INORGANIC CHEMISTRY DIVISION COMMITTEE OF IUPAC

Meeting at Sheffield 4th and 5th September 2002

MINUTES

Attendance: Present were President, Gerd Rosenblatt, Vice-President, Anthony West, Past President and Acting Secretary, John Corish; Titular Members: Ty Coplen and Norman Holden; Associate Members: Alan Chadwick and Herb Kaesz, and National Representative, Kazuyuki Tatsumi.

Apologies were received from Leonard Interrante, Bernard Meunier, Venceslav Kaucic and Philip Taylor who could not attend.

1– Introductions

The President welcomed members to the Meeting, especially those attending at the Division Committee for the first time. He thanked West for acting as host and for the excellent facilities that had been made available in the Department.

2 – Agenda

The Agenda was accepted as circulated. The President described it as full and felt that it would require an intensive effort to get through all the business in the time available.

3 - Minutes from Brisbane

The President explained that the Committee Secretary had found it necessary to resign since Brisbane and he informed the Meeting that following consultation he had asked Interrante to become Secretary. He had agreed but could not, because of prior commitments assume office until after the General Assembly at Ottawa. Corish had agreed to be Acting Secretary until that time and the President thanked him for preparing the Brisbane Minutes. The minutes were accepted as presented and signed. It was suggested that in future lists of current projects and of publications from the Division be included as further appendices. It was agreed that copies of the draft minutes would be sent to everyone who had been asked to contribute to the Meeting.

4 - Reports of IUPAC Bureau and Executive actions (President, Past-president)

The President reported on items of correspondence relating to the election of Division committees and sent by the Secretary General for discussion at the Bureau Meeting in Paris. The Committee agreed with the President that he should support the proposal that the Chair of the Nominating Committee need not come from outside the Division Committee and also the other proposals. With respect to the electorate Division II felt that it was essential to increase the size of
the electorate so that it would be made substantially larger than the size being proposed for Ottawa i.e., the Division Committee and Nominating Committee members. The ensuing discussion focussed on the need to increase interaction between the Division and the international chemistry community and it was agreed to begin the process of forming an Advisory Group for the Division. This could be based on former members of the Division Committee and of the Commissions, unsuccessful candidates, referees, Presidents of the other Divisions and any other interested scientists. Active communication and exchange of ideas with such an Advisory Group would be essential and Kaesz agreed to produce a newsletter for email circulation. It would be based on the minutes of the Division Committee and would also incorporate news of the projects, conferences and other activities of the Division. He would send it first to the Division President and Secretary for approval. This Advisory Group might ultimately be used as an electorate for the Division Committee.

*Publication in Journals other than PAC:* This subject was also due for discussion at Paris. It was felt to be important to enhance the image of IUPAC within the international chemistry community that articles/reports/recommendations be published in the leading journals in the relevant areas. The Division President should be empowered to grant such permission after consultation with the Executive Director. PAC could remain as a secondary place of publication and thus act as an archive for IUPAC work.

5 - Organization of Division, and procedures for project oversight and generation

The Committee discussed the organisation of the work of the Division with the three areas of atoms, molecules and materials, as defined by the Co-ordinating Groups. It confirmed the determination of the Division to maintain worthwhile activities in each of these areas while noting: (i) that the work on atoms, with the exception of that relating to the naming of new elements, should be promoted by the new Commission II.1; (ii) that virtually all the work relating to molecules was in the area of nomenclature and had been moved to Division VIII; and (iii) that a new Sub-committee of Materials Chemistry, which has representatives from four of the Divisions, would be seeking to secure an appropriate place for Materials Chemistry within the Union.

The major current problem was the need to set up procedures to generate new projects in these areas and also to oversee their progress and completion through the IUPAC system. It should be accepted as part of the TMs’ responsibilities to stimulate the generation of projects in their own areas of expertise. Each current project would be assigned a TM to assist its completion including publication of the results. In this context it was essential that every TM clearly understood the types of projects that constituted good IUPAC practice and the differences between these and standard research projects. Strenuous but unsuccessful attempts had been made to build up the ‘molecules’ area. The lack of a Commission structure to foster such activities would make it more difficult to succeed but the elections should be used to renew and reinforce these efforts.

It was agreed that the Co-ordinating Groups would meet again at Ottawa as they provided foci for the work of the Division.

6 - Review of Division budget allocations and expenditures

The President reviewed the budget provision for the 2002/2003 biennium. The $51,200 allocated was to cover all expenses with the exception of travel and subsistence of the Division TMs at the Ottawa GA. The guidance suggested that 25% be used for the operations/administration
leaving a balance of $12,800 in each of the three principal areas for the support of projects. The President proposed and it was agreed that the Division should seek in the first instance to ensure that its scientific programme was correct: the budgetary decisions would then follow.

Atoms: The projects proposed were very large and with expenditures in excess of the funds available. The President was anxious to know what provisions, if any, had been made to allow the members of the Commission to meet. It was agreed that Holden and Coplen would consult with the Commission Chair, Taylor, to (i) obtain a considered opinion on how much should be committed to projects and (ii) be forewarned on any other expenditures/projects anticipated within the biennium. Coplen was further asked to revise current projects in line with the informal suggestions made by Professor Lorimer and to seek clarification of their timing before resubmission.

Molecules: There were as yet no proposals and the need to assign the funds within a reasonable timescale was recognised.

Materials: $4800 had been allocated to Balducci for a project on the teaching of High Temperature Chemistry at Third Level. Of the other requests to hand it was agreed that that from Kizilyalli (on the Classification, Terminology and Nomenclature of Borophosphates) needed to be considered in conjunction with Division VIII. In particular it was essential to avoid a piecemeal approach to nomenclature in this area. Coplen was asked to request the Kizilyalli and Kniep be asked to complete the form and to define a more general approach that could then be discussed with Division VIII. The Division would fund, jointly on a 50:50 basis with Division VIII, any project that emerged.

7 - Report from Commission II.1

Note: No report had been received prior to the meeting nor was any information available on how the Commission intended to operate during the current biennium. The Committee asked Coplen and Holden to request a report from Taylor within one month and also a copy of the minutes from the Commission Meeting at Brisbane. The Report will then be appended to these minutes. In particular, the Division Committee needs clarification with respect to the manner in which the Commission wished to use that part of the budget available to it.

The Report received on October 10th 2002 is given in Appendix II

8 - Reports from sub-committees

(All the Reports summarised here – from Sub-committees, other IUPAC bodies and Projects are, where available, shown in full in Appendix III)

Sub-committee on Extra-Terrestrial Isotopic Ratios

A Report by Ebihara dated September 7th was received after the meeting. At Brisbane the sub-committee had decided that its members would survey all existing literature data on isotopic abundances of rare-earth elements in extra terrestrial materials. They planned to meet again at the next GA to prepare a review paper that was intended to be the first in a series on isotopic abundances in extra-terrestrial materials. An interim review meeting was planned for the Pacific Basin at year-end. This work related directly to project 2001-042-1-200 (see below).
Sub-committee on Isotopic Abundance Measurements

Bolke and Peiser reported that a paper summarising the history and status of the atomic weights of the elements had been drafted, reviewed and revised by members of the Commission. Its title was “AtomicWeights of the Elements, Review 2000” by J de Laeter, J. R. Böhlke, P. DeBievre, H. Hidalea, H. S. Peiser, K. J. R. Rooman and P. D. P. Taylor: a copy of the draft manuscript was presented to the meeting by Coplen. This is directly related to Project 1999-043-1-200 (see below). This paper will be submitted for publication in PAC within the next few months.

Sub-committee on Applications of Isotopic Specific Measurements

No report was received.

Sub-committee on Characterization of Carbonaceous Materials and New Carbons

No report was received at the meeting and it was agreed to resend the request by regular mail. Boehm reported on September 12th (after the meeting) that little progress had been made and requested assistance to enable him to continue the work of the Sub-committee.

Sub-committee on Materials Chemistry

Corish reported that an intended meeting of the Sub-committee planned to coincide with the Meeting of the Division Committee had proved impossible to realise because of the non-availability of members. A smaller meeting comprising the Executive of the Sub-committee (Chadwick, Corish, Rosenblatt and West) had met on September 3rd and had agreed (i) that the full Sub-committee should meet before the next GA probably coupled with a major topical conference; (ii) that the Sub-committee would continue to manage the HTMC Conferences and the WAM series; (iii) that an Interest Group be identified and canvassed to seek views and input to the Sub-committee and (iv) that the ultimate objective was the establishment of a Materials Chemistry Division in IUPAC. Kaesz warned against the danger of completely running down the Division but the importance of Materials Chemistry in modern chemistry was acknowledged as was the need to get away from the disciplinary stigma by eventually establishing a Division.

9 - Reports from other IUPAC bodies

Committee on Chemistry Education

No report was received. The President agreed to discuss the activities of the Committee with its Chairman, Atkins, at the Bureau in Paris.

Division VIII: Nomenclature and Structure Representation

Kaesz presented a Report, originally sent to the ACS Committee on Nomenclature, Terminology and Symbols, and authored by McNaught, President of Division VIII. The new Division had made an auspicious start: its membership and a review of current projects are listed in the Report. Two items were of particular interest to the Division Committee. The first was the work on preferred names. There were irreconcilable incompatibilities between the practices in Organic and Inorganic Chemistry in respect of some preferred names and the new Division was working to establish principles to rationalise naming recommendations in areas of overlap. The President requested Kaesz to seek to ensure that insofar as was possible all difficulties be caught during the review stages of the new Red and Blue books and that users seeking guidance not encounter conflicting recommendations from different IUPAC sources. He also thanked Kaesz for
the truly effective collaboration with Division VII. The second item of major interest was the work on the IUPAV Chemical Indentifier. Here the prototype algorithm for well-defined, discrete covalent organic structures had been tested and work was continuing so that a single name and structure would always be equivalent regardless of the direction taken between then.

10 - Project-by-project review of project status

(Please note that the name of the Division Committee member to whom responsibility for each project has been assigned is given in parenthesis after the project title).

1999-001-1-200 - Nomenclature of inorganic chemistry - Revised 'Red Book' - Part I. (Kaesz)

Connelly had reported that almost everything had now been revised. Comments on Chaper 6 had been received but the nomenclature of the solid state needed a complete rethink and Kaesz agreed to bring this need to the attention of Leigh. The President suggested that Metselaar, who had contributed to the original volume, should again be approached. The revised Red Book I is expected to be ready for review by the end of October.

1999-043-1-200 - Element by element review of atomic weights to the year 2000. (Coplen)

See Item 8 – Subcommittee of Isotopic Abundance Measurements - above

1999-049-1-200 - Thermodynamic characterization of high-temperature superconductors in the yttrium-barium-copper-oxygen system. (West)

Voronin had sent a written report stating that the first stage of the project, giving a description of data for the Y123 solid solution, had been published in PAC 72, 463-477 (2000). The second stage, comprising data for the Y247 and Y124 phases was also complete and had been reviewed by Commission II.3 at Brisbane. Work was in progress on the final stage – thermodynamic simulation, data compilation and description for solutions in the Y-Ba-Cu-O system. The publication of the final report had been planned for March 2003 but would most likely be delayed by three to six months because of delays in some primary publications. West was asked to write to encourage Voronin and to enquire as to the utilization of the budget.

2000-020-2-200 - Collecting, testing and dissemination of experiments in solid state and materials chemistry (Corish)

Kizilyalli had sent a written report on changes in the members of the group and the addition of two new members and on the progress in testing the experiments. This was not yet sufficient to warrant a meeting but the work of testing and retyping the experiments, where this was necessary, would continue. Corish was asked to write to acknowledge the report, encourage the project and ask for details of budgetary planning

2000-022-1-200 - Characterization of carbon materials (Rosenblatt)

See Item 8 above – Subcommittee on the Characterisation of carbonaceous Materials and new Carbons. Rosenblatt was asked to write to seek ways to make completion possible.
2000-024-2-200 - Teaching high temperature materials chemistry at University (Rosenblatt)

Balducci sent a written report detailing only modest progress and proposing that the group members might meet at HTMC-XI in Tokyo. Rosenblatt will write to encourage the work and seek a more explicit plan for the completion of the project.

2001-019-2-200 - Guidelines for mass spectrometric isotope ratio measurements (Coplen)

It is the aim of this project to provide basic guidelines for isotope ratio measurements by inorganic mass spectrometry to improve data quality and comparability. Consensus building within the community is critical to ensure that guidelines are finally adopted. The internet may serve here as an ideal tool.

The last Goldschmidt Conference in Davos successfully created awareness that guidelines are needed for quality control and the reporting of high precision isotope-ratio measurements. As a first step it has been agreed to set up a list server on the internet which will (i) allow users to discuss directly quality control and data reporting in isotope ratio mass spectrometry, (ii) attract scientists outside the IUPAC task group to contribute actively to guideline definitions, and (iii) provide a mechanism for discussing and criticising proposed guidelines as well as other IUPAC recommendations openly. Access will be such as to ensure that interests of the entire inorganic mass spectrometry community are considered properly. This list server will be used to publish a draft version of the guidelines proposed by the task group members, which is in preparation. None of the financial resources allocated by IUPAC to the project have been used yet.

2001-042-1-200 - Review of Isotopic Abundances in Extraterrestrial Materials: Part 1 (Holden)

See Item 9 Subcommittee on Extra-Terrestrial Isotopic Abundances

2000-002-2-100 - Standardization of methods for the characterization of inorganic membranes (with Division 1) (Chadwick)

This project had been reviewed at Dublin and additional referees had been nominated. Corish was asked to check records. An extensive report was received from Yi Hua Ma, the project coordinator, including a tentative schedule for its completion that would see publication of the Final Report in January 2004. Five sub-groups have been appointed with reprints expected from their leaders within 3 to 4 months.

2000-007-1-400 - Glossary of terms relating to polymeric gels and networks, hybrid inorganic polymeric materials and the processing thereof (with Division IV) (Chadwick)

A written report dated 4th September was received from Chadwick. The bulk of the work had been completed. Jones and Chadwick had drafted a glossary that had been reviewed during the meeting of Division IV at Beijing. Revisions suggested at that time are being incorporated into a final version for review. It was suggested that some informal reviews be sought prior to sending it out to the fifteen official reviewers.

2001-015-1-100 - Standard potentials of radicals (with Division I) (Rosenblatt)

It was noted that Wilson (Division I) will monitor this project. No report was received and Rosenblatt was asked to contact Wilson requesting that the Division receive a report from Stanbury – possibly through Koppenol.
2001-031-1-800 - Alignment of nomenclature in areas of overlap between the preferred names for organic nomenclature and the revision of the nomenclature of inorganic chemistry (with Division VIII) (Kaesz)

See Item 8 above Report from Division VIII. A written note was received from Damus stating that his final report from this project was being posted on the Division VIII web board with the following links.

www.rec.org/IUPACS/attachments/Cambridge 01012.rtf
www.rsc.org/IU3umopxfh/PAC8/attachments/Cambridge 0102.pdf

High temperature mass spectrometry: accuracy of the method and influence of the ionization cross-sections (Rosenblatt)

The President rehearsed the long history of this project, which was not within the new structure and therefore did not have a number. Chatillon had written that an extensive report was now in the final states of preparation and publication was imminent.

11 - Reports on upcoming Division-sponsored conferences

HTMC-XI in 2003 Tokyo

A written report was received from the local organizer, Yamawaki. The dates for the meeting are 19-23 May 2003 at the Sanjo Kaikan Hall of the University of Tokyo and the First Announcement has been distributed. Twelve sessions with plenary and keynote speakers for each session are planned with a closing date of September 13th for contributed papers.

HTMC-XII in 2006 (Spear, Rosenblatt)

A written report was received from Spear, Chair of the Division’s Planning Committee for the HTMC Series. Twenty-four letters of invitation to host HTMC-XII in 2006 had been sent out in April 2002 and five positive responses had been received from Atlanta (USA), St. Petersburg (Russia), Rio (Greece), Vienna (Austria) and Orleans (France) Preliminary discussions had taken place among Committee members on the proposals and a decision would be made before the Tokyo meeting.

12 - Report on discovery and naming of new elements.

A written report on the progress made by the Joint IUPAC/IUPAP Working Group was received from its chairman, Karol. The Report on elements of atomic number >110 is currently being drafted. Karol also requested that there be no further delays in the process of naming element 110.

Corish reported that the Koppenol paper on the naming of the Elements had appeared in PAC. He then presented a letter from Marinov in which he proposed changes in the procedures that had been used following the publication of the Joint Working Group Report on element 110. The Committee could find no basis for such changes and requested that Corish convey this decision to Marinov.

They also requested that Corish write to Hofman at GSI enclosing a copy of the Koppenol publication and requesting that the group propose a name for element 110 within one month and
stating that the Division Committee would much prefer that they propose a name rather than activate the default procedure that placed the onus on the Division Committee to do this.

13 - Formation of Nominating Committee for new members

The Committee thoroughly discussed the future needs of the Division and decided that of the five vacancies that would be filled at Ottawa 3 or 4 should ideally go to members whose interests lay in the area of molecules and 2 or 1 to members with interest in atoms.

The following were proposed as members of the Nominating Committee: Internal; West (Chairman) and Corish, External Prof. Hitoshi Ohtake (Japan), Dr. H. Tom-Dieke (Germany) and Prof. J. Casavo (Spain). Rosenblatt would seek approval for this membership from the Secretary General at Paris. Prof. A. Sargeson (Australia) and Prof. W. Roper (New Zealand) were nominated as reserves.

The need to achieve a balance in the Geographical distribution of the membership was stressed, as was the need to seriously consider the names of those nominated by the NAOs as NRs for the current biennium, current AMs and names from the Advisory Group that will be established.

14 - Status of pending project proposals

2000 – 018 – 1 Vapour deposition terminology - Carlsson

There had been no response to requests to revise this application: the Committee decided that the process of application should be formally discontinued.

Balducci - Thermochemistry of carbides

A decision on this project was deferred until the rate of progress with project 2000-024-2-200, which was also led by Balducci has been clarified. Rosenblatt was asked to convey this decision to Balducci.

Kizilyalli - Classification, Terminology and Nomenclature of Borophosphates

See discussions under Item 9 Division VIII and also Item 10 Project-1999-001-1-200 above. This project would be held until Division VIII identified directions within the broader context of nomenclature of the solid state. Kaesz was asked to take the request to Division VIII via Leigh and ask that a holding letter be sent to Kizilyalli.

2000 – 049 – 1 Taylor - RICE and TSAW

See discussions under Items 6 and 7 above. As part of their enquiries with the Commission Coplen and Holden will seek to redefine budgets for these projects as part of an overall plan for expenditure by the Commission.

Taylor/Papadakis - IMEP-17 and IMEP-19

There had been no further progress but the Committee felt that there remained a need to inform applicants of the nature of IUPAC projects. In particular, IUPAC was not a funding agency in the usual sense and could not be expected to respond positively to requests that lay well above the limits of available funding.
15 - Review of any new project proposals

No new proposals were received.

16 - Discussion on solicitation of new projects

The President stressed that under the new system the only way to keep the Division alive and healthy was through the execution of an adequate number and variety of funded projects. It was therefore essential to find a method to solicit, encourage and nurture such projects to bring them to the stage at which they could successfully seek funding. The decision taken earlier that each TM be given responsibility to oversee the generation of projects in their areas was a first step but additional effort would be required. The challenge was to define the mission of IUPAC and to make use of its imprimatur to attract potential participants. It had to be recognized that its ability to fund projects was very limited.

One change brought about by the restructuring was the loss of the 'nucleation' stage of projects, which had in the past typically occurred within the Commissions. West suggested that it might be possible to use workshops – perhaps associated with conferences – to define/generate project proposals. For example such workshops might be bolted on to meetings such as the Faraday, Dalton and Materials Discussions organised by the RSC. The Division Committee would need to be proactive and to target the relevant community wherever it saw the need and opportunity for a project. A much shortened (half A4 page) and sharper summary of what could constitute a project should be written and circulated – list servers could be developed for this purpose. The President was asked to determine whether the operational budget could be used for publicity to generate projects.

17 - Leadership and generation of proposals in molecules area (President)

The generation of projects in the molecules area represented a particular challenge because heretofore all activity had pertained to nomenclature and terminology. Kaesz, Kazuyuki and Suk faced a serious challenge and would need to enlist the assistance of the new TMs to be elected at Ottawa. The President emphasized the need for meetings to promote team building and suggested that it might be possible to bring some NRs to Ottawa. It was vital that a nucleus of interested and active people be established as quickly as this was feasible.

18 - Division Report for Bureau at Paris

The Committee agreed the content of this presentation, which was to be made orally by the President to the Bureau. The President and Acting Secretary agreed to prepare the presentation on the following date – a copy of the viewgraphs is provided in Appendix IV.
19 – Next meetings

The next two General Assemblies were scheduled for:

**Ottawa 2003** 9 – 17 August; and

**Beijing 2005** 13 – 21 August

A number of venues was mooted for the Division Committee Meetings in 2004. These included Maine, Dublin, Grenoble and New York but no decision was taken.

20 - Any other business

(i) **Publication listing.**

It was decided the minutes of the Annual Division Committee Meetings should contain an appendix listing all the publications that appear. Members will be asked to send details of all publications over and above those listed in the Report to Council appended to the Brisbane Minutes.

(ii) **Advisory Committee and Newsletter**

All members were requested to send suggested names for the Advisory Committee to Kaesz who had undertaken to compile a listing of members and prepare a newsletter.

(iii) **IUPAC Website**

Chadwick, Coplen, Holden, Kaesz and Kazuyuki agreed to visit the Divisions pages on the IUPAC website with a view to advising how our representation might be upgraded.

**Conclusion:**

The President thanked all present for their participation and all those who had sent written reports to the Committee. The meeting expressed its appreciation to West for his generous hosting of his colleagues and for the facilities provided by his Department.

John Corish
Acting secretary
Dublin January 2003
**APPENDIX I**

*Inorganic Division Committee, Commission II.1 and Subcommittees*

2002-2003

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**Inorganic Chemistry Division Committee**

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9TM, 5AM, 6NR
## Commission on Isotopic Abundances and Atomic Weights

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### Subcommittee for Materials Chemistry (SMC)

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APPENDIX II

Report form Commission II.1 Isotopic Abundances and Atomic Weights.
(Received October 10th 2002)

- CAWIA Brisbane meeting in Aug 2001
At the Brisbane meeting in Aug 2001, the Commission on Atomic Weights and Isotope Abundances reviewed the published data for the period Aug 1999 up to June 2001. As a consequence, several changes were carried out to the Table of Isotopic Compositions (TIC), which SIAM decided not to publish in 2001. Publications for the elements Zn, Ge, Kr, Mo, Dy were reviewed. Additionally, a discussion was held on the variability of Fe, Zn, Se, Ca, Mo due to biological fractionation. Recommendations to the Atomic Weights Commission were not to modify the Ar(Fe), although new data on the natural variation of iron isotopic composition were available (but revealing smaller uncertainties than previously reported). It was decided to modify the Ar(Zn) to 65.409 (4) because of calibrated measurement by Chang et al. (01CHA1; 65.4087(38)). It was decided to modify the Ar(Kr) to 83.798 (2) because of calibrated measurement by Aregbe et al. (83.79802(24)). The uncertainty was increased, as no natural samples were measured and only tank gas was measured. The new uncertainty was based on assuming a 0.001 fractionation effect, and taking difference with unfractionated value. It was decided to not modify the Ar(Ge) despite the new data from Chang et al. (72.6390(34)), as these are basically measurements carried out on the same samples of his 1999 measurements (but using other equipment). Furthermore, during the 1999 discussion, the value of Kipphardt et al. 99KIP1 data of type ‘F’ (leading to 72.628 (19)) differed significantly. The Ar(Fe) was only been changed in 1999. To modify the Ar(Mo) 95.94(2) based on data by Wieser et al. (01WIE1; 95.938(16)). This leads to an increase in the uncertainty. This is due to the fact that the present uncertainty estimate was not calculated using the presently valid SIAM statistical guidelines. It was decided to modify the Ar(Dy) to 162.500(1) because of calibrated measurement by Chang et al. 99CHA3 (162.4995(12)). It was decided that CAWIA requests SIAM to set up a mid-term meeting within 1 year to prepare a draft of a combined SNIF/TICE, to be called ICE (Isotopic Composition of the Elements for Normal Terrestrial Samples). It was decided to that this draft may then be distributed to all members for comments. It was decided that CAWIA promotes itself more actively in the field of isotopic measurements as an authoritative and expert body. It was decided that a recommendation be issued to realise the delta scale for iron using IRMM-014. It was decided to approach and get on board suitable people from life sciences & biogeochemistry to join SNIF/SIAM.

A report summarizing the history and status of the atomic weights of the elements has been drafted, reviewed, and revised by members of the Commission on Atomic Weights and Isotopic Abundances for publication by IUPAC: "The Atomic Weights of the Elements, Review 2000" by DeLaeter, J.R., Böhlke, J.K., DeBievre, P., Hidaka, H., Peiser, H.S., Rosman, K.J.R., and Taylor, P.D.P.
Part 1: History, continuing significance, and assessment of atomic weight determinations
Part 2: Element by element review of the standard atomic weights

Part 1 gives a brief history of the science of atomic weight measurement, a discussion of the evolving emphasis in the field from defining constants to investigating variations, and descriptions of the methods used. Part 2 summarizes for each element the history and motivation for changes in the standard atomic weight recommended by the Commission, with notes on causes of atomic
The manuscript is currently being formatted and rechecked before final submission to PAC, which should occur within the next couple months.

- **Guidelines for mass spectrometric isotope ratio measurements: started August 2002 (Project No.: 2001-019-2-200)**

  It is the aim of this project to provide basic guidelines for isotope ratio measurements by inorganic mass spectrometry to improve data quality and comparability. As noted by one of the reviewers, consensus building within the community is critical to ensure that guidelines are finally considered in routine work. The internet may serve here as an ideal tool. At the recent Goldschmidt Conference in Davos (Aug 2002), the major scientific meeting of the isotope geology community, has been used successfully to create awareness that guidelines are needed for quality control and reporting of high precision isotope ratio measurements. As a first step it has been agreed to set up a list server on the internet which will allow

  - to involve users directly in discussions regarding matters of quality control and data reporting in isotope ratio mass spectrometry
  - to attract scientists outside the IUPAC task group to contribute actively to guideline definition
  - to discuss and criticise proposed guidelines as well as other IUPAC recommendations openly between users

  The list server will not be limited to isotope geologists as the major user group. This will ensure that interests of the entire inorganic mass spectrometry are considered properly. The host of the biggest internet forum on inorganic mass spectrometry (Mike Cheatham, Syracuse University, NY) has agreed to set up a new list server dedicated to these topics. This list server will be used to publish a draft version of the guidelines proposed by the task group members which is in preparation. None of the financial resources allocated by IUPAC to the project have been used yet.

- **Review of isotope abundances in extraterrestrial materials (Project No.: 2001-042-1-200):**
  project has not started, but a meeting is planned in Nov 2002.

- **The 2001 Table of Standard Atomic Weights (Project No.: 210/3/81 ?):**
  a draft is under preparation and is expected to be completed by Oct 2002. It will be circulated amongst Commission members and prepared for publication in PAC by Jan 2003

- **RICE project proposal:** project to review isotopic composition & atomic weights. Project submitted, on halt until green light for funding.

- **from Sub-committee Isotopic Specific Measurements as Traceable References:** no activity.
Appendix III

Reports from Sub-Committees, other IUPAC Bodies and Project updates

Report from Sub-committee on Extra-Terrestrial Isotopic Ratios

This report covers the following two items:
(1) Subcommittee on extra-terrestrial isotopic ratios, and

Current status
At the subcommittee meeting in Brisbane, we discussed the future activity of our subcommittee and agreed that the subcommittee members would survey all existing data in the literature on isotopic abundances of rare earth elements in extra-terrestrial materials. It is expected that such efforts are being continued currently.

Future plan
We will meet at the occasion of the next IUPAC General Assembly in Ottawa and finalize our project. Our final goal at the Boston meeting is to prepare the manuscript of a review paper on isotopic abundances of REE in extra-terrestrial materials. This publication is regarded as the first issue in a series of isotopic abundances of elements in extra-terrestrial materials. Before meeting in Ottawa next year, I will plan to have a meeting in this year, possible in December, or early next year. Considering members countries, we will meet somewhere in Pacific Basin countries. At this meeting, we will discuss details of the review paper. Until this meeting, we will continue to survey literature data. However, after the meeting, we will be supposed to quit surveying and switch to writing a draft of the review paper.

Mitsuru Ebihara
Chairman of subcommittee on extra-terrestrial isotopic ratios

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Report from Sub-committee on Isotopic Abundance Measurements

Bolke/Peiser  Project 1999-043-1-200 - Element by element review of atomic weights to the year 2000

A report summarizing the history and status of the atomic weights of the elements has been drafted, reviewed, and revised by members of the Commission on Atomic Weights and Isotopic Abundances for publication by IUPAC:
"The Atomic Weights of the Elements, Review 2000"

Part 2: Element by element review of the standard atomic weights.

Part 1 gives a brief history of the science of atomic weight measurement, a discussion of the evolving emphasis in the field from defining constants to investigating variations, and descriptions of the methods used.

Part 2 summarizes for each element the history and motivation for changes in the standard atomic weight recommended by the Commission, with notes on causes of atomic weight variations for some elements. The manuscript is currently being formatted and rechecked before final submission to PAC, which should occur within the next couple months. If possible, Tyler Coplen will bring a copy of this report to the meeting in Sheffield.

John Karl Bohlke
US Geological Survey
431 National Center
12201 Sunrise Valley Drive
Reston, VA 20192
703-648-6325

Report from Sub-committee on Materials Chemistry

IUPAC
Sub-Committee on Materials Chemistry

Meeting of Officers: 3rd September 2002
Sir Robert Hadfield Building, Department of Engineering Materials,
University of Sheffield

Present:- J Corish, G Rosenblatt, A R West, A V Chadwick (Secretary)

I. The Materials Chemistry Sub-Committee – the Future

Corish began the meeting by reviewing briefly the background to the formation of the Sub-Committee. It had grown from an ad-hoc inter-divisional Committee on Materials that had met
Sheffield Minutes

several times – most recently at Brisbane. He and Rosenblatt had discussed the status of Materials Chemistry in the Union with the senior officers who had expressed their support for a more visible and active role for the area, which they recognised as being of ever-increasing importance in modern chemistry.

The Materials Chemistry Sub-Committee had been established after the Brisbane GA as an outgrowth of the meetings there. It is currently a sub-Committee of the Inorganic Chemistry Division but has members representing three of the other Divisions. The Officers of the Union concur that a greater emphasis on Materials Chemistry would enhance IUPAC, particularly in its links with industry, and have agreed informally to provide funding for a meeting of the Sub-Committee before the General Assembly at Ottawa - the Sub-Committee will also meet at Ottawa.

There followed a general discussion on the best way forward in IUPAC for the Material Chemistry interest. The Sheffield participants agreed with the meeting of the ad hoc Committee in Brisbane that the ultimate objective should be the formation of a Materials Chemistry Division and felt that given the state of scientific interest and activity in Materials Chemistry this would be fully justified. The members present discussed the effect that a potential new Materials Division might have on the present disciplinary divisions. They concluded that the major impact might be on the Inorganic Division but that with good planning this could be accommodated.

II Membership

Since Brisbane two additional names had been brought forward: Joachim Maier (Stuttgart) and Ron Weir (Kingston). They were both welcomed as very appropriate new members of the Sub-committee.

III Projects in Materials Chemistry

Rosenblatt reminded the members that there was a need to generate good projects in materials chemistry and that links with industry need to be fostered. These would be the basis of the case to the Bureau for the formation of a new Division. The current activity in materials chemistry in the Union was briefly reviewed. All of the divisions represented had projects in different areas of materials chemistry. The Inorganic Chemistry Division was also responsible for a very successful conference series; High Temperature Materials Chemistry. In addition, IUPAC has had two workshops on advanced materials (the last one in Bangalore, 2002), supported to the level of $25,000, that in the future could be part of a new Materials Chemistry Division activity.

IV Contact with the Materials Chemistry Community and Industry

The need to establish contact with and seek input for the wider Community of Materials Chemistry and from relevant industries was recognised. It was agreed to circulate a letter to a group of chemists to seek to generate interest – it would be necessary to put together a circulation list for this purpose. West and Chadwick agreed to draft the letter; Corish would co-ordinate the establishment of the circulation list, which was intended to draw entries from across the spectrum of materials chemists. The letter would define Materials Chemistry in a positive way, outline the possible role of IUPAC and explain how IUPAC would be used to support projects. It would include the list of topics in Materials Chemistry drawn up at Brisbane with an invitation to comment on or add to that list. Rosenblatt suggested that a few of the people who responded positively might be invited and funded to attend the Materials Chemistry Sub-Committee meeting at Ottawa.
V Next Meeting of the Sub-Committee

A letter outlining the outcome of the Sheffield meeting should be sent (Action: Corish) to all current members of the Sub-Committee and a meeting set up before Ottawa. Suggestions for a suitable time and venue might be sought, e.g., in conjunction with a major topical conference in the area to try to maximise attendance.

Alan V. Chadwick
Secretary

Report from Division VIII: Nomenclature and Structure Representation

IUPAC DIVISION (VIII) OF CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION

Report prepared by Alan McNaught and presented to the ACS Committee on Nomenclature, Terminology and Symbols, Boston, MA, 17 August 2002;
The present copy was presented by H.D. Kaesz to Div. II (IUPAC), Sheffield, UK, 4 Sept. 2002.

• Establishment of the new Division. Established in January 2002, the new IUPAC Division VIII consists of a Division Committee (twelve members and six National Representatives) and an Advisory Subcommittee (40 people). Membership lists are attached. Division members have access to a Web Discussion Board, on which minutes of meetings and current draft recommendations are posted for comment. The Joint IUPAC-IUBMB Commission on Biochemical Nomenclature reports to the Division Committee; however its future is under review. The IUPAC Bureau will consider at its September meeting how the work of this body should be handled, and will then begin discussions with IUBMB.

• Current projects

• IUPAC Chemical Identifier. The prototype algorithm for well-defined, discrete covalent organic structures was distributed for testing in March 2002. The project group reviewed feedback at a meeting in Columbus on June 30th. No problems were apparent, and release of a further version is planned for the end of 2002. News items reporting the software release appeared in Nature:


and The Alchemist:

http://www.chemweb.com/alchem/articles/1015947904091.html

A CAS/IUPAC Conference on Chemical Identifiers and XML for Chemistry was held in Columbus on July 1st. This meeting was devised following discussions with Chemical Abstracts staff when the IUPAC Chemical Identifier project was initiated. The speakers
reviewed various types of identifier, and explored their relationship with potential XML schemas for molecular data. The conference abstracts are available at:

http://www.rsc.org/IUPAC8/attachments/CAS-IUPACConf.doc

- **Organic preferred names.** Work on the new Nomenclature of Organic Chemistry (IUPAC Blue Book), including recommendations for identifying IUPAC-preferred names, is approaching completion. The project team will review a complete draft in Boston on August 14-15.

- **Alignment of recommendations for inorganic and organic nomenclature.** Principles for rationalising naming recommendations in areas of overlap were discussed at meetings in Cambridge in September 2001 and January 2002, and decisions were made on how to proceed with the revision of the Red Book (Nomenclature of Inorganic Chemistry; to be published by RSC next year) and the new Blue Book.

- **Fullerene nomenclature Part II.** Extension of the recently published recommendations to larger and more complicated molecules.

- **Rotaxanes and catenanes**
- **Cyclic macromolecules**
- **Macromolecular rotaxanes**
- **Dendritic and hyperbranched polymers**
- **Chemically modified polymers**

- **Scoping exercises**

  - **Stereochemistry.** Requirements for future development of stereochemical nomenclature in all disciplines are being reviewed, and project proposals will be formulated towards the end of 2002.

  - **Structure representation.** Jonathan Brecher (CambridgeSoft) is investigating what kind of general guidelines for drawing chemical structures on a computer might be helpful to the community. A project proposal is expected to emerge later this year.

*Alan McNaught*

9 July 2002

**Division Committee membership**

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<td>Prof Michael Hess</td>
<td>(Gerhard-Mercator U, Duisberg)</td>
<td>2 years</td>
</tr>
<tr>
<td>Prof Herb Kaesz</td>
<td>(UCLA)</td>
<td>4 years</td>
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<tr>
<td>Prof Jeff Leigh</td>
<td>(Sussex)</td>
<td>2 years</td>
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<tr>
<td>Dr Gerry Moss</td>
<td>(Queen Mary, U of London)</td>
<td>4 years</td>
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<td>Dr Bill Town</td>
<td>(ChemWeb)</td>
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<td>Dr Tony Williams</td>
<td>(ACD Labs)</td>
<td>4 years</td>
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<tr>
<td>Dr Michael Dennis</td>
<td>(Chemical Abstracts)</td>
<td>2 years</td>
</tr>
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</table>
### Associate members:
- Dr Steve Heller (NIST) 2 years
- Prof Sandy Lawson (Beilstein/MDL) 2 years
- Prof Bruce Novak (North Carolina State) 2 years

### National Representatives:
- Prof Osman Achmatowicz (Poland), Prof Roberto de Barros Faria (Brazil), Dr Jean Toullec (France), Prof Yohsuke Yamamoto (Japan), Prof Jiasong He (China), Prof Bernardo Herold (Portugal)

### Advisory Subcommittee membership
- Dr Hidetsugu Abe (Toyohashi U of Technology, Japan)
- Prof Steven M Bachrach (Trinity U San Antonio, USA; Editor, Internet Journal of Chemistry)
- Dr Byron J Bossenbroek (Chemical Abstracts, USA)
- Mr Jonathan Brecher (CambridgeSoft, USA)
- Dr John Brennan (European Patent Office, Netherlands)
- Prof Neil G Connelly (Bristol, UK)
- Prof Richard Cammack (Kings, London, UK; Chairman IUPAC-IUBMB Joint Commission on Biochemical Nomenclature)
- Dr Ilaria Campagnari (GSK, Italy)
- Prof Chong Shik Chin (Seoul, Korea)
- Prof Franco Cozzi (Milan, Italy)
- Dr Ture Damhus (Novozymes, Denmark)
- Prof Bernadette Donovan-Merkert (U of North Carolina, Charlotte, USA)
- Prof Andreas Dress (Bielefeld, Germany)
- Dr Andrey Erin (ACDLabs, Russia)
- Dr Geoff Fairhurst (BASF, Germany)
- Prof Henri A Favre (Montreal, Canada)
- Dr Piroska Fodor-Csányi (Budapest, Hungary)
- Dr Patton M Giles (Chemical Abstracts, USA; ACS Nomenclature Committee)
- Dr Jonathan M Goodman (Unilever Centre for Molecular Informatics, Cambridge, UK)
- Prof Richard M Hartshorn (Canterbury, New Zealand)
- Dr Karl-Heinz Hellwich (Beilstein, Germany)
- Prof Bernardo J Herold (Lisbon, Portugal)
- Dra. Rita Hoyos de Rossi (Cordoba, Argentina)
- Dr Alan T Hutton (Cape Town, South Africa)
- Dr Wolf-Dietrich Ihlenfeldt (Computer Chem Center, Erlangen-Nurnberg, Germany)
- Prof Aubrey D Jenkins (Sussex, UK)
- Prof Jaroslav Kahovec (Prague, Czech Republic)
- Prof Alan R Katritzky (Florida Center for Heterocyclic Compounds, USA)
- Professor Risto S Laitinen (Oulu, Finland)
- Dr Graham F McCann (Royal Society of Chemistry, UK; Editor, Dalton Trans. and J Materials Chem)
- Dr W Val Metanomski (Chemical Abstracts, USA)
- Prof Ebbe Nordlander (Lund, Sweden)
- Prof Vincent L Pecoraro (Michigan, USA; Assoc Editor, Inorg Chem)
- Prof C Dale Poulter (Utah, USA; Editor, J Org Chem)
- Prof Damon D Ridley (Sidney, Australia)
- Dr Paolo Righi (Milan, Italy)
- Ms Helen Schofield (Manchester, UK)
- Dr Steve Stein (NIST, USA)
- Dr Sarah Thomas (Royal Society of Chemistry, UK; Editor, ChemComm)
Mr Kevin Thurlow (LGC Nomenclature Advisory Service, UK)
Dr Edward S Wilks (ex-Dupont, USA)
Dr Janusz L Wisniewski (MDL, Germany)
Dr Shen-Gang Yuan (Shanghai, China)


Gerd Rosenblatt has asked me to send a report on the Red Book. I have just sent one to Alan McNaught so this is very much the same.
I have attached a list of chapter headings, etc. as an rtf file, (please let me know if you cannot open it). The list also says who has done what and also what remains to be done.

Basically, almost everything has been revised several times and is waiting final checking before being sent for review. I expect to receive Chapter 6 in the next two days, and Ture Damhus is working on the extended Table VIII which I have no doubt he will deliver very soon. The only remaining chapter is that on organometallic chemistry, which I have yet to see since Brisbane. The version considered there was very near completion and I hope to see one I can finally edit in the next few weeks. (I have being continually chasing the author).

When I have everything I intend to meet with Ture Damhus, and maybe others, to go over everything for consistency. It will then go out for review.

In summary, we are a little behind schedule. I am here this week, away for a week, back for one more week, then away for one month. In other words I have two weeks available before the beginning of September. After that I am very likely to be the new Dean of Graduate Studies for the Science Faculty here so that I will have less time to finish the Book. However, once I have the organometallic chapter and get together with Ture it should not take long to finish. With luck it may be in a fit state for review by the end of October. I will keep you informed. Incidentally, I think the revised version will be changed much more than originally envisaged. It should therefore be a lot better for that!

Professor Neil Connelly
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Tel: 0117 9288162
FAX: 0117 9290509
mail: School of Chemistry
University of Bristol
Bristol BS8 1TS
UK

See report from Subcommittee of Isotopic Abundance Measurements - above

Report from Project 1999-049-1-200 - Thermodynamic characterization of high-temperature superconductors in the yttrium-barium-copper-oxygen system.

The aim of the project is to obtain and recommend for use in chemical researches, design and practical calculations a set of self-consistent thermodynamic data for three high-temperature superconductors in the Y-Ba-Cu-O system. The work has to be done includes: (1) critical assessment and accommodation of existing thermodynamic data for solid phases Y123, Y247, Y124 and liquid solutions of components, (2) analytical representation of the Gibbs energy functions for these phases, and (3) computer-assisted optimisation analysis to obtain a set of functions parameters with the best fitting to the experimental results and fulfilment of thermodynamic relations.

PROGRESS:

(1) The first stage of this project concerning description of data for the Y123 solid solution is completed and the corresponding technical report is published in Pure Appl. Chem. 72(3), pp. 463-477, 2000

(2) The next stage concerning of data for the Y247 and Y124 phases is successful completed in the second quarter 2001; its results were presented on the Commission II.3 meeting in Brisbane in July 2001.

(3) Now is going the work on the last stage of the project - thermodynamic simulation, data compilation and description for liquid solutions in the Y-Ba-Cu-O system. It is planned to be ended in the first quarter 2003. Preparedness of draft version of the final report and second publication for the PAC were planned in March 2003. But, it seems, the time-table of the last action should be shifted on one-two quarters later because of delay of some primary publications, which have to be used in the work with technical report for PAC.

Task Group Chairmen
G. F. Voronin
July 30, 2002
Report from Project 2000-020-2-200 - Collecting, testing and dissemination of experiments in solid state and materials chemistry.

1. After Brisbane meeting Dr. Aysen Yılmaz apologized for withdrawing from the task force because moving to the in USA to take up a post-doctoral position.

2. No response was received from Prof. Carlsson to our e-mail messages. We think that he has withdrawn from the group.

3. Two new names were added to the list, Prof. Subba Rao from Singapore and Prof. U.V. Varadaraju from India. Prof. Rao is the scientist who submitted some previous experiments to Prof. Kihlborg. He suggested Prof. Varadaraju, who also volunteered to test some of the experiments. Prof. Rao also promised to collect some new experiments.

4. I received a negative response from several people that Prof. Kihlborg suggested from Sweden for testing the experiments originated from Stockholm University. We will try to check some of them in our University.

5. Prof. H. Mandal is going to send 3 new experiments. Others from our University promised to contribute.

6. Prof. Art Ellis and Prof. R Kniep stated that they do not have facilities to test these experiments.

7. At the moment only 7 experiments have been checked, 3 more are being investigated and will be finished soon in our Department. Some of these will require retyping.

8. I consider that at the moment it is not necessary to arrange a meeting. We should meet when there is a considerable progress in the project.

Prof. Dr. Meral Kizilyalli
Department of Chemistry
Middle East Technical University
06531, Ankara Turkey
Tel: 90 312 2103208
Fax: 90 312 2101280

Report from Project 2000-024-2-200 - Teaching high temperature materials chemistry at University.

This is a very short report on status and plans for IUPAC Project "Teaching High Temperature Materials Chemistry at University"(#2000-024-2-200)

Approval of the project and allocation of corresponding budget (for 3-year lifetime of the project, starting 1 January 2002) has been notified on January 30th 2002.

Present status and plans:
Among Task Group members A. Navrotsky has informed me that due to other very demanding engagements she most probably couldn’t take part actively in the project. F.Hodaj with C.Chatillon (who made himself available to help in the project) sent a programme of topics on high temperature and solid-state materials taught at ENSEEIG in Grenoble. This is to be added to my collection in the framework of the project. Next autumn I will submit to Task Group members a list of topics and
bibliographic references as a basis for future work. No expenditure on the budget has been made so far.

In addition to the exchange of materials by e-mail, perhaps some of the Task Group members could meet and discuss on the project in the occasion of the HTMC-XI Conference next May in Tokyo.

Gianni Balducci


Interim Report August 2002

Project Start: Jan 1, 2002
Project Lifetime: 2 years
Allocated Budget: 2,000 USD

Task Group Members: T. Walczyk, M. Berglund, J. K. Böhlke, K. G. Heumann, P. Taylor

It is the aim of this project to provide basic guidelines for isotope ratio measurements by inorganic mass spectrometry to improve data quality and comparability. As noted by one of the reviewers, consensus building within the community is critical to ensure that guidelines are finally considered in routine work. The internet may serve here as an ideal tool. The last Goldschmidt Conference in Davos, the major scientific meeting of the isotope geology community, has been used successfully to create awareness that guidelines are needed for quality control and reporting of high precision isotope ratio measurements. As a first step it has been agreed to set up a listserver on the internet which will allow

• to involve users directly in discussions regarding matters of quality control and data reporting in isotope ratio mass spectrometry
• for attracting scientists outside the IUPAC task group to contribute actively to guideline definition
• for discussing and criticizing proposed guidelines as well as other IUPAC recommendations openly between users

Access to the listserver should not be limited to isotope geologists as the major user group interested in isotope ratio measurements. This will ensure that interests of the entire inorganic mass spectrometry are considered properly. The host of the biggest internet forum on inorganic mass spectrometry (Mike Cheatham, Syracuse University, NY) has agreed to set up a new listserver dedicated to the above topics. This listserver will be used to publish a draft version of the guidelines proposed by the task group members which is in preparation. None of the financial resources allocated by IUPAC to the project have been used yet.

Ty Coplen

See Report from Subcommittee on Extra-Terrestrial Isotopic Abundances

Report from Project 2000-002-2-100 - Standardization of methods for the characterization of inorganic membranes (with Division 1)

The notification of the approval of the project was received at the end of January, 2001. A workshop was held in Montpellier, France on Thursday, June 26, 2001 with seven (7) invited oral presentations, which included Microstructure, Structure and Defect Structure, in Mixed Conductor Membrane Materials (R. Bredsen of Norway), Present Status of the “CHARMME” Network, Harmonization of Characterization Procedure for Porous Membranes (C. Guizard of France), An Overview of Techniques for Membrane Characterization (T. Tsotsis of USA), Characterization of Inorganic Membranes by Radiation Scattering and Spectroscopic Techniques (J. Ramsay of France), Status of Zeolite Membrane Characterization (R. Noble of USA) and Characterization of Pd and Pd/alloy Membranes (J. D. Way of USA). There were about 80-100 people attended the Workshop and participated in the discussions.

The project coordinator, Y.H. Ma, attended the 41st IUPAC General Assembly and made a brief summary of the Workshop at the Commission I.6: Colloid and Surface Chemistry Including Catalysts meeting. A tentative schedule for carrying the project was also discussed in the Commission meeting and it was decided that the following tentative schedule would be appropriate:

2. End of 2002, first draft report for comments.
3. Middle of 2003, second draft report for review.

At the time of the formation of the tentative schedule, it appeared to be reasonable. However, at the present, it seems to be rather ambitious although it is still the project coordinator’s intent to do his best to meet the schedule.

The leaders of five subgroups have either appointed or being appointed. They are:

1. Zeolite Membranes: R. Noble of University of Colorado, USA.
2. Mixed Conductor Membranes: J. Lin of University of Cincinnati, USA
3. Porous Inorganic Membranes: D. Fain of USA
4. Metal Membranes: to be appointed
5. Radiation and Spectroscopic Techniques for Membrane Characterization: to be appointed.
Reports of subgroups are expected to be completed within three – four months. These will then be put together for comments.

Yi Hua Ma
June 16, 2002

___________________________________

Report from Project 2000-007-1-400 - Glossary of terms relating to polymeric gels and networks, hybrid inorganic polymeric materials and the processing thereof (with Division IV)

The bulk of the work on this project has been performed. Early meetings of the task group collected a long list of the relevant terms. A meeting of the task group earlier this year drew up classifications for the terms and considered any omissions. Jones and Chadwick worked further on the glossary in the Spring of 2002 and it was put into a first draft form. Division IV met in Beijing this Summer and Jones held a meeting with other members of the task group to review the draft. Further revisions were suggested. Jones and Chadwick will address the revisions and prepare a version for internal evaluation before it goes to the final approval procedures.

Alan V. Chadwick
September 4th 2002

___________________________________

Report from Project 2001-031-1-800 - Alignment of nomenclature in areas of overlap between the preferred names for organic nomenclature and the revision of the nomenclature of inorganic chemistry (with Division VIII).

THE final report for the project mentioned below has been posted or is being posted on the Division VIII web board and the IUPAC web site by Alan McNaught and Fabienne Meyers. The following links will enable you to download a copy in either Word rtf or Adobe pdf format.

www.rsc.org/IUPAC8/attachments/Cambridge0102.rtf
www.rsc.org/IU3UMOpxhrf PAC8/attachments/Cambridge0102.pdf
Brief summary of meeting of IUPAC project group,
Cambridge, January 27-28, 2002
Project # 2001-031-1-800

Participants
Henri Favre (HF), Warren H. Powell (WHP), Richard Hartshorn (RH), Ture Damhus (TD; chairman), Gerry P. Moss (GPM); Alan D. McNaught (ADM), Neil G. Connelly (NGC), Herbert D. Kaesz (HDK) (GPM, NGC, HDK only January 27).

The first five participants on the list constitute the project group with HF and WHP representing the former Commission on Nomenclature of Organic Chemistry and its project on writing a new Blue Book to replace the Blue Book from 1979 and the Blue Guide from 1993, GPM representing the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature, and RH and TD representing the team working at a revision of the Red Book from 1990 (Red Book I). NGC is editor-in-chief of the revised Red Book I and HDK was chairman of the former Commission on Nomenclature of Inorganic Chemistry (CNIC) where the Red Book I revision project was initiated. ADM is president of Division VIII on Chemical nomenclature and structure representation and also hosted the meeting at the facilities of The Royal Society of Chemistry in Cambridge.

(Chairman's comment: Most attendees considered the meeting to have provided useful discussions and clarification of a number of issues. Attempts were made to compose proper minutes after the meeting, but failed due to disagreement on a number of details in the wording. The present summary is the sole responsibility of the chairman and is mostly kept rather brief.)

1. Review of production plans for the Red and Blue Book
NGC explained that the current timetable for the Red Book I revision called for submission of the manuscript for review in June 2002 and submission to the RSC for publication in December 2002. RB I is out of print and further delays in the production of the revision should be avoided. As a consequence, the RB I team stood firmly on the decision that inorganic preferred names will not be given in the revision, but must be left for a future project group to deal with.
The Blue Book timetable involves completion of a technically edited draft by April 2002 (could be postponed a couple of months); reviews in by September 2002; final draft December 2002; copyediting completed March 2003; galley proofs corrected September 2003. A publisher has not yet been chosen. Several attendees pointed out that it would be advantageous to have The Royal Society of Chemistry also publish the Blue Book.
The review process was also discussed. One part of the public review could be posting the entire Red and Blue books on the notice board of the Division VIII advisory subcommittee for its 40-odd members to review. In addition, NGC suggested to consider actually offering individuals a modest compensation, e.g. £ 100, for reviewing one of the books.
When the books are presented for review, a cover letter should clearly state where substantial changes have been made relative to previous recommendations (e.g. 'chloro' to 'chlorido' in additive nomenclature). NGC is collecting items for such a cover letter for the Red Book.
In some cases, it may still be necessary to just state that "further work on this topic is in progress" (e.g. metallacycles, cf. item 4 below).
2. Preferred names and preselected names

The point of this discussion was to ensure that later work on preferred names in inorganic nomenclature (cf. above) was not unduly anticipated in the Blue Book, i.e. to ensure that no inorganic (non-carbon-containing) compounds were given preferred names in the Blue Book.

A device was discussed which would enable the organic rules to institute certain inorganic hydride parent names (such as 'hexasilinane') and inorganic oxoacid parent names (such as 'phosphinic acid') as preselected for the specific application as parent names for providing preferred names of organic derivatives by substitutive or replacement or functional class nomenclature, without designating them as preferred names for the inorganic compounds themselves at the present time.

It is important to stress that the intention here was just to free the present Red Book I revision team from any considerations about preferred names at this time. It may well be that the parent names now preselected by the Blue Book team, or a number of them, will later be preferred names (for example, 'trisiloxane', 'diphosphoric acid'). Furthermore, the names of parent oxoacids to be used in organic nomenclature will also be mentioned (and indexed) in the revised Red Book I, in some cases in the text and in all cases in the revised and enlarged Table VIII.

Whereas the above concepts were applauded as useful and a major step ahead, there were varying opinions on the terms 'preferred' and 'preselected' themselves. It was suggested that the Division (VIII) should take responsibility to eventually consult more widely with the community and ask for better alternatives.

3. Hydrogen names for acids and partially dehydronated acids

Correspondence after the meeting has shown that this long-standing issue is not yet fully resolved. The discussion at the meeting dealt with

(1) inorganic names with 'hydrogen' joined directly to the name of an anion, e.g. 'dihydrogenphosphate' or, fully systematically (in a format currently proposed in the revised Red Book I), 'dihydrogen(tetraoxidophosphate)(1−)';

(2) partially dehydronated organic acids, by present rules named with the word 'hydrogen' separate from the rest of the name, e.g. 'hydrogen phthalate';

(3) partial esters in the names of which 'hydrogen' is also a separate word, e.g. 'methyl hydrogen sulfate', 'ethyl hydrogen phthalate';

It may happen that there will continue to be a difference between the naming of inorganic and organic compounds here. It was pointed out that in certain languages (Finnish, Scandinavian languages, German), the chemical names in question are written in one word anyway, so some of the above problems disappear, but also the possibility of using the space for any kind of distinction is absent.

4. Organometallic nomenclature

Chapter 11 of the revised Red Book I and Sections P-68 and P-69 of the new Blue Book are planned to address the nomenclature of organometallic compounds in the broad sense of the term, i.e. compounds with carbon bonded to elements of groups 1,2,12,13,14,15,16, and the transition elements.
A special subject is metallacycles, *i.e.* carbocyclic compounds in which one or more carbon atoms have been replaced by transition metal atoms. A subgroup of the former CNIC had been assigned the task of working out the rules for metallacycle nomenclature (that is, names based on using 'a' replacement terms for the elements substituting carbon), and they had encountered certain problems that would probably only be resolved later when the a project group on organometallic nomenclature started working. That is, the revised Red Book would not give a full treatment of this subject at this time.

5. Red Book chapter on substitutive nomenclature

This chapter, in a draft form, was reviewed on January 28. Numerous specific rules and names were inspected and hopefully brought into correspondence with what will be prescribed in the revised Blue Book. WHP provided a number of references regarding boron nomenclature, including the treatment in Chapter 11 of *P. Block, W.H. Powell, W. C. Fernelius: Inorganic Chemical Nomenclature – Principles and Practice* [ACS, Washington, 1990]. If not for the brief treatment foreseen in the revised Red Book I, this input will be of use in the later project of providing a fuller update on advanced nomenclature of boron hydrides and their derivatives.

6. Red Book table of ligand abbreviations and ligand names

This table was likewise examined in the January 28 session and a number of queries dealt with.

TureDamhus

2002-06-30

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Report on HTMC-XI, Tokyo, 19th – 23rd May 2003 (Yamawaki)

SUMMARY OF THE STATUS OF PREPARATION FOR HTMC-XI

The date and place of HTMC-XI have been decided as 19-23 May 2003 and Sanjo Kaikan Hall of the University of Tokyo, Tokyo, Japan. The First Announcement has been printed and distributed, and also put up on the Internet: http://www.q.t.u-tokyo.ac.jp/public/HTMC_XI

Twelve sessions have been hosted to cover the topics of HTMC-XI. About 10 plenary lecturers have been nominated, while 2 or so keynote speakers will be decided for each session in the near future. The closing date for the submission of abstracts of paper will be 13th September 2002. I hope as many would-be attendees as possible to be informed of HTMC-XI and be suggested to submit abstract of paper by this date.

Michio Yamawaki
Chair, Organizing Committee of HTMC-XI

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Michio Yamawaki (Prof.)
Department of Quantum Engineering and Systems Science,
Reports on HTMC-XII in 2006

IUPAC Inorganic Chemistry Division Committee Meeting

Report on
IUPAC-sponsored High Temperature Materials Chemistry Conference, HTMC-XII, 2006
Submitted by: Karl Spear, Chair of Committee for Choosing Host/Site for HTMC-XII

This report is from the committee charged with selecting the host/site for the IUPAC-sponsored High Temperature Materials Chemistry Conference, HTMC-XII, to be held during the year 2006. Members of the IUPAC HTMC-XII Host/Site Selection Committee are listed below:

Gianni Balducci, Dept. Chim - Univ. Roma, Italy
Klaus Hilpert, Research Centre Juelich (KFA), Germany
Rudolf Metselaar, Techn. Univ. Eindhoven, The Netherlands
Gerd Rosenblatt, Lawrence Berkeley Nat. Lab., CA, USA
Karl E. Spear (Chair), Penn State University, PA, USA

High Temperature Materials Chemistry Conferences have been regularly held since 1977 under IUPAC sponsorship, with guidance from IUPAC’s Inorganic Chemistry Division, its subcommittee on Materials Chemistry, and its former commission on High Temperature Materials and Solid State Chemistry.

The next High Temperature Materials Chemistry Conference, HTMC-XI, will be held in Tokyo, Japan on 19 – 25 May 2003. It will be chaired by Michio Yamawaki, and follows a very successful HTMC-X in Juelich during April 2000, hosted by Klaus Hilpert. Meetings already held in this series are as follows:

- 2000, Juelich, Germany (Hilpert, Froben & Singheiser)
- 1997, University Park, PA USA (Spear)
- 1994, Vienna, Austria (Komarek, Mikula & Ipser)
- 1991, Orleans, France (Coutures)
- 1989, Gaithersburg, MD USA (Hastie & Bonnell)
- 1987, Rome, Italy (DeMaria & Balducci)
- 1984, Santa Fe, NM, USA (Rosenblatt & Skaggs)
- 1981, Harwell, United Kingdom (Potter & Rand)
- 1979, Toronto, Canada (Alcock & Skaggs)
- 1977, Odeillo, France (Coutures)

Twenty-four letters of invitation to submit proposals to host HTMC-XII in 2006 were sent in April 2002. An example copy of this letter is attached, and illustrates the guidance for writing a proposal that was given to potential hosts. Letters were not sent to potential hosts in the Far East since the 2003 conference will be held in Tokyo. In general, consecutive conferences are not held on the same continent.

By the middle of July, we had received five positive responses to our invitation to submit a proposal for hosting HTMC-XII, 2006. These proposals were submitted by:

J. Gole, Georgia Tech, Atlanta, GA USA
V. Stolyarova, St. Petersburg, Russia
G. Papatheodorou, Rio, Greece (proposed possible joint HTMC/Molten Salts conference)
A. Mikula, Vienna, Austria
M.-L. Saboungi, Orleans, France

Discussions and information gathering on these proposals occurred among committee members during the first half of August 2002. We concluded that we have several excellent possibilities from which to choose the host/site for HTMC-XII. The committee also agreed that we did not want to combine HTMC-XII with the Molten Salts conference in 2006. This was communicated to G. Papatheodorou, and he has been given the opportunity to submit another proposal by mid-September for hosting HTMC-XII.

Our committee discussions will continue the later in September. A host/site for HTMC-XII will definitely be chosen before the HTMC-XI conference is held in Tokyo, May 2003.
April 19, 2002


Dr. Christian Chatillon
Domaine Universitaire, B.P. 75
LTPCM-ENSEEG, 1130, Rue Piscine
38402 St. Martin d’Heres CEDEX
France

Re: Invitation for a proposal to host the IUPAC-sponsored High Temperature Materials Chemistry Conference, HTMC-XII, in the Year 2006.

Dear Christian,

This letter is an invitation and request for you to consider hosting the IUPAC-sponsored High Temperature Materials Chemistry Conference, HTMC-XII, in the Year 2006, perhaps in collaboration with some colleagues. This invitation is being sent to about a dozen or so selected colleagues.

As you no doubt know, we will have a High Temperature Materials Chemistry Conference, HTMC-XI, in Tokyo, Japan on 19 – 25 May 2003. It will be chaired by Michio Yamawaki. This follows a very successful HTMC-X in Juelich on April 2000, hosted by Klaus Hilpert.

The previous meetings in this series are as follows:
- 2000, Juelich, Germany (Hilpert, Froben & Singheiser)
- 1997, University Park, PA USA (Spear)
- 1994, Vienna, Austria (Komarek, Mikula & Ipser)
- 1991, Orleans, France (Coutures)
- 1989, Gaithersburg, MD USA (Hastie & Bonnell)
- 1987, Rome, Italy (DeMaria & Balducci)
- 1984, Santa Fe, NM, USA (Rosenblatt & Skaggs)
- 1981, Harwell, United Kingdom (Potter & Rand)
- 1979, Toronto, Canada (Alcock & Skaggs)
- 1977, Odeillo, France (Coutures)

Although all of the work and funding of these conferences has fallen upon the local organizers, their success and international stature has been aided by formal sponsorship by the International Union of Pure and Applied chemistry (IUPAC). In addition, traditionally each conferences international advisory committee has had participation from members of IUPAC’s Inorganic Chemistry Division, its subcommittee on Materials Chemistry, and its former commission on High Temperature Materials and Solid State Chemistry. This has provided a mechanism by which IUPAC members can give help and advice to meeting organizers. Also, to assist with the continued success of these meetings, IUPAC established a committee to help identify future conference organizers and
locations, and to facilitate communication between the conference organizer and IUPAC. I am writing to you in my capacity as chairman of that committee.

Most of the meetings in this distinguished series have been highly successful. In looking back over the most successful conferences, some key factors are apparent: (i) early and clear communication with IUPAC members and the IUPAC Secretariat, (ii) an early start on physical arrangements and conference publicity, (iii) adequate local funding, (iv) tight local organization (often it has been helpful to have conference co-chairs), (v) early announcement of the meeting dates, (vi) reasonably early announcement of plenary lectures, (vii) broad publicity.

Your name has been suggested as a potential organizer of HTMC XII (2006), perhaps in collaboration with some colleagues. If you are interested in organizing this meeting, and we hope you are, we request that you send me a short one-paragraph to one-page letter or email expressing your willingness, and giving a broad outline of plans for the meeting. It would be helpful if the letter described such things as the (a) location, (b) time of year, (c) anticipated meeting and housing facilities, (d) anticipated cost to participants (low, medium, or high) relative to previous meetings in this series and to similar international conferences, (e) sources of funding and/or the natures of the institutional and organizational support that would be provided, (f) relevant experience in hosting this type of meeting, (g) description of transportation to/from the meeting and to/from the airport.

After receiving responses to this letter, the IUPAC committee (Balducci, Hilpert, Metselaar, Rosenblatt, and myself) will discuss the responses. I will present a report to the president of the Inorganic Chemistry Division of IUPAC, and to the chairman of its subcommittee on Materials Chemistry. Notification of the site selected for HTMC-XII (2006) is anticipated to be no later than the summer of 2003.

We hope, and past experience indicates, that this is an effective and fair process. I look forward to hearing from you by June 30, 2002. If you have any questions or comments please contact me by email, mail, fax or phone, whatever is most convenient to you. The heading of this letter provides all of the pertinent communication information.

Sincerely,

Karl Spear


**Appendix IV**

**Publications of The Inorganic Chemistry Division**

**Publications since July 1999.**

Names for muonium atoms and ions (II.2)

Chemical research needed to improve high-temperature processing of advanced ceramic materials (II.3)
*Pure Appl. Chem.*, 72(8), pp. 1425-1448, 2000

Establishment of SI-traceable reference ranges for the content of various elements in the IMEP-9 water sample (II.4)
*Accred Qual Assur* 5 (2000) 8, 331-338

Contribution to the certification of B, Cd, Mg, Pb, Rb, Sr, and U in a natural water sample for the International Measurement Evaluation Programme Round 9 (IMEP-9) using ID-ICP-MS (II.4)
*Accred Qual Assur* 5 (2000) 7, 272-279

Thermodynamic characterization of high-temperature superconductors in the yttrium-barium-copper-oxygen system. The Y123 solid solution.(II.3)

Names for inorganic radicals (II.2)

Terminology for compounds in the Si-Al-O-N system (II.3)
*Pure Appl. Chem.*, 71(9), pp.1765-1769, 1999

Atomic weights of the elements 1997 (II.1)
*Pure Appl. Chem.*, 71(8), pp.1593-1607, 1999

Nomenclature of organometallic compounds of the transition elements (II.2)
*Pure Appl. Chem.*, 71(8), pp.1557-1585, 1999

Definitions of terms for diffusion in the solid state (II.3)
*Pure Appl. Chem.*, 71(7), pp.1307-1325, 1999

Practitioner's report: International Measurement Evaluation Programme IMEP-7: Inorganic components in human serum (II.4)


**In press**

Red Book II, to be published by the Royal Society of Chemistry

Atomic weights of the elements 1999, by T. B. Coplen (*PAC* Apr. 01)

**In review**


Element by Element Review of Atomic Weights to the Year 2000
Appendix V

The Division Report to the Bureau at Paris is in the attachment

Bureau Paris.ppt
INORGANIC CHEMISTRY DIVISION

REPORT TO IUPAC BUREAU

Paris 2002

Gerd M. Rosenblatt
REPORT TO BUREAU

- Division summary and status
- Division strategy and plans
- The materials initiative
- Issues
DIVISION SUMMARY AND STATUS

- See Division input into Strategic Plan
- Mesh with Division VIII
- Industry – cf. materials initiative
- Twelve current projects:
  - 4 (+1) data projects
  - 2 chemical education projects
  - 6 materials projects
  - 2 nomenclature projects
  - 4 projects with other Divisions

Bureau - Paris
DIVISION STRATEGY AND PLANS

- Atoms
  - Commission II.1
  - Naming of new elements

- Molecules

- Materials
THE MATERIALS INITIATIVE

- Materials Chemistry: an important and growing area
  - involves all classical chemical disciplines

- Formed Sub-committee for Materials Chemistry
  - membership from Divisions I, II, IV and V

- Near–term activities
  - meeting of Sub-committee and others including industry before Ottawa
  - canvas community to ascertain interest and ideas for the area in IUPAC
  - develop portfolio of new projects to add to existing projects

- Organize and run HTMC Conferences and WAM

- Long-term: IUPAC Division of Materials Chemistry
ISSUES

- Sources of projects
- Communications with the community
- Division between workers and Bureau
- Diversity of Division Committee
- Procedures not as simple as they seem
- Workload needed to run Division
- Project reviews – review project not the proposal
Appendix VI

A listing of Current Projects is in the attachment

Status Div Proj in Jan 2003.xls
<table>
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<th>Project #</th>
<th>Submitter</th>
<th>Division Shepherd</th>
<th>Amount Allocated</th>
<th>Committed As of Aug 2002</th>
<th>Comment</th>
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<td>West</td>
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<td></td>
<td></td>
<td></td>
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Nomenclature of inorganic chemistry - Revised 'Red Book' - part I.

Element by element review of atomic weights to the year 2000

Thermodynamic characterization of high-temperature superconductors in the yttrium-barium-copper-oxygen system

Standardization of methods for the characterization of inorganic membranes and networks, hybrid inorganic polymeric materials and the processing thereof

Glossary of terms relating to polymeric gels and networks, hybrid inorganic polymeric materials and the processing thereof

Collecting, testing and dissemination of experiments in solid state and materials chemistry

RICE--Making a new comprehensive Report on the Isotopic Compositions of the Elements for global user communities

Alignment of nomenclature in areas of overlap between the preferred names for organic nomenclature and the revision of the nomenclature of inorganic chemistry

Accuracy of the method and influence of the ionization cross-sections