the sessions on materials chemistry have been the largest component of the scientific programs. Also, the RSC has approved the creation of a Division of Materials Chemistry and has been holding biennial meetings for many years in this area that have been attended by hundreds of scientists from all over the world. Finally, the ACS and RSC have established two major journals in materials chemistry that currently receive thousands of papers each year. Thus, it is clear that IUPAC is now very under-represented in Materials Chemistry and a fundamental change is needed to bring it into sync with the reality of chemistry in the 21st Century.

A detailed account of the history of materials chemistry and its relationship within IUPAC, along with a proposed "working definition" for this subject, can be found in an article in *PAC* (2009, Vol. 81, Issue 9, p. 1707-1717) and a summary in *Chemistry International* (May-June 2009, pp. 4-8), which resulted from a recently completed Project (2005-001-1-200 - Towards defining materials chemistry) led by Peter Day.

An extended discussion followed this presentation in which various possible alternatives for reforming and/or redefining the Subcommittee were considered. Interrante suggested forming an interdivisional task group to look into options for accomplishing this goal. Corish indicated that we could perhaps develop a Project that would consider the options and formulate a proposal for a new Division of Materials Chemistry. Interrante proposed that the Division allocate \$2,000 to partially fund a meeting involving our Division and members of Divisions I (Physical) and IV (Macromolecular), as well as any other interested Divisions, to come up with a proposal to IUPAC. Reedijk made a motion that we form a committee consisting of two members of Division II and four others from two other Divisions to meet to discuss the options for a new structure that would best stimulate more IUPAC projects in materials chemistry. We would allocate up to \$2,000 of Division II funds to allow two members of the Division to attend this meeting. This motion passed unanimously. Interrante agreed to take the lead on this (**Action Item**).

Subsequent discussions with members of Divisions I and IV and their respective Presidents, that were carried out after this Division meeting, resulted in the reconstitution of the Subcommittee as an Interdivisional Subcommittee on Materials Chemistry, comprised of an equal number of members (2 each) from the initially participating three Divisions. West and Interrante agreed to represent Division II, with Interrante as the new Chair of this Subdivision. The initial meeting of this reconstituted Subcommittee was scheduled for October, 17, 2009 at Cornell University in New York State, and would be

hosted by Chris Ober, President of Division IV and one of the two members of that Division (along with Richard Jones) on the Subcommittee. The remaining two members, representing Division I, were Angela Wilson and Michel Rossi.

The meeting was adjourned for the day at ca. 5:30pm and reconvened the next day (Saturday) at 9:15am.

13- Reports from other IUPAC bodies and Affiliated Organizations **Chemical Nomenclature and Structure Representation Division (Reedijk)**

Reedijk, who is our Division's representative on Division VIII, reported that the Division discussed the question of the proposed name and symbol for element 112, which was suggested by the Darmstadt group and announced publicly prior to their approval by Division II. The early (and bad) publicity on Cp and Copernicium was regretted by the Division. Div. VIII recommended to Div. II NOT to accept Cp.

Regarding the issue of the use of Wolfram as an alternative name for Tungsten^{*}, the following observations were noted,

1. The reply made by Ture Damhus to the 2005 paper in Chem. Intl. by Pilar Goya and Pascual Román (Vol. 27 No. 4 July-August 2005), was reconfirmed as still valid in its entirety. This reply noted that IUPAC nomenclature recommendations are issued in, and intended for use in, the official language of the union, i.e., English, and that the official name for element 74 in English is tungsten. This does not prevent the use of Wolfram, in Spanish, Danish, or other languages, to refer to this element but for reasons of nomenclature in English, Tungsten is the only name for that element that is valid.
2. The text in the old red book was primarily meant as a service to the reader that also "Wolfram" occurs but was not intended to be used as an IUPAC-approved "alternative name" in English for this element.
3. The 2008 memo written by Norman Holden (see Appendix 4 on page 28 of the Helsinki Minutes) was well received and highly agreed with.
4. The use of Wolfram in Mexico is not occurring.
5. The accepted PIN system (Preferred IUPAC Names for compounds) will NOT allow a name for W different from tungsten.
6. As before, in other languages one is free to use names based on Wolfram; (like for K, Na, Hg...)

^{*} This issue was raised originally by Division II members Oro and Garcia from Spain, after wolfram had been removed as an allowed alternative name for element number 74 from the last edition of the "red book". This removal caused some concern/frustration among the Spanish community, homeland of the discoverers of this element, who asked that it should be reinstated as an alternative name for tungsten.

Moreover, a July 31 search on the web of science (2000-2009) for wolfram or wolframate revealed only 1 paper in English relating to wolframate. In particular, Tungsten or tungstate received 19416 hits, Wolfram or wolframate 598 hits (most of which are NOT chemistry, like "wolfram syndrome"), Wolfram or wolframate (and a Spanish address): only 21 (from which only 3 are chemistry: 2 from a journal written in Spanish, Revista de Metallurgia; this left only one paper that was in English: JOURNAL OF PHYSICAL CHEMISTRY A 111 (2007) Pages: 9969-9977 Mixed-valence polyoxometalates: Spin-coupling and electron distribution in the decawolframate anion reduced by two electrons).

Other items from Division VIII:

- PINs: There is now agreement between organic and inorganic (substitutive nomenclature, vs. additive nomenclature): for example, tetrachlorosilane vs. tetrachloridosilicon; i.e. a line in the Periodic Table and certain types of compounds.
- The Blue Book: It is approaching the end (up to some 1400 pages), including PINs and rules to make a PIN

Committee on Chemistry Education (Garcia, P. Mahaffy)

Garcia, our Division's representative, gave a brief report on the CCE. A more detailed report was presented later in the morning by the Chair and Secretary of CCE, after the start of Coplen's Project-by-project review of project status; however, for the sake of the continuity of the subject matter, this report is given below.

Report by Peter Mahaffy (Chair) and Eva Akesson (Secretary) CCE

A major current focus of this Committee is on planning for the International Year of Chemistry in 2011 and the organization of events worldwide that are connected with this. They urged the Division members to become involved at the national and local level with activities that celebrate the achievements of chemistry and its contributions to the well being of humankind. As is noted on the website (<http://www.chemistry2011.org/about-iyf/introduction>), "the Year of Chemistry is intended to reach across the globe, with opportunities for public participation at the local, regional, and national level."

This interactive website features, among other things, an article by Div. II TM Javier Garcia on the Spanish Year (of chemistry). This article is reprinted from the website and attached to these minutes as **Appendix 6**. Akesson acknowledged Garcia's contributions to the work of the CCE, especially in connection with publicizing the IYC within Spain.

Garcia was asked by the Div. Pres. Tatsumi to serve as our representative in planning for the IYC and to develop some options for our consideration at the next Division meeting (**Action Item**).

Akesson also noted that one of the key priority areas identified by CCE for the current biennium was the promotion of a learner-centered chemistry curriculum throughout the world, i.e.,

- *To foreground the importance of learner-centered chemistry curriculum, both in the developed and developing world. The extent to which this is done should be one criterion used to assess educational projects.*

This is being done through Projects in various areas and also as part of the biennial International Conferences on Chemical Education, which are organized through the CCE and attract a large audience of teachers and students from all over the world. The biennial International Conferences on Chemistry Education are flagship activities for CCE. We seek to more fully integrate ICCE activities into the work of CCE and use ICCE conferences to report the outcomes of CCE projects and bring participants together to implement CCE strategies and to build chemistry education networks, using fully the multicultural competence within CCE. The next ICCE, the 21st International Conference on Chemical Education - Chemistry Education and Sustainability in the Global Age, is scheduled for August 2010 in Taipei, Taiwan.

Mahaffy noted that another of the key priority areas for the CCE is increasing the public understanding of chemistry:

- *Increasing the public understanding of chemistry is also of central importance to CCE. In this biennium we plan to work closely with COCI and divisions to obtain broad IUPAC approval for and implementation of our report proposing a niche for IUPAC in public understanding of chemistry. One measure of success will be for Public Understanding of Chemistry to be seen as everyone's responsibility, tied into all IUPAC projects and activities in appropriate ways.*

The CCE meets tomorrow (Sunday) and on Monday, with focus groups continuing on Tuesday. They urged interested Division members to attend these meetings and to think of a global experiment connected to our fields to which students can contribute. Sustainability is one big issue that will be of central importance in the IYC and beyond. They noted that it was important to think beyond the IYC and to develop ideas and projects that might benefit from the international focus on chemistry during the IYC, but would have continuing benefits to chemistry education and society going forward.

YO Miki Hasegawa then gave a short PP presentation on her current efforts to translate from Japanese into other languages and disseminate an illustrated book for children on the elements that was quite popular in Japan a number of years ago.

Committee on Chemistry and Industry (COCI)

This report was also presented out of sequence, in the middle of Coplen's Project-by-project review of project status; however, it is placed here instead, so as to group the different reports received from other IUPAC bodies together under item 13 to avoid confusion.

Mark Cesa, the COCI Chair, presented a report on "Recent activities in COCI", which was also received in electronic form. This is attached as **Appendix 5** of these minutes.

Report on Chemistry International by Fabienne Meyers, Editor

Fabienne stopped by the meeting to give us a short report on *Chemistry International*, the newsmagazine of IUPAC. News about IUPAC, its chemists, publications, recommendations, conferences and the work of its commissions and committees is published bimonthly in CI, both in hard copy form and on the web. Currently ca. 10,000 copies of each issue, which averages 32-36 pages, are distributed worldwide. A series of regular features relating to the IYC are planned for 2011. She welcomed our contributions to CI, which could provide a very effective vehicle for the international dissemination of news, events and general interest articles relating to chemistry.

Report from A. Fajgeli, Vice-President, Division V (Analytical)

In the afternoon, during the following presentations by Coplen and Holden, we received a visit from Ales Fajgeli who gave a short presentation on the activities of Division V.

- In the current biennium (2008-2009) the core bodies of the Analytical Chemistry Division remain the Division Committee, the Interdivisional Working Party on Harmonization of Quality Assurance (WPHQA) and the Subcommittee on Solubility and Equilibrium Data (SSED)
- The Division continues to successfully run a number of divisional and interdivisional projects.
- The Division keeps and actively supports its key publication/databases, namely *The Compendium of Analytical Nomenclature - Orange Book*, the *Solubility Database* and the *Stability Constants Database*.

The Orange Book:

The Officers confirmed the need to maintain the Orange Book as a major ACD and IUPAC product. It was agreed that:

- The Orange Book shall be updated.
- The ACD committee will take responsibility of revising the Orange Book.
- The revision of the Orange Book will be proposed as a major ACD project to IUPAC.
- Each ACD TM shall be involved in the revision, and will be required to take responsibility for a sub-project.
- Selection of candidates by the Nominating Committee should take into account their capacity for contributing to the revision of the Orange Book.
- It was agreed that the Orange Book is a compilation of the present IUPAC terminology. If it is found that sections need revision of terms, separate projects will be required to create IUPAC recommendations published in PAC.
- The Officers supported the 'glossary format' in which alphabetical arrangement of terms would include a definition (in appropriate ISO format), and appropriate brief notes and examples.

- The product will be published as a book, and as an electronic product. The material will be able to be extracted for the Gold Book.

The Stability Constants Database:

The agreement reached with the Bureau is that data collection will terminate at the end of the current project (which will complete data compilation from the literature to the end of 2006) and that the database will be made available through IUPAC as a frozen compilation, until such time as interested parties within IUPAC identify a need to continue the work in what is then seen as a timely fashion and format for identified end-users.

- For the current biennium the Division has established focus (interest) groups on Communication, Critical evaluation of data, Electronic resources for IUPAC terminology work, Emerging analytical issues, Metrology, and the Analytical potential of nuclear techniques.
- The Division continues publishing its newsletter *Teamwork*, which serves for communication within the Division and with other IUPAC members and bodies.
- The Division is actively involved in global harmonization and standardization activities, where in the current biennium a special emphasis was put to metrology in chemistry. This is considered as very important, and for the GA in Glasgow, meetings with other Divisions are planned, mainly on the information about the project on Metrological Traceability of Measurement Results in chemistry.
- The Division actively cooperates with number of international organizations and bodies (e.g. BIPM, CITAC, EURACHEM, IAEA, IAM, IUPAP, UNIDO, etc.)
- Based on a good geographical distribution of its members, and on the above mentioned cooperations, the Division is continuing its efforts in supporting chemists in developing countries and economies.

14- Reports on recent, planned and proposed Division-sponsored conferences
High Temperature Materials Conference (HTMC-XIII) (West)

HTMC XIII is scheduled for 14-18 September 2009 in Davis, California. Prof. Dr. Alexandra Navrotsky is the chair of the local organizing committee. This is the 13th Conference in a series of triennial meetings, with the previous two held in 2003 in Tokyo (Japan) and in 2006 in Vienna (Austria). Former Division II President Gerd Rosenblatt was planning to attend on behalf of the Division and IUPAC, and to give a brief presentation on IUPAC and the Conference series. The next conference in this series, HTMC XIV, will be held in 2012 in Beijing, China.

Next Workshop on Advanced Materials (WAM IV)

The last WAM (WAM III) was held in Stellenbosch, South Africa in 2005, and WAM IV was originally planned for 2008; however, these plans fell through and Mathur had agreed to try to revive this series and find an alternative location and conference organizer. Mathur was unable to attend this GA and no report was received regarding the outcome of these efforts. We must therefore consider this Workshop series to be at least temporarily suspended.

Reedijk reported on ICCC 39, the 39th International Conference on Coordination Chemistry, which is scheduled to be held in Adelaide, Australia on July 25-30, 2010 (<http://iccc2010.eventplanners.com.au/>). According to the website, "the conference will bring together the world's leading coordination chemists to showcase the latest developments in this field of science. This will include fundamental coordination chemistry through to chemistry specifically addressing the pressing concerns of the 21st century, exemplified by energy, environmental, and medicinal chemistry."

15 - Project-by-project review of project status (Coplen)

Part I: Review of Funded Projects

Project Coordinator Coplen reported that the Division currently has 17 1/2 funded projects, 5 of which are extending past their planned ending date, but are almost completed. In comparison, at our Helsinki meeting, we had 15 funded projects, 7 of which were extended past their planned ending dates. We are currently in the middle of the pack among the Divisions in terms of overdue projects, but it is better than it appears, as several of these projects have completed their work and submitted reports, but are awaiting their publication in PAC to be considered "officially" complete.

2000-024-1-200 Balducci

Teaching High Temperature Materials Chemistry

Division Monitor, G. Rosenblatt; \$4,800 allocated, \$4,508 spent

status: Completed

2001-015-1-100 Stanbury

Standard potentials of radicals

Planned Ending Date: 30-Jun-2009

Allocated: 21,000 (with Div I); Spent: 20,525

Div Monitor: Rosenblatt (Replacement needed?)

Comment: Extended by a year from June 2008 to June 2009

Progress:

Stanbury reported that: "Progress on this IUPAC project has been slow this year, but I believe that we are nearing completion. The greatest challenge in the inorganic component of the Radical Potentials project has been assignment of the dioxygen/superoxide potential. Although this potential is reasonably well-known, assignment of a "best" value has been contentious within the Task Group. The value is derived from measurements of equilibrium constants of electron-transfer reactions with other "reference" redox couples. The problem is that the reference couples are not as reliable as has been widely believed. We have now assessed the reliability of the reference couples. Last month I traveled to Zurich to visit Wim Koppenol (a Task Group member), and we reviewed the data and arrived at a consensus. The next step will be to prepare a document regarding this consensus,

circulate it to the other Task Group members and solicit their opinions. Hopefully all will be in agreement and we can proceed to preparation of the final reports."

2001-019-1-200 Walczyk

Guidelines for mass spectrometric isotope ratio measurements

Planned Ending Date: 31-Dec-2007

Allocated: 2,000; Spent: 2,000

Div Monitor: Coplen

Comment: Waiting for publication of two reports in PAC

Submitted to PAC: "Explanation of terms used in expression of relative isotope ratios and gas ratios (IUPAC Recommendation)", by T. Coplen; 25 reviews were received;

Revised: 9 reviews; Revised again, 2 reviews; Revised a third time, 1 15-page review;

How do we get it published?

2003-031-1-200 Berglund

Isotopic Compositions of Selected Elements

Planned Ending Date: 31-Dec-2007

Allocated: 12,000; Spent: 13,026

Div Monitor: Loss

Comment: Revision of final report nearly complete—sent to PAC and waiting for publication

Submitted to PAC: Atomic Weights of the Elements 2007, IUPAC Technical Report by M.E. Wieser and M. Berglund; this is the Final report for: 2003-033-1-200, Wieser; 2003-031-1-200, Berglund; 2001-019-1-200, Walczyk; 2005-027-1-200, Berglund

2003-033-1-200 Weiser

Determination of Atomic Weights Using New Analytical Techniques

Planned Ending Date: 1-May-2008

Allocated: 14,800; Spent: 14,800

Div Monitor: Loss

Comment: Revision of final report submitted to PAC, waiting for publication

2003-034-1-200 Kniep

Classification, Terminology and Nomenclature of Borophosphates

Allocated: 16,000; Spent: 0

Div Monitor: West

Comment: Completed. The Task Group concluded that because the borophosphates are a very diverse group of compounds with complex structures that span 0-3 dimensions in nature and occur with a variety of compositions, that it would be extremely difficult to propose a systematic nomenclature covering all possibilities. The Task Force therefore regards its project as complete.

2005-001-1-200 Day

Towards Defining Materials Chemistry

Planned Ending Date: 31-Dec-2007

Allocated: 8,000; Spent: 4,583

Div Monitor: West

Comment: essentially complete, with articles in Chemistry International and PAC (see Item 11 for full details)

2005-022-1-200 Brand/Coplen

Calibration of Organic and Inorganic Oxygen-bearing Isotopic Reference Materials

Allocated: 12,000; Spent: 10,546

Div Monitor: Coplen

Comment: Completed; Publication in Rapid Communications in Mass Spectrometry

The Goal: Measurement of the same homogeneous sample by any laboratory worldwide should yield the same isotopic composition within analytical uncertainty.

The fraction of ^{18}O in many naturally occurring substances can be used to infer the origin, source, or history of the substance. Relevant to forensic and environmental applications.

The aim was to calibrate 3 waters, 3 sulfates, 3 nitrates, and 3 organic oxygen-bearing isotopic reference materials. This turned out to be far more difficult analytically than anticipated; involved 5300 measurements by six laboratories.

2005-027-1-200 Berglund

Evaluated Published Isotope Ratio Data (2005-2007)

Planned Ending Date: 31-Dec-2007

Allocated: 9,800; Spent: 8,750

Div Monitor: Loss

Comment: Final report submitted to PAC. Authors are Wieser and Berglund

2005-043-1-400 Ober

Terminology for self-assembly and aggregation of polymers

Planned Ending Date: 1-Apr-2009

Joint with Div IV; Allocated: 6,000 (2k from Div II); Spent: 5,719

Div Monitor: Chadwick

Comment: no update was received from Ober

2006-016-1-200 Renne

Recommendations for Isotope Data in Geosciences

Planned Ending Date: 31-Dec-2009

Allocated: 4,900; Spent: 0

Div Monitor: Holden

Comment: Object is to update and harmonize recommendations on half-lives and isotopic compositions

Progress: Bilateral meetings were held in Beijing, Berkeley, & Upton (NY).

Issues Identified: The standard and symbol used for the measurement of the half-lives of long-lived radionuclides used for age determinations.

A standard unit of time is needed;

A year is not a defined quantity in SI; instead the second is.

- A year decreases by 0.530 s per century.
- For the symbol of time unit, year, the IUPAP's SUN (Symbols, Units and Nomenclature) and IUPAC's "Green Book" recommend "a" for annum. Problem: Others don't.
- Definitions of time in terms of seconds
 - The Julian Year = 365.25 days = $3.155\,760\,(10)^7$ seconds.
 - The Gregorian Year = 365.2420 days = $3.155\,690\,88\,(10)^7$ seconds.
 - The Sidereal Year = 365.256 360 417 days = $3.155\,814\,954\,(10)^7$ seconds.
 - The Calendar Year (non-leap year) = 365.00 days = $3.1536\,(10)^7$ seconds.
 - The Calendar Year (leap year) = 366.00 days = $3.162\,24\,(10)^7$ seconds.

Uncertainty: For a publication on a half-life measurement for which no specification is given for the standard unit of the year, the uncertainty could be as large as +0.07% for a non-leap year measurement, while the uncertainty could be as large as – 0.21% for a leap year measurement merely due to the uncertainty in the standard.

The quoted half-life value would have an inherent "type B" uncertainty of 0.21% (see the International Organization for Standardization, ISO, Guide to the Expression of Uncertainty in Measurement, GUM), independent of any other type A or type B uncertainties.

This could limit the accuracy of age determinations to no better than 0.2%, depending on the half-life measurement used.

Results: Publication submitted to Pure and Applied Chemistry and comments from the editor of PAC are being resolved now.

Future Plans: Due to the problems associated with the standard unit, year, an effort to reevaluate the major publications on half-lives being used for age determinations will begin to assess the type A and type B uncertainties in these publications

Recommendations (**Action Item**)

It is recommended that Division II and IUPAC extend the deadline (by 15 months) for this Task Group to December 31, 2009 (at no additional cost to IUGS or IUPAC) to allow time for the reevaluation of the half-life publications.

A similar request is being made to the IUGS Executive Committee to extend their funding period for this Task Group to December 31, 2009 also.

2006-025-1-200 Holden

Assessment of fundamental understanding of isotopic abundances and atomic weights of the chemical elements (SNAFU for short)

Planned Ending Date: 31-Dec-2009

Allocated: 9,800; Spent: 6,861

Div Monitor: Holden

Comment: Object is to review fundamental issues and concerns that have been raised by members of the Commission on Isotopic Abundances and Atomic Weights.

Holden gave a PowerPoint presentation on this Project and on the work of the Subcommittee on the Natural Assessment of Fundamental Understanding (SNAFU).

- Meeting 18-20 July, 2007 at the BIPM (Bureau International des Poids et Mesures), Sèvres, France
- Meeting 20-21 July, 2009 at International Atomic Energy Agency in Vienna, Austria

Participants

N. E. Holden, Chairman

T. B. Coplen, Secretary

P. De Bièvre

J. K. Böhlke

J. de Laeter

E. Roth (2007 meeting and participant through early 2009)

- The Committee started with understanding the key issues/ problems and questions that needed to be answered.
- Using expertise of Senior Task Force members (cumulative 188 years experience on IUPAC) addressed key problems, reviewed reports/ meeting minutes
- Identified Options
- Created recommendations
- Analyzed/Discussed recommendations with Commission
- Continuing approach with additional issues generated from Commission discussion

Key Problems/Issues 2007

- Discussion of Multiple Audiences for the work of CIAAW
- Are data products different for potentially different CIAAW audiences?
- Potential publication time scales and other recommended details
- Do radioactive elements require an atomic weight value?
- Does the definition of atomic weight require a revision?
- Uncertainty treatment for recommended atomic weights and abundances
- Treatment of natural variations for potentially different CIAAW audiences
- Status and recommendations for a CIAAW website and design
- Should CIAAW prepare an ISO VIM subdocument for isotope measurements?

2007 Recommendations

A list of 24 recommendations that were made and their status was presented. The first of these recommendations was the establishment of a CIAAW website for the scientific public having data and publications from published Commission reports. This website is now up and running (<http://www.ciaaw.org/>) and contains much useful information about the Commission, its history and purpose, as well as data on atomic weights and isotopic abundances and publications that can be downloaded as pdf files.

A key point made was that the atomic weights of the elements are not constants of nature but depend on the relative abundance of the various isotopes of that element, which can vary significantly depending on the source of that element. The single value is selected to be near the middle of the range of variation and therefore may not correspond to any measured value.

Key Problems/Issues 2009

- Advantages and Disadvantages of “Range” versus Atomic Weight; contrast the range of values with standard values and uncertainties.
- If a “range” of atomic weight values is recommended, how should a user select a preferred value from a range?
- What footnotes and annotations are needed for the Table of Atomic Weights and the Table of Isotopic Compositions?
- What is meant by a calibrated system for isotopic measurements?
- What requirements should be placed on the use of reference materials in isotopic measurements?
- How can the Commission develop a comprehensive system for isotopic literature coverage?
- What should be the required publication cycle for the Table of Isotopic Compositions?
- Is there a need for a new definition of a Standard Atomic Weight?

2009 Recommendations

Issue:

Advantages and Disadvantages of “Range” or Atomic Weight; contrast the range of values with standard values and uncertainties.

Recommendation:

SNAFU recommends that TSAW 2009 include ranges of atomic weights and recommended (reference) values for polynuclidic elements when the range exceeds the measurement uncertainty.

Issue:

If a “range” of atomic weight values is recommended, how should a preferred value be selected and provided to the reader?

Recommendation

SNAFU recommends that the preferred value of an atomic weight for elements with an evaluated range that exceeds the measurement uncertainty be the TSAW 2007 standard atomic weight value without an uncertainty value attached.

Issue:

What footnotes and annotations are needed for the Table of Standard Atomic Weights and the Table of Isotopic Compositions?

Recommendation

- SNAFU recommends that non-mass dependent variations of isotopes be identified in TICE by a footnote, which is explained in the rubric.
- SNAFU recommends that elements with radiogenic isotopes be identified in TICE by a footnote, which is explained in the rubric.
- A unique footnote is recommended to cover elements with anomalous isotopic compositions from the 2 billion-year-old natural nuclear reactor at Oklo, Gabon.
- Ensure that footnotes and annotations are consistent between TSAW and TICE.

Issue:

What is meant by a calibrated system for isotopic measurements?

Recommendation

SNAFU recommends that a project proposal be prepared to form a task group headed by John de Laeter to prepare a document on guidelines on atomic weight and isotopic abundance measurements.

This document should be published by PAC and educational journals.

Issue:

What requirements should be placed on the use of reference materials in isotopic measurements?

Recommendation

SNAFU recommends that the Commission needs to provide a priority list of isotopic reference materials for elements that do not presently have isotopic reference materials, taking into consideration the physical form of the material. (This might be an outcome of the project on isotopic reference materials.)

SNAFU recommends that the scope of future work of the Commission incorporate isotopic reference material value assessment. This could be a Subcommittee. The Commission might consider preparing a project proposal, working in cooperation with other international and national organizations involved with isotopic reference materials.

Issue:

How can the Commission develop a comprehensive system for isotopic literature coverage?

Recommendation

SNAFU recommends that the Commission should develop a set of keywords for identifying papers involving new standard atomic weights and/or ranges.

Issue:

What should be the required publication cycle for the Table of Isotopic Compositions?

Recommendation

- SNAFU recommends that the Commission prepare a TICE 2009 document for publication.
- SNAFU recommends that TSAW and TICE be published concurrently whenever the TICE data change.
- SNAFU recommends that current atomic masses be incorporated into each new TICE publication after 2009.

Issue:

Is there a need for a new definition of a Standard Atomic Weight?

Recommendation

SNAFU recommends that the Commission take up a discussion for a new definition of standard atomic weight. It should be noted that a new definition could impact several disciplines (Divisions) within IUPAC, and a change could take half a decade over many general assemblies.

Additional Recommendations

SNAFU recommends that the Chairman of the Commission indicate to the Division and the Secretariat that the 2007 Atomic Weights Report be published under the old rules. Paul De Bièvre will make the same request to Division V (Analytical Chemistry Division).

The Commission should include a statement on measurement uncertainty in its regular reports; all measurement uncertainties are measurement uncertainties with coverage factor $k=2$ unless otherwise noted (Std Dev = 2 sigma). This implies that the annotations C, F, L, and N might be eliminated in column 6 (best measurement) of the TICE table for future updates, retaining the historical information.

- SNAFU recommends that Paul De Bièvre prepare a proposal to the JCGM Working Group on the VIM on the contribution of the uncertainty evaluations of the Commission.
- The Commission should prepare a project proposal on TICE for the 21st Century that would be database intensive.
- The Commission should alert members that 2/3 funding of travel (lodging, meal and incidentals, and air travel) might be the rule in the future with exceptions in some necessary cases.
- The Commission should make its publications compliant with GUM, which means compliant with metrological concepts. This may involve preparation of a project proposal.
- SNAFU recommends that its members provide the Commission with a proposed TSAW in revised format for the 2009 meeting, and that this update be provided Tuesday July 28.

Next Steps

Consider evaluating the uncertainty in the atomic mass tables and its impact on the standard atomic weight values of mononuclidic and near mononuclidic elements, which

account for approximately 1/4 of the first 92 elements. This might require a project proposal.

Conclusion

The SNAFU project has identified more than 40 major issues facing the Commission and suggested solutions for the majority of these issues.

2006-028-1-400 Vohlídal (new)

Terminology for conducting, electroactive and field-responsive polymers

Planned Ending Date: 1-Sept-2009

Allocated: 6,000 total (with Div IV); Spent:4,431

Div Monitor: Chadwick

Comment: With recent advances in the realm of organic electronics for displays, solar cells, and other applications, the entire field of electroactive polymers is of growing importance. This project is aimed at proposing a list of terms and definitions to be accepted and respected by chemists and others working as materials scientists within academia and industry.

2006-046-1-200 Karol

Priority claims for the discovery of elements with atomic number greater than 111

Planned Ending Date: 1-Aug-2009

Allocated: 10,200; Spent: 7,290

Div Monitor: Corish

Claims for the discovery of elements of atomic number greater than 111 have been invited and the scientists name below have submitted the following claims:

Dr. Amnon Marinov, The Hebrew University, Jerusalem, Israel; for element 112

Dr. Kosuke Morita, The Institute of Physical and Chemical Research, Riken, Japan; for element 112 (in part) and element 113

Dr. Sergey Dimitriev, Joint Institute for Nuclear Research, Dubna, Russia; for elements 112, 113, 114, 115, 116, and 118

Dr. Sigurd Hofmann, Gesellschaft fur Schwerionenforschung mbH, Darmstadt, Germany; for element 112

2007-028-1-200 Berglund

Evaluated Published Isotope Ratio Data (2007-2009)

Planned Ending Date: 31-Dec-09

Allocated: 12,800; Spent: 0

Div Monitor: Loss

Comment: Meeting in Vienna, Austria (2009)

Data Evaluation contributing to Table of Isotopic Compositions of the Elements (TICE) and Table of Standard Atomic Weights of the Elements (TSAW)

2007-029-1-200 Zhu

Evaluated Published Isotope Ratio Data (2007-2009)

Planned Ending Date: 31-Dec-09

Allocated: 12,800; Spent: 0

Div Monitor: Loss

Comment: Meeting in Vienna, Austria (2009)

Data Evaluation contributing to Table of Isotopic Compositions of the Elements (TICE) and Table of Standard Atomic Weights of the Elements (TSAW)

2007-031-1-200 Schönberg

Evaluated Compilation of International Reference Materials for Isotope Abundance Measurements

Planned Ending Date: 31-Dec-2010

Allocated: 13,750; Spent: 0

Div Monitor: Coplen

Comment: Making excellent progress.

2007-038-3-200 Holden

Development of an Isotopic Periodic Table for the Educational Community

Planned Ending Date: 31-Dec-2010

Allocated: 11,000; Spent: 0

Div Monitor: Holden

Comment: Recently funded along with the Committee on Chemical Education (CCE)

2007-040-2-200 Garcia-Martinez

Analysis of the Usage of NanoScience and Technology in Chemistry

Planned Ending Date: 31-Dec-2009

Allocated: 4,000; Spent: 0

Div Monitor: Garcia

A brief oral report on this Project was received from Garcia. The main focus of this Project is on tracking the usage of the prefix "nano" and its connections with other key words, e.g., catalysis, etc. in scientific publications. He expects to write a report on his findings soon and may possibly finish by the end of this year.

2008-006-3-100 Sun

Thermodynamic study on hydrogen storage materials: metal organic frameworks and metal or complex hydrides

Planned Ending Date: 30-Jun-2011

Allocated: 15,000 (1,000 from Div II); Spent: 0

Div Monitor: Needs to be assigned

Comment: Recently funded

2008-040-1-200 Karen

Towards a comprehensive definition of oxidation state

Planned Ending Date: 1-Mar-2011

Allocated: 4,200; Spent: 0

Div Monitor: Karen

Comment: Making excellent progress

Part II: Review of Project Proposals

Current Division II Budget

Total biennial allocation: USD 53,200

Expenditures (as of 3-Jul-09): USD 16,340

2007-031-1-200, Schönberg, USD 5,750

2007-038-3-200, Holden, USD 1,000

2007-040-2-200, Garcia-Martinez, USD 4,000

2007-006-3-100, Sun USD 1,000

2008-040-1-200, Karen USD 4,200

One project proposal could be funded immediately

2007-030-1 Wieser, Evaluation of Radiogenic Abundance Variations in Selected Elements 8,500; This project received three very suitable reviews in 2007, but it could not be funded at that time. The only negative comment was that one reviewer suggested that younger task group members be added, noting that three of the members were over 70 years of age.

One of the proposed task members, Dr. Etienne Roth, passed away earlier this year. Dr. Holden has also removed his name from this proposal, and two younger task members have been added.

It could be funded immediately.

Proposals submitted

2009-012-1 Öhrström Coordination polymers and metal organic frameworks: nomenclature guidelines 13,615

This project looked very good even though it has not gone to outside reviewers. It was funded for about 5 to 6 k so that task members could meet in Glasgow.

2009-020-1 The Development of International Standards for Editors, Authors and Reviewers of Chemical Publications Interrante, Task Group Chairman
3 yr 12,500

ACS will provide 12,500 for a total of 25,000. We encouraged that this proposal be submitted in Helsinki. Coplen provided that information to Dr. Fabienne Meyers and recommended that it be sent out for review.

Technical Guidelines for Isotope Abundances and Atomic Weight Measurements (Prof. John de Laeter) 1 yr 2,500

Prepare a document on guidelines on isotope abundance and atomic weight measurements in a form suitable for publication.

This document is directed at the mass spectrometric community.

Recent experience at Commission meetings has indicated that there is a lack of understanding in mass spectrometric protocols and uncertainty determinations.

The intention of this project is to improve the quality of the reporting isotopic measurements in the international literature. The quality of isotope publications should be improved so that there will be an increase in the number and quality of isotopically based papers for consideration by the Commission.

Online evaluated isotope ratio database for user communities (2010-2011) (Dr. Michael Berglund) 2 yr 6,000

Facilitate and streamline the management of isotope data as used by CIAAW and its subcommittees during data evaluation, numerical processing, and provide customized isotope related output for the CIAAW members, IUPAC, and wider user communities.

The online database will improve the speed and accuracy of the data evaluation, retain historical information and explanation, and provide instant specific access for user communities of approved data.

Assessment of Stable Isotopic Reference and Inter-Comparison Materials (Dr. Willi Brand) 2 yr 9,600

The objective of this project is to compile a list and evaluate isotopic composition values of available reference materials suitable for stable isotope analysis.

The resulting compilation listing all relevant information for user communities will also be useful in identifying which materials are missing. A second objective is to evaluate newly published measurements and assess the validity of new results as a means to establish new values for the community.

Compilation and evaluation of isotopic fractionation factors for environmental investigations (Dr. Tiping Ding) 3 yr 6,000

The objective is fostering the application of isotope techniques in environmental studies. Isotopes are in fact among the most powerful tracers for investigating deterioration, contamination and remediation of water resources, air, the biosphere, etc. There is no doubt that these problems will be crucial in 21st century.

Values of isotopic fractionation factors for reactions and processes of interest for environmental investigations will be reviewed and evaluated. The isotopic fractionations for which there are no values available in the scientific literature will be identified.

Recommendations for Isotope Data in Geosciences (Dr. Paul Renne) 3 yr 4,900

Update & harmonize recommendations on half-lives & isotopic compositions.

A specific goal of the project is to reconcile current inconsistencies between values used in geological and planetary sciences on the one hand, and those used in the nuclear physics and chemistry communities on the other. The project will draw on complementary expertise present in IUGS and IUPAC. Previous work by IUGS (Working Group “Decay constants in geochronology”) and IUPAC (Commissions II.1 “Isotopic abundance” and V.7 “Radiochemistry and Nuclear Techniques”) will be included, harmonized, and updated. IUGS-IUPAC interaction will be tightened. Phase II (2010-2011) focuses on 7 nuclides used in geochronology (40K, 87Rb, 138La, 147Sm, 176Lu, 187Re, 232Th).

Evaluated Published Isotope Ratio Data (2010-2011) (Dr. Takafumi Hirata) 2 yr 13,200

Evaluate isotope ratio publications between 2009 and early 2009 and early 2010 to determine “best isotope ratio measurements” for compilation and publication in a 2011 TICE, recommend “new” standard atomic weights, and publish “Atomic Weights of the Elements 2011” in Pure & Applied Chemistry, which will also include a table of relative atomic masses.

Nuclidic mass evaluation (2010-2011) (Dr. Norman Holden) 2 yr 2,500

Evaluate nuclidic masses, which has not been done for nearly a decade.

Preparing the IUPAC Commission on Isotope Abundances and Atomic Weights for uncertainty budgeting in light of the GUM (2010-2011) (Dr. Paul De Bièvre) 3 yr 4,000

To prepare the introduction of measurement uncertainty budgets that follow the GUM approach in the documents, reports and publications, released by IUPAC-CIAAW (including its Subcommittees), thus ensuring that CIAAW works in consistency with the ISO Guide on the “Expression of Uncertainty in Measurement”), JCGM 100-2008 (“GUM”). IUPAC is one of the eight international organisations (BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, OIML) which have unanimously approved the GUM as prepared by the Joint Committee on Guides for Metrology, JCGM.

Preparing the IUPAC Commission on Isotope Abundances and Atomic Weights for uncertainty budgeting in light of the VIM (2010-2011) (Dr. Paul De Bièvre) 2 yr 6,000

To prepare the introduction of VIM-compliance of the documents, reports and publications, released by IUPAC-CIAAW (including its Subcommittees), thus ensuring that CIAAW works in full consistency with the “International Vocabulary of Metrology – basic and general concepts and associated terms (VIM) edition 3, JCGM 200-2008 (“VIM3”). IUPAC is one of the eight international organizations (BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, OIML), which have unanimously approved VIM3 as prepared by the Joint Committee on Guides for Metrology, JCGM.

Summary of Proposals in progress:

2007-030-1 Wieser (can decide to fund today)	8,500
2009-012-1 Öhrström funded)	13,615 (already part.
2009-020-1 Interrante	12,500
Technical Guidelines for Isotope Abundances and Atomic Weight Measurements (de Laeter)	2,500
Online evaluated isotope ratio database for user communities (2010-2011) (Berglund)	6,000
Assessment of Stable Isotopic Reference and Inter-Comparison Materials (Brand)	9,600
Compilation and evaluation of isotopic fractionation factors for environmental investigations (Ding)	6,000
Recommendations for Isotope Data in Geosciences (Renne)	4,900
Evaluated Published Isotope Ratio Data (2010-2011) (Hirata)	13,200
Nuclidic mass evaluation (Holden)	2,500
Preparing the IUPAC CIAAW for uncertainty budgeting in light of the GUM (De Bièvre)	4,000
Preparing the IUPAC CIAAW for uncertainty budgeting in light of the VIM (De Bièvre)	6,000

Total, about USD 89 k

The Division decided to fund the Weiser Proposal for USD 8,500 and to send the others out for review.

16 – Other Business

Appointment of Division representatives (Tatsumi)

Tatsumi announced that Norm Holden had agreed to take the place of L. Oro as our Division's representative on ICTNS.

Status of the Information Packet for New Division Members

Loss has put together a draft of the Information Pack for new/prospective Division members which is attached to these Minutes as **Appendix 7**.

This Information Pack is intended to provide information for new/prospective members to be better prepared to participate effectively in Divisional meetings or assist them in deciding on becoming Divisional members. The members were urged to look this over and give him their suggestions for changes or additions.

Other Reports and Potential Projects

Ken Sakai gave a Power Point presentation relating to a proposed project for providing technical guidelines for the luminescence quantum yield determination of inorganic compounds. He first explained what he had proposed and was discussed in the previous off-year meeting in Helsinki. Although the project proposed in Helsinki was to accurately re-evaluate the luminescence quantum yield of $\text{Ru}(\text{bpy})_3^{2+}$, he ultimately decided not to do so but to prepare a document suggesting that the use of this compound as an international standard for the luminescence quantum yield should be avoided because of its too high sensitivity towards the change of temperature and the change in the O_2 concentration in solution. The former effect was explained to be due to the fact that the emitting state (triplet metal-to-ligand charge transfer state; i.e., triplet MLCT state) is in a thermal equilibrium with another triplet excited state called a triplet d-d state. The latter was explained to be due to the energy-transfer quenching of the triplet MLCT state by O_2 . His new proposal from this division is to prepare a document on guidelines for the luminescence quantum yield determination of inorganic compounds. He suggests that the document be directed to the broad area of luminescent molecules. The document is intended to be published in an IUPAC Technical Report together with a Web page of IUPAC. The anticipated impact of this project is that the luminescence quantum yields reported in scientific papers can be made more trustworthy by using the guidelines that are to be generated under this project.

YO Dan Rabinovich presented an interesting slide show that he had developed on "chemistry in stamps" in connection with the IYC. He was encouraged by the members to submit a proposal for creation of a website that would illustrate chemistry through stamps.

The meeting was adjourned at ca. 4pm.

Appendix 1

ACTION ITEMS GLASGOW August 2009

1. Javier agreed to be the Div II representative to San Juan meeting & IYC 2011 liaison.
2. Bob Loss will resurrect a nominating committee after a week or so should it be needed to address the changes in Div. II officers required if K. Tatsumi is elected as President of IUPAC.
3. Len will deliver a press release to the Secretariat on behalf of the Comission this week.
4. Everyone should distribute the newsletter to their respective communities.
5. Len will coordinate a meeting of 2 people from Div II with 2 people from Div I and 2 from Div IV to write up a justification for a new Materials Chemistry entity.
6. Division II and IUPAC needs to extend the deadline (by 15 months) for Project 2006-016-1-200 to December 31, 2009 (at no additional cost to IUGS or IUPAC) to allow time for the reevaluation of the half-life publications.

Appendix 2

Inorganic Chemistry Division Committee 2010-2011

Name	Proposed Status	Proposed Term	NAO
Prof. Robert D. Loss	TM - President	2010-2013	Australia
Prof. Jan Reedijk	TM - Vice President	2010-2013	Netherlands
Prof. Leonard V. Interrante	TM - Secretary	2008-2011	United States
Prof. Kazuyuki Tatsumi	TM - Past President	2010-2011	Japan
Prof. Tiping Ding	TM	2008-2011	China/Beijing
Dr. Norman E. Holden	TM	2010-2013	United States
Prof. Pavel Karen	TM	2010-2013	Norway
Prof. J. García-Martínez	TM	2008-2011	Spain
Prof. Sanjay Mathur	TM	2010-2013	Germany
Prof. Ken Sakai	TM	2010-2013	Japan
Dr. Tamara V. Basova	AM	2010-2011	Russia
Dr. Milan Drábik	AM	2010-2011	Slovakia
Prof. Markku Leskelä	AM	2010-2011	Finland
Prof. Ling-Kang Liu	AM	2010-2011	China/Taipei
Prof. Lars R. Öhrström	AM	2010-2011	Sweden
Dr. Tyler Coplen	AM	2010-2011	United States
Prof. Md. T. Hossain Tarafder	NR	2010-2011	Bangladesh
Prof. N. Trendafilova	NR	2010-2011	Bulgaria
Prof. V. Chandrasekhar	NR	2010-2011	India
Dr. R. Gonfiantini	NR	2010-2011	Italy
Prof. Tara Dasgupta	NR	2010-2011	Jamaica
Prof. K. Yoon	NR	2010-2011	Korea
Prof. Lai-Yoong Goh	NR	2010-2011	Malaysia
Prof. A. Kilic	NR	2010-2011	Turkey
Prof. Anthony West	NR	2010-2011	UK
Prof. Aldo Bologna Alles	NR	2010-2011	Uruguay
	10 TMs, 6 AMs, 10 NRs		

AM = Associate Member

NR = National Representative

TM = Titular Member

Appendix 3

Draft report for the Inorganic Division Commission on Isotope Abundances & Atomic Weights (CIAAW) Report for 2008-2009

The Titular and Associate members, National Representatives and Observers present at the Commission on Isotope Abundances and Atomic Weights Meeting in Vienna were: R. Gonfiantini (Chair, Italy), M. Wieser (Secretary, Canada), M. Berglund (Belgium), M. Gröning (Austria), N. Holden (USA), T. Walczyk (Singapore), S. Yoneda (Japan), W. Brand (Germany), T. Hirata (Japan), R. Schönberg (Norway), X. Zhu (China), P. De Bièvre (Belgium), J.R. De Laeter (Australia), J.K. Böhlke (USA), T.B. Coplen (USA), T. Ding (China), R. Loss (Australia), R. Kessel (USA), J. Meija (Canada)

The Commission on Isotopic Abundances and Atomic Weights met at the International Atomic Energy Agency in Vienna, Austria from the 28th to the 29th of July, 2009 under the chairmanship of Prof. Roberto Gonfiantini. This was a historic meeting of the Commission on Isotopic Abundances and Atomic Weights. In anticipation of the International Year of Chemistry IYC-2011, the Commission focussed on the educational needs of Chemistry students worldwide with its attempt to emphasize the non-constancy (variability) of the atomic weight values of many elements. The variation in the isotopic composition of various terrestrial samples of these elements leads to a range of atomic weights for these elements. The atomic weights of these elements are now listed with ranges rather than a value with a large uncertainty, which could imply that a measured value with a measurement uncertainty was being provided.

Following up on the topic of educating the Chemistry student for the IYC, the Commission has prepared a first draft of a Periodic Table of the Isotopes. This table should help to inform students that chemical elements are made up of stable isotopes and unstable isotopes, while displaying their properties and applications in everyday experiences. The theme of atomic weight variations in nature for many elements will be displayed on the element page of the "IUPAC Periodic Table of the Isotopes".

The third initiative of the Commission at this year's meeting dealt with Isotope Reference Materials (IRM) for which a subcommittee has been formed. These IRMs are used to normalize the results from the analysis of isotopic composition of materials and are necessary to allow intercomparison of data. This subcommittee will perform assessments of IRMs via project proposals to IUPAC.

In addition, the Commission has resubmitted the Subcommittee for Natural Assessment of Fundamental Understanding, which was inadvertently omitted by the Division previously. The group has worked without formal status over the past few years and has addressed

over forty challenges facing the Commission and has suggested solutions to most of these obstacles.

The standard atomic weights of 23 chemical elements are under review for change based on determinations of isotopic abundances and reviews of previous isotopic abundances and atomic masses (IUPAC, Pure and Applied Chemistry, vol. 74, pp 1987-2017, 2002). The Commission will consider changing the Standard Atomic Weights of the following 22 elements as follows:

hydrogen: from 1.007 94 +/- 7 to the range 1.007851 – 1.008010
helium: from 4.002 602 +/- 2 to the range 4.002600 – 4.002603
lithium: from 6.941 +/- 2 to the range 6.9387 – 6.9959
boron: from 10.811 +/- 7 to the range 10.8062 – 10.8207
carbon: from 12.0107 +/- 8 to the range 12.00966 – 12.01150
nitrogen: from 14.0067 +/- 2 to the range 14.00643 – 14.00727
oxygen: from 15.9994 +/- 3 to the range 15.99904 – 15.99976
magnesium: from 24.3050 +/- 6 to the range 24.3046 – 24.3055
silicon: from 28.0855 +/- 3 to the range 28.08522 – 28.0878
sulfur: from 32.065 +/- 5 to the range 32.059 – 32.075
chlorine: from 35.453 +/- 2 to the range 35.4472 – 35.4553
argon: from 39.948 +/- 1 to the range 39.948 – 39.962
calcium: from 40.078 +/- 4 to the range 40.0778 – 40.0784
chromium: from 51.9961 +/- 6 to the range 51.9961 – 51.9982
iron: from 55.845 +/- 2 to the range 55.84477 – 55.84532
nickel: from 58.6934 +/- 4 to the range 58.6930 – 58.6938
copper: from 63.546 +/- 3 to the range 63.542 – 63.549
zinc: from 65.38 +/- 2 to the range 65.36 – 65.40
selenium: from 78.96 +/- 3 to the range 78.93 – 78.99
strontium: from 87.62 +/- 1 to the range 87.62 – 87.91
lead: from 207.2 +/- 1 to the range 207.184 – 207.293

The Standard Atomic Weight of germanium was also changed from 72.64 +/- 1 to 72.63 +/- 1.

These changes in the atomic weights will be published in a new Table of Standard Atomic Weights 2009, which will be submitted for publication in Pure and Applied Chemistry (PAC) by the end of 2009.

Commission Members 2010 - 2011:

(a) Titular Members

Dr. M. Berglund

Dr. Willi Brand (Chair)

Prof. R. Gonfiantini

Dr. M. Gröning

Dr. Takafumi Hirata

Dr. Ronny Schönberg

Dr. M. E. Wieser (Secretary)

(b) Associate Members:

Dr. Juris Meija
Dr. Thomas Prohaska
Dr. Paul Vallenga
Dr. T. Walczyk
Dr. Xiang Kun Zhu

(c) Proposed National Representatives:

Dr. John Karl Böhlke (USA)
Prof. Paul De Bièvre (Belgium)
Prof. John R. De Laeter (Australia)
Dr. Shigeku Yoneda (Japan)

(d) Membership of subcommittees

1. Subcommittee for Isotopic Abundance Measurements (SIAM)

Dr. Michael Berglund
Dr. Robert D. Loss (Secretary)
Dr. John Karl Böhlke
Dr. Willi Brand
Dr. Tyler B. Coplen
Prof. Paul De Bièvre
Prof. John R. de Laeter
Prof. Tipping Ding
Dr. Roberto Gonfiantini
Dr. Manfred Gröning
Dr. Takafumi Hirata (Chair)
Dr. Norman E. Holden
Dr. Juris Meija
Dr. Thomas Prohaska
Dr. Ronny Schönberg
Dr. Paul Vallenga
Dr. Robert Vocke
Dr. Thomas Walczyk
Dr. Michael Wieser
Dr. Shigeku Yoneda
Dr. Xiang Kun Zhu

2. Subcommittee for Natural Assessment of Fundamental Understanding. The purpose of this Subcommittee is to promote and provide educational materials on the significance and use of Isotope Abundances and Atomic Weights.

Dr. John Karl Böhlke
Dr. Tyler B. Coplen
Prof. Paul De Bièvre
Prof. John R. de Laeter

Dr. Norman E. Holden (Chair)
Dr. Michael Wieser

3. Subcommittee for Stable Isotope Reference Material Assessment.

Dr. Michael Berglund
Dr. John Karl Böhlke
Dr. Willi Brand (Chair)
Dr. Tyler B. Coplen
Prof. Tiping Ding
Dr. Manfred Gröning
Dr. Thomas Prohaska
Dr. Ronny Schönberg
Dr. Jochen Vogl
Dr. Robert Vocke
Dr. Thomas Walczyk

Michael E. Wieser
Secretary IUPAC Commission on Isotopic Abundances and Atomic Weights.

Appendix 4

International Union of Pure and Applied Chemistry Subcommittee of Isotope Abundance Measurements (SIAM)

Vienna, July 23-24 and July 27.

SIAM members Present

J.K. Böhlke, United States Geological Survey, USA jkbohlke@usgs.gov
Willi Brand, Max Planck Institute for Biogeochemistry, Germany wbrand@bgc-jena.mpg.de
Ty Coplen, United States Geological Survey, USA tbcoplen@usgs.gov
Paul De Bièvre, Metrology Consultant, Belgium paul.de.bievre@skynet.be
John de Laeter, Curtin University of Technology, Australia J.DeLaeter@curtin.edu.au
Tiping Ding, Chinese Academy of Geological Sciences tding@cags.net.cn
Roberto Gonfiantini, Inst. Geosciences and Georesources, Italy Roberto.Gonfiantini@yahoo.it
Manfred Gröning, International Atomic Energy Agency, Austria M.Groening@iaea.org
Takafumi Hirata, Tokyo Institute of Technology, Japan hrt1@geo.titech.ac.jp
Norman Holden, Brookhaven National Laboratory holden@bnl.gov
Bob Loss, Curtin University of Technology, Australia R.Loss@curtin.edu.au
Ronny Schönberg, University of Bergen, Norway ronny.schoenberg@geobio.uib.no
Thomas Walczyk, National University of Singapore walczyk@nus.edu.sg
Michael Wieser, University of Calgary, Canada mwieser@ucalgary.ca
Shigekazu Yoneda, National Museum of Nature and Science, Japan s-yoneda@kahaku.go.jp
Xiangkun Zhu, Chinese Academy of Geological Sciences xiangkun@cags.net.cn
Michael Berglund, 27/07 – 29/07 IRMM, Belgium Michael.BERGLUND@ec.europa.eu

Observers/Other Participants

Rüdiger Kessel, NIST, USA , ruediger.kessel@nist.gov
Paul Vallelonga, 23/07 – 24/07 Consiglio Nazionale delle Ricerche, Italy
vallelonga@unive.it
Jochen Vogl, BAM, Germany jochen.vogl@bam.de
Thomas Prohaska, 23/07– 24/07 Univ. Nat. Res. and App. Life Sciences, Austria
thomas.prohaska@boku.ac.at

Apologies

Robert D. Vocke, NIST, USA , robert.vocke@nist.gov

Invited but did not attend

Wolfgang Pritzkow, BAM, Germany wolfgang.pritzkow@bam.de

Definitions:

TICE: Table of Isotopic Compositions of the Elements

TICE2009: an updated TICE to be published using the current format

TICE21: 21st century TICE, new look, new data etc.

SOP: standard operating procedure

GUM: Guide to the expression of Uncertainty in Measurement

GUMWB: Uncertainty calculation software

July 23: TICE2009 session

Chair: Weiser; *Secretary:* Loss

9:30 Meeting opened by Manfred Groening, IAEA Local Host

Opening address by Prof Werner Burkart, Director IAEA Stable Isotopes Laboratory.

Deliverable: Updated text, list of elements, References

Action items: Berglund, Wieser and Loss to prepare TICE2009 (project 2007-028-1-200)

Prepare a "normal" TICE a la 1997.

- Review publications since 2007. → Task group
 - Review the text of the last TICE and update(draft 2001?) → Task group
 - Make a list of elements that needs to be updated in TICE including values for col. 1 to 9.
 - [Berlin(99), Brisbane(01), Ottawa(03)] → Task group
 - [Beijing(05), Pisa(07), Vienna(09)] → Task group
 - Update the list of references → Task group (maybe done by the above groups)
-

9:50

Opening summary of the day's activities by MW

Major Outcome is to produce a new TICE

Tackle 2005/2007 IC published data (no evaluated data from 2003)

Plan is to break out into groups to review the IC data from pervious years.

PDB. The Commission and it's subcommittees produces the "best evaluated data" of any of the Codata evaluated data.

TW and JDL: Urgent need to produce new TICE

PDB: Problem of natural variability feeding into GUM calculations

MW: In absence of new data we should concentrate on the new TICE.

RL: What about previously evaluated data in the RICE projects?

JKB: Most of the RICE evaluated elements are no different from the current way .

Problem arises of what is GUM compliant – this needs to be defined.

SIAM 2009 Working Groups

These groups to revisit and review data from the 2005/2007 SIAM and report back on entries for TICE2009

2007

Ar	PDB, RK, JKB, MG, NH	x End SIAM.DONE what column to pick for the data in column 9?
Yb	SY, NH, RL, PV	x fix DONE
Zn	TW, MW, RS, XZ, TP, JV	x DONE
Lu	RL, JDL	x check if 3s is necessary end of SIAM
Mo	TW, MW, RS, XZ, TP, JV	x done
Ni - change $U[A_r(\text{Ni})]$		
O (mass independent effects)	WB, TC, JKB	x From SNAFU report
Ge	JDL	
Cd	SIAM group	X Friday am

2005

C (Reference Material Rec)	TC, WB, RG, MG, TD	x stick with present rec in TICE, NBS19.
Nd	TC, WB, RG, MG, TD, MW	x need to verify AW uncertainty, Reference Materials?
Sm	TC, WB, RG, MG, TD, MW	x Reference Materials?
Pt	JDL, TH, NH, PV, SY	x Recalculation of col 9 data
Ta	JDL, TH, NH	x okay
La	TW, MW	x Monday

Column 4 content discussion on Monday

ARGON recommendations for TICE (JKB 20090727)

PDB, RK, JKB, MG, NH

Column 4- "G" [range not quantified]

Column 6- Insert new best measurement (1s, F)

Column 7- New reference:

Lee, J.-Y., Marti, K., Severinghaus, J.P., Kawamura, K., Yoo, H.-S., Lee, J.B., Kim, J.S. (2006) A redetermination of the isotopic abundances of atmospheric Ar. *Geochimica et Cosmochimica Acta* 70, 4507–4512.

Column 9- Insert new values and uncertainties (in air)

Column 9- Add superscript "g" at ^{40}Ar for radiogenic isotope

			NEW Column 6 (1s, F)	NEW Column 9		
	2001 best (Nier)	2001 Col 9	Lee fractions (after GUM) 1s	Expanded (GUM 6s) (40/36 = 296.7- 300.5) does not include Nier values	<i>Expanded range to include Nier (about $\times 10^+$) (40/36=295- 302 JKB</i>	<i>Recalc to match 2001 Ar(Ar) JKB</i>
36Ar	.003365(6)	.003365(30)	0.0033361(35)	.003336(21)	0.00334(4)	.00329(24)
38Ar	.000632(1)	.000632(5)	0.0006289(12)	.000629(7)	0.00063(1)	.00062(2)
40Ar	.996003(6)	.996003(30)	0.9960350(42)	.996035(25)	0.99604(4)	.99609(26)
Ar(Ar)	39.947677	39.947677	39.947798(15)	39.94780(9)	39.9478(2)	39.948(1)

Cd New BAM ref material BAM- I012 – is being produced

- Existing BM in TICE is based on Rosman and Barnes not calibrated.
- Problem with published paper showed little technical data about how measurements were made so no changes were made.
- Proposal was made that a letter be requested from BAM outlining these details.
- Outcome: BAM will publish a letter outlining these details that can be considered at the next Commission meeting

Ge

Reconsideration by Holden, de Laeter, De Bièvre, and Coplen 7/24/2009

The Commission has changed the recommended value for the standard atomic weight of germanium to $A_r(\text{Ge}) = 72.63(1)$, based on (i) a re-evaluation of lattice parameter measurements of Smakula and Kalnajs [1], density measurements of Smakula and Sils [2], and atomic weight calculations by Smakula, Kalnajs and Sils [3] on the basis of updated crystallographic data, and (ii) a re-assessment of the mass spectrometric measurements of Kipphardt et al. [4] and Chang et al. [5]. The previous value of $A_r(\text{Ge}) = 72.64(1)$ was assigned by the Commission in 1999 [6], which selected the calibrated mass spectrometric measurements of Chang et al. [5]. Historical values of $A_r(\text{Ge})$ include [7]: 1894, 72.3; 1897, 72.48; 1900, 72.5; 1925, 72.60; 1961, 72.59; 1969, 72.59(3); and 1999, 72.64(1).

1. A.Smakula and J.Kalnajs : Phys.Rev. 1955, **99**, 1737
2. A.Smakula and V.Sils : Phys.Rev. 1955, **99**, 1744
3. A.Smakula, J.Kalnajs and V.Sils : Phys.Rev. 1955. **99**, 1747
4. H.Kipphardt, S.Valkiers, F.Henriksen, P. De Bièvre, P.D.P.Taylor and G.Tölg : Int.J.Mass Spectrom. 1999, **189**, 27
5. Tsing-Lien Chang, Wen-Ju Li, Guang-Sheng Qiao, Qui-Yu Qian and Zhu-Ying Chu : Int.J.Mass Spectrom. 1999, **189**, 205
6. TSAW 1999
7. T. B. Coplen and H. S. Peiser. *Pure Appl. Chem.* **70**, 237-257 (1998).

New Data for column 6 and 9

Column 6 data [4] 3s C	Col 9
20.57(1)	0.2057(27)
27.45(11)	0.2745(32)
7.75(4)	0.0775(12)
36.50(7)	0.365(2)
7.73(4)	0.0773(12)

GUM calc at wt 72.6277(99)

Pt, (see 2005 SIAM minutes for detailed notes)

- 5 synthetic Isotope corrected measurement.
- Col 6 values as per pub with 3S STATUS Undecided,
- Column 9 as per TSAW 2005

Mass #	4	5	Col 6	7	8	Col 9
190				13	IRMM 010	0.00012 (1)
			0.0001172 (58) 2S F			
192			0.007818 (80)			0.00782 (16)
194			0.3286 (14)			0.3286 (28)
195			0.33775 (79)			0.3378 (16)
196			0.25210 (110)			0.2521 (22)
198			0.07356 (43)			0.07356 (86)
A.W.			195.0844 (58)			1.000000

13. Briche , et al (2002)

La, (see 2005 SIAM minutes for detailed notes)

- 2005 TSAW Recommended changing BM
- Linearity checked using K, fractionation corrected measurements using Yb. N
- Col 6 values as per pub with 2s N
- Unusual Case – Uncertainty in F can be as large as F and it makes no difference
- Column 9 as per TSAW 2009

Mass #	4	5	Col 6	7	8	Col 9
138			0.000 888(2) 2s N			0.000 888(6)
139			0.999 112(2)			0.999 112(6)

Delater and Bukilic (2005)

Lu, (see 2007 SIAM minutes for detailed notes)

- Linearity checked using K, fractionation corrected measurement using Yb. N
- Col 6 values as per pub with 2s
- Unusual Case – Uncertainty in F can be as large as F and it makes no difference
- Column 9 as per TSAW 2009
- The 2007 working party proposed the use of the reported fractionation value rather than that determined from $(m_1/m_2)^{0.5}$. A Uf of $\pm f$ or 5.2 (rather than ± 0.05 permil/amu) was proposed since this retains the concept of using the $\pm f$. This translates to a 100 times increase on the stated Uf but still generates a UAW = 0.0001 on the using GUM. Why this is the case is believed to be due to GUM not being used by D and B in calculating their AW.

Mass #	4	5	Col 6	7	8	Col 9
175		g	0.974013 (12) 2s,N	10		0.97401 (12)
176			0.025987 (12)			0.02599 (12)
A.W.						174.9668 (1)

De laeter, J.R. and Bukilic, N., (2006) Solar Abundance of ^{176}Lu and s-process nucleosynthesis. (2006) Physical Review C, 73,

Mo, (see 2007 SIAM minutes for detailed notes)

- Transfer data from SIAM calculation into column 9
- Transfer data from publication into column 6 (1s + F)
- Cross-checked that data in column 9 (incl. uncertainties) result in current Standard Atomic Weight and uncertainty
- Effect of known isotope variations well within uncertainty range of current Standard Atomic Weight
- No additions to column to column 8
- New BM for M with a 6x extended U in Abundances

Mass #	4	5	Col 6 (1s, F)	7	8	Col 9
92		g	0.145 246(15) but actually: 0.145 25(15)	12		0.1453 (31)
94			0.091 514(74)			0.0915 (9)
95			0.158 375(98)			0.1584 (11)
96			0.166 72(19)			0.1667 (15)
97			0.095 991(73)			0.0960 (14)
98			0.243 91(18)			0.2439 (37)
100			0.098 24(50)			0.0982 (31)
A.W.						95.96 (2)

Nd, (see 2005 SIAM minutes for detailed notes)

Notes needed

Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8	Col 9
60	Nd	142	delete	g	0.271 53(19)	*		0.2715(5)
		143			0.121 73(18)			0.1217(2)
		144			0.237 98(12)			0.2380(3)
		145			0.082 93(7)			0.0829(1)
		146			0.171 89(17)			0.1719(3)
		148			0.057 56(8)			0.0576(1)
		150			0.056 38(9)			0.0564(2)

M. Zhao, T. Zhou, J. Wang, H. Lu, F. Xiang, C. Guo, Q. Li, C. Li. *Rapid Commun. Mass Spectrom.* **19**, 2379-2382, (2005).

Ni, (see 2007 SIAM minutes for detailed notes)

- New paper shows variability in Ni outside current U limits.
- U AW should be increased to cover variability – corresponds to a 6s
- Recommend 58.6934 (5) cf (2)
- Changes to column 4 and 9 , 6 stays as is
- Natural variation (delta values) given relative to the best meas material (NIST 986)
- **“0.000001” added to mass 62**

Mass #	4	5	Col 6	7	8	Col 9
58		g	Stays the same			0.68077 (19)
60						0.26223 (15)
61						0.011399 (13)
62						0.036346 (40)
64						0.009255 (19)
A.W.						58.6934 (4)

Tanimizu , M. & Hirata, T. (2006) Determination of natural Isotopic variation in Nickel using inductively coupled mass spectrometry. *J. Anal. Atomic Spectroscopy.* **21**, 1423 – 1426.

Ta, (see 2005 SIAM minutes for detailed notes)

- ½ linearity checked, ½ fractionated corrected measurement.
- Col 6 values as per pub with, 6S
- Column 9 as per TSAW 2005

Mass #	4	5	Col 6	7	8	Col 9
180			0.0001201 (8) 2se N	11		0.000120 (3)
181			0.9998799 (8)			0.999880 (3)
A.W.						OK

11. J.R. De Laeter and N. Bukilic. *Physical Review C*, **72**, 025801 (2005)

Yb, (see 2007 SIAM minutes for detailed notes)

Non linearity checked, fractionation corrected measurement. F

Col 6 values as per pub with 2se F,

Column 9 as per TSAW 2009 with an F (6S) and a minor change to 168

Mass #	4	5	Col 6	7	8	Col 9
168		g	0.001232(4) 2se F			0.00123(3)
170			0.02982(6)			0.02982(38)
171			0.14086(20)			0.14085(134)
172			0.21686(19)			0.21685(128)
173			0.16103(9)			0.16103(62)
174			0.32025(12)			0.32026(78)
176			0.12995(13)			0.12996(81)
A.W.						OK

de laeter, J.R. and Bukilic, N., (2006) The isotopic composition and atomic weight of Ytterbium, *International Journal of Mass Spectrometry*, 252, 222 - 227

Zn, (see 2007 SIAM minutes for detailed notes)

- Calibrated Meas 2s C
- Column 9 as per TSAW 2009 with U expanded (180s) to cover fractionation variability in reference materials
- Transfer data from SIAM calculation (Element Reviews 2007) into column 9
- Transfer data from publication into column 6 (2s + C)
- Cross-check that data in column 9 (incl. uncertainties) result in current Standard Atomic Weight and uncertainty

- Effect of known isotope variations well within uncertainty range of current Standard Atomic Weight
- Add IRMM-3702 in column 8

Mass #	4	5	Col 6	7	8	Col 9
64	TBD	r, g	0.491704(83)	16	IRMM-3702	0.49170 (25)
66			0.27731 (11)			0.27731 (33)
67			0.040401(18)			0.04040 (5)
68			0.184483 (69)			0.18448 (21)
70			0.006106 (11)			0.00611 (3)
A.W.						65.38 (0.02)

Ponzevera, E., Quétel, C., Bergland, M., Taylor, P., Evans, P., Loss, R.D., Fortunato, G. (2006) Mass Discrimination during MC-ICPMS Isotopic Ratio Measurements: Investigation by means of synthetic isotopic Mixtures (IRM-007 Series) and Application to the Calibration of Natural-like Zinc Materials (Including IRMM-3702 and IRMM-651). J Am Soc Mass Spect (17) 1412 – 1427.

July 24 Morning: Uncertainty session

11:20; Presentation By Jochen Vogl (BAM) on isotopic Reference Materials.

Group discussion on

- need for certain standards
- ways of and amount to be stored
- Standard homogeneity
- business of operation and cosy recover

Recommendation that SIAM recommends to the Commission that some form of recommended use of reference materials be discussed in the report. PDB; Direct letters of support to institutions preparing reference materials can lead to major problems.

12:20: Discussion on TICE Column 4.

TW SUGGESTED ADDITIONS TO COLUMN 4

- a) Range in isotopic abundances in accordance with SNIF (as is)
- b) No sufficient evidence from peer reviewed scientific publications exists to date for variations in isotope abundances in terrestrial samples for this element

- c) Sufficient evidence for variations in isotope abundances exist for this element in the peer reviewed scientific literature but reported variations can currently not be converted into an abundance range for each individual isotope

JDL – comprehensive literature review is too large a task.

RK – Accept only data sent to the Commission.

TW – Just give an indication that there is a variation or not.

JKB - combine column 4 and 5.

Need to remove non-evaluated data in column 4

RG – variations can be caused by Radiogenic causes.

MW – these to be included in next but not this version of TICE.

PV – remove all non referenced entry

WM – await

July 24 3pm : Uncertainty session

Chair: Schönberg; *Secretary:* Loss

Objective: Uncertainty presentation by R. Kessel, Discussion on uncertainty in TICE21

Deliverable: Recommendations on how to treat uncertainty in TICE21.

Action items: Schönberg, Kessel and Berglund to add recommendations to the TICE21 SOP.

Presentations by Dr. Kessel

- Uncertainty and use of GUMWB (45 min + discussion)
- GUM supplement 1, Monte Carlo and the future of uncertainty (30 min + discussion)
- discuss CIAAW needs in terms of consistency, transferability. Discuss possibilities of non-symmetrical uncertainties and uncertainty of ranges in view of TICE21.

3:30 pm Coffee break

TICE21 – Where too next

Chair: Walczyk, *Secretary:* Loss

Objective: Decide how TICE/TSAW will look and be managed in the future

Deliverable: SOP for retrieving data for TICE21

Action items: Walczyk, Berglund and Loss to finalize the TICE21 SOP.

To do: Answer the questions WHAT? HOW? and WHERE?

WHAT:

What data do we want to put in a future TICE: delta(ratio) ranges materials for different matrixes/compounds (SNIF style), all available reference materials, delta 0 material(s), col. 1-9, TSAW values and its deltas, ref to calibration schemes, etc.?

Review experiences from SNIF → Ty and JK.

HOW:

- How will we retrieve all the information we want in view of the workload assuming approx 5 to 50 articles to review per element and numerous calculations?

Some ideas to discuss:

- A snapshot of 3-4 elements (2 year project) keeping the workload approximately as it is today
- One element per member (2 year projects): reviewed at the next CIAAW meeting. No budget hassle for CIAAW meetings, you work yourself there.
- web forum Wikipedia style, the community enters the data for us: increasing our community interaction and boost the educational aspect of CIAAW/IUPAC

WHERE:

Where do we want to publish our retrieved and calculated data:

- journals (paper form)
- on the web
 - pure database interaction (updated continuously or biannually)
 - forum based discussion and acceptance of data (updated continuously)

Lively discussion

RK – GUM WB is an ideal tool for this problem

MG – demonstrated use of GUM/EXCEL U prop calculations

RK - GUM/EXCEL ok for routine use of one calculation but not suitable for all

SIAM/CIAAW needs. Other tools besides GUM can be used but important to keep all data in the one calculation otherwise correlations may be lost.

MW – supports use of xml data format

General support for use of XML – GUM – XML system.

TW presented a possible presentation format for TICE 21 and what data should be included

Session closed at 5:55 pm

July 27 morning 1: TICE2009 roundup

Chair: Wieser; *Secretary:* Loss

9:15 start

Element by Element Check.

Ar decision made to go with Lee et al. results. Data to come from JKB
Data still needed for Pt and data needs checking for Yb.
All other elements OK

Discussion on TICE table column 4

SUGGESTED ADDITIONS TO COLUMN 4 by TW

- a) Range in isotopic abundances in accordance with SNIF (as is)
- b) No sufficient evidence from peer reviewed scientific publications exists to date for variations in isotope abundances in terrestrial samples for this element
- c) Sufficient evidence for variations in isotope abundances exist for this element in the peer reviewed scientific literature but reported variations can currently not be converted into an abundance range for each individual isotope

JDL: problems with radiogenics.

MW: Some entries have no “r” or “g” yet have a range of Abundances (eg Hf and Nd)

NH : TICE 21 should re-evaluate ranges done outside the SNIF project.

Proposal to add “No observed variation” to col 4 header

Add reference to SNIF publication.

TW: suggest adding “No observed variation or range not evaluated” footnote to column 4

So 3 entries will be possible for column 4

- No entry for MonoNuclidics
- Range when available
- “No observed variation or range not evaluated”

TW: Column4 explanatory text on current TICE (p58) will need 2nd line removed

Summary:

SIAM recommendations for Col. 4

- add “Observed” to Col. 4 header
- add reference to SNIF to relevant data in column
- leave existing range data
- add reference to TICE when range first appeared in the table.
- add “No observed variation or range not evaluated” for those polyisotopic elements where current Col. 4 entry is blank.
- Modify Col 4. Explanation in text to agree with these changes (delete 2nd sentence in this paragraph).

11:15

July 27: Follow up on TICE21 with a roundup

Chair: Walczyk; Secretary: Loss

APPENDICES:

Presentations

What is Gum compliant

Rüdiger Kessel, NIST, USA,
ruediger.kessel@nist.gov

Agenda

GUM and Metrology
State of Knowledge Concept
The GUM 1993 Calculation Rules
The Supplement 1 Calculation Rules
Model Development

GUM and Metrology

The GUM is a calculation standard
The supports the metrology system
The metrological concepts define the model

- Traceability
- Coherent conclusions
- Limited knowledge

“GUM compliant” is often the synonym of “the model equation is compliant with metrological concepts”

State of Knowledge Concept

The GUM calculations are derived from a state of knowledge Concept.
The symbols in the model equation represent the sate of knowledge about a metrological effect.
Symbols not define nature, but the state of knowledge about nature.
The model equations represents the knowledge about the relations in nature.

The GUM 1993 Calculation Rules

The model is given
Use type A or type B evaluation methods to calculate the standard uncertainty based on the kind of data
Propagate standard uncertainty
Use a coverage factor to calculate the expanded uncertainty
Document the uncertainty budget and use the defined report format for the result and uncertainty.

The Supplement 1 Calculation Rules

The model is given

Use specific random generators to sample from different distributions to generate a large number of random input sets.

Calculate a set of results of the model for the random input sets.

Sort the results and evaluate the standard uncertainty and the coverage interval.

Use the defined report format for the result and uncertainty.

Model Development

Key problem I metrology

Better support is needed

Cause-effect-chain should be the basis

Metrology concepts must be implemented

...

Appendix 5

Recent activities in COCI (Committee on Chemistry and Industry)

COCI had the off-year meeting in Marl, Germany, April 26-27, 2008. The meeting dealt with regular issues topics like: functioning of COCI., budget, reports from Bureau and Executive Committee, report from the on-going projects, and possible new projects.

COCI will be active for IYOC (international year of chemistry) and try to find sponsors. This will be an important action for the coming three years. COCI has the following on-going projects:

- Chemistry in a changing world - new perspectives concerning the IUPAC family (2006 -)
- Responsible Application of Chemistry -- An Introduction to Responsible Care (2006 -)
- IUPAC-UNESCO-UNIDO Safety Training Program Workshop, Turin, Italy (2007 -)
- Future Energy: Improved, sustainable and clean options for our planet (2007 -)
- Options for IUPAC engagement in SAICM implementation (2008 -) (SAICM = Strategic Approach to International Chemicals Management) (Intergovernmental Forum on Chemical Safety).

The Safety Training Program (STP) is an important action in COCI. In that chemists from developing countries are visiting and practicing in American and European chemical companies. The main focus in the training is in safe working. New companies are needed for this program.

The following new project ideas were discussed in the Marl meeting:

- Nanotechnology and Human Health. Preparation is going-on.
- Biomonitoring. The topic was discussed with Analytical division but they were not interested in. Next discussions with division VI.
- Biofuels. Discussions will continue with CHEMRAWN.
- STP (Safety Training Program) Internet Modules. This has been done first in Uruguay and will be distributed in industry in South America. English version is still missing. Further collaboration will be made with CCE.
- IUPAC Industrial Chemistry Prize. The prize should be for innovation that had developmental capabilities to piloting and commercial exploitation. The award would be presented to a maximum of three persons with the same value as the Richter prize. The first award would be presented in Glasgow in 2009. Needs sponsors and acceptance of IUPAC.

Next, the status of the programs in COCI was discussed. The programs are:

- Public Appreciation of Chemistry Program. A new PAC-related Web-site in collaboration with CCE will be developed.
- NGO/IGO/Trade Associations Program. NGO status of IUPAC in UNESCO, CEFIC etc. should be strengthened.
- Division/Standing Committee Collaborations Program. Only a few divisions were present in Marl. In Glasgow the divisions get 15 min for presentations.
- NAO/CA Program. In connection to this program an European regional workshop was held in Marl before COCI meeting ("Workshop in a changing world – new perspectives concerning the IUPAC family"). NAOs, CEFIC, RSC were present. In that meeting one message was: new company members needed in COCI: Asia is developing well, Europe is setting back, companies in developing countries are not interested in IUPAC. Many other topics interesting industry were discussed.
- Health, Safety and Environment Program. This is still the most important program. New ideas for further development are needed.

Appendix 6

From: <http://www.chemistry2011.org/participate/ideas/show?id=5>

Spanish Year

Idea by Javier Garcia-Martinez | Nov 30, 2009 06:56PM

In 2007, Spain celebrated its Year of Science honoring Mendeleev in many different ways and choosing the Periodic Table, Mendeleev 's iconic legacy. This was an excellent opportunity to raise public awareness and promote science and technology.

The Mendeleev's Year began formally on 2 February 2007 with the launch of a very special stamp entitled Tabla Periódica de Elementos de Mendeléiev (Mendeleev's Periodic Table of Elements).

A few months later, the University of Jaén decided to decorate the wall of its Experimental Science Department with a large version of the Periodic Table of this stamp. The large version of the periodic table (3.80×2.70 m) is made of beautiful ceramic tiles, and replicates the table featured on the stamp.

A Design Competition to Spark the Imagination

The Periodic Table is not only the fixed organization of elements hanging on the chemistry classroom, but a living creature that grows and changes over time. There are literally hundreds of versions of the Periodic Table, each one emphasizing a different aspect of the Periodic Law. So, why not give everyone the opportunity to have his or her own version? With this objective, the First Periodic Table Design Competition was launched in June 2007 to promote science and art, especially among the young. Once again, young people showed they are full of creativity and excitement about chemistry when given the opportunity.

Also, in July 2007, the 1st Summer School on the History of Chemistry Dedicated to Mendeleev was held at the University of La Rioja. In October, the Spanish Royal Society of Chemistry (RSEQ, Real Sociedad Española de Química) launched a competition for high school and college students for the best comic about Mendeleev's life. Twenty-four comics were received from Spain, Mexico, and Argentina from students with ages ranging from 14 to 25 years old.

Appendix 7

Draft of Information Packet for new Division Members



IUPAC

International Union of Pure and Applied Chemistry

Inorganic Chemistry Division (II)

Welcome Pack 2009

[illegible]

Dear Observer/New/Prospective member,

Welcome to the IUPAC Division of Inorganic Chemistry. As you are probably well aware, Inorganic Chemistry continues to be an ever expanding and evolving science, particularly in areas such as materials, metallo-organic and nano chemistry, which like all areas of chemistry require ongoing support from International Organizations such as IUPAC, and associated national adhering organizations (NAOs).

This information pack is provided to you as either an observer, or prospective and new member to help you to understand the structure, operations, scope and business of the Division of Inorganic Chemistry, and I hope you find it useful. In addition, the information contains a number of lists, links to relevant websites and sample forms and documents that are used by Divisional members.

I would also like to draw your attention to the importance of projects to our overall operation, as they are the primary reason for the existence of the Division. Since you do not need to be a member of the Division to generate a suitable project I strongly encourage you to generate and submit new projects that draw on both the internal expertise of the Division but also involve external members of Chemical community. I would also encourage you to promote the IUPAC project system to members of the wider scientific community. Relevant application forms and information about how to apply are provided in this pack.

We look forward to your continuing involvement with IPUAC and the Division.

Sincerely



Robert Loss,
Division II Vice President
John de laeter Centre for Mass Spectrometry
Department of Imaging and Applied Physics
Curtin University of Technology
Kent St Bentley 6102 WA
Australia
r.loss@curtin.edu.au

1. The Division Structure and membership.

The Division of Inorganic Chemistry is one of 8 Divisions within IUPAC

The 8 divisions are

1. [Analytical Chemistry Division](#) (V)
2. [Chemical Nomenclature and Structure Representation Division](#) (VIII)
3. [Chemistry and Human Health Division](#) (VII)
4. [Chemistry and the Environment Division](#) (VI)
5. [Inorganic Chemistry Division](#) (II)
6. [Organic and Biomolecular Chemistry Division](#) (III)
7. [Physical and Biophysical Chemistry Division](#) (I)
8. [Polymer Division](#) (IV)

The primary task of the Division is to evaluate projects and recommend funding of successful projects. It also contributes to cross divisional projects and provide advice to the other IUPAC Divisions on inorganic chemistry related matters.

The Division also coordinates the operation of 3 subcommittees and a Commission:

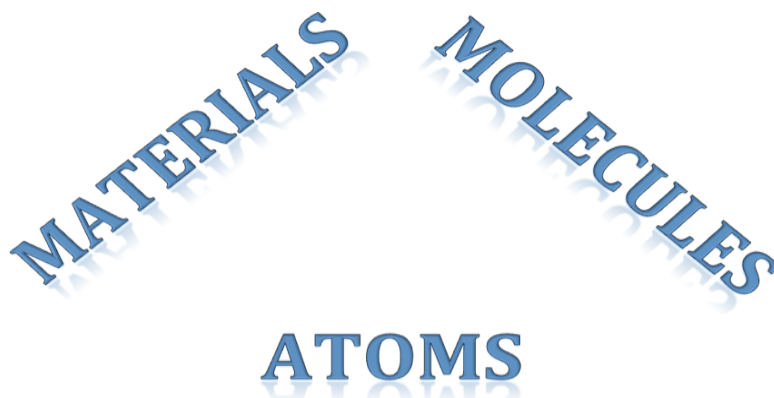
- Subcommittee on Isotopic Abundance Measurements
- Subcommittee on Characterization of Carbonaceous Materials and New Carbons
- Interdivisional Subcommittee on Materials Chemistry
- Commission on Isotopic Abundance and Atomic Weights

Membership of the Division is determined by election and selection to cover the main areas of chemistry (see next section) dealt with by the Division, or in the case of the subcommittees, based on the relevant expertise of members.

The Division has 3 categories of membership.

1. Titular Membership (TM), where members are elected for either two or four year terms. Officers of the Division are normally elected from existing membership.
2. Associate Membership (AM): which are normally selected to serve for two years
3. National Representatives (NR) Nominated by their National Adhering Organizations and selected to serve for two years. When a country is already represented by either a TM or AM, no NR is selected from that country.

1. **The Current membership of the Division is as follows:**
(new list to be inserted)



2. **The Scope of the Division.**

The Division covers 3 broad areas of inorganic chemistry and divisional members are normally associated with at least one of these areas. The fact that there are only three areas does not mean that other areas of inorganic chemistry are not recognised or important or not dealt with by the Division.

Atoms:

This covers the areas of the isotopic abundances of each element and the resulting Atomic Weights. This work is primarily done through the Commission of Isotopic Abundances (CIAAW and the Subcommittee on Isotopic Abundances (SIAM).

Molecules: Javier – maybe you can write something here

Materials

Covers the broad spectrum of the area of materials chemistry. A useful definition for Materials Chemistry can be found here. The Interdivisional Subcommittee for Materials Chemistry draws on members from this area of the Division

One area of Inorganic Chemistry that is not dealt with by the Division is that of inorganic nomenclature, which is dealt with by Division VIII.

3. A list of the Active projects and their coordinators.

Task Group Chair	Project Title	Nominal Area
Stanbury	Standard potentials of radicals	Molecules
Walczyk	Guidelines for mass spec meas	Atoms
Berglund	Isotopic Compositions of Selected Elements	Atoms
Wieser	Determination of Atomic Weights Using New Analytical Techniques	Atoms
Kniep	Classification, Terminology and Nomenclature of Borophosphates	Molecules
Day	Towards Defining Materials Chemistry	Materials
Brand/Coplen	Calibration of Organic and Inorganic Oxygen-bearing Isotopic Reference Materials	Atoms
Berglund	Evaluated Published Isotope Ratio Data (2005-2007)	Atoms
Ober	Terminology for self-assembly and aggregation of polymers	Molecules
Renne	Recommendations for Isotope Data in Geosciences	Atoms
Holden	Assessment of fundamental understanding of isotopic abundances and atomic weights of the chemical elements	Atoms
Vohlídal	Terminology for conducting, electroactive and field responsive polymers	Molecules
Karol	Priority claims for the discovery of elements with atomic number greater than 111	*
Berglund	Evaluated Published Isotope Ratio Data (2007-2009)	Atoms
Zhu	Evaluation of Isotopic Abundance Variations in Selected Heavier Elements	Atoms
Schönberg	Evaluated Compilation of International Reference Materials for Isotope Abundance Measurements	Atoms
Holden	Development of an Isotopic Periodic Table for the Educational Community	Atoms
Martinez	Analysis of the Usage of NanoScience and Technology in Chemistry	Molecules
Sun	Thermodynamic study on hydrogen storage materials: metal organic frameworks and metal or complex hydrides	Molecules
Karen	Towards a comprehensive definition of oxidation state	Molecules

In conjunction with IUPAP

(current list to be inserted in place of this one)

4. **If the Red Book is not available any more a pdf copy or instructions on how to get it.**
-

5. **A list of useful URLs within IUPAC**

The official website of the International Union of Pure and Applied Chemistry

<http://www.iupac.org/>

IUPAC Divisions

<http://www.iupac.org/Organization/Divisions>

IUPAC Committees

<http://www.iupac.org/Organization/Committees>

General information on the IUPAC Project System

<http://www.iupac.org/publications/ci/2001/january/SG-report.html>

Guidelines for IUPAC projects

http://old.iupac.org/general/handbook/guidelines_projects.html

http://old.iupac.org/projects/faqs_projects.html

http://old.iupac.org/projects/form_guide.html

IUPAC publications

<http://www.iupac.org/Publications>

IUPAC electronic resources

<http://old.iupac.org/publications/epub/index.html>

IUPAC sponsored conferences

<http://www.iupac.org/indexes/Conferences>

IUPAC Compendium of Chemical Terminology - the Gold Book

<http://goldbook.iupac.org/>

6. Procedures for claiming expenses.

To apply to have travel and other expenses reimbursed you need to obtain a travel expenses claim form (See Sample claim form below) as an email that can be obtained from the Secretariat. Once you have completed the entries you should submit to the Secretariat in the case of Divisional meetings, or, in the case of a project, to the project Leader. Please also note the instructions at the end of the sample claim form shown below.

IUPAC SAMPLE CLAIM FORM

Instructions for completion of this form are given at the bottom of the form. Please return this form either by return e-mail, by fax to +1 919 485 8706 or by mail to the Secretariat at the address below:

IUPAC Secretariat

P.O. Box 13757, Research Triangle Park, NC 27709-3757, USA

MEETING TITLE: XXXX

Date: XX/XX/XXXX

Place:

Charged to: Project XXXXX

ALLOCATION: The amount is determined in consultation with the Divisional President or Project Task Group Leader.

PAYMENT

Please indicate the preferred method of payment.

Bank transfer in national currency

Bank transfer in USD

USD check

Check in national currency

Use previous bank information? yes/no?

Bank Transfer information:

Swift Code:

Bank Sort Code or Bankleitzahl, as applicable:

Account number (EU residents please use IBAN):

Account name:

Bank Name and Address

MAILING ADDRESS (For check payments.)

Date:

Signature:

Approved by Executive Director on behalf of the Treasurer

For reimbursements by bank transfer or check before the meeting, the claim form must reach the IUPAC Secretariat four weeks before the meeting.

Instructions for completion of the Claim Form:

Please check to see if all pre-printed information is correct.

Provide Project number and title if applicable.

Provide bank transfer information. Wire transfers are the preferred method of payment, except for those who can use a check in USD.

Approval must be obtained from the Division President or Task Group Chairman either by having the form signed or by an e-mail or fax message to the Secretariat from the Division President or Task Group Chairman as appropriate.

Please remember that IUPAC will pay only for economy airfares unless special circumstances exist and specific permission is given by the Division President.

IUPAC will pay for extra per diem if a longer stay is required to obtain a lower fare and the result is a lower total cost.

7 A copy of the project submission form

(attached)

8 Some samples of a successful project

I would suggest to ask Ty Coplen to provide this information. I would suggest the project "Towards Defining Materials Chemistry"

<http://www.iupac.org/web/ins/2005-001-1-200>

9 A list of references/reports;

List of past and current Inorganic Chemistry Division Projects:

<http://www.iupac.org/indexes/Projects/bodies/200>

A good example of a DivII project report can be found in:

http://www.iupac.org/publications/ci/2009/3103/1_day.html

APPENDIX (to Information Pack)

List of Abbreviations Commonly used within IUPAC

AACC - American Association of Cereal Chemists
ACS - American Chemical Society
AIQ - Advance Information Questionnaire re symposium sponsorship by IUPAC
AMP - Affiliate Membership Programme of IUPAC
AO - Associated Organization of IUPAC
AOAC - Association of Official Analytical Chemists
AOCS - American Oil Chemists Society
ASTM - American Society for Testing and Materials

BIPM - International Bureau of Weights and Measures (Bureau International des Poids et Mesures)
BS - Blackwell Science Ltd.

CA - Company Associate of IUPAC
CAC - Codex Alimentarius Commission of Joint FAO/WHO Food Standards Programme
CCE - IUPAC Committee on Chemistry Education
CCFA - Codex Committee on Food Additives
CCMAS - Codex Committee on Methods of Analysis and Sampling
CCPR - Codex Committee on Pesticide Residues
CEBJ - IUBMB Committee of Editors of Biochemical Journals
CEC - Commission of the European Communities
CEFIC - Conseil Européen de l'Industrie Chimique (European Chemical Industry Council)
CGPM - Conférence Générale des Poids et Mesures and its Committees
CHEMRAWN - Chemical Research Applied to World Needs
CI - *Chemistry International*, news magazine of IUPAC
CIPAC - Collaborative International Pesticides Analytical Council
CIPM - Comité International des Poids et Mesures (International Committee on Weights and Measures)
COCI - IUPAC Committee on Chemistry and Industry
CODATA - ICSU Committee on Data for Science and Technology
COSPAR - ICSU Committee on Space Research
COSTED-BIN - ICSU Committee on Science and Technology in Developing Countries and International Biosciences Networks
CPEP - IUPAC Committee on Printed and Electronic Publications
CTC - IUPAC Committee on Teaching of Chemistry (superseded by CCE)
CTS - ICSU Committee on Teaching of Science

EC - IUPAC Executive Committee
ECCLS - European Committee for Clinical Laboratory Standards
EFB - European Federation of Biotechnology

EFC - European Federation of Corrosion
EFCE - European Federation of Chemical Engineering
EMEP - Co-operative Programme for Monitoring and Evaluation of the Long Range Transmission of Air Pollutants in Europe
EPA - European Photochemistry Association
ESNA - European Society of Nuclear Methods in Agriculture
EU - European Union
EvC - Evaluation Committee
EWPCA - European Water Pollution Control Association

FACS - Federation of Asian Chemical Societies
FAO - United Nations Food and Agriculture Organization
FC - IUPAC Finance Committee
FOSFA - Federation of Oils, Seeds and Fats Association Ltd.

HSE - Health and Safety Executive

IACIS - International Association of Colloid and Interface Scientists
IACST - International Association for Cereal Science and Technology
IAEA - International Atomic Energy Agency
IAGC - International Association of Geochemistry and Cosmochemistry
IARC - International Agency for Research on Cancer
IAWQ - International Association on Water Quality
ICAME - International Commission on Application of Mössbauer Effect
ICC - International Congress on Catalysis
ICCC - International Conferences on Coordination Chemistry
ICO - International Carbohydrate Organization
ICOMC - International Conferences on Organometallic Chemistry
ICSC - International Conferences on Solution Chemistry
ICSU - International Council for Science
ICTAC - International Confederation for Thermal Analysis and Calorimetry
ICTNS - IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols
IDCNS - IUPAC Interdivisional Committee on Nomenclature and Symbols (superseded by ICTNS)
IDF - International Dairy Federation
IEC - International Electrotechnical Commission
IFCC - International Federation of Clinical Chemistry
IGAC - International Global Atmospheric Project
IGCAIC - International Group for Correlation Analysis in Chemistry
IMA - International Mechanochemical Association
IOBB - International Organization for Biotechnology and Bioengineering
IOCC (OICC) - International Office of Cocoa and Chocolate (Office Internationale du Cacao et Chocolat)
IOCD - International Organization for Chemical Sciences in Development
IOCG - International Organization of Crystal Growth
IOOC - International Olive Oil Council

ISE - International Society of Electrochemistry
ISHC - International Society of Heterocyclic Chemistry
ISMAR - International Society of Magnetic Resonance
ISO - International Organization for Standardization
ISO/TC12 - ISO Technical Committee on Quantities, Symbols, and Conversion Factors
ISO/TC61-SC/4 - ISO Technical Committee on Burning Behaviour
ISPP - International Society of Plant Pathology
ISS - Istituto Superiore di Sanità
IUBMB - International Union of Biochemistry and Molecular Biology
IUCr - International Union of Crystallography
IUFOST - International Union of Food Science and Technology
IUGS - International Union of Geological Sciences
IUIS - International Union of Immunological Societies
IUMS - International Union of Microbiological Sciences
IUNS - International Union of Nutritional Sciences
IUPAB - International Union of Pure and Applied Biophysics
IUPAP - International Union of Pure and Applied Physics
IUPHAR - International Union of Pharmacology
IUTOX - International Union of Toxicology
IZA - International Zeolite Association

JAOAC - Journal of Association of Official Analytical Chemists
JCBN - IUBMB-IUPAC Joint Commission on Biochemical Nomenclature
JMPR - Joint FAO/WHO Expert Committee (Meeting) on Pesticide Residues

NAFTA - North American Free Trade Association
NC-IUBMB - Nomenclature Committee of IUBMB
NAO - National Adhering Organization of IUPAC
NIOSH - US National Institute of Occupational Safety and Health
NIST - US National Institute of Science and Technology

OIML - International Organization for Legal Metrology (Organisation Internationale de Métrologie Légale)
OSHA - Occupational Safety and Health Association

PAC - *Pure and Applied Chemistry*, Official Journal of IUPAC
PC - Project Committee

REMCO - ISO Committee on Reference Materials
RIVM - Rijksinstituut voor Volksgezondheid en Milieuhygiene (The Netherlands)
RSC - Royal Society of Chemistry (UK)

SCOPE - ICSU Scientific Committee on Problems of the Environment

SCOWAR - ICSU Scientific Committee on Water Research

SUNAMOCO - IUPAP Commission on Symbols, Units, Nomenclature, Atomic Masses, and Fundamental Constants

UNEP - United Nations Environment Programme

UNESCO - United Nations Educational, Scientific and Cultural Organization

UNIDO - United Nations Industrial Development Organization

US-NIH - US National Institutes of Health

WHO - United Nations World Health Organization

Coding for IUPAC Bodies

010 Bureau

013 Project Committee

014 Evaluation Committee

015 Union Advisory Committee

020 Executive Committee

021 CHEMRAWN Committee

022 Committee on Chemistry and Industry (COCI)

024 Committee on Printed and Electronic Publications (CPEP)

026 Finance Committee (FC)

027 Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

028 IUBMB-IUPAC Joint Commission on Biochemical Nomenclature (JCBN)

034 SC on Spectroscopic Data Standards

040 Representatives on Other Organizations

050 Committee on Chemistry Education (CCE)

051 SC on Chemistry Education for Development

052 SC on Public Understanding of Chemistry

100 Physical and Biophysical Chemistry Division Committee (I)

104 Advisory Subcommittee (of Div I)

110 Commission on Physicochemical Symbols, Terminology, and Units (I.1)

200 Inorganic Chemistry Division Committee (II)

201 SC on Extra-Terrestrial Isotopic Ratios

202 SC on Isotopic Abundance Measurements

204 SC on Characterization of Carbonaceous Materials and New Carbons

205 Interdivisional SC on Materials Chemistry

210 Commission on Isotopic Abundance and Atomic Weights (II.1)

300 Organic and Biomolecular Chemistry Division Committee (III)

- 301 SC on Organic Synthesis
- 302 SC on Biomolecular Chemistry
- 303 SC on Green Chemistry
- 304 SC on Photochemistry
- 305 SC on Structural and Mechanistic Chemistry
- 306 SC on Biotechnology

400 Macromolecular Division Committee (IV)

- 401 SC on Macromolecular Terminology
- 421 SC on Structure and Properties of Commercial Polymers
- 428 SC on Modeling of Polymerization Kinetics and Processes

500 Analytical Chemistry Division Committee (V)

- 501 Interdivisional Working Party on Harmonization of Quality Assurance
- 502 SC on Solubility and Equilibrium Data

600 Chemistry and the Environment Division Committee (VI)

- 601 SC on Food Chemistry
- 602 SC on Biophysico-Chemical Processes in Environmental Systems
- 603 SC on Chemistry of Environmental Compartments
- 604 SC on Crop Protection Chemistry

700 Chemistry and Human Health Division Committee (VII)

- 702 SC on Nomenclature, Properties and Units in Laboratory Medicine
- 703 SC on Drug Discovery and Development
- 720 SC on Toxicology

800 Chemical Nomenclature and Structure Representation Division Committee (VIII)

- 801 Advisory Subcommittee (of Div. VIII)

CODING - OFFICER STATUS AND CATEGORY OF MEMBERSHIP

AM - Associate Member

CC - Commission Chairman

CS - Commission Secretary

DP - Division President

DS - Division Secretary

DVP - Division VicePresident

DPP - Division Past President

NR - National Representative

OF - Representative **of** Other Organization

ON - Representative **on** Other Organization

PR - Provisional Member

SCC - Subcommittee Chairman

SCS - Subcommittee Secretary

SCVC - Subcommittee Vice Chairman

STCC - Standing Committee Chairman

STCS - Standing Committee Secretary

STCVC - Standing Committee Vice Chairman

TGC - Task Group Chairman

TGM - Task Group Member

TM - Titular Member

WPC - Working Party Chairman