

INORGANIC CHEMISTRY DIVISION COMMITTEE OF IUPAC

Meeting at Seattle 13th and 14th August 2006

MINUTES

Attendance: Present were *President*, Anthony West; *Vice President*, Kazuyuki Tatsumi; *Secretary*, Leonard Interrante; *Titular Members*: Alan Chadwick, Tyler Coplen, Marku Leskela, Robert Loss; *Commission II.1 Chairman*, Tiping Ding; *Associate Members*: Javier Garcia-Martinez, Norman Holden, Luis Oro, and Gerd Rosenblatt; and National Representative, John Corish.

Apologies were received from Titular Members Jan Reedijk, and Myunghyun Pik Suh, NR Joe Takats, and Past IUPAC President, Leiv Sydnes, who could not attend. TM Claudio Biancini also did not attend.

1– Introductions and Announcements

The meeting commenced at ca. 9:40 a.m. on Tuesday, August 13, 2006 in the U.S. Federal Building. President West welcomed the members to the meeting. Each of the attendees then introduced themselves and described their professional affiliations and areas of expertise. After a brief discussion regarding the arrangements and logistics for our Division dinner that evening, West presented a brief overview of IUPAC and the Division II structure, which was especially informative to first-time attendees.

2 – Agenda

The previously distributed Agenda was modified by 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 Beijing

Copies of a draft of these minutes were previously distributed by email, but apparently were not received by some of the Division members, judging from their comments at the meeting. Based on the minor comments that were received from those participants that did receive the minutes, a final copy was submitted to the IUPAC Secretariat in November 2005 and are now available on the IUPAC Division II web page.

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

The Bureau met in Beijing, at the IUPAC General Assembly and meets next in Madrid, Spain in October of 2006. At the meeting in Beijing, the Bureau approved the membership of several new National Adhering Organizations and approved the location of the 2009 G.A. in Glasgow, Scotland. The formal recognition of Commission II.1, with its own guaranteed biennial funding of \$10K (\$8.5K from Division II), was approved for another 2-year period.

5- Budget Allocations and Expenditures

This discussion was deferred until Project Coordinator Coplen's presentation later in the agenda.

6- Report from other IUPAC bodies – Committee on Chemistry Education (Interrante) and the Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS) (Corish)

Interrante reported on the meeting of the CCE which was held in Beijing as part of the IUPAC GA. He had attended a session of this meeting together with Daniel Rabinovich, a Young Observer at the G.A., who had discussed with the Division a possible project relating to the development of inorganic chemistry curricula for Latin American countries. Daniel presented his idea to the CCE and received a rather mixed reaction in which several members of the Committee felt that the emphasis on “curriculum development” was misplaced and that IUPAC should not be in the business of recommending, or advocating, specific curricula but instead should emphasize the importance of learner-driven curricula, with a focus on the desired overall and specific educational outcomes. We went away with the feeling that a properly directed proposal that had such a focus would receive the support of the committee. Unfortunately, despite subsequent urgings from Interrante, a project proposal has not been forthcoming from this contact. The CCE was also scheduled to meet at the biennial International Conference on Chemical Education in Seoul, Korea, to be held virtually simultaneously with the Division II meeting on August 12-17, 2006. The Division representatives on CCE were invited to participate in this, and future, ICCE’s and to present a poster or talk relating to the main educational priorities of our respective Divisions. A copy of a message received from CCE Chair Peter Mahaffy proposing improved communications with the Divisions, and their increased involvement in the mission of the CCE, is attached to these minutes as **Appendix I**.

Corish reported on the role and recent actions of the ICTNS, which reviews recommendations from the various IUPAC Committees. Two proposals from Division II, relating to the “Atomic Weights of the Elements” and “Definition of Terms Relating to Polymer Gels and Networks”, were approved by the ICTNS. A new edition of the Green Book (of physical chemistry nomenclature) was approved and is in the process of publication. A written report was received from Corish and is attached to these minutes, along with a report from the ICTNS Chairman, Jack Lorimer, on the status of all Technical Reports and Recommendations submitted since 2004 (**Appendix II**).

7- Naming of New Elements (Corish)

Corish noted that one of the responsibilities of this Division was to oversee evaluation of claims for the discovery of new elements, which is carried out by a joint IUPAC/IUPAP Working Party. The membership of this Working Party is periodically reviewed and approved by both organizations and meets when needed to go over the claims and make recommendations. Claims for the discovery of elements 112, 113, 114, 115, 116 and 118 have been submitted. Further details are contained in the written report submitted by Corish after this Division meeting was concluded (see **Appendix III**).

8- Reports from Other IUPAC Divisions and Committees

(a) Chemical Nomenclature and Structure Representation Division (VIII) – G. Leigh

The following brief report was received from Jeff Leigh

- The new Red Book (Nomenclature of Inorganic Chemistry – IUPAC Recommendations 2005) is now published and obtainable from the RSC
- A project on revising the Principles of IUPAC Nomenclature is about to start, and the results should be published in 2008.
- A project on developing inorganic PINs (Preferred IUPAC Names) is currently under way, but it may be difficult to establish a reliable methodology to select them.
- A Technical Report on the extension of the use of polyhedral symbols and configuration indices to coordination numbers greater than 7 is almost ready for submission. One conclusion is that for coordination numbers > 8 there is not much value in trying to extend this usage, since polyhedral geometries often cannot be easily and reproducibly assigned.
- Division VIII meets in Prague in early September, 2006

b) COCI

West noted that COCI (the IUPAC Committee on Chemistry and Industry) had requested that we appoint a Division representative to participate in their meetings. Leskela agreed to act in this capacity.

Alan Smith of COCI had prepared a draft summary of those Division II activities that might be of interest to industry. With some amendments, this was approved (attached to these minutes as **Appendix IV**) and will be combined with similar summaries from other Divisions into a COCI report for the IUPAC Bureau in Madrid.

9- Reports on Other IUPAC-Affiliated Organizations

a) EuCheMS

Oro reported on the 1st European Chemical Congress and EuCheMS, the European Association for Chemical and Molecular Sciences. EuCheMS promotes co-operation in Europe between non-profit-making scientific and technical societies in the field of chemistry whose membership consists largely of individual qualified chemical and molecular scientists and whose interests include the science and/or practice of chemistry. In answer to a request for a representative from the Inorganic Division on the EuCheMS Working Party on Inorganic Chemistry, Oro was nominated and accepted by EuCheMS. This newly-created international organization of chemists had its first meeting (the 1st European Chemical Congress) on August 27-31 in Budapest (www.euchems-budapest2006.hu/). Over 3,000 participants from more than 50 countries worldwide attended this Congress. The second European Chemistry Congress will be held in Torino, 16-20 September 2008.

b) IUGS

Holden reported on his contacts with the International Union of Geological Sciences, IUGS, which had asked him to help move along efforts to settle inconsistencies in the accepted isotope half-life values between IUPAC and IUGS. Holden attended their last meeting in Florence and will serve as the IUPAC liaison with **IUGS**.

c) IOCG

West received an enquiry from the International Organization for Crystal Growth regarding a proposed cooperation with IUPAC. Their original proposal was to have an IOCG member sit on the Executive Committee of IUPAC. It was not possible to grant this request; however, IOCG was encouraged to send an observer to the IUPAC General Assembly meetings.

10- Report on the Materials Chemistry Subcommittee (S. Corish)

The last full meeting of the Materials Chemistry Sub-Committee was held in Beijing at the GA Assembly in August 2005. The minutes of this meeting can be found in **Appendix V**. As has been the practice in the last few years, the members of this Subcommittee who were attending the Division II Committee Meeting in Seattle met informally just prior to the Division Committee meeting, on August 14th. Professor Charles Campbell, of the Department of Chemistry at the University of Washington, hosted the meeting. A set of draft minutes are given in **Appendix VI**.

Among the principal matters discussed were reports on and future planning for the series of High Temperature Materials Conferences (HTMC) and the Workshops on Advanced Materials (WAM), both of which are handled by the Sub-Committee. Both these IUPAC-sponsored events continue to prosper and plans were approved for future meetings in the series. Corish's report on WAM III is attached to these minutes as **Appendix VII**.

The project on Defining Materials Chemistry, led by Professor Peter Day, organised a one-day workshop at the Royal Society of Chemistry in London on April 14th, attended by a group of approximately thirty-five invited scientists, including the Division Chairman, Secretary and the Chairman of the Materials Chemistry Sub-Committee. Professor Day, who was prevented from attending the Division II meeting in Seattle by travel difficulties associated with heightened security at UK airports, submitted a report on the Workshop, which is attached to these minutes as **Appendix VI, Annex I** (see also, report on Project #2005-001-1-200 below). The Sub-Committee decided to recommend that the project be further advanced by organising a joint meeting of the Sub-Committee with the Task force for the project. The Sub-Committee also reviewed other projects, which it had initiated, and discussed how best it could contribute to the session designated for Materials Chemistry at the Congress at Turin in 2007.

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

Commission Chairman Ding gave an oral report, accompanied by PowerPoint slides, on the state of CIAAW and the activities of the Commission during the past year. Two new projects (see below) were submitted and subsequently approved involving the work of the Commission. Ding noted that, at least as far as the IUPAC web site is concerned, the two Subcommittees that carry out the work of the Commission, i.e., the Subcommittee on Extra-Terrestrial Isotopic Ratios and the Subcommittee on Isotopic Abundance Measurements, are still listed as two of four Subcommittees of the Division as a whole, rather than part of the Commission and that the relationship between these two Subcommittees and the Commission was not indicated. Moreover, the Subcommittee for Natural Assessment of Fundamental Understanding (SNAFU) of the Commission does not appear on the list of Subcommittees for the Division at all. There was some discussion among the Division members regarding the proposed name and acronym (SNAFU) of this new Subcommittee and it was the consensus of the Division Committee that the Commission members should seek an alternative name that would be more informative regarding the actual scope and activities of this Subcommittee. West also asked Holden, the Subcommittee

Chairman, to provide a more detailed description of the scope and need for this Subcommittee. Holden had submitted to the Secretary in advance of this meeting a report on the activities of this Subcommittee, which is attached to these minutes as **Appendix VIII**. He reported briefly about this Subcommittee and agreed to come up with an alternative name for it.

Ding and Loss indicated that the activities of the currently-listed Subcommittee on Extra-Terrestrial Isotopic Ratios had been effectively terminated with the proposed abandonment of Project #2001-042-1-200 (see below) and that the Commission recommended replacement of this Subcommittee by the new one (currently called SNAFU, within the Commission, but hopefully soon to change) on the Division web page. Moreover, it should be made clear on our web page, which Subcommittees are under the jurisdiction of the Commission and which report directly to the Division. It should be noted that this problem with the Subcommittee listings that are currently on the Division web page also extends to the currently listed Divisional Subcommittee on Characterization of Carbonaceous Materials and New Carbons, now that our only remaining Project in this area (#2000-022-1-200, see below) is no longer being actively pursued and should be considered abandoned.

In the discussion of this report, Interrante suggested that the Commission might wish to prepare a general interest article to publicize its work and to bring to the attention of the broader chemistry profession and perhaps even to the general public, the ways in which information concerning elemental isotope ratios have been used in many areas of chemistry, environmental science, geology, etc. This perhaps could be written for Chemistry International or another chemistry news magazine such as CE&N.

12- Project-by-Project Review

The Division Project Coordinator, 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.

Of the 16 Projects that are currently listed as funded Division II Projects, 10 are extending past their planned ending date, tying us with Division VII as the Division with the worst completion record. Of the total biennial allocation for the Division (USD 53,200), we have currently committed \$2,000 and have already spent \$14,954 in operational costs and need to set aside \$10,000 of Divisional funds for support of Commission II.1. This leaves a maximum of \$26,000 potentially available for projects; however, a significant proportion of this will be spent on the current Division Meeting. Two new Project proposals have been submitted this year. We requested that Sanjay Mathur resubmit a project proposal with a lower cost; however, we have not yet seen it. A breakdown of the current status of, and expenditures on, the currently listed Division Projects follows.

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

The originally-planned ending date of this project was December 31, 2002. The first stage of this project concerning the Y123 solid solution was completed and the corresponding technical report was published in Pure Appl. Chem. 72(3), pp. 463- 477, 2000. In 2004, Voronin indicated that the work on 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; however, since that time, \$5,764 was spent on the project. We have not yet received a final report for this Project; however, prior to this meeting Interrante received the following interim report from Voronin:

Within the framework of the project the following work is done: (1) critical assessment and accommodation of thermodynamic data for two solid solutions $\text{YBa}_2\text{Cu}_3\text{O}_{6+z}$ ($0 < z < 1$), $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_{14+w}$ ($0 < w < 1$), and one compound $\text{YBa}_2\text{Cu}_4\text{O}_8$ in the system Y-Ba-Cu-O, (2) an analytical representation of the Gibbs energy functions for these phases, and (3) a computer-assisted optimization analysis with obtaining a set of model parameters for the best fitting to the experimental results and fulfilment of all rigorous relations between thermodynamic functions. More than 3500 experimental points obtained in miscellaneous experiments published in 110 papers have been processed in order to obtain the most reliable thermodynamic functions of the phases in the temperature range from 250 to 1300 K and pressures up to 100 kbar. Obtaining such results was the purpose of the project. Therefore, it is possible to say, that the scientific program of work for the project is completed.

The first part of these results, related to the properties of the solid solutions Y123, has been published as a PAC Technical Report in 2000. There are several publications in other journals. The remaining part will be presented at the conference, HTMC-XII at Vienna in August 2006. In connection with this conference a meeting of the project Task Group is scheduled. During this meeting the content of the final report and the expediency of a new publication in PAC will be discussed. The final report will be presented to the Division this year.

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; planned ending date: February 1, 2003.

Corish submitted the following written and oral report regarding his (unsuccessful) efforts to get this project restarted after the unfortunate death of the Project Leader in 2005.

Following the Beijing General Assembly, information, including the files to date, were supplied to Dr. Tamara Basova, who undertook to try to carry forward the project from the point to which it had been taken by Professor Meral Kizilyalli before her death in July 2005. During July Dr. Basova reported that despite her best attempts, including reopening contact with members of the task force who had earlier contributed to the project, she did not see any prospect of completing the task. A further reason for this was that there were no longer suitable students at her institution who could test and validate the experiments. She recommended that the project should not be continued.

Rosenblatt believes that the project is still of considerable value to the solid state community but that it could be successful only if some well-known and established senior figure was willing to take it on and carry it to completion.

Given all the difficulties, including the possibility of responsibility for the safety of experiments that might be published by the Division, he recommended that the project be closed. However a considerable amount of work has been done, a valuable file exists, and this should be retained so that the project could be reinstated later should the opportunity to do this present itself.

On the basis of this report the Division Committee agreed that this project would be officially listed as abandoned.

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

As was noted at our last meeting in Beijing, this is another case of a project that has apparently been abandoned after much of the work had been completed (with none of the allocated funds expended) due to the illness of the Project Leader. We agreed that this project would also be officially listed as abandoned. As was noted above, under Item 11-, the current Subcommittee on Characterization of Carbonaceous Materials and New Carbons should also be eliminated from the current list of Division Subcommittees.

2000-024-2-200 Balducci; Teaching of high temperature materials chemistry at universities; G. Rosenblatt, Project Monitor; allocated: \$4,800, spent \$0. Planned ending date: December 31, 2004.

Rosenblatt reported that considerable progress has been made on this project despite the lack of any funds spent. In February of 2006, Balducci sent the Secretary and the Task force members a report (attached to these minutes as **Appendix IX**), which indicated that the Project was near completion and asked for assistance with a second draft of the Project report. We have received no further updates on this project since that time; however, it appears that the work on this project is very much in progress and that we should maintain it in the “active project” category despite the 2-year delay in its completion.

2001-015-1-100 Stanbury; Standard potentials of radicals; G. Rosenblatt, Project Monitor; Planned ending date: December 31, 2004.

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 has been spent thus far. The last update received on this project was in February 2005; however, a poster was presented at the Beijing IUPAC Congress in July 2005. No report was received in response to a request put out to all Project Leaders for updates in advance of this meeting.

2001-019-2-200 Walczyk; Guidelines for mass spectrometric isotope ratio measurements; T. Coplen, Project Monitor; allocated \$2,000, spent: \$0. Planned ending date: December 31, 2003.

This project was last updated on the IUPAC web site in January 2002. No information regarding this project was received from the Project Leader (who has four other active – and no completed - projects listed on the IUPAC web site) since 2005, when it was reported that “: Dr. Walczyk has been very frugal, attending 3 meetings and publishing 1 paper on the topic.” Coplen reported that he had been in contact with Dr. Walczyk and that Dr. Walczyk expects to expend remaining funds and complete the project by December 2007.

2001-042-1-200 Ebihara; Review of isotopic abundances in extraterrestrial materials; Holden, Project Monitor; allocated: \$6,000, spent \$6,000; planned ending date: December 31, 2003

This was the main project of the Subcommittee for Extra Terrestrial (ET) Isotope Ratio measurements. The function of this Subcommittee was to compile/review ET Isotopic Compositions of the Elements for relevant user communities. The recent findings were reported as a subsection of the CIAAW reports. In 2001, Schultz, Ebihara, Weiser, Yoneda, Hidaka and Loss proposed a project, Review of Isotopic Abundances in ET materials (RIAETM). RAIETM 2002/3 involved a review of isotopic abundance in ET materials for two groups of elements: the Rare Earth Elements and the Noble Gases. A project was proposed in July 2001 and partially funded in 2002. The funds were used to assist the SETIR group to attend the CIAAW in Ottawa in 2003. Schultz, Ebihara, Weiser, Yoneda, and Hidaka developed a draft data treatment/presentation and the elements were divided up for preliminary review (Schultz - noble gases; Yoneda, Hidaka - REE). At the meeting in Beijing in 2005 Weiser and Yoneda were the only attendees. The Chairmanship was taken up unofficially by Yoneda who agreed to contact Hidaka and try to complete the project.

A preliminary report and a copy of the database (1200) was submitted by chairman Yoneda - but essentially no significant progress in project objectives were made. CIAAW recommends closure of the project.

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 was attached to the minutes of the Beijing meeting. Work continues on this topic as project #2003-031-1-200.

2003-006-1-100 Harris/Becker; NMR chemical shifts – updated conventions; Chadwick, Project Monitor; allocated: \$7,000(\$2,000 Div II), spent 6,477; Planned Ending Date: 31-Mar-2005.

A written report was received from Prof. Harris on this continuing active project, which is attached to these minutes as **Appendix X**. To sum up this report: “Currently a draft final report is in existence. This requires approval and final comments from members of the Task group, after which it will be ready for submission.”

2003-031-1-200 Berglund; Isotopic compositions of selected elements; Loss, Project Monitor; allocated: \$12,000, spent \$12,513; Planned Ending Date: 31-Dec-2005.

An oral report was given by Loss. The major purpose of this long-term, continuing, project, which constitutes a major current task of Commission II.1, is to make a new comprehensive **Report on the Isotopic Compositions of the Elements (RICE)** for global user communities. [emphasis on Isotope Ratios]; in particular, 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 21st Century. This project was proposed in July 2001 and partially funded in late 2002. At the task force meeting held in Ottawa in 2003, they developed draft protocols and presentation (Ni S, Os), with an emphasis on thoroughness vs pragmatism. The major outcome was that this is going to be a very difficult task! RICE II, Isotopic Compositions of Selected Elements (RICSE), was

proposed on August 20, 2001, funded, December 2003, and was anticipated to be completed in Dec 2005. The objective was to design, compile and produce a new Report on the Isotopic Compositions of Selected Elements, containing updated data with uncertainties that conform to ISO 9001 requirements. The tasks were: to develop and implement new guidelines for data evaluation and presentation; to review and evaluate the isotope ratio data publications for ~10 selected elements; to prepare a new layout of the spread sheet style data base and sample extracted tables; and to issue the new tables and widely distribute it using suitable channels. Two workshops were held in 2004 (3 days at the U.S. Geological Survey, Reston, VA) and 2005 (2 days at the CAGS, Beijing, China). Accomplishments included the development of a working/presentation spreadsheet and data processing protocols. Considerable time was spent on how to handle uncertainties when not stated/dealt with adequately in the original literature. Case studies from the original literature on Ba, Br, Cd, Cr, Dy, Fe, H, Zr were chosen (only Dy completed). This continued to raise more problems than were solved. Check sheets and forms were developed on procedures and uncertainties present in each publication. These discussions continued at the Beijing SIAM meeting, concerning C, Dy, La, Nd, Ne, Pt, Sm, Si, Ta and Zn. After the Beijing RICEII meeting a number of unresolved issues remained. The final report is awaiting feedback from the RICEII members. The final outcomes are to be distributed for consideration of approval by the CIAAW 2007. Publication guidelines for authors of IC/AW publications are to be developed.

2003-033-1-200 Wieser; Determination of atomic weights using new analytical techniques; Loss, Project Monitor; allocated \$14,800, spent, \$2.190. Planned Ending Date: 1-May-2008

This ongoing core project of Commission II.1 was funded in early 2004 by Leiv Sydnes (IUPAC President) at no cost to Div II.

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. Planned Ending Date: 31-Dec-2006 (will have to be extended).

Coplen has requested Prof. Jing-Tai Zhao, a task group member, to provide both the Secretariat and Division II with the names of new task group members.

2005-001-1-200 Day; Towards defining materials chemistry; West, Project Monitor; allocated \$8,000 (shared with Division VIII), spent \$571; Planned Ending Date: 31-Dec-2007.

A written report on this new project was submitted by Prof. Day (see **Appendix VI Annex 1**), who was unable to attend this meeting due to difficulties in travelling from the UK (see Item 9 above).

2005-022-1 Brand/Coplen; Calibration of Organic and Inorganic Oxygen-bearing Isotopic Reference Materials, amount requested: \$12,000, duration: 24 months; received July 22, 2005; Coplen, Project Monitor; Planned Ending Date: 31-Dec-2007.

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. The goal is that measurement of the same homogeneous sample by any laboratory worldwide should yield the same delta value within analytical uncertainty. This is a brand new project that was funded partially from Div II funds and mostly from the IUPAC Treasurer.

2005-027-1 Berglund; Evaluated Isotope Ratio Data (2005-2007); amount requested: \$9,800; received August 19, 2005; Loss, Project Monitor; Planned Ending Date: 31-Dec-2007.

The objective of this newly-funded project is to evaluate isotope ratio publications between 2005 and early 2007, to determine "best isotope ratio measurements" for compilation and publication in a 2009 TICE, recommend "new" standard atomic weights, and publish "Atomic Weights of the Elements 2007" in Pure and Applied Chemistry, which will also include a table of relative atomic masses and half-lives of selected radionuclides. The evaluated data will be incorporated into the CIAAW* Table of Isotopic Composition of the elements (TICE) and Table of Standard Atomic Weights. This project is an interim step in the evaluation of isotopic data production for the next proposed publication of TICE in 2009.

2005-043-1-400 Ober; Terminology for self-assembly and aggregation of polymers; Allocated 6,000; Joint with Division IV (2k from Div II); Planned Ending Date: 1-Apr-2009.

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 in the area of aggregation and self-assembly in polymers. Its connection to Division II is primarily through the Interdivisional Materials Chemistry Subcommittee.

The meeting was adjourned for the day at 5pm and reconvened the next morning at 9:30am.

13- New Project Proposals

2006-028-1-400 Ober; Terminology for conducting, electroactive and field-responsive polymers; Joint with Division IV (2k from Div II).

After some discussion, in which the relevance of this topic to the Materials Chemistry Subdivision was cited as a justification for its partial funding by the Division, Division II decided to contribute \$2,000 to this project.

2006-016-1- Renne; Recommendations for Isotope Data in Geosciences; Requested from IUPAC, USD 4,900, USD 4,900 also being sought from IUGS; Objective: Update & harmonize recommendations on half-lives & isotopic compositions.

This proposal was reviewed favorably by Divisions II and V. Division V has agreed to support this project at the level of USD 2,000. Therefore, Division II will provide support of USD 2,900.

2006-025-1-200 Holden; Assessment of fundamental understanding of isotopic abundances and atomic weights of the chemical elements; Requested from IUPAC: USD 9,800; Planned Ending Date: 30-Sept-2008.

The objective of this proposal is to review fundamental issues and concerns that have been raised by members of the Commission on Isotopic Abundances and Atomic Weights (CIAAW). The basis for this proposal and the need for the study were described by Holden (see Appendix VII for further details). Division II voted to approve this Project, which had been favorably reviewed by four Division Committee members.

14- Discussion regarding potential new projects

- i) Interrante had received a draft document from Prof. G. Girolami at the Univ. of Illinois relating to an issue of chemical terminology that he was considering sending somewhere. This was a proposal for standardization of terminology relating to what is meant when a chemist uses the terms “electron-rich” or “electron-poor”. He had asked for advice regarding where to send this proposal and wondered if IUPAC would be interested in it. His enquiry was forwarded to Alan McNaught, Past President of the Chemical Nomenclature Division, who agreed with Girolami that there is a need for clarification. Alan indicated that, “if Division II were to produce agreed definitions (perhaps as a part of a glossary of terms used in inorganic chemistry?), they could be reviewed and approved by the usual IUPAC procedure, published, and added to the Gold Book”. Interrante told Girolami that he would take this up with the Division Committee in Seattle. After some discussion, which included a warning from Rosenblatt that the use of the term “electron-deficient” is already well established and has a specific meaning in solid state chemistry (as well as in other areas of chemistry) and one would have to be careful in specifying the areas of application, it was agreed that Interrante should encourage Girolami to prepare and submit a project proposal on this subject. Interrante agreed to do this and to assist him in developing this proposal if he were interested.
- ii) Following an earlier suggestion from Javier Garcia, there was some discussion of another terminology issue that has arisen in the area of nanotechnology, where terms such as meso-, that has a well-defined meaning in the area of porous materials, was becoming widely used in the nanoparticle area and associated with structure (e.g., “mesostructured materials”) in a manner that has no clear scientific basis. Given the general lack of standardization in the nanomaterial area in general and the still viable possibility that Division II would receive a revised proposal relating to terminology in the nanomaterials area from Mathur, further discussion of this suggestion was deferred.
- iii) Tatsumi described an idea for a proposal in the organometallic area that was suggested by a colleague from Japan, relating to the development of tables for use in designing catalysts, etc. that would list the cone angles and basicity of selected ligands. After some discussion, it was agreed that the individual should be encouraged to write/submit a proposal describing the proposed effort in more detail and with better justification.
- iv) Oro suggested possible projects in nomenclature on cluster chemistry. He was advised, in the first instance, to make contact with Division VIII to clarify the boundaries between Divisions II and VIII and find out what, if anything, is being carried out in this area.
- v) Leskela suggested a potential project relating to the standardization of terminology in the area of Chemical Vapor Deposition. Interrante agreed that standardization was needed in this area.

Rosenblatt noted that C. Spear had started a project along these lines but never completed it. Leskela was encouraged to proceed with formulating such a proposal or get someone else to put one together.

vi) Garcia gave a short PP presentation entitled "Division II: Too Few Projects" and proposed the preparation of a "Call for Proposals" which would be circulated by the Division Committee members using all available means within their chemical societies and other organizations. A draft of this proposed "Call for Proposals" was submitted by Garcia, and following subsequent slight modifications after the meeting by Division Committee members, it is attached to these minutes as **Appendix XI**. The Division Committee members and NRs were encouraged to use this in an effort to stimulate further proposal activity within our Division.

15. Newsletter

As part of the discussion on projects, Rosenblatt raised the question of whether the Division should start its own Newsletter, analogous to the one that the Analytical Division had started recently. Such a newsletter would be circulated outside, as well as inside, IUPAC and could be quite useful in attracting interest in the Division's activities and as a means of stimulating the generation and submission of new project proposals in the area of inorganic chemistry. The Division Secretary agreed to handle the assembly and distribution of such a newsletter, if other members of the Division Committee could supply the content. Everyone agreed that this would be a good idea and that this coming December would be a good time to launch the first edition.

16. Division Finances

West summarised, in general terms, the status of Division finances for this biennium. At present, we do not know the final cost of the Seattle meeting, but there should be sufficient funds available (just) to cover all the projects submitted/approved so far in this biennium, including the two that are relevant to the Materials Subcommittee and the joint IUPAC-IUGS project, together with funds to support attendance of key AMs and NRs at Turin.

17- Torino IUPAC General Assembly and Chemical Congress, August 4-10, 2007

The Division II meeting at this GA will be held on August 4th and 5th (Sunday and Monday). We discussed how we might obtain Division input into the program of the Chemical Congress. Gerd agreed to contact Fabienne and Della Gatta to suggest J. Garcia as co-chair for one of the symposia.

18- Nominations committee for Division Committee Titular Members

West discussed the procedures used to select the nominations committee and the nominees and the general timing for the election process. The names of the Nominations Committee members are to be submitted to the Secretariat for Approval by December 1, 2006 and the names of the nominees (2 for each of 3 positions in the area of Atoms, Molecules and Materials) are due by March 1, 2007. The election will be carried out by the Secretariat by email prior to the Torino Meeting next summer. West appointed Holden as the Nominations Committee Chairman and asked Tatsumi and Interrante to also serve on this Committee. Three additional outside members

would also be asked to serve. Suggestions were received for potential outside members in the 3 main areas of interest within the Division.

19. Info packs for new members

Following a discussion with new members Garcia, Oro and Leskela, it was suggested that the Division Officers should ensure that all new members receive, at the beginning of each biennium, the following:

1. A welcome letter.
2. The Division member list and structure (including all committees and subcommittees).
3. The scope of the Division (including what is not within the scope of the Division, for example, nomenclature of inorganic compounds).
4. A list of the ongoing projects.
5. A copy of the Blue Book. If a hard copy is no longer available, a pdf copy or instructions on how to get it should be provided.

The Meeting was closed at 11:30 am on August 16th.

Appendix I

Message from the Chair and Division Liaison, CCE

March 22, 2006

Dear CCE AMs and Division Presidents,

This letter is to introduce myself and Prof. Eva Åkesson respectively, as the new chair and division liaison officer/secretary of the Committee on Chemistry Education (CCE). We invite you as associate members of CCE and division presidents to think creatively about your educational roles, and how we can work together to advance the public understanding of chemistry, particularly in educational contexts.

Following on the initiative of past chair Peter Atkins, we intend to place high priority on strengthening channels of communication with the divisions and other standing committees. We hope to continue the practice of meeting briefly with each division every two years at IUPAC general assemblies, and would like to actively work with you on an ongoing basis to identify and collaborate on educational initiatives. We hope to dialogue further with division presidents about educational initiatives at the Bureau meeting in October 2006.

We have recently held a strategic planning meeting for CCE, in which we outlined the following priority areas for 2006.

- ❑ Emphasize the role for chemistry education in sustainable development. Working through the CCE Chemistry Education for Development (CED) subcommittee we will initiate new projects as well as review and support current initiatives such as our Flying Chemist's Program. We see bright possibilities for collaboration with other partners, including ICSU and UNESCO on Chemistry Education for Development initiatives.
- ❑ Use CCE global networks to address pedagogy in chemistry education, emphasizing the importance of learner driven, outcome oriented curriculum. The multi-cultural competence within CCE (TMs, AMs, NRs) should be fully utilized in these initiatives.
- ❑ We intend to build on the 2005 Public Understanding of Chemistry Subcommittee's report on IUPAC's niche in public understanding, and facilitate review and broad ownership within IUPAC of the key recommendations.
- ❑ International networks and partnerships are the primary mechanisms by which we achieve our goals. We intend to support existing successful partnerships with organizations such as Science Across the World (YAC Program) and the Organization for Prohibition of Chemical Weapons (ethical issues in chemistry, including multiple use chemicals).
- ❑ Within IUPAC we will continue to strengthen communication channels with divisions and standing committees.
- ❑ The biennial International Conference on Chemical Education (ICCE) is a key mechanism for bringing together global and regional expertise and also addressing CCE strategic areas. We will work closely with the organizers for the 19th ICCE in Seoul (August 2006) and the 20th ICCE in Mauritius (2008, with a satellite meeting in Sub-Saharan Africa) to address CCE priority areas as well as regional issues in the conferences. We would like to have as

full participation as possible in ICCE conferences from all CCE members, including AMs and NRs.

Prof. Åkesson is also the CCE secretary for 2006 and will distribute copies of our minutes to AMs in the future, so you are aware of CCE initiatives.

We invite your responses to the following suggestions for your role as AMs:

- To represent the educational dimension of your divisional activities to CCE.
- To promote CCE strategies and resources to your division.
- To identify and promote interdivisional educational projects.
- To identify activities within your division that have educational and/or public understanding spin-off.
- To help CCE identify regions and countries where chemistry education for development activities might be focused.

Finally, two requests for your immediate consideration.

1. On August 12 – 17, CCE will meet in Seoul during the 19th ICCE. We would ask you to place this meeting on your calendars and seriously consider contributing a poster or talk to the ICCE and attending the CCE meeting. Perhaps your division will consider supporting your attendance as an AM at the meeting.
2. Please identify and inform us of what you consider to be the two highest educational priorities for your division. These could then be discussed at the CCE meeting in Seoul and also presented in a poster at the conference. They might also be included in division president reports to the Bureau to encourage interdivisional cooperation.

We look forward to getting to know each of you personally, and to working with you in the coming year.

Best regards,



Peter Mahaffy
Chair, CCE



Eva Åkesson
Division Liaison and Secretary, CCE

Appendix II

Report from ICTNS to Division II Committee

Seattle, August 2006

The ICTNS has functioned efficiently and effectively during the past year under the chairmanship of Professor Jack Lorimer. The most recent Status Report from the Committee lists approximately thirty publications of which two relate to contributions from Division II. These are:

- (i) PAC-REC-06-02-01. Definitions of Terms Related to the Structure and Processing of Inorganic and Polymer Gels and Networks, and Inorganic-polymeric Materials (Jones). Received 2006-02; and
- (ii) PAC-REP-06-03-01. Atomic Weights of the Elements 2005 (Wieser). Received 2006-03-21.

Members of the Division have also contributed to the new Green Book

PAC-REC-05-11-10. Quantities, Units and Symbols in Physical Chemistry, 3rd ed. ("Green Book") (Quack). Rec'd 2005-11-10. Public comment period ends 2006-03-31. ICTNS comments by 2006-02-28. Accepted with revisions to come 2006-03-07.

The most recent status report is attached as ITCNS Summary 2006-04-05

John Corish
Trinity College Dublin
August 2006

Date: 2006-04-05
To: All Members, ICTNS
From: Jack Lorimer
Re: Updated Summary of TRs and Recommendations to date (E&OE)

The following is a list of the status of all TRs and Recommendations that were:

- (a) submitted before 2004-01-05 but not completed by that date;
- (b) submitted between 2004-01-05 and current date.

Summary

1.0 Recommendations and Technical Reports Submitted Before 2004-01-01 and Not Published by 2006-03-31 – total 5

- 1.0.1 Recommendations Submitted Before 2004-01-01 and Not Completed or Accepted by 2006-03-31 – total 0**
- 1.0.2 Technical Reports Submitted Before 2004-01-01 and Not Completed or Accepted by 2006-03-31 – total 5**

2.0 Recommendations Submitted Between 2004-01-01 and Current Date and Not Published by 2006-03-31 – total 17

- 2.0.1 Recommendations Submitted, Accepted and Published Between 2004-01-01 and Current Date – total 1**
- 2.0.2 Recommendations Submitted and Accepted Between 2004-01-01 and Current Date but Not Published – total 1**
- 2.0.3 Recommendations Submitted and Accepted Between 2004-01-01 and Current Date but Awaiting Final Manuscript or Final Review by ICTNS – total 5**
- 2.0.4 Recommendations Submitted Between 2004-01-01 and Current Date and Not Accepted by Current Date – total 10**

3.0 Technical Reports Submitted Between 2004-01-01 and Current Date – total 11

- 3.0.1 Technical Reports Submitted, Accepted and Published Between 2004-01-01 and Current Date – total 5**
- 3.0.2 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Not Published – total 1**
- 3.0.3 Recommendations Submitted and Accepted Between 2004-01-01 and Current Date but Awaiting Final Manuscript or Final Review by ICTNS – total 2**
- 3.0.4 Technical Reports Submitted Between 2004-01-01 and Current Date and Not Accepted by Current Date – total 3**

1.0 Recommendations and Technical Reports Submitted Before 2004-01-01 and Not Published by 2006-01-01 – total 5

1.0.1 Recommendations Submitted Before 2004-01-01 and Not Completed or Accepted by 2006-03-31 – total 0

1.0.2 Technical Reports Submitted Before 2004-01-01 and Not Completed or Accepted by 2006-03-31 – total 5

81 Melt rheology (Plochocki). 17 pages comments JWL to BJH 2003-11-03. Reminder by BJH 2004-10-07. Query to R. Stepto 2005-04-21.

878/PAC-REP-04-06-08 IR & Raman at High T, p (Heyns). Corrected ms requested 2002-09-04. Comments by BJH, TC, JWL sent 2004-06-22. New ms. sent to Secretariat 2005-10-15 as a pdf file. Author asked how he intends to proceed 2006-04.

1137 Exposure...Logbook Method (Olsen). Comments sent JWL to BJH 2003-11-19. Reminder by BJH 2004-10-07. Another reminder 2005-04-21.

67 X-ray emission analysis (Gohshi). JWL to Gohshi 2004-03-05 asking for report on status; reply from Gohshi indication revised ms will be supplied. Further reply to K. Powell reporting progress. No further information.

877 Thermochemistry (da Silva). New ms being prepared. Reminder by JWL 2004-05-07. Author will prepare revision in September, 2005. No further information.

2.0 Recommendations Submitted Between 2004-01-01 and Current Date– total 17

2.0.1 Recommendations Submitted, Accepted and Published Between 2004-01-01 and Current Date– total 1

PAC-REC-05-09-13 JCAMP-DX for EMR (Lancashire). Received 2005-09. ICTNS reviews due 2005-12-31. Recommended acceptance with minor corrections 2005-12-20. Revised ms accepted 2005-12-30. Public comment ends 2006-01-31. ICTNS comments by 2005-12-31. Published PAC **78**, 613-631 (2006).

2.0.2 Recommendations Submitted and Accepted Between 2004-01-01 and Current Date– total 1

PAC-REC-05-08-11 XML-based IUPAC~Standard for Experimental, Predicted and Critically Evaluated Thermodynamic Data Storage and Capture (ThermoML) (Frenkel). Received 2005-08. ICTNS reviews due 2005-12. Accepted with major revisions 2005-12-18. Final acceptance 2005-12-29. Public comment ends 2006-01-31. ICTNS comments by 2005-12-31.

2.0.3 Recommendations Submitted and Accepted, but Awaiting Final Manuscript Between 2004-01-01 and Current Date or Final Review by ICTNS – total 5

PAC-REC-05-10-23 Compendium on Macromolecular Terminology and Nomenclature (The Purple Book), 2nd ed. (Wilks). Received 2005-10. Reviewed by ICTNS. Accepted with minor changes 2005-12-18. Final ms 2006-03-22 under review.

PAC-REC-04-12-04 Terminology of Polymers Containing Ionizable or Ionic Groups and of Polymers Containing Ions (Kubisa). 9 reviews. Public comment period ends 2005-05-31. Letter 2005-04-20 major revision. Author (2005-04-21) notes final review by Division will be done in Beijing in August. Final version received 2005-12. Accepted with major revision 2006-01-24. More revisions sent to authors 2006-03-22.

PAC-REC-05-11-10. Quantities, Units and Symbols in Physical Chemistry, 3rd ed. (“Green Book”) (Quack). Rec'd 2005-11-10. Public comment period ends 2006-03-31. ICTNS comments by 2006-02-28. Accepted with revisions to come 2006-03-07.

PAC-REC-05-10-26 Glossary of Terms Used in Photochemistry (Braslavsky). Received 2005-10. Public comment period ends 2006-03-31. ICTNS comments by 2006-02-28. Accepted with major revisions 2006-03-07.

PAC-REC-05-03-01 Graphical Representation of Stereochemical Configuration (Brecher). Public comment period ends 2005-07-31. Letter of acceptance with minor revision (revised ms required) 2005-08-04. Revision under review September, 2005. Accepted with minor revision 2006-03-12.

2.0.4 Recommendations Submitted Between 2004-01-01 and Current Date But Not Accepted by Current Date– total 10

PAC-REC-04-05-03 Guide to Expression of Uncertainty (GUM), Supplement 1 (ISO/BIPM). 1 review by 2004-06-23. Public comment ends 2004-09-30, ICTNS 2004-08-31. Accepted on behalf of IUPAC with minor editorial revisions to IUPAC and Wallard 2004-09-27 – but again under revision. ISO Document JCGM-WG1-SC1-N10. Status queried with A. Thor 2005-04-21 – reply not yet published. Still under revision March, 2006.

PAC-REC-04-05-02 International Vocabulary of Metrology (VIM) (ISO/BIPM). Accepted on behalf of IUPAC with minor editorial changes to Wallard 2004-10-05. Status queried with A. Thor 2005-04-21 – reply not yet published. Again under revision by VIM working group 2006-03.

PAC-REC-04-10-24 Nomenclature of Cyclic Peptides (Moss). 2 reviews. Public comment period ends 2005-03-31. Letter asking for major revision, 2005-03-15.

PAC-REC-04-11-03 Nomenclature of Organic Chemistry (“Blue Book”) (Powell). Public comment period ends 2005-03-31. Complete revision underway.

PAC-REC-05-07-05 Guidelines for Potentiometric Measurements in Suspensions (Oman). Received 2005-07-18. Public comment period ends 2006-01-31. ICTNS comments by 2005-12-31. Subsequently, ms being reconsidered by Div. V.

PAC-REC-05-07-04 Use of the Terms “robust” and “rugged” and the Associated Terms “robustness” and “ruggedness” in descriptions of analytical procedures (Burns). Received 2005-07-15. Public comment period ends 2006-01-31. ICTNS comments by 2005-12-31. Subsequently, ms being reconsidered by Div. V.

PAC-REC-05-12-09. Nomenclature of Rotaxanes (Yerin). Rec'd 2005-12-16. Public comment period ends 2006-04-30. ICTNS comments by 2006-03-31.

PAC-REC-06-01-01. Glossary of Terms Relating to Pesticides (Stephenson). Rec'd 2006-01-05. Public comment period ends 2006-05-21. ICTNS comments by 2006-04-21.

PAC-REC-06-01-06. IUPAC Explanatory Dictionary of Key Terms in Toxicology (Nordberg). Rec'd 2006-01-24. Public comment period ends 2006-06-24. ICTNS comments by 2006-05-24.

PAC-REC-06-02-01. Definitions of Terms Related to the Structure and Processing of Inorganic and Polymer Gels and Networks, and Inorganic-polymeric Materials (Jones). Received 2006-02.

3.0 Technical Reports Submitted Between 2004-01-01 and Current Date– total 11

3.0.1 Technical Reports Submitted, Accepted and Published Between 2004-01-01 and Current Date– total 5

Project (to be submitted to JPCRD) Reference Data for the Density and Viscosity of Liquid Aluminum and Liquid Iron (Assael). ICTNS review (JWL, R. Weir) sent to author 2005-04-24; final version accepted (with minor corrections) 2005-04-25. Published JPCRD **35**, 285-300 (2006).

PAC-REP-04-05-06 The International Harmonized Protocol for the Proficiency Testing of Analytical Chemistry Laboratories (Ellison). Two more reviews requested 2004-10-07 (one received) to confirm adherence to BIPM standards. Reviews sent to author 2004-12-09. Revised ms received, returned for minor correction of symbols 2005-07-11. Accepted 2005-09-20. Published PAC **78**, 145-196 (2006).

PAC-REP-04-04-04 NMR for pKs (Popov). Revised ms received 2005-07-28. New review September, 2005. Accepted 2005-10-21. Published PAC **78**, 663-675 (2006).

PAC-REP-05-05-03 Guidelines for Calibration in Analytical Chemistry. Part 3. Uncertainty Estimation and Figures of Merit for Multivariate Calibration (Olivieri). Last rev. due 2005-05-03. JWL review complete. 2005-06-11. Revision under review, September, 2005. Accepted 2005-10-22. Published PAC **78**, 633-661 (2006).

PAC-REP-05-09-16 (formerly PAC-REC-05-09-16) Guidelines for Terminology for Microtechnology in Clinical Laboratories (Wilding). Rec'd 2005-10. Re-classified as a TR. Accepted with minor changes 2006-01-20. Published PAC **78**, 677-684 (2006).

3.0.2 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Not Published by Current Date– total 1

PAC-REP-04-08-05 Standards, Calibration and Guidelines in Microcalorimetry. Part 2. Calibration Standards for Differential Scanning Calorimetry (Della Gatta). 4 reviews (3 ICTNS). Returned to author for minor revision 2004-11-25. Reminder 2005-04-21. Revised ms received 2006-03-07. Accepted 2006-03-22.

3.0.3 Technical Reports Submitted and Accepted Between 2004-01-01 and Current Date but Awaiting Final Manuscript or Final Review by ICTNS– total 2

PAC-REP-04-10-25 Properties and Units in the Clinical Laboratory Sciences. Part XX. Properties and Units in Clinical and Environmental Toxicology (Duffus). Request for revised ms. showing what materials are to be archived on web site 2004-11-20, expanded 2005-01-25. Revised ms September, 2005. Accepted provisionally subject to major revision 2006-01-21. Revision received 2006-03, under review.

PAC-REP-05-12-12. Cytokine Profiles in Human Exposure to Metals (Stephenson). Rec'd 2005-12-22. Received 2005-12-22. Accepted with minor revisions 2006-03-14.

3.0.4 Technical Reports Submitted Between 2004-01-01 and Current Date and Not Accepted by Current Date– total 3

PAC-REP-06-01-07. Structure and Properties of Polyester Elastomers Coposed of poly(butylenes terephthalate) and poly(ϵ -caprolactone) (Takigawa). Received 2006-01-29.

PAC-REP-06-01-06. Solute Movement in Soils with Potential Rapid By-pass Transport (Pesticide Movement in Soils) Actual title: Transport of Pesticides via Macropores (Kördel). Received 2006-01-30.

PAC-REP-06-03-01. Atomic Weights of the Elements 2005 (Wieser). Received 2006-03-21.

Appendix III Report on the Naming of New Elements

A new round in the naming of new elements is in progress. The first step is the assignment of the discoveries to claimant laboratories. This is done by an IUPAC/IUPAP Joint Working Party. A new JWP was appointed by the Presidents of the Unions and comprises the following members:

Prof. Erich Vogt
University of British Columbia
TRIUMF
4004 Westbrook Mall
Vancouver, V6T2A3
Canada
TEL: 604-222-1074
FAX: 604-822-3118
E-MAIL: vogt@triumf.ca

Prof. Heinz W. Gäggeler
Paul Scherrer Institut
Würenlingen und Villigen
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Prof. Paul J. Karol
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Chemistry Department
4400 Fifth Avenue
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FAX: 412-268-6945
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Prof. Robert C. Barber
International Union of Pure & Applied Physics
Department of Physics & Astronomy
University of Manitoba
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TEL: 204-474-9817
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Prof. Hiromichi Nakahara
Tokyo Metropolitan University
Department of Chemistry
1-1 Minami Ohsawa Hachioji
Tokyo 192-0364
Japan
TEL: [81] 426 77 2552
FAX: [81] 426 77 2525
EMAIL: nakahara-hiromichi@c.metro-u.ac.jp

Prof. Emanuele Vardaci
Universita' degli Studi di Napoli "Federico II"
Dipartimento di Scienze Fisiche
Istituto Nazionale di Fisica Nucleare - sezione di Napoli
Complesso universitario di Monte Sant'Angelo
Edificio G, Via Cinthia
Napoli 80126
Italy
TEL: not known
FAX: not known
EMAIL: vardaci@na.infn.it

The Group will again be chaired by Professor Paul Karol.

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 Hewbrew University,
Jerusalem,
Israel
For Element No. 112;

Dr Kosuke Morita,
The Institue of Physical and Chemical Research,
Riken,
Japan.
For Element 112 (in part) and Element 113;

Dr Sergey Dimitriev,
Joint Instituite for Nuclear Research,
Dubna,
Russia
For Elements 112, 113, 114, 115, 116, and 118; and

Dr. Sigurd Hofmann,
Gesellschaft für Schwerionenforschung mbH,
Darmstadt,
Germany
For element 112.

These have been distributed by the Secretariat to the JWP whose report is now awaited. Originally hopes were that this round might be completed in time for the Council Meeting at Turin to consider any recommendations that might emerge. However, due to a number of delays, and the steps that remain to be carried through after the JWP report is received, this now seems unlikely.

In an effort to prevent a reoccurrence of some of the delays encountered this time in appointing the JWP the Secretary General, Professor David Black, consulted with me and I have made some suggestions to him as to how this could be avoided in future.

John Corish
Trinity College Dublin
August 2006



Appendix IV- RECENT ACTIVITIES OF DIVISION II – INORGANIC CHEMISTRY

RECENT BOOKS

[Nomenclature of Inorganic Chemistry - IUPAC Recommendations 2005](#), Connelly, N.G, Damhus, T., Hartshorn, R.M., and Hutton, A.T., The Royal Society of Chemistry, 2005 [ISBN 0 85404 438 8]

KEY RESPONSIBILITIES

Division II is responsible for the Commission on Isotopic Abundances and Atomic Weights, which keeps such data up to date.
It takes overall responsibility for the authentication and naming of new elements, including the assignment of priorities for discovery, via a joint IUPAC/IUPAP working party.

PROJECTS NEAR COMPLETION OR IN PRESS

[High-temperature mass spectrometry: Instrumental techniques, ionization cross-sections, pressure measurements, and thermodynamic data](#) (IUPAC Technical Report), *Pure Appl. Chem.* **77**(4), 683-737, 2005

[Name and symbol of the element with atomic number 111](#) (IUPAC Recommendations 2004), *Pure Appl. Chem.* **76**(12), 2101-2103 (2004)

[Name and symbol of element of atomic number 110](#) (IUPAC Recommendations 2003), *Pure Appl. Chem.* **75**(10), 1613-1615 (2003)

[On the claims for discovery of elements 110, 111, 112, 114, 116, and 118](#) (IUPAC Technical Report), *Pure Appl. Chem.* **75**(10), 1601-1611 (2003)

[Atomic weights of the elements 2001](#) (IUPAC Technical Report), *Pure Appl. Chem.* **75**(8), 1107-1122 (2003)

[Atomic weights of the elements. Review 2000](#) (IUPAC Technical Report), *Pure Appl. Chem.* **75**(6), 683-799 (2003)

SELECTED CURRENT PROJECTS

[Isotopic compositions of selected elements](#)
[Determination of atomic weights using new analytical techniques](#)
[Classification, terminology and nomenclature of borophosphates](#)
[Towards defining materials chemistry](#)
[Calibration of organic and inorganic oxygen-bearing isotopic reference materials](#)
[Evaluated published isotope ratio data \(2005-2007\)](#)

RECENT AND FORTHCOMING CONFERENCES

Workshop on Advanced Materials III, South Africa, September 2005
 High Temperature Materials Chemistry XII, Austria, September 2006
[Coordination Chemistry](#), 13-18 Aug 2006, Cape Town, South Africa
[Organometallic Chemistry](#) and Organic Synthesis, 2-6 Aug 2007, Nara, Japan
[Phosphorus Chemistry](#), 15-21 Apr 2007, Xiamen, China
[Transactinide Elements](#), 23-28 Sep 2007, Davos, Switzerland

Appendix V

Sub-Committee on Materials Chemistry

15 August 2005

Beijing

DRAFT 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 R, CC, F Adams (JC to provide complete list).

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, Fe_3O_4 and possible applications of these in the technique of magnetic hyperthermia 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 (SC 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 Torino 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
Interdivisional Sub-Committee on Materials Chemistry
Informal Meeting on 14th August 2006 in Seattle
Room 105, Department of Chemistry, University of Washington

DRAFT MINUTES

Present: J. Corish (Chairman), A.V. Chadwick (Secretary), L.V. Interrante, A.R. West, G. Rosenblatt, J. Garcia-Martinez, M. Leskela, C. Campbell (Local host).

1. Welcome

The Chairman welcomed the members of the Sub-Committee to the meeting and thanked Charlie Campbell from the Chemistry Department for acting as the local host and providing facilities for the meeting.

2. Minutes of the last meeting

The minutes of the last meeting of this Sub-Committee at Beijing were tabled and discussed. It was not clear how many members of the group had received electronic copies of the minutes, therefore they should be re-circulated.

[Action: Secretary to e-mail minutes of the Beijing minutes out to members]

The matters arising from the Beijing minutes mainly concerned progress on projects and will be covered elsewhere in the agenda for the meeting.

3. Reports of progress on projects

a. Defining Materials Chemistry

This is an accepted and funded project led by Peter Day (Chemistry, Oxford, UK) as the Task Group leader.

Professor Day had initiated a meeting in London earlier this year organised by the Royal Society of Chemistry and there was a report from this meeting (Annex 1). Unfortunately Professor Day could not attend the present meeting because of travel difficulties associated with increased security. The meeting appreciated the report but were unclear about what the next stage of the project would be and noted that the Task Group had not yet formally met. Tony West is the monitor for this project. The Chairman suggested that it would be useful for the Task Group to meet with members of this Sub-Committee with a view to bring the project to completion because the outcome of the project was so fundamental to the work of the Sub-committee. Tony West thought that the project still had sufficient funds to finance such a meeting possibly at the next General Assembly (The project was funded \$8k, and most of this was still available for such a meeting). The Sub-Committee endorsed the proposed meeting.

[Action: Tony West to contact Peter Day to discuss plans for the completion of the project]

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

This is a proposed project from Sanjay Mathur. There had been considerable discussion of this proposal at Beijing. There were concerns that the cost was initially too high and the project did not have sufficient focus. At Beijing it was left to Sanjay to follow up with a revised proposal. This has not yet been completed although some progress had been made and the Sub-Committee was sympathetic to the difficulties in producing a proposal on this subject. It was noted that some good starting points for the nomenclature; the book by Ozin and the Vocabulary PAS 71:2005 produced by British Standards. Tony West suggested a workshop on the topic could be held in conjunction with GA at Turin. It was clear that Sanjay would need help in preparing the proposal. After much discussion the following procedure was proposed to forward this project.

Step 1: The Chairman to ask Sanjay Mathur if he would be willing (with assistance from other members of the Sub-Committee) to run a workshop in Turin and still wishes to run the project that might be defined there. The aim of the workshop would be to assess the scope and viability of the project.

[Action: The Chairman to contact Sanjay Mathur to discuss plans for the project]

Step 2: Tony West and Javier Garcia-Martinez to assist Sanjay Mathur by (i) distilling information from the available glossaries of nanomaterials terminology (see above) and (ii) compiling a list key people who could eventually form a Task Group for the project. Potential Task Group members within IUPAC could be identified from the Blue Book.

[Action: Tony West and Javier Garcia-Martinez to distil glossaries and find potential members and convey the information to Sanjay Mathur]

Step 3: Tony West will publicise this plan to have the workshop at the Bureau Meeting in Madrid. This will inform IUPAC and the other Division Presidents of the plan and will help identify other people within IUPAC who could be on the Task Group.

[Action: Tony West to publicise plans at the Bureau Meeting]

Step 4: (Added after the meeting). Since the above steps involve several people it seems appropriate for the Secretary to monitor progress on the steps.

[Action: The Secretary to monitor the steps]

c. Experiments in Materials Chemistry

Dr. Bosova, who was asked to coordinate the project, feels the project should be dropped as the task force has disintegrated. In addition she has no students to test the experiments. Gerd Rosenblatt gave the history of the project describing it as still being of potentially great value to the community if it could be completed in the future.. However, in the present circumstances it does look as though this project should be terminated. This will be reported at tomorrow's meeting of the Division Committee.

4. HTMC-XII Vienna

All information on this meeting is on the Web. It is IUPAC sponsored. There will be approximately 150 attendees, similar to the previous meeting in Japan. A presentation from IUPAC is normally given at this meeting; however there does not appear to be an attendee who is an IUPAC member. It could be possible that Hilpert or Chatillon are attending and he could give the presentation.

[Action: Gerd Rosneblatt to contact Hilpert and Chatillon to ascertain his attendance at the conference]

4. HTMC-XIII (2009)

The venue selection committee, chaired by Hilpert, considered five to six good applications to hold meeting. Within the established schedule it was time to hold the meeting in the US and it will be organised by Alexander Navrotsky at Davis.

5. WAM III (Workshops on Advanced Materials)

This was held in Stellenbosch, South Africa in September 2005. A full report, written by Piet Styne and the Chairman, is available on the Web and was published in Chemistry International. The Chairman attended the workshop and reported that it was a very successful meeting with wide representation of students from African countries. Sanjay Mathur had organised a mini-symposium jointly funded by National Research Foundation (South Africa) and the Deutsche Forschungsgemeinschaft (Germany) in conjunction with the meeting. All of the presentations at this symposium were given by research students.

6. WAM IV

An offer had been received from Thailand to host this meeting, to be organised by Joydeep Dutta at Asian Institute of Technology in Klong Luang Pathumthani. Sanjay Mathur will be involved in assisting the organisers. This application was reviewed and was considered to be an excellent and well thought out proposal and should be endorsed.

[Action: Chairman to contact the organisers and provide assistance in seeking IUPAC funding for the meeting]

7. New Projects

7.1. Terminology for conducting, electroactive and field-responsive polymers

This is a proposal submitted from Division IV, coordinated by Prof Ober. Gerd Rosenblatt said that it was good and needs to proceed, but we (the Sub-Committee) have no budget. But the Sub-Committee could give it support as being a good project. However, there is no inorganic chemistry in the project, hence the Division might not agree to fund it. Gerd Rosenblatt suggested we give it the backing of this Sub-

Committee, such that The Chairman could write to the Secretariat strongly endorsing the proposal. The Sub-Committee was happy with this course of action.

7.2 Nomenclature for mesoporous materials

Javier Garcia-Martinez felt that there is confusion in nomenclature. It is a much focused area and is part of the nanomaterials area. A lot of work done by IUPAC in the area of porous materials nomenclature (as early as 1985) but area is now getting confused with the new materials and nanotechnology. Thus there is room for a focused project. To pursue this it the interest of other Divisions should be assessed. Tony West will consult Division Heads at the Bureau meeting in Madrid.

[Action: Tony West to consult at Bureau meeting]

8. Future of Sub-Committee

The Chairman pointed out that this Sub-Committee was formed in Brisbane and it was time to review the status. Several members commented that materials chemistry is a growing area, but where does it fit into the current structures of IUPAC? There is no funding, so how does the Sub-Committee continue? There have not been a lot of projects in the materials chemistry area and no outstanding successes despite the fact that Materials Chemistry had formed significant parts of recent IUPAC Congress Programmes and will feature again in Turin. Gerd Rosenblatt said it would be hard to start a Division for Materials Chemistry; a strong case could not be made and Inorganic Division itself is not currently one of the stronger divisions. Tony West pointed to the experience of the Royal Society of Chemistry in setting up its very successful Materials Forum suggested that it was necessary to move carefully and slowly in building up successful structures that could effectively assist this subject. The future of the Sub-Committee will be raised at the Division II meeting to seek a wider view.

9. Presentation

Charlie Campbell gave a short presentation on the research in chemistry at the University of Washington.

10. Conclusion

The Chairman thanked the attendees for their participation and Charlie Campbell again for being a splendid local host.

12. Date of next meeting

The Sub-Committee will meet at the Turin General Assembly.

Alan Chadwick - 23 September 2006

ANNEX 1**IUPAC Inorganic Chemistry Division Committee**

Seattle, USA, 15-16 August 2006

Defining Materials Chemistry: IUPAC Project – Prof. Peter Day**Background**

In the last 10-15 years materials chemistry has rapidly emerged as a distinct discipline within the broad family of chemical sciences. A significant fraction of all publications in chemistry claim to form part of this new field. Two examples will suffice: Googling 'materials chemistry' results in no fewer than 175M hits, while the number of articles submitted to one of the major journals in the field has increased almost 15-fold in 15 years. Nevertheless, finding an agreed definition of what constitutes 'materials chemistry' is not easy. Materials chemistry transcends the traditional sub-divisions of chemistry. So can we devise an inclusive but meaningful definition? To date the discipline has developed organically and to a large extent, the common idea of what constitutes materials chemistry is circularly linked to the type of work that those calling themselves materials chemists do.

Faced with these facts IUPAC set up a project to furnish a succinct definition of the subject area covered by materials chemistry and recommend how this new discipline might best be represented within the IUPAC structure. Apart from collecting information from practitioners and from the journals principally devoted to the subject, one of the key tools in the project was a Workshop, kindly organised by the Materials Chemistry Forum of the UK's Royal Society of Chemistry. The MCF brings together representatives, not only of the relevant subject groupings in the RSC but also from contiguous disciplines like physics and materials science, all of which contributed, in addition to international speakers. The workshop aimed to provide a definition and discuss the nature of the discipline. The opinions and ideas collected provide valuable feedback to the publishing and funding communities, as well as the IUPAC project. The brief comments that follow draw heavily on that discussion. I am grateful to Dr Rachel Brazil of the RSC for her notes.

What is a Material?

In defining materials chemistry, it becomes clear that one of the most difficult tasks would be defining what constitutes a material in contrast to just a chemical. This would be the key to defining materials chemistry. The dictionary defines a material as 'a physical substance which things can be made from'. To devise a more technical definition many felt that the idea of functionality or application needed to be considered. A material is something that has properties which give it a particular useful application, either structural, as with a building material, or functional, as with materials used to make devices (electronic, optical or magnetic). A material is generally thought of as a

solid or highly viscous phase where interactions between the entities forming the aggregate play a large role, rather than a liquid or gas.

Another key concept is that of 'emergent properties' Materials are assemblages of sub-units. The properties of a material emerge from the way these sub-units are put together. Whilst a single molecule will have properties related to its chemical structure which remains constant, the properties of a material are dependent on how its subunits are assembled. In fact, properties can arise from structural defects and materials made of the same chemical sub-units can have different properties. This relationship between structure and property could be used to define a material and differentiate it from a chemical. An example of a material would be a nanotube, whose properties will vary depending on its structure. This can be compared to a molecule of benzoic acid, which is a chemical whose properties are related only to its chemical make-up.

The work of a materials chemist

To develop ideas about the sub-discipline it is useful to look at some of the processes and priorities of researchers in the discipline.

- *application as motivation*

Much materials chemistry is motivated towards discovery and development of materials that may be exploited for desired applications. Whilst this is an essential motivating factor, there does also need to be some scope for purely studying the structure and properties of materials. Chemists will generate new materials before their potential applications may have been conceived. The discipline must include the ability to synthesise, study and assess new materials.

- *structural or functional*

Today, the work of most materials chemists is focused on producing functional device materials and the discipline is often seen as being focused on the production of materials with function – electrical, optical or magnetic. The production of structural materials such as alloys, composites and plastics has been seen as the province of materials scientists. Polymer science, whilst carried out by chemists was not always historically strongly connected to other materials chemistry, largely due to the number and strength of journals devoted to macromolecular chemistry alone. However, with the development of the field of conducting polymers, the materials chemistry and polymer science communities are moving closer together. The development of new nanostructured and smart materials is also uniting communities and bringing the science involved in functional and structural materials together. Materials chemistry can encompass both structural and functional materials. Structural properties such as strength or flexibility can be considered as another type of functionality. At the moment chemists are more interested with other types of functionality but this may change in the future.

- *designing and processing materials*

The concept of 'design' was seen as very important in defining the work of materials chemists. Rather than purely investigating properties, the materials chemist tries to manipulate the synthetic process to produce a desired end product. The relationship between method of synthesis and design of the final end product is crucial for a materials chemist.

- *Characterisation and analysis*

Characterisation techniques are important to the work of all chemists. However, whilst many mainstream chemists are primarily concerned with characterising the chemical or molecular structure, materials chemists are often interested in looking at higher level structure in addition. Microscopy is an important element of the work of many materials chemists.

The difference between materials science and materials chemistry

In defining materials chemistry, the differences between materials science and materials chemistry were examined. Many materials science departments have appointments in materials chemistry. However the areas of study described as materials chemistry can differ from the materials chemistry practised within chemistry departments. Materials chemistry from the chemistry perspective should be considered a sub-discipline of chemistry.

Materials chemistry does share some common elements with materials science, but often the scale of elements studied differ, with materials chemistry being concerned with a molecular understanding of materials, whilst materials scientists are looking at a larger scale. Materials chemistry can be concerned with properties up to the micron scale though.

It must be recognised that there is a big overlap and many materials scientists will be working to the same end as many materials chemists.

Another element that may differentiate materials chemistry from materials science is the interdisciplinary nature of the work. Materials chemistry may require an understanding of the principles of both chemistry and materials science and sometimes physics and biology.

A working definition of materials chemistry

Some definitions suggested at the workshop:

Materials chemistry is the chemistry of the design, synthesis and characterisation of assemblies of molecules whose properties arise from interactions between them.

Materials chemistry is the understanding, synthesis, processing and exploitation of compounds or substances in their assembled form.

Materials chemistry is the synthesis, processing, characterisation, understanding and exploitation of compounds that have useful or potentially useful properties and applications.

What is *not* materials chemistry?

It may be agreed that simply synthesising a new chemical substance in nano- or macroscopic form is not materials chemistry but just chemical synthesis. For it to be considered materials chemistry there needs to be an element of application, function or novel design. Work on novel materials that may show potential applications must be included as materials chemistry since chemists may generate new types of materials with previously unknown properties leading to unimagined applications.

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

Inevitably there are areas of contention when trying to define the sub-discipline materials chemistry. Would catalysis be considered part of the field? Homogeneous catalysis would certainly not fit the definition above, but would heterogeneous catalysis? The synthesis of novel catalyst materials does certainly fit the parameters by which materials chemistry has been described.

There are other areas that could be debated, in which the chemical synthesis is of a precursor to the material itself. Examples are CVD precursors, new liquid crystal molecules (synthetic chemistry or materials chemistry?) or the ball milling of ceramics (materials science or materials chemistry?).

Materials Chemistry in IUPAC

It is abundantly clear that materials chemistry impacts on, and requires input from, many of the traditional sub-groups of chemical science (physical, organic, inorganic, macromolecular etc). At present the interests of the subject are overseen by a Materials Chemistry Working Group that is formally a sub-committee of the Inorganic Chemistry Division Committee. It could be argued that this arrangement no longer responds adequately to the size and reach of the materials chemistry community. IUPAC should address this deficiency. One model to study is that of the 'Special Interest Group' in the RSC structure, of which the Materials Chemistry Forum is one example.

22 July 2006

Appendix VII

IUPAC WORKSHOP IN ADVANCED MATERIALS - WAM III

The University of Stellenbosch, South Africa, September 4th to 8th 2005

A very successful IUPAC New Directions in Chemistry Workshop in Advanced Materials (WAM III), funded under the Union's programme for conferences in emerging regions and organised by the University of Stellenbosch UNESCO Associated Centre for Macromolecules and Materials, attracted more than one hundred and fifty participants to South Africa, in September. Responsibility for this series of Workshops, the first and second of which were held in Singapore and Bangalore, respectively, was vested in the Sub-committee for Materials Chemistry at the Ottawa General Assembly. WAM III focussed on Nanostructured Advanced Materials with the Local Organising Committee chaired by Professor Ron Sanderson. The eight sessions ranged from new synthetic routes for the production of nanostructured materials, through nano-electronics, nanotubes and fibres, design and self assembly, bio-related materials and carried through all the way to include device characterisation and applications. The Workshop was opened, on behalf of IUPAC by its past- President, Professor Piet Steyn. Another former President and the organiser of WAM II, Professor C. N. R. Rao also participated and presented a plenary lecture. The plenary and invited lectures will be published in a special edition of Pure and Applied Chemistry and the editor, Professor James Bull, also attended.

The Workshop concentrated on the vital role played by chemists in the design and fabrication of nanostructured materials, with a particular emphasis here on soft chemistry. The presentations covered an exhaustive range of established as well as novel synthetic techniques for the preparation of nanoparticles as well as nanotubes and a variety of nanostructured films, nanocomposites and nanoporous materials. All of the principal characterisation techniques were also covered with particularly impressive presentations on the latest developments in the use of STM and AFM microscopy on silicon surfaces. The current and future technological utilisation of nanomaterials as coating materials, electrocatalysts and electronic components, as well as applications in chemical separations, fuel cells and other novel energy technologies and in medicine were also discussed as was the potential offered by autonomous nanoscale motion through catalysis.

The WAM III programme incorporated a Bilateral German-South African Mini-symposium organised by Prof. Sanjay Mathur and Professor Sanderson and jointly funded by National Research Foundation (South Africa) and the Deutsche Forschungsgemeinschaft (Germany). All of the presentations at this symposium were given by research students.

The South African Department of Science and Technology generously sponsored Poster Awards for young chemists at the Workshop. The first prize was won by Ziboneni Godongwana, South African Institute for Advanced Materials, University of the Western Cape for a poster entitled: "Inexpensive production of graphitic mesoporous carbon material" The second prize was awarded for a poster entitled "Preparation and characterisation of proton conducting

membranes for direct methanol fuel cell (DMFC) applications” by Rushanah Mohamed and Ziboneni Godongwana from the same Institute.

The success of WAM III in terms of its educational objective can perhaps best be judged by the fact that many more students than established scientists attended. The current rapid growth in interest in materials chemistry in general and in nanoscience was reflected in the fact that the workshop was also very significantly larger than its predecessors. It was attended by delegates and students from the following African countries: Algeria, Ethiopia, Lesotho, Libya, Nigeria, Mozambique, Senegal and South Africa.

The IUPAC Sub-committee for Materials will at its meeting in 2006 select a location for WAM IV, which will be held in 2008. Anyone interested in submitting a bid to host the workshop, bearing in mind its objective of bringing the cutting edge of the science of advanced materials chemistry to emerging countries, should contact its Chairman, Professor John Corish, School of Chemistry, Trinity College, Dublin 2, Ireland, (jcorish@tcd.ie).

***Report by Piet Steyn and John Corish
October 2005***

Appendix VIII

Report of the Sub-committee on the Natural Assessment of Fundamental Understanding (The first annual progress report to the Commission on Isotopic Abundances and Atomic Weights, CIAAW, and to the IUPAC Inorganic Chemistry Division Committee)

Norman E. Holden
Chairman

The Commission on Isotopic Abundances and Atomic Weights (CIAAW) proposed the formation of this sub-committee for IUPAC approval, to the Inorganic Chemistry Division Committee, during the Beijing General Assembly in August 2005. The work of this group began in January 2006. The task assigned to the sub-committee by the CIAAW was to address and answer a series of rather fundamental questions that continuously face the Commission but for which there is never adequate time available at the Commission meetings for proper discussion and for any potential recommendations for resolution.

A quarter of a century ago, IUPAC imposed a 12-year membership rule that now requires a complete turnover of all Commission members in slightly over a decade. Commission members, who in the past had the opportunity to raise and discuss fundamental questions about atomic weight values and their uncertainties, the methods by which these quantities were determined and expressed in reports to the general chemical scientific community for maximum understanding of these concepts, have long since been replaced as Titular and Associate members on the Commission. As a result, present CIAAW members have very limited knowledge of the arguments or the discussions or the reasoning behind many of the Commission's rules and technical guidelines that they must follow. Preservation of a consistent continuity of knowledge is an important duty of CIAAW, and justification for the Commission's existence.

This subcommittee is preparing possible approaches to many longstanding questions that Commission members have had over the past decade or two. The subcommittee's report will hopefully become a source for the Commission's discussion of various options in the presentation of the contents, definitions and support information for future Commission's tables and their interpretation. The sub-committee will shortly propose a Task Group to undertake a detailed discussion of many of the most significant of these topics.

The working members of this subcommittee are senior scientists, who have experience within IUPAC in the scientific areas of atomic weight values and isotopic compositions of the chemical elements. The more senior members in this group have between thirty-five and forty-five years worth of IUPAC experience, while the "newcomers" in the group have between fifteen to twenty-five years of IUPAC experience in the field. All of the members have been officers of either the Commission or one of its subcommittees or both. Their history and knowledge of working methods and techniques of Commission's past work and the rationale for past decisions will be drawn upon during the course of this effort.

The questions that the sub-committee and its proposed Task Group will be discussing fall into one of the following categories: either historical, technical, scientific, administrative, procedural, or philosophical. Members will attempt to answer the questions raised as they map out the direction for the future of the Commission.

The list of potential topics for the sub-committee's work included about two-dozen issues raised by various Commission members during the past two decades. Members of this sub-committee added another dozen topics to the list. In the initial discussions of the sub-committee over the past half year, it was determined that the most significant ones would be addressed by a Task Group of the sub-committee. These topics will be listed separately in the Project description portion of the Task Group's Project Proposal to the Inorganic Chemistry Division Committee.

The other topics that were not included in the Project Proposal were considered either to be of a lesser significance to the Commission, or each topic would require a much larger effort, that would require a separate Task Group Project Proposal or the topic might depend on the conclusions that would be reached on issues in the Project Proposal or that topic might be incorporated into the detailed discussion of the topics already included in the Task Group Project Proposal.

Some of the topics that were initially discussed by the sub-committee and then were eventually postponed to a later time included the following issues:

What constitutes a naturally occurring element versus a synthetically produced element, specifically the case of the element "technetium"?

How does one treat the issue of the absolute isotope abundance ratio measurements and the relative isotope abundance ratio measurements and the inter-connection of these two types of measurements via the "delta" scale of values, also called differences between the isotope amount ratio measurements of a sample and a reference sample for a particular chemical element?

Have the Commission determine the zero point of all "delta" scales for each chemical element, with the use of Reference Materials for each chemical element.

Must a bank of Reference Materials for all chemical elements be created and should the Commission serve as a clearinghouse for the database on Reference Materials?

Must a discussion be held on the new definitions that will be proposed for the "kilogram" and the "mole" in 2011 and must the possible impact of these new definitions on the work of the Commission be evaluated? The Commission is directly involved in providing the link between mass and the amount of substance.

Must a database be developed of information on the measurement of the variability of isotope amount ratios for all chemical elements?

Must a database be developed for information on isotope amount ratio measurements for each non-terrestrial sample of a chemical element?

Must data be reviewed on non-mass dependent isotope fractionation of the chemical elements and determine how they might be applied for correcting isotope amount ratio measurements?

Must the sub-committee on natural isotopic fractionation, SNIF, be reconstituted for the elements with more than two isotopes and must a method be determined to apply isotope fractionation corrections, when only one isotope amount ratio has been measured for that element?

Must the issue of radiogenic isotopes be addressed with respect to the need for isotope fractionation corrections in measurements on these isotopes, for example, in the cases of rubidium-strontium and of samarium-neodymium?

Must the paradox be addressed that as the uncertainties in the very best measurements of the isotope amount ratios become smaller, uncertainties in recommended atomic weight values become larger, due to the variability of isotope amount ratios measured in nature? Significant figures are added to the atomic weight values of mono-nuclidic elements, at the same time that significant figures are being removed from two isotope light elements.

The majority of the Commission's audience would be unsophisticated users, who would have difficulty understanding the scientific reasons for this result.

Must the continuing issue be addressed of symmetric and asymmetric uncertainties, when reporting data? What type of effort would be required by the Commission to educate users to accept the concept of asymmetric measurement uncertainties in recommended values?

Must a standardized method for evaluating measurement uncertainty be developed for measured isotope amount ratio values and also for the natural variation in isotope ratio measurements? Must rules be developed for the combining of the two uncertainties?

Must such uncertainty rules be recommended in order to obtain recommended isotope abundance values and the resulting atomic weight values?

Have the CIAAW begin to work on a sub-document, which would be based on, and derived from the Vocabulary of Basic and General Concepts in Metrology (VIM) of the International Organization for Standardization (ISO), applicable in the field of isotope measurements. This VIM sub-document could provide scientific language and methods for use in texts in applied fields such as food regulations and environmental regulations. The treatment of light isotopes and their use in brand food and drug authentication, the authentication of food origin, the falsification of food and drinks and the illegal use of drugs in sport would benefit from the development of such a document.

Must an explicit statement be prepared and added to CIAAW tables and other products of the Commission, which would clearly state how to properly cite these items or how to obtain permission to republish them? This statement would eliminate the present practice of republishing freely the tables and other products without any attribution to CIAAW or IUPAC.

Further work by the sub-committee on any of these above topics would, of course, await a decision by the Division Committee on funding the Project Proposal of the Task Group to perform work on the more significant issues that are included in that Project Proposal.

Sub-committee Membership

N. E. Holden (USA)

J. K. Boehlke (USA)

T. B. Coplen (USA)

P. J. DeBievre (Belgium)

J. R. de Laeter (Australia)

E. Roth (France)

Appendix IX

IUPAC Project 2000-024-2-200

“Teaching high temperature materials chemistry at university”

Dear colleagues and friends,

After a forced interruption due to health issues, these improved much satisfactorily to allow me to work for an update of the status of the IUPAC Project 2000-024-2-200 entitled “Teaching high temperature materials chemistry at university”.

The document has been revised and implemented in respect to the first draft submitted to you in the past. The arrangement of the topics and the explanation for each topic have been somewhat refined and useful bibliography pertinent to each topic has been selected and appended.

Topics are arranged in such a way that the first part represents, I would say, the “core” of the traditional high-temperature chemistry subjects and thermodynamic issues relevant to high temperature materials. In a second part under “special topics” are grouped a number of subjects relative to materials processes and properties where high temperature science plays a fundamental role. Some of these “special topics” might be taught as optional according to the level and type of students (undergraduate, near graduate, specializing in materials chemistry etc). The present arrangement reflects in large part my personal experience having taught a lecture course in high temperature physical chemistry topics for very many years at the Department of Chemistry, University of Rome. The list of topics (in particular those listed under special topics) and the relative explanation might be lacking and, also, the bibliography appended reflects my personal knowledge of literature available to me and therefore may be in some cases lacking or incomplete.

Therefore I ask any of you according to your expertise and experience suggestions for adding or deleting topics, improving short explanations and useful bibliography and, finally, improving language. For example I was suggested to insert in the topics subjects concerning liquids, sintering, reactions with containers. In the present version of the document explanations and bibliography for these subjects are, it seems to me, in an embryonic stage and need to be improved. I trust in you.

I would very much appreciate your effective contribution in giving comments, suggestions how to improve the attached report. We are late in respect to the planned time for the completion of the project. I feel that the document must be finalized and then we have to decide on some dissemination actions. As usually requested by the Division I would intend to submit a written update of the status of this IUPAC project to the Division Committee within a short time.

Thank you for your collaboration.

With my best regards and wishes for the year 2006

Gianni Balducci

Rome, February 2006

Appendix X

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

Task Group Chairman: Robin Harris (University of Durham)

Progress report, 2 July 2006

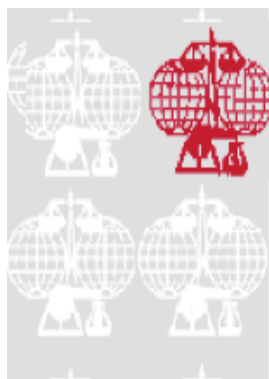
Objective: To update *IUPAC Recommendations 2001: NMR Nomenclature, Nuclear Spin Properties and Conventions for Chemical Shifts* [PAC 73, 1795 (2001)] by addressing several issues still to be resolved in setting standards for chemical shifts, including temperature variation of the NMR signals of reference 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 was 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 has now been published in *J. Magn. Reson.* **176** (2005) 87. Two further relevant papers, on susceptibility corrections and solvent effects, again by Dr. Hoffman, have also now been published, in *J. Magn. Reson.* **178** (2006) 237 and *Magn. Reson. Chem.* **44** (2006) 606 respectively. The IUPAC report relies in part on these papers. Two meetings between Professor Harris and Dr. Becker have taken place in London in July 2005 and 2006. The strategy for completing the project was discussed, with schedules set. Currently a draft final report is in existence. This requires approval and final comments from members of the Task group, after which it will be ready for submission. However, one table requires data which are not yet available; a decision will have to be made as to whether it is sensible to wait for the data or to omit the table.

Robin K. Harris
Task Group Chairman

Appendix XI



I U P A C

**Call for proposals
Inorganic Chemistry Division (II)**

The IUPAC Division of Inorganic Chemistry is seeking outstanding consortia of international research groups, associations, and individuals that would like to establish standardized terminology, procedures, or data in their respective fields that are also relevant to the broad aims of IUPAC.

Funded projects will be required to produce reports that on approval and publication will become IUPAC recommendations to the international chemical community.

For more information on how to produce an IUPAC project proposal:
http://www.iupac.org/general/handbook/guidelines_projects.html

Contact person:
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