

# INORGANIC CHEMISTRY DIVISION COMMITTEE OF IUPAC

Meeting at Beijing 13<sup>th</sup> and 14<sup>th</sup> August 2005

## MINUTES

**Attendance:** Present were *President*, Anthony West, *Past President*, Gerd Rosenblatt, *Secretary*, Leonard Interrante; *Titular Members*: Tyler Coplen, Norman Holden, Robert Loss, and Kazuyuki Tatsumi; *Commission II.1 Chairman*, T. Ding, *Associate Members*: John Corish and Myunghyun Suh; *IUPAC President*, Leiv Sydnes, Young Observers Tamara Basova (Russia), Shaowei Chen (U.S.A.), Evgeny Koltsov (Russia), Richard Layfield, (U.K.), Daniel Rabinovich (U.S.A.), and Zhiping Zheng (U.S.A.), and visitors Ling-Kang Liu (China/Taipei), A. Tshavhungwe (S. Africa), G. McCann (G.B.), G. Leigh (G.B.), and Jing-Tai Zhao (China/Beijing).

**Apologies** were received from Titular Members Claudio Biancini, Alan Chadwick and Christian Chatillon who could not attend.

### 1- Introductions and Announcements

The meeting commenced at ca. 9:20 a.m. on Saturday, August 13, 2005. President West welcomed the members, Young Observers and IUPAC President Sydnes to the meeting. He then presented a brief overview of IUPAC and the Division II structure for the benefit of the first-time attendees. Each of the attendees then introduced themselves and described their professional affiliations and areas of expertise. West then continued with his introduction to the Division and discussed the schedule and locations for the Division II meeting at this GA today and tomorrow and the Materials Chemistry Subcommittee meeting on Monday. He asked TM R. Loss to describe briefly the activities of Commission II.1. Loss described the use of isotopic abundances: information in nutrition, geology, etc., and the Commission's role in taking published isotopic abundance data, evaluating these data, considering uncertainties, methods, and in conducting case studies. S. Corish was then asked to describe the Division's role in the process of verifying claims for new elements and assigning names and symbols. Corish used the recent case of element 111, Roentgenium (Rg) to describe this process. A report entitled "The name and symbol of the element with atomic number 111", by Corish and Rosenblatt was prepared in 2004 and has subsequently appeared in *Pure & Applied Chemistry* (*Pure Appl. Chem.* 76(12), 2101-2103, 2004). The role of the Division in generating, supporting (through small grants mainly used for travel) and organizing projects and in sponsoring conferences and workshops was outlined by West, and G. Rosenblatt described, as an example, a recently completed project on the use of mass spectrometric techniques in determining thermodynamic values. West indicated that one of the objectives of this meeting is to propose and discuss ideas for new projects and he encouraged the participants in general, and the new attendees in particular, to think about and propose for consideration such new projects. One of the Young Observers in particular, Daniel Rabinovich, indicated his potential interest in a project involving inorganic chemistry curriculum development in Latin American countries, where he felt that there was an interest in sharing ideas about course content and teaching methods in inorganic chemistry among the educators in several countries in North, Central and South America. Interrante agreed to work with him to help develop a project proposal and to discuss these ideas with the members of the Committee on Chemistry Education at their meeting later this week.

## **2 – Agenda**

The previously distributed Agenda was modified by President West and at the suggestion of the members present to include some changes in the order of discussion of certain topics and additional topics.

### **3- Minutes from Division Meeting in Grenoble**

Copies of these minutes were previously distributed and can be found on the IUPAC Division II web page. These minutes were approved by unanimous vote and accepted without change.

### **4 - Reports of IUPAC Bureau and Executive Actions (President West)**

The Bureau met in Bled, Slovenia on Oct. 2, 2004 and will be meeting again at the G.A. on Aug 17-18. At the meeting in Bled, the Bureau approved a proposal from Prof. Black that gave the Divisions the option to increase the Division electorate by including members of the subcommittees or advisory committees if desired by the Division. The Bureau also voted to continue having ten NRs on Division Committees for 2006-7. Other items of potential interest to Division II include the approval of a proposal to change the name of Division IV from the “Macromolecular Division” to the “Polymer Division”, to change the guideline set by the Treasurer for the proportion of the total Division budget which should be spent on operational expenses from up to 25% to up to 30%, and the name and symbol for the element of atomic number 111 as roentgenium and Rg, as was proposed in the Provisional Recommendation. The Bureau also ratified the appointment of Prof. A.R West, as President, and Prof. Kazayuki Tatsumi, as Vice President, of Division II. The formal recognition of Commission II.1, with its own guaranteed biennial funding of \$10K (\$8.5K from Division II), was also obtained.

### **5- Report by IUPAC President Leiv K. Sydnes**

President Sydnes gave a brief report on the IUPAC and the project system, indicating that most of the Divisions were functioning effectively under the new project system. He mentioned that some of the Divisions had been successful in pursuing joint funding of projects with other agencies. One such agency is the International Council for Scientific Unions (ICSU), which is a non-governmental organization that was founded in 1931 and includes both national scientific bodies (101 members) and international scientific unions (27 members). The ICSU acts as a forum for the exchange of ideas, the communication of scientific information, and the development of scientific standards. ICSU’s members organize scientific conferences, congresses, and symposia all around the world and also produce a wide range of newsletters, handbooks, journals, and proceedings. The ICSU Grants Programme, which is co-funded by UNESCO, seeks to support international and interdisciplinary issues that, because of their complex nature, are difficult to address through national or disciplinary channels. Although the overall budget is relatively small (USD850 000 for 2004), ICSU support often helps recipients attract additional funding from other sources. Over the past three years, ICSU has taken steps to improve the program by initiating a competitive peer-review process and identifying five broad priority areas: emerging science and technology, science and technology for sustainable development, capacity building and science education, dissemination of information on science and technology, and the science/policy interface. N. Holden gave an example of a prior joint project involving IUPAC and the Geological Union, involving half-lives of isotopes in geology, that was funded by this council.

## **6- Report regarding the 2005 TM elections (President West)**

West explained that the nominations process had become bogged down during the process of assembling the nominations committee and that, as a result, the selection of nominees and the election of the Division TMs had not been completed prior to the current meeting as was previously planned. It was suggested by Interrante and Rosenblatt that more detailed guidelines, including deadlines for the various stages of the nominations and elections process, be established by the Division, so as to avoid the repetition of problems such as this one in the future. Interrante agreed to set up such a timetable for the different stages in this process and to present it to the Division Committee at its next meeting. Corish noted that one problem we have is that some of our elected TMs never show up for our meetings. Sydnese agreed that it was most important that we get dedicated people who are willing to perform. Interrante and Rosenblatt suggested that if an elected TM fails to show up for two consecutive meetings we should ask them to resign. It was generally agreed that we should do this and Interrante was asked to prepare a letter to be sent to TMs who we find to be in this position. West raised the question of who we should consider as the electorate for our election of TMs. Rosenblatt pointed out that the Division now has the flexibility to establish the electorate. It was decided that the electorate should include the people who are on the agenda (project leaders, subcommittee chairs, TMs, AMs, NRs). Project leaders would be allowed to vote only for the duration of the project as originally defined. West had obtained the agreement of the IUPAC President that we could complete the nomination process this time by using the current Division officers as an ad-hoc nominations committee and that we would present the names and biographies of the nominees to the IUPAC Secretariat in time for completion of the election before the end of October.

## **7- Review of Division Budget Allocations and Expenditures**

The Division Project Coordinator, Coplen, presented the Division budget allocations and expenditures for Projects for the current biennium. The following single project was funded so far by the Division: 2005-001-1-200 P. Day, "Towards defining materials chemistry", \$8,000. [The Project 20003-033-1-200, Weiser, Determination of atomic weights using new analytical techniques, was funded by the Treasurer this biennium]. In the current biennium, \$51,200 was originally allocated, of which \$20,680 was spent on operations and \$8,000 on projects, leaving \$22,520 left to be allocated by the end of this year.

## **8- Membership and Terms of Office of the Inorganic Division Officers and Titular Members**

Owing to the resignation of Division II Past President Rosenblatt in 2004, and the subsequent uncertainty regarding the terms of office for the current Division President and Vice-President, clarification was sought from IUPAC regarding the terms of all of our Division officers. In an email message subsequent to the IUPAC Bureau meeting in Bled, Slovenia on Oct. 2, 2004, where this question was raised by A. West, Prof. David Black indicated that the IUPAC Bylaws have two relevant provisions: (1) the term of a Division President is no more than four years and (2) service as an officer, TM or AM cannot total more than 12 years. Thus it was suggested that West would serve as President for the remaining two years of Rosenblatt's term and then be eligible to serve another two years. Rosenblatt does not reach the 12 year limit until 2007, so he is eligible to serve a further two years as TM or AM. Further discussions with the IUPAC President during this meeting were planned to clarify this situation and, in particular, to appeal

for a full 4-year term for West after the initial 2-year completion of Rosenblatt's term. This would allow Tatsumi the usual full four years as Vice-President, prior to his assuming the President's position. Pending the results of these discussions, of upcoming election of new TMs, and a decision on the part of the Division Executive committee regarding the choice of AMs and NRs for the coming biennium, a new list of members for the Inorganic Division Committee will be prepared and submitted to IUPAC Secretariat by the Division President prior to the end of 2005.

### **9- Report from other IUAPC bodies – Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS) (Sean Corish)**

The ICTNS, under the Chairmanship of Professor Lorimer, has been working very well during the past biennium. The current status list of Technical Reports and Recommendations 2004 – 2005, of which a copy is available at the IUPAC web site, contains forty-seven entries of which three refer to this Division. All of these three are published or are in course of publication: Name of Element 111 (Corish); HT Mass Spectrometry (Drowart); and Red Book (Connelly). Another which originated in this Division and remains of relevance concerns the numbering of Fullerenes. The ICTNS will this year discuss the Periodic Table and the Division Committee should also now discuss any of our forthcoming reports that we need to be referred to ICTNS for approval prior to its publication. He will bring these to the attention of the ICTNS meeting here at Beijing (none were subsequently forthcoming). A copy of the report from Division II to ICTNS, that was prepared by Corish for this meeting, is attached to these minutes as *Appendix I*.

### **10- Report from Commission II.1 (and Sub-committees on Extra-Terrestrial Isotopic Ratios, Isotopic Abundance Measurements, and Applications of Isotopic Specific Measurements) (T. Ding)**

A written report was submitted by Commission Chairman Ding, which includes a complete list of the current Commission and Subcommittee members, and is attached to these minutes as *Appendix II*. The Commission met in Beijing immediately preceding this GA and was attended by the following members: T. Ding (Chair, China), J.K. Böhlke (USA), M. Berglund (Belgium) T. Coplen (USA), T. P. De Bièvre (Belgium), M. Ebihara (Japan), A. R. Gonfiantini (Italy), M. Gröning (Germany), N. E. Holden (USA), R.D. Loss (Australia), P.D.P. Taylor (Belgium), N.E. Holden (USA), K.J.R Rosman (Australia), T. Walczyk (Switzerland), M Wieser (Canada), S. Yoneda (Japan), M-T Zhao (China) and Y-K Xiao (China). The meeting consisted of a two day ICEII Proj Workshop on Aug 5-6, a one day Isotope Symposium on Aug 7, a two day SIAM meeting on Aug 9 – 10, and a two day meeting of the overall CIAAW on Aug 11 – 12. The Subcommittee for Isotopic Abundance Measurements (SIAM) continues to be the major activity of the Commission. The participants in the SIAM meeting evaluated isotopic abundance data in 12 publications covering 11 elements and made recommendations to change or modify entries for several polyisotopic elements. An evaluation of 2003 published data on atomic mass determinations resulted in recommended changes to the 11 monoisotopic elements. These results were the subject of a press release that subsequently appeared in the News & Notices section of the IUPAC website ([http://www.iupac.org/news/archives/2005/atomic-weights\\_revised05.html](http://www.iupac.org/news/archives/2005/atomic-weights_revised05.html)) and which was reported in Chemistry International in its November-December 2005 issue. A copy of this notice is appended to these minutes as *Appendix III*. The recommendations will be reflected in the publication Table of Atomic Weights 2005, which will be submitted for publication in PAC before the end of the year. G. Rosenblatt promised to update the IUPAC

Periodic Table to reflect the new atomic weights, leaving the timing and format of the Table's dissemination to the Secretariat. The Commission also resolved to investigate setting up a web presence on the IUPAC website and would seek the support of IUPAC to establish a secure "members only" area. Following their meeting, the members of CIAAW formed working parties to work on several projects most of which will be submitted to IUPAC before the end of the Assembly period.

### **11- Report of Materials Chemistry Subcommittee (S. Corish)**

S. Corish submitted a written report, which is attached to these minutes as *Appendix IV*. The last official meeting of this Subcommittee was in Ottawa, at the 42<sup>nd</sup> GA in August 2003; however, there was an unofficial meeting of the Division II members of this Subcommittee that were in attendance at the August 2004 Division meeting in Grenoble, France. Among the significant accomplishments of the sub-committee during the past year was the solicitation, and subsequent submission and approval, of a *Project to Define Materials Chemistry*, with Professor Peter Day as the Project Leader and the submission of another proposal, on a *Project to Produce a Glossary of Terms used in Materials Chemistry*, by Dr Sanjay Mathur, which is now ready for review by the Division Committee at Beijing. A third Workshop on Advanced Materials (WAM III) was also initiated by this Sub-committee, which was the subject of a separate report at this Division Meeting (see following). The Sub-Committee was scheduled to meet on Monday August 15<sup>th</sup> during the current GA in Beijing (a copy of the minutes of this meeting, subsequently prepared by, and obtained from, A. West, are attached to these Minutes as *Appendix V*).

### **12- Workshop on Advanced Materials, Stellenbosch South Africa, September 4<sup>th</sup> to 8<sup>th</sup> 2005, WAM III (S. Corish)**

This workshop was initiated by the Sub-Committee after Ottawa, via Professor Piet Steyn. It has been organised by Professor Ron Sanderson and has been supported by IUPAC. It has been the subject of a separate report to the Division committee, which is also appended here (see *Appendix VI*). Prof. Corish will report further on this at the Subcommittee meeting on Monday.

### **13- Project-by-Project Review**

Coplen gave a PowerPoint presentation that summarized the current status of the various Projects that are being pursued under the management of the Division Committee, and of the funding that had been allocated to these projects. Following are the key points from this presentation, along with other input received by the Secretary directly from the relevant Project Leaders.

#### **1999-001-1-200 Connelly; Nomenclature of Inorganic Chemistry – Revised ('Red Book', Part 1); H. Kaesz, Project Monitor**

\$9,930 was originally allocated to this project, \$10,521 was spent; Sep 2005 – the Project is now completed – The Red Book will be published by the RSC this fall [ISBN 0 85404 438 8] (see item 16).

**1999-049-1-200 G.F. Voronin; Thermodynamic characterization of high-temperature superconductors in the yttrium-barium-copper-oxygen system; A. West, Project monitor.**

At the time of our last Division meeting in Grenoble, Voronin had submitted a brief written report to the Secretary, which was appended to those minutes. At that time (July 2004) Voronin had indicated that the work at the project was in the completion phase and that he wanted to add another task force member and use the available funds allocated to the project (\$5,000) for the future work. As of the time of the Beijing meeting, no further report had been received and none of the funds had been spent. West agreed to contact Voronin and check regarding the status of this project.

**2000-002-2-100 Y.H. Ma; Standardization of methods for the characterization of inorganic membranes, A. Chadwick, Project Monitor**

The last report on this project was received in June 2004 and is attached to the Minutes of the Division II Grenoble meeting. At that time, Ma indicated that most drafts had been received but that considerable rewriting was required and that this had not yet been completed. After attending two meetings in June-July 2004, where many of the task force members would be present, he expected to provide the Secretary with a report on his discussions with the group leaders and other leaders in the field and also to give his assessment and recommendations on the feasibility of continuing the project. As of this time, no such report had been received and none of the original funds (\$5,000 Division I) had yet been spent.

**2000-007-1-400 R. Jones; Definitions of Terms Relating to the Structure and Processing of Inorganic and Polymeric Gels and Networks, and Inorganic-Polymeric Materials; A. Chadwick, Project Monitor; allocated: \$11,500 (Div. IV), spent \$10,237**

A report was received from R. Jones and is attached to these minutes as *Appendix VII*. This project has been completed and a formal report has been written. Its content was to be reviewed by members of the Subcommittee on Macromolecular Terminology and by external experts. S. Corish indicated that this now needs to go to ICTNS and that he would handle it (as our Division's ICTNS representative).

**2000-020-2-200 Kizilyalli (deceased); Collecting, testing and dissemination of experiments in solid state and materials chemistry; S. Corish, Project Monitor; allocated: \$8,600, spent \$225**

Corish gave an oral and the following written report on this project "I learned with great sadness on July 21<sup>st</sup> of the death of our colleague Professor Meral Kizilyalli who had been the leader of this Project and who had made considerable progress in bringing it forward. Given the nature of this project and of the work that Professor Kizilyalli had done to date, both in the collection and in the testing of the experiments in the portfolio, I believe that it will be difficult to find someone to take her place. The best initial option would be to seek a volunteer from within the current members of the Task Force." Subsequent to this report, Corish discussed with two of the guests who had attended the Division meeting, Drs. Basova and Koltsov, the possibility that they could complete this project and, after they had expressed interest in doing so, he undertook to send them copies of the work that had been accomplished to date.

**2000-022-1-200 Boehm; Characterization of Carbon Materials; G. Rosenblatt, Project Monitor; allocated: \$5,500, spent \$0**

No report was received from Boehm, who was reported to be ill as of a year ago by G. Rosenblatt. Rosenblatt indicated that this is another project that is ca. 80% completed but that none of the funds had been spent and nothing was published. He advised dropping it from the list of current projects.

**2000-024-2-200 Balducci; Teaching of high temperature materials chemistry at universities; G. Rosenblatt, Project Monitor; allocated: \$4,800, spent \$0**

Balducci submitted in an email message to the Secretary that “after a forced interruption due to my protracted illness in the last months, work aimed to prepare an improved version of the document started again and is progressing. The basis for the improved version has been indicated in the Inorganic Division Project Review (Review 2) submitted a few months ago to T.B. Coplen (*Appendix VIII*). In particular, work is presently focused on refining explanations for the topics and on selecting and updating the useful bibliography pertinent to each topic. When the revision work will be completed the document will be circulated among the task group members and other colleagues expert in the field (I plan within 2-3 months)”.

**2001-015-1-100 Stanbury; Standard potentials of radicals; G. Rosenblatt, Project Monitor**

This Project, whose objective is “to evaluate standard potentials ( $E^0$ ) and related quantities for important aqueous organic and inorganic radicals”, was jointly funded with the Physical Chemistry Division (I) (primary sponsor) at the level of \$15,000, of which \$13,446 had been spent thus far. Rosenblatt reported that this project was “alive and on-going”. From the IUPAC website: “Feb- 2005: So far, a set of evaluations and seven summary tables have been prepared, including: Inorganic Standard Potentials, Gibbs Energies of Formation for Radicals, Inorganic Radical  $pK_{as}$ , Hemicolligation Equilibrium Constants, Organic Standard Potentials, Radical Henry's Law Constants, and Inorganic Radical Equilibrium Constants. Linked to these tables are the individual evaluation sheets. At present we have prepared about 140 evaluation sheets.” This project was presented at a poster session at the current IUPAC Congress in Beijing.

**2001-019-2-200 Walczyk; Guidelines for mass spectrometric isotope ratio measurements; T. Coplen, Project Monitor; allocated \$2,000, spent: \$0**

Coplen reported that this project is on-going and will be finished in the next few months

**2001-042-1-200 Ebihara; Review of isotopic abundances in extraterrestrial materials; Holden, Project Monitor; allocated: \$6,000, spent \$6,000**

Coplen reported that the money has been spent, and that the work is finished but not yet published. Yoneda plans to publish within next 6 months.

**2002-049-2-200 Taylor (Loss); A new comprehensive report on the isotopic compositions of the elements for global user communities. Phase 1; Coplen and Holden, Project Monitors. Allocated \$8,000, spent: \$5,699**

A final report on this project was received from Loss, and is attached to these minutes as *Appendix IX*. Work continues on in this mainline Commission project, as project 2003-031-1-200 (see below, as well as the CIAAW report in *Appendix II*).

**2003-006-1-100 Harris/Becker; NMR chemical shifts – updated conventions; Chadwick, Project Monitor; allocated: \$7,000(\$2,000 Div II), spent 5,054.**

A written report was received from Prof. Harris on this continuing active project, which is attached to these minutes as *Appendix X*.

**High temperature mass spectrometry: accuracy of the method and influence of the ionization cross-sections Drowart, Project Leader; Rosenblatt, Project Monitor**

This project was started in the early 1980's under the auspices of the previous Commission II.3 on High Temperature and Solid State Chemistry and has long since used up its funding from IUPAC and is no longer "on the books"; nonetheless, the task force members have continued work on it and in 2005 completed a comprehensive (54 page) report entitled "High Temperature Mass Spectrometry: Instrumental Techniques, Ionization Cross-sections, Pressure Measurements, and Thermodynamic Data", which was recently published in *Pure and Applied Chemistry* [Vol. 77, No. 4, pp. 683-737 (2005) (<http://www.iupac.org/publications/pac/2005/7704/7704x0683.html>)]. The Secretary was asked to prepare a letter to the authors of this report (J. Drowart, C. Chatillon, J. Hastie, and D. Bonnell) to thank them for their extraordinary effort on this project, which can now be listed as "completed" in every sense of the word (the letter that was subsequently prepared and sent to these authors is attached to these minutes as *Appendix XI*).

**2003-029-1-200 DeLaeter; "Element by element review of atomic weights to the year 2000 – Extension of 1999-043-1-200" ; Loss, Project Monitor; allocated: \$4,000, spent \$4,706**

The purpose of this project, which is now completed, was to provide 1000 reprints of of the well received report "Atomic Weights of the Elements: Review 2000" by J. R. de Laeter, J. K. Böhlke, P. De Bièvre, H. Hidaka, H. S. Peiser, K. J. R. Rosman, and P. D. P. Taylor, *Pure Appl. Chem.*, **75**, 683-800 (2003).

**2003-031-1-200 Berglund; Isotopic compositions of selected elements; Loss, Project Monitor; allocated: \$12,000, spent \$12,513.**

An oral report was given by R. Loss; the written version submitted to the Secretary states that: "(the) Task group members have been continuing to evaluate selected elements and participating in email communication/discussion with the task group and other CIAAW members. The guidelines for evaluation of scientific publications has been discussed and reviewed continuously during the spring of 2005. In August 4-5, a two-day workshop was held in Beijing. The current status was presented and discussed. A number of elements were scrutinized and the guidelines were evaluated. A schedule was set up for finishing the project in December 2005. This project

was reviewed at the CIAAW meeting. A number of action items have to be dealt with by the members and the final report of this project is still expected to be completed by the end of 2005”.

**2003-033-1-200 Wieser; Determination of atomic weights using new analytical techniques; Loss, Project Monitor; allocated \$14,800, spent, \$2,190**

This core project of Commission II.1 was funded in early 2004 by Leiv Sydnes (IUPAC President) at no cost to Div II. See the Commission II.1 report (*Appendix II*) for an overview of these projects on isotopic composition and atomic weight determination.

**2003-034-1-200 R. Kniep (previously, Kizilyalli (deceased)); Classification, terminology and nomenclature of borophosphates (4-year project); Rosenblatt, Project Monitor; allocated \$16,000, spent \$0**

An oral report was presented by Prof. J-T. Zhao, a task force member, at this meeting. Prof. Zhao indicated that “Since the sad sudden death of Prof. M. Kizilyalli a year ago, this project has been postponed and not much effort was put into it. The project is worthwhile carrying out and the task group members are still interested in it. Therefore, at the request of Prof. Kniep, I am attending this the IUPAC meeting to explain the situation to the sponsoring Division. I hope that the project will be carried out more efficiently in the near future and expect progress in the next year.”

**2005-001-1-200 Day; Towards defining materials chemistry; West, Project Monitor; allocated \$8,000 (shared with Division VIII), spent \$0.**

This new project has as its objective: “To assemble, collate and disseminate information about the scope of the newly-emerging discipline of materials chemistry, leading to an authoritative definition of the subject within the family of chemical sciences”. G. McCann, Managing Editor of the Journal of Materials Chemistry, gave an oral report on behalf of Prof. Day, who could not attend the meeting (*Appendix XII*). Dr. McCann gave his perspective on the background to this project and on the subject of materials chemistry and offered the following draft definition of materials chemistry to “help get the ball rolling”: “The synthesis, processing, characterisation and exploitation of compounds that have useful, or potentially useful, properties and applications. The focus of the research is the creation, understanding and development of compounds or systems with improved properties that will impact positively on business and personal life. To use chemistry to create compounds that may lead to new technological opportunities or significant improvements in existing technology. Research in (non-materials) Chemistry is focused on adding to our understanding of chemistry, of how matter is composed, interacts and how fundamental properties arise.” The first face-to-face meeting of the task force for this project has been proposed for April 2006.

#### **14- Review of New Project Proposals**

**2005-020 -1 Corish and Mathur; Glossary of Terms in Materials Chemistry – I; amount requested: \$38,250; received July 19, 2005**

The major goal of this project is “to generate accurate definitions of research and technical terms along with their contextual uses to enhance the cognisance of materials chemistry with other

related disciplines". This proposal is at the Division Committee evaluation stage, for internal evaluation and identification of outside reviewers.

**2005-022-1 Coplen; Calibration of Organic and Inorganic Oxygen-bearing Isotopic Reference Materials, amount requested: \$12,000, duration: 24 months; received July 22, 2005**

The purpose of this work is to carry out laboratory analytical measurements and convene a workshop to assess the relative amounts of oxygen isotopes in internationally distributed organic and inorganic isotopic reference materials and publish "reference" values and uncertainties for these materials. Reviews have been obtained and, subsequent to this meeting, were communicated to the Division for final action on 27-Sep-05.

**2003-027-1 Ebihara; Review of Isotopic Abundances in extraterrestrial materials – Part II, amount requested \$8,000; received August 17, 2005**

The Subcommittee did not meet in 2005 and Coplen and Holden recommended that a decision on this proposal be deferred due to the fact that the previous project on this topic (2001-042-1-200) has not yet been completed.

**2005-021 Berglund; Evaluated Isotope Ratio Data (2005-2007); amount requested: \$9,800; received August 19, 2005**

Reviews have been obtained and, subsequent to this meeting, were communicated to the Division for final action on 26-Sep-05.

**15- Reports on recent and planned Division-sponsored conferences (Rosenblatt, Corish) (See item 12 for Corish's report on WAM III)**

Rosenblatt reported on the progress to date on the organization and planning for HTMC-XII, the 12<sup>th</sup> in a series of triennial Division-sponsored conferences on High Temperature Materials Chemistry, which will be held in Vienna, Austria on September 18-22, 2006. Ca. 120-250 attendees are expected at this latest - of what has become the premier - conference on high-temperature materials chemistry. The chairmen of the meeting will be Adolf Mikula and Herbert Iperser from the University of Vienna and Ulrich Schubert from the Vienna University of Technology. The scope of the conference will focus on new developments of High Temperature Chemistry in various fields of material science. Further details regarding this conference can be obtained at the conference website: <http://www.univie.ac.at/htmc06/>.

**16- Reports from Other IUPAC Bodies - Chemical Nomenclature and Structure Representation Division (VIII) – G. Leigh**

Neil Connelly had reported in an email message to the Secretary that "the revised Red Book is with the RSC. We have corrected the proofs and I am waiting for a second set from which to construct the subject index. (At the same time I, and Ture Damhus, will check that the corrections have been made and that there are no other errors). If all goes well I expect the book to be in press by the end of September (I was hoping it would be in the book stores on July 16 to compete with the latest Harry Potter!)". Prof. G. Jeffery Leigh (Division VIII AM) also gave an oral report to the Division at this meeting. The anticipated publication of the IUPAC Red Book

on Inorganic Nomenclature (noted above) was discussed as well as other continuing activities of potential interest to our Division. He indicated that the formation of the new Division had not yet resolved the conflicts between the Organic and Inorganic Divisions regarding the nomenclature in overlapping areas of interest, such as organometallic chemistry, acids, etc. but that they were still working toward agreement on these matters. Rosenblatt noted that this disagreement between the organic and inorganic people regarding the nomenclature of compounds of common interest was not new and was one of the factors that led to the creation of a combined Nomenclature Division. Leigh then described the ongoing efforts to develop the IUPAC International Chemical Identifiers (INChIs), which are strings of numbers that are used to identify a particular compound, assign its structure, etc. These Chemical Identifiers have already been adopted by several organizations and there is a version of this on the IUPAC web site which covers organic and inorganic compounds and which is being extended to polymers. These INChIs are not necessarily the ultimate solution to identifying compounds, for example, there are unsolved problems with tautomers and mixtures, but have advantages over the CAS Registry numbers, which are arbitrary numbers, in that they are derived from the chemistry of the materials involved and can be used both to identify a substance and to derive its structure. He also indicated that a complete revision of Boron nomenclature was still needed, along with that for metallocycles, and that efforts were underway to meet these needs. Another active problem mentioned was the extension of the system of polyhedral symbols beyond the current coordination number 6 to general methods for coordination numbers 7, 8 and 9 (one runs into problems in identifying polyhedra when one gets to 10-12). Finally, he asked for input from this Division regarding the development of a new version of the book, "Principles of Chemical Nomenclature. A Guide to IUPAC Recommendations" by G.J. Leigh, H.A. Favre, and W.V. Metanovski (Edited by G. Leigh); Blackwell Science Ltd., (1998). This book provides an introduction to chemical nomenclature that is especially directed towards students. The need for a revision has become particularly acute due to the impending arrival of the three new "color books" this next year. He would like anyone who is interested in working with them in preparing this new version to contact him.

### **17- Adjournment**

The Meeting was adjourned at 5:30 pm on Sunday, August 14, 2005

## **Appendix I – Report to ICTNS from Division II**

### **IUPAC General Assembly, Beijing, August 2005 - John Corish, August 15<sup>th</sup> 2005**

The Division Committee has completed a very successful meeting at Beijing with an average attendance of sixteen. It had proved impossible to complete the election process prior to the General Assembly but the results of the elections are now expected to be known by the end of September. The election will be used to strategically strengthen the Division by electing two in the area of molecules and one each in materials and atoms. The meeting considered five proposals for new projects and the approval of some of these will enable the funding for the current biennium to be fully committed.

#### ***The Red Book***

The new edition of the Red Book, a project initiated in the Division and now coordinated by Division VIII is now in the very final stages of editing of proofs and is expected to be published before the end of this year.

#### ***Commission II.1***

This Commission and some of its subcommittees met at Beijing prior to the General Assembly. The publication of some revised atomic weights is awaiting Council approval and a new project to continue this work during the next two years was discussed and approved in principle at the Division Committee meeting. The Commission continues to make substantial progress in the projects currently in its portfolio.

#### ***The naming of new elements***

The name for the element with atomic number 111 was approved during the current biennium. The joint IUPAC/IUPAP Working Party with responsibility for the assignment of priorities for the discovery of new elements had decided that there was not sufficient new published data to justify a re-examination of claims for the discovery of elements above number 111 during the past twelve months but the Division Committee decided at Beijing to now invite it to carry out another review. This request will be initiated immediately it is intended to again follow the new naming procedures, which have worked satisfactorily for elements numbers 110 and 111.

#### ***Sub-Committee on Materials Chemistry***

This is an Interdivisional Sub-Committee and invitation to membership has been extended to all interested Divisions. The area of Materials Chemistry remains fast growing as is evident from the exceptional growth in interest in and contributions to the journals now dedicated to the area by both the ACS and the RSC. The editors of both of these journals attended the meeting of the Sub-committee held at Beijing. Work has commenced on a project initiated by the sub-committee, under the leadership of Professor Peter Day, to define the area of Materials Chemistry. A second project aimed at producing a glossary of terms for nanotechnology has been formulated involving Divisions I, II and IV and will be initiated during this biennium. The Sub-Committee has also carried forward the series of Workshops in advanced Materials and WAM III, organised by a local committee led by Professor Ron Sanderson, will take place in Stellenbosch, South Africa, September 4<sup>th</sup> to 8<sup>th</sup> 2005. The Sub-committee will shortly set up a website linked to the IUPAC site.

## Appendix II - Commission II.1 Report

### Draft report for the Inorganic Division (13 – 8 – 05) Commission Isotope Abundances & Atomic Weights (CIAAW) Report for 2003-2005

The Titular and Associate members, National Representatives and Observers present at the Commission on Isotope Abundances and Atomic Weights Meeting in Beijing were: T. Ding (Chair, China), J.K. Böhlke (USA), M. Berglund (Belgium) T. Coplen (USA), T. P. De Bièvre (Belgium), M. Ebihara (Japan), A. R. Gonfiantini (Italia), M. Gröning (Germany), N. E. Holden (USA), R.D. Loss (Australia), P.D.P. Taylor (Belgium), N.E. Holden (USA), K.J.R Rosman (Australia), T. Walczyk (Switzerland), M Wieser (Canada), S. Yoneda (Japan), M-T Zhao (China), Y-K Xiao (China),

An evaluation of published isotope abundance measurements for the period 2001 – 2005, review of the atomic weights, based on the reports from the Subcommittees for Isotopic Abundance Measurements (SIAM), continues to be the major activity of the Commission. The SIAM met on August 9 and 10, 2002 at the CAGS in Beijing and evaluated isotopic abundance data in 12 publications covering 11 elements and made recommendations to change or modify entries for the following polyisotopic elements: Sm, Nd, Ta, La and Pt. In addition an evaluation of 2003 published data on atomic mass determinations has resulted in recommended changes to 11 monoisotopic elements (Na, Al, P, Sc, Mn, Co, Cs, Tb, Au, Bi and Th) These recommendations will be reflected in the publication *Table of Atomic Weights 2005*, which will be submitted for publication in PAC before the end of the year. This publication will also contain recommendations for scientists measuring absolute isotope abundances with the view to making.

The task of the Subcommittee on Isotopic Abundance Measurements (SIAM) has become increasingly important with the emergence of new analytical techniques that enable the analyst to measure isotope amount ratio measurements to very high precision (reproducibility) and the widespread adoption of isotopic techniques in science and technology. The challenge for SIAM is to ensure that these high precision measurements and associated uncertainty calculations that lead to published representative isotopic compositions and Standard Atomic Weights adequately cover systematic as well as statistical uncertain. SIAM is collaborating with outcomes from the Isotopic Composition of Selected Elements project, which is developing systematic and comprehensive evaluation criteria to account for systematic uncertainties during sample preparation and measurement. In addition, the Isotopic Composition of Selected Elements project is developing a database that presents the evaluated isotopic compositions, range of variation of isotopic composition, and the atomic weight as decided by CIAAW. These evaluation tools are of immediate use to SIAM and are fundamental to the ongoing work of SIAM.

The Subcommittee for Extra-Terrestrial Isotope Ratios did not meet during the period 2003 - 2005 and hence did not contribute to Commission proceedings.

The Commission also resolved to investigate setting up a web presence on the IUPAC website and would seek the support of IUPAC to establish a secure “members only” area.

Following the meeting the members of CIAAW formed working parties to work on several projects most of which will be submitted to IUPAC before the end of the Assembly period:

- 1: Evaluation of newly published isotopic abundance data (2005 – 2007)..
- 2: An investigation into the extent of Natural Isotopic Variation.
- 3: A Non-constancy of Atomic Weights Poster.

**Commission Members 2006 - 2007:**

(a) Titular Members

Prof. Tiping Ding (Chair)  
Dr Michael Wieser (Secretary)  
Dr. Michael Berglund  
Dr. Thomas. Walczyk  
Dr. Shigeku Yoneda

(b) Associate Members:

Dr. A. M. Foulliac  
Dr R. Gonfiantini  
Dr M. Gröning  
Dr. H. Hidaka  
Dr. X. Zhu

(c) National representatives

Dr. P. de Bièvre  
Dr. J. R. de Laeter

(d) Membership of subcommittees

1. Subcommittee for Isotopic Abundance Measurements (SIAM)  
Dr. Michael Berglund (Chairman)  
Dr John Karl Böhlke  
Dr Tyler B. Coplen  
Prof Paul De Bièvre  
Prof John R. De Laeter  
Prof Tiping Ding  
Dr Roberto Gonfiantini  
Dr Manfred Gröning

Dr Norman E. Holden  
Dr Robert D. Loss  
Prof Etienne Roth  
Prof Kevin J. R. Rosman  
Dr Thomas Walczyk  
Dr Michael Wieser  
Prof Motian Zhao  
Dr Xiang Kun Zhu

2. Subcommittee for Extra-Terrestrial Isotopic Ratios (SETIR)

Prof Mitsuru Ebihara (Chair)  
Dr Hiroshi Hidaka  
Dr Robert D. Loss  
Dr Michael Wieser (Secretary)  
Dr Shige Yoneda

3. Subcommittee for Extra-Terrestrial Isotopic Ratios (SETIR)

Prof Mitsuru Ebihara (Chair)  
Dr Hiroshi Hidaka  
Dr Robert D. Loss  
Dr Michael Wieser (Secretary)  
Dr Shige Yoneda

4. 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  
Dr Norman E. Holden (Chair)

## Appendix III

## Standard Atomic Weights Revised

The Commission on Isotopic Abundances and Atomic Weights (II.1) met for two days, on 10-11 August 2005, during the 43rd IUPAC General Assembly in Beijing. Following its meeting, the Commission released the changes to the standard atomic weights,  $A_r(E)$ , of 16 chemical elements. The following changes are based on new determinations of isotopic abundances and reviews of previous isotopic abundances and atomic masses:

	From	To
Aluminium	26.981 538 (2)	26.981 5386 (8)
Bismuth	208.980 38 (2)	208.980 40 (1)
Caesium	132.905 45 (2)	132.905 4519 (2)
Cobalt	58.933 200 (9)	58.933 195 (5)
Gold	196.966 55 (2)	196.966 569 (4)
Lanthanum	138.9055 (2)	138.905 47 (7)
Manganese	54.938 049 (9)	54.938 045 (5)
Neodymium	144.24 (3)	144.242 (3)
Phosphorus	30.973 761 (2)	30.973 762 (2)
Platinum	195.078 (2)	195.084 (9)
Samarium	150.36 (3)	150.36 (2)
Scandium	44.955 910 (8)	44.955 912 (6)
Sodium	22.989 770 (2)	22.989 769 28 (2)
Tantalum	180.9479 (1)	180.947 88 (2)
Terbium	158.925 34 (2)	158.925 35 (2)
Thorium	232.0381 (1)	232.038 06 (2)

The values are presented in a concise notation whereby the standard uncertainty is given in parenthesis next to the least significant digits to which it applies; for example,  $A_r(\text{Al}) = 26.981\ 538\ (2)$  is the concise form of the expression  $A_r(\text{Al}) = 26.981\ 538 \pm 0.000\ 002$

These changes in the atomic weights will be published in a new Table of Standard Atomic Weights 2005, which will be submitted for publication in *Pure and Applied Chemistry* by the end of 2005. The commission also continued its review of publications of variations in the natural isotopic abundances. For more details about the Commission meeting in Beijing, see *Chem. Int. Nov/Dec 2005 issue*, Division Roundups on p. 7, or contact Michael E. Wieser <[mwieser@ucalgary.ca](mailto:mwieser@ucalgary.ca)>, secretary of the Commission.

<release published in [Chem. Int. Nov/Dec 2005 issue](#)>

## **Appendix IV - Report on the Materials Chemistry Sub-Committee**

### **Beijing General Assembly August 2005**

The Committee had last met at the GA at Ottawa. Plans to hold a meeting in conjunction with the 2004 Division Committee in Grenoble did not materialise though much of the business of the Sub-Committee was discussed at that meeting but only by the members from Division II.

Of the work programme set out at Ottawa most of the major items had been accomplished or are in progress.

#### **Projects**

*Project to Define Materials Chemistry:* This project had been initiated under the leadership of Professor Peter Day, a Task Force had been assembled, although some members may be added and initial discussions were scheduled for Beijing although, unfortunately, Professor Day will be unable to attend. Dr. Graham McCann will make a presentation on Monday.

*Project to Produce a Glossary of Terms used in Materials Chemistry:* An application prepared by Dr Sanjay Mathur has been submitted and is now ready for review by the Division Committee at Beijing. Dr. Mathur will make a presentation on Monday.

#### **Workshop on Advanced Materials, Stellenbosch South Africa, September 4<sup>th</sup> to 8<sup>th</sup> 2005, WAM III**

This workshop initiated by the Sub-Committee after Ottawa via Professor Piet Styne is will take place. It has been organised by Professor Ron Sanderson and has been supported by IUPAC. It has been the subject of a separate report to the Division committee which is appended here. Prof. Corish will report on Monday.

#### **Website for the Sub-Committee:**

This was the final action proposed at Ottawa and, in so far as I am aware no work has been done as yet to establish this site which it is intended will be linked to the IUPAC site.

Although some of the objectives of the Sub-Committee have been achieved and others are under way it has in general been a less active biennium than might have been ideal. This has been due in part to slow responses from members and collaborators and in part to the uncertainties in the Division during the first year.

The Sub-Committee is scheduled to meet on Monday August 15<sup>th</sup> during the GA at Beijing.

John Corish  
Trinity College Dublin  
28<sup>th</sup> July 2005

**Appendix V**  
**Sub-Committee on Materials Chemistry**  
**15 August 2005**  
**Beijing**  
**MINUTES**

**Present [Division membership, young observer or other status]:** J Corish (Chairman) [II], A R West (Acting Secretary) [II], L V Interrante [II], D Rabinovich [YO], G McCann [RSC representative], A M Tshavhungwe [South Africa, capacity building], R Jones [IV], C Gorman [YO], Z Zeng [YO], R Weir [I], G Rosenblatt [II], S Mathur [II].

**Apologies:** A V Chadwick, J Maier, E Reichmanis, C Chatillon, F Adams.

**1. Minutes of Ottawa Meeting**

These had previously been circulated electronically. JC gave a summary of the meeting and said that all actions arising had been completed, apart from preparation of the website. To do this should now be relatively easy since IUPAC (Fabienne) are setting up a web system to allow members to input information in a convenient format. **Action: RJ to pursue, with assistance from JC.**

**2. Project to Define Materials Chemistry**

This has received IUPAC approval with Prof P Day as Project Leader. In his absence, Dr G McCann updated the subcommittee on progress. The project will run for 2 years. The objective is to produce a statement showing how Materials Chemistry can fit within the overall IUPAC structure.

PD has met with a) ARW for preliminary discussions about the mechanism and scope of the project and b) the RSC Materials Chemistry Forum, following which GM prepared an initial statement.

GM's presentation had two main features, a) the target audience for the IUPAC project and b) the content of the definition of Materials Chemistry. First, GM indicated that primarily the audience was the IUPAC organisation and membership. Following discussion over this, which included also the appropriate home of the Materials Chemistry sub-committee, it was agreed that Materials Chemistry is clearly an interdisciplinary area that crosses the borders of several Divisions within IUPAC, although Division II Inorganic is its current principal home.

GR commented that if the prime audience is the IUPAC community then an article for CI should form one of the main outputs. LVI and GM also indicated that their respective journals could well highlight the result of the IUPAC project in, for instance, an editorial as well as on their respective websites. JC commented that it is very important to integrate Materials Chemistry within the IUPAC organisation, as well as to make public statements about Materials Chemistry. GM then spoke about his initial efforts to define Materials Chemistry and the difficulties that

were likely to be encountered, especially at the fuzzy interfaces with other disciplines of Chemistry.

To promote discussion, GM then presented the first draft of a definition of Materials Chemistry based on his experience as Editor of the Journal of Materials Chemistry, as follows:

“The synthesis, processing, characterisation and exploitation of compounds that have useful, or potentially useful, properties and applications. The focus of the research is the creation, understanding and development of substances or systems with improved properties that will impact positively on business and personal life. To use chemistry to create compounds that may lead to new technological opportunities or significant improvements in existing technology.

As expected and hoped, this generated a considerable amount of positive discussion, including the following points:

The word ‘compounds’ may be falling out of use somewhat in Material Chemistry and for the moment, the word ‘substances’ is used instead.

CG commented that, from the draft definition, the remit of Materials Chemistry could easily include Medicinal Chemistry with medical applications of Materials and questioned whether it is worthwhile to try and distinguish Medicinal from Materials Chemistry. By contrast, JC stated that, at his University (Trinity, Dublin), there are two Chemistry degree programmes in a) Advanced Materials and b) Medicinal Chemistry, with essentially no overlap in content. After considerable discussion, there was no consensus as to whether Medicinal Chemistry would be ‘in’ or ‘out’, but it was felt that the interface was fuzzy; areas such as the PEGylation of materials of possible pharmaceutical application could possibly fall within the scope of Materials Chemistry since this would not necessarily fall within the focused remit of pharmaceuticals.

Questions were raised as to whether catalysts (ZZ), structural materials (RJ) and organometallic compounds as precursors to inorganic solids (GM) belong within the remit of Materials Chemistry. There was considerable discussion as to the distinction between Materials Science and Materials Chemistry (GM, ARW), since both areas target properties/applications; the difference may well come down to the level of chemistry content, but this was not agreed upon definitely. The distinction between molecular and solid state inorganic materials was highlighted (ARW) and the point made that many established areas of what could be legitimately regarded as Materials Chemistry already have a home for publishing elsewhere, e.g. Catalysts and Solid State Chemistry/Physics.

The point was made that the ACS journal, *Chemistry of Materials*, and the RSC journal, *Journal of Materials Chemistry*, both arose to fill an identified need for chemists to be able to publish work that does not clearly fall within the remit of conventional inorganic/organic/physical chemistry journals; as a result, the remit of these journals has effectively been decided by the readership/authorship. One point to emphasise and about which there was no dissension, is that Materials Chemistry is now certainly a major branch of Chemistry. This is illustrated by the facts that: the two journals referred to above are now among the largest journals published by the ACS and the RSC; the Journal of Materials Chemistry is certainly the most rapidly-growing

journal within the RSC; the Chemical Congress in Beijing has a major Materials Chemistry programme with a huge poster session. GR commented that IUPAC has already recognised the significance and growth of Materials Chemistry and that he had received an immediate and positive response from IUPAC for setting up the Materials Chemistry sub-committee.

### **3. Project to Produce a Glossary of Terms Used in Materials Chemistry: Nano-related Terminology**

By way of introducing himself, Dr Sanjay Mathur gave a presentation on some of his research interests in the area of nanoparticles and their incorporation into composites to achieve modified properties such as, for instance, loading polymers with oxide particles with applications, for example, as abrasion-resistant paints. He also presented some key results on preparation of precursor materials for magnetite,  $\text{Fe}_3\text{O}_4$  and possible applications of these in the technique of magnetic hypothermia to kill cancer cells; work is already at the stage of clinical trials and represents a very good example of collaboration between Chemists, especially Materials Chemists, Biologists and Medical Practitioners.

He then described his attempts, following the Ottawa GA at which he was encouraged to consider preparing a Glossary in Materials Chemistry, to generate some interest in this project. It became clear that the project was probably over-ambitious and that it could be difficult to get potentially-interested parties to participate in a project that rather lacked focus.

He therefore reconsidered his options and is now proposing a nano-related project to collate an agreed glossary of terms which, perhaps, have the prefix 'nano'. This suggestion was received with much enthusiasm from the sub-committee; in particular, a focused project on nano-related terminology could perhaps form the first step in a much wider glossary of terminology in Materials Chemistry. Considerable helpful discussion followed concerning how to establish an agreed terminology in an emerging area such as this (CG, GR). A 'straw horse' approach was suggested, in which, in the first instance, SM would circulate a rough draft listing nano-related terms that he had encountered from an initial literature survey, to a selected group of individuals for comment, with the hope that a focused request such as this should receive a good response, especially from people who themselves have proposed new terms. RJ commented on the mammoth nature of the task that preparing a glossary can become, from his personal experience of an almost-completed project associated with sol-gel and hybrid material terminology.

Following some discussion/uncertainty about the status of any recommendations that arise from this, or any other project, JC commented that IUPAC has a clear ratification procedure in which any project outcome is submitted to the ICTNS, who consult with fifteen independent referees, before something such as a glossary becomes an established IUPAC recommendation. The question of having an active website to allow the public to input comments was discussed and felt to be worthwhile, but that at the conclusion of the project, an active website would necessarily close, since IUPAC would not wish their recommendations to be updated in an *ad-hoc* manner. RJ commented that Division IV has a polymer-related project on aggregation and self-assembly and that the proposed Mathur project on nano terminology could be done in parallel, with some interaction between the two projects. JC commented that the proposed nano

terminology project would require discussion with other Divisions, especially Physical (RW) and should involve as many as possible of the well-known figures within the nano community.

Division VIII had received an approach from Rice University about a possible project/conference in nano terminology, but as yet nothing had been finalised; presumably Division VIII would also be interested in this proposed project. ZZ suggested including appropriate ACS Editors/Board members in any Task Force. It was commented that this proposal for work on terminology at the frontiers of Materials Chemistry, at which changes occur spontaneously, had many similarities to the recently terminated project on terminology of 'Fullerenes'. The Fullerene project took considerable time, but was eventually successful and is good for giving IUPAC a high profile in this developing area of chemical research.

The following action plan was proposed:

SM indicated that he could quickly revise his proposal with a scaled-down budget, probably in the £8-10k range, for a 3-year programme. This should be submitted to Materials members of Division II for initial help and comment, following which the final version should be submitted to Division II (ARW), who would then forward it to Fabienne requesting that all Divisions be invited to comment and offer support if interested.

#### **4. Course Development in Materials Chemistry**

LVI has received comments about the lack of text books and established curricula in Materials Chemistry and made the observation that there is a clearly defined need for appropriate undergraduate course material. After some discussion it was felt that preparation of a draft curriculum could well form the basis of an IUPAC project and LVI was given the go-ahead to contact David Avnir about the possibility of preparing a project submission.

#### **5. Workshops on Advanced Materials**

The status of WAM III, due to be held in South Africa in September 2005, was discussed. JC commented on the difficulties of establishing an easy form of communication with R Sanderson. SM indicated that, from his recent visit to South Africa, there exists the possibility of a joint Germany-South Africa Symposium, to be attached to WAM III. Notwithstanding difficulties over communication with the organisers of WAM III, a programme is now available, although perhaps has not been publicised as widely as it could have been; it was felt that the principle behind the WAM activities is good and that following conclusion of WAM III, plans could be made for WAM IV, with China or South America as two possible locations (JC to contact DR to determine possible interest).

#### **6. The Future of the Materials Subcommittee**

Several of the subcommittee members have continued membership on Division II and therefore the immediate future is assured. However, new recruits are certainly needed. There was much dismay that the organisers of the Congress did not respond to the suggestions from the Materials Chemistry Subcommittee, of possible involvement in the organisation of the Materials Chemistry

programme. Following Ottawa it had been the intention of the Materials Chemistry Subcommittee to hold a Materials Chemistry Workshop at some stage during the Beijing meeting, but with zero interaction with the Chinese organisers, this proved impossible.

## **7. Future Meetings**

Since the bulk of the membership of the Materials Subcommittee is also associated with Division II, it is proposed that the next meeting of the Materials Subcommittee be held just before/after the off-year meeting of Division II, which, at this stage, is likely to take place in Seattle, USA in August 2006.

## **8. Other Actions**

- i) ARW to raise the question of possible involvement of the Materials Chemistry Subcommittee in the Turin Congress.
- ii) JC to send copies of these Minutes to other Division Presidents for their information and requesting that, if interested, they nominate new members for the Subcommittee.

## **Appendix VI**

### **Report on Workshop on Advanced Materials**

**Stellenbosch, September 4<sup>th</sup> to 8<sup>th</sup>, 2005**

### **WAM III**

The third in the series of Workshops on Advanced Materials (WAM III) is scheduled to take place in Stellenbosch, South Africa between Septemebr 4 and 8<sup>th</sup> 2005. This conference was proposed at the Meeting of the Materials Sub-Committee in Ottawa and suggested to the then President, Professor Piet Styne who was asked to find a suitable location in South Africa for the workshop to be held during 2005. Professor Styne arranged for the conference to be organised by Professor Ron Sanderson who chaired a local organising Committee in Stellenbosch, and also put together an International Advisory Committee. The Workshop will be supported financially by IUPAC through its scheme to support conferences. Full information on the meeting is available from its website at <http://academic.sun.ac.za/unesco>.

The meeting will run from its September 4<sup>th</sup> to 8<sup>th</sup> with two sessions each on Monday, Tuesday and Wednesday and Thursday with the closing scheduled for 15.50 on the last afternoon. There will be Plenary Lectures from leading scientists to open each of these sessions followed by invited and contributed papers and a Poster session on the Tuesday evening. There are reduced rates for students and for scientists for developing countries.

The programme is wide ranging but is based on nanostructured advanced materials. The sessions are entitled:

1. Nanoparticles: centres in application I.

2. Nanoparticles: centres in application II.
3. Nano-electronics
4. Nanotubes and fibres
5. Nanostructures: Bottom-up design and assembly.
6. Nanostructured: Biorelated and general
7. Device application and characterisation I.

Device application and characterisation II.

John Corish  
Trinity College Dublin  
28<sup>th</sup> July 2005

### **Appendix VII – Report on Project 2000-007-1-400**

Dear Colleagues,

For the past few years, Professor Alan Chadwick and I have been involved with an IUPAC Polymer/Inorganic interdivisional project directed to defining the terminology relevant to sol-gel and inorganic/organic hybrid materials.

After a number of iterations, the project is now called, "Definitions of Terms Relating to the Structure and Processing of Inorganic and Polymeric Gels and Networks, and Inorganic-Polymeric Materials", which is rather a mouthful. However, under this title it has reached its final stages.

It is standard IUPAC practice to send a finished project to experts for their observations and to offer them the opportunity to make recommendations for improvement. Accordingly, if you can find the time to review the content, attached to this e-mail is the project as it presently stands and I would welcome your comments, preferably by 8 August in time for me to convey them to members of the Subcommittee on Macromolecular Terminology at the IUPAC General Assembly in Beijing (13-18 August).

In advance I should like to thank you for your valuable advice.

Yours sincerely,

Dick Jones

### **Appendix VIII – Report on Project 2000-024-1**

The proposed project will provide a resource book of topics in the area of properties and behaviour of high temperature materials for those teaching materials science or physical or inorganic chemistry at various levels. The recommended topics will be accompanied with a bibliography of helpful references and a short introduction or explanation, including the areas of application.

A second draft report prepared by G. Balducci has been discussed and reviewed in a meeting (G. Rosenblatt, C. Chatillon and G. Balducci) at the Gordon Research Conference last August. Considering the suggestions emerged in the discussion, the list of topics has been grouped in two parts. The first group encompasses topics of general nature relevant to the peculiar properties and reactivity of materials at high temperature (e.g. vaporization and decomposition reactions: thermodynamic and kinetic aspects; presence of complex species at high temperature; gas-solid reactions and their role in the behavior of materials in extreme environments, etc.). The second group of topics pertains to the processes important for applications where high temperature chemistry plays its role (e.g. special methods of inorganic synthesis, production and use of high temperature materials, pyrometallurgical processes). The useful bibliography appended to each topic has been reduced where applicable inserting textbooks or monographs and review articles more readily available to the readers. The general list of the references arranged in chronological order should constitute an appendix useful on the one hand as a source of references and on the other hand to show the evolution of high temperature materials chemistry over the time. On this basis, a new draft report is being prepared and will be resubmitted to the task group members and experts in the field.

With very best wishes

Gianni Balducci

\*\*\*\*\*

Prof. Giovanni Balducci  
Dipartimento di Chimica  
Università di Roma La Sapienza  
P.le Aldo Moro 5 00185 ROMA 34 Italia

## **Appendix IX**

### **FINAL PROJECT REPORT**

**Project number 2002-049-2-200, Isotopic Composition of the Elements for Global User Communities.**

**Prepared by:** Dr. Bob Loss

Curtin University of Technology, Department of Imaging and Applied, Kent St Bentley, Western Australia, 6102.  
+61 89266 7192

#### **Original Objective:**

To design, compile and produce a new Report on the Isotopic Compositions of the Elements, containing updated data and in a format fit for the 21<sup>st</sup> Century

#### **Original Description:**

CAWIA produced in the past several tables of the isotopic compositions of the elements (last one in 1997) with data representing the best available measurements and representative materials corresponding to the standard atomic weights.

With increasing importance of isotope ratio measurements in chemistry, environmental sciences, product authentication, forensic and life sciences, there is a need for an expanded and revised database on isotopic abundances in normal terrestrial materials and associated reference materials.

For this reason CAWIA proposes to issue a new authoritative document to update and spread this information. This is a major modification and expansion of the present compilations.

The Subcommittee on Isotope Abundance Measurements (SIAM) will therefore meet and

- Review and evaluate new data published since 1997
- Develop and implement new guidelines for data evaluation and presentation
- Prepare a new layout of this table

Issue the new table and widely distribute it using suitable channels

### **Goals and directions**

- Prepare a Report on Isotopic Composition of the Elements (RICE) as the basis of an active dissemination of the current best knowledge on isotopic information to the global user communities in all sciences
- Improving the comparability of isotopic measurements, by linking absolute and relative measurement scales
- Improve understanding of the atomic weight concept in the chemical measurement community

### **Task Group Members**

R. Loss, J.K. Bohlke, K. Rosman, T. Coplen, T. Walczyk, M. Berglund, P. Taylor

### **Progress Review**

This project was first proposed in July of 2003 with a budget of ~\$20 over 4 years under Task Group Chairmanship of Dr P Taylor. The project proposal assumed that the Commission of Isotope Abundances and Atomic Weights would receive a comparable level of funding to support 3 additional workshops over that 4 year period.

Following a number of revisions the project was eventually partially funded by the Division in early 2003 to assist with travel funds for task members to attend a workshop in Ottawa to begin the development of an urgent major revision of the Table of Isotopic Composition of the elements taking into account natural isotopic variability.

The Ottawa workshop (was held sans the project Chairman) prepared several prototype tables using evaluated data for nickel, sulfur and osmium. The Ottawa workshop rapidly revealed just how difficult this task would be to perform for all the polyisotopic elements especially because;

- This project proposed reporting evaluated data as isotope ratios as well as abundances (rather than absolute abundances), which is a major departure from previous reporting of only isotope abundances. This created major difficulties in evaluating and determining isotope ratio uncertainties from those publications that only reported abundances especially those with unclear or non-existent uncertainties.
- The amount of time required to review the literature and evaluate isotope data for all of the proposed parameters was much greater than first thought (~ 2.5 person days per element/paper). Also the degree of interpersonal interaction involved in evaluating the data at the workshop clearly demonstrated the need for workshop time/facilities to make satisfactory progress with this major evaluation.

Recognizing the difficulties involved in the re-evaluation of the literature for all polyisotopic elements, the task group proposed a new proposal ( 2003-031-1-200 - Isotopic Compositions of Selected Elements). This project was partially funded in early 2004 and resulted in a workshop in Reston, Virginia in April 2004 and in Beijing in 2005, in which substantial progress was made and is reported elsewhere. This is now estimated to be a four to six year project that should lead to improved consistency between the Table of Isotopic Compositions and the Table of Standard Atomic Weights.

### **Outcomes**

There are no publicly available outcomes although this is not unexpected due to the level of funding provided and the vast underestimation of the extent of the task. The evaluation templates and experience gained for the task force members was invaluable and are being well used in project 2003-031-1-200.

### **Funds**

I understand there are residual funds allocated to this project, which I believe should either be transferred to project 2003-031-1-200, or used to fund travel and per diem to the Beijing workshop.

## **Appendix X**

### **Project 2003-006-1-100: NMR Chemical Shifts - Updated Conventions**

*Task Group Chairman: Robin Harris (University of Durham)*

#### **Progress report, 20 July 2005**

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

**Status:** Following a Discussion Forum held during the International Meeting on NMR organised by the Royal Society of Chemistry in Cambridge (England) in the summer of 2003, five of the six task group members were each assigned one of the relevant topics listed above (plus the question of notation for shielding tensors) and were asked to prepare a briefing paper on it. Progress has been made with all of these, with comments sought from all members of the task group and from some other experts in the field.

In the case of temperature variations of chemical shifts, it was decided to undertake some new measurements with respect to the He-3 nuclide, and one of the task group members (Dr. Roy Hoffman) has done this. The funds supplied by IUPAC for the project sufficed to obtain the necessary helium gas. This work is now in press in *J. Magn. Reson.* A second relevant paper, on susceptibility corrections, again by Dr. Hoffman, has also been submitted for publication. The eventual IUPAC report will rely in part on these papers. A briefing paper on shielding tensors has been sent to several experts for comment prior to the drafting of recommendations. Responses have been received and the document has been revised for inclusion as a section of the IUPAC report. In fact, a first draft of the full report is now approximately two-thirds complete. An additional section on alternative standards (especially for nitrogen) is now planned, in addition to those determined at the Discussion Forum mentioned above.

A meeting between Professor Harris and Dr. Becker in London took place in July 2005 and the strategy for completing the project was discussed, with schedules set.

Robin K. Harris  
Task Group Chairman

## Appendix XI



# Rensselaer

Professor Leonard V. Interrante  
Department of Chemistry  
Troy, NY 12180-3590

J. Drowart, Brussels  
Dr. Christian Chatillon, Grenoble  
J. Hastie, NIST  
D. Bonnell, NIST

October 22, 2005

Dear Drs. Drowart, Chatillon, Hastie and Bonnell :

On behalf of the Inorganic Division of IUPAC, I would like to thank you for your extraordinary effort, over 19 years, in bringing to a successful completion the Project "High temperature mass spectrometry: accuracy of the method and influence of the ionization cross- sections", and to complement you on your excellent, comprehensive, report on this project, that was published in Pure Appl. Chem. Vol. 77(4) (2005) pp. 683-737. It is clear, even to a non-expert in this area, that this paper will have a major impact on the fields of high temperature inorganic chemistry and HT thermodynamics in the future. Your careful and detailed analysis of the sources of inaccuracies in the HTMS determination of absolute or relative partial pressures, the limitations and scope of this method, as well as the tables of atomic and molecular ionization cross-sections, will remain a valuable resource for workers in this area for many years to come. The fact that this project was continued well after the funds allocated by IUPAC were exhausted, attests to your personal dedication to this task and your perseverance in seeing it through to a successful conclusion, some 19 years after the project was originally started.

Thank you again for your contribution to the advancement of worldwide chemistry.

Sincerely yours,

Leonard V. Interrante  
Secretary, Division II, IUPAC  
c.c. Prof. A. West, Division II President, Prof. D. Black, IUPAC Secretary  
General

## Appendix XII - Defining Materials Chemistry

### Graham McCann, Journal of Materials Chemistry

The Editorial Board of Journal of Materials Chemistry has been developing their definition of “Materials Chemistry” since the journal was founded.

The current scope of the journal is:

*Journal of Materials Chemistry* is a weekly, international journal that publishes high impact work on the chemistry of novel materials. The journal has a broad readership, covering all areas of materials research. It covers the chemistry of materials *in all forms*, particularly materials associated with new technologies. Coverage is broad and includes the design and synthesis of materials, their characterisation, processing, modelling, properties and applications. Papers covering interdisciplinary research and papers from related disciplines are encouraged, in particular those addressing emerging and quickly developing fields.

To establish the suitability of the articles for *Journal of Materials Chemistry* they must highlight the novel properties or applications (or potential properties/applications) of the materials studied. Papers that report primarily structural studies (such as crystallographic, NMR or IR studies) will be considered for publication only where the materials have interesting properties or are of potential interest for the materials community.

### Defining Materials

What is a Material? Currently our definition is that it a material is a compound in any form that has properties/applications or potential properties/applications.

Every compound has properties, so terms such as ‘advanced technologies’, ‘interesting properties’, ‘interest for the materials community’ are included to elaborate. A property here should be potentially exploitable and desired for an application.

Chemistry is likely to be the science that generates new materials, before properties and applications are fully realized. We therefore think it is important that potential applications are included in the journal scope, to ensure that the newest materials are reported in the journal. This aspect of Chemistry, creating compounds with potentially interesting or useful properties, may be an important one for the IUPAC group

### Defining Chemistry

Around 2000, the journal guidelines were altered to discourage purely structural/characterisation studies of materials that show no properties or applications. This was in response to large numbers of papers characterizing solid state compounds with few (or no) applications or interesting properties. It is clear that structural and characterisation work is an important part of Materials Chemistry. Knowledge generated from detailed structural studies is important for the understanding of properties and, ultimately, the potential applications of materials. However, in isolation structural and characterisation work alone would not fall within our definition of Materials Chemistry. A clear link to how the work aided the understanding of properties/applications would be necessary.

## **Materials Science**

Articles we receive that develop the science of materials but not the chemistry or applications of materials fall outside the scope of the journal. Examples might be improvements in experimental setups.

## **History**

Members of the IUPAC working group will have a better knowledge than I do of how the perception of Materials Chemistry has changed over the years. When the journal was founded, the focus was on liquid crystals, conducting/magnetic organics, extended solids, inorganic synthesis and characterisation. This has moved more into nanomaterials, organic materials, bio-related materials, applications in devices and medical applications.

## **Definition of Materials Chemistry**

To help get the ball rolling, here is a draft definition of Materials Chemistry.

The synthesis, processing, characterisation and exploitation of compounds that have useful, or potentially useful, properties and applications. The focus of the research is the creation, understanding and development of compounds or systems with improved properties that will impact positively on business and personal life. To use chemistry to create compounds that may lead to new technological opportunities or significant improvements in existing technology.

Research in (non-materials) Chemistry is focused on adding to our understanding of chemistry, of how matters is composed, interacts and how fundamental properties arise.

## **Materials Chemistry or Not?**

Molecular catalysts (pure chemistry, or materials chemistry?)

Ball milling of ceramics (could be materials science or materials chemistry)

Synthesis of new liquid crystalline compounds (organic synthesis?)

Potential new CVD precursors (inorganic synthesis?)

Graham McCann; 13-Jul-05