

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

REPORT OF THE INORGANIC CHEMISTRY DIVISION TO

COUNCIL

Berlin General Assembly – August 1999

1. Introduction

The past biennium has been a particularly active period for the Inorganic Division as, in parallel with its usual full programme of work, it devoted substantial effort and resources to responding to the Report of the Strategy Development and Implementation Committee (SDIC). The major changes proposed in the structure and organisation of the Union rendered redundant some of our discussions at the Division Meetings at Geneva. Consideration of the implementation of the new proposals was viewed as a welcome opportunity to assess the work programme of the Division and for a planned approach to our future development and growth. During the biennium the Division instigated a process of consultation with its four Commissions to determine the response of each to the specific changes and to examine how their very varied work programmes might be affected by the proposed new *modus operandi*. Two special meetings took place. The Division Executive met on September 10th 1998 in Berkeley, California to consider responses from the Commissions and to formulate a plan for the future. We were greatly assisted by the attendance of Secretary General Becker at that meeting. In December 1998 the Division Committee met at the IUPAC Secretariat, NC. The principal outcomes of that meeting in terms of planning for the future of the Division are outlined in Section 5 below.

The current work programme of the Division has continued apace. The highlights will be detailed below in brief reports from each of the Commissions and, where applicable, from their sub-committees. The decision taken a few years ago regarding the reduction in the membership of the Division Committee has been proved to work well. Membership has been continued at five TMs (including the President, Vice-President and Secretary) and with the Chairmen of the Commissions, together with some former officers, being Associate Members. This inclusion of direct representation of the Commissions together with the practice of attendance at the opening Divisional Meeting of each General Assembly by Commission Secretaries has greatly enhanced the cohesion of our effort. The release of some TM positions to the Commissions has further increased the overall capacity of the Division to undertake project work. The lessons learned by this redeployment will be relevant in our planning for the new structures and functions proposed for the Division Committees.

This direct input from the Commissions to the Division Committee has also been vital because the activities of Division II are very diverse and it would be unrealistic to expect that any small group of scientists however experienced could critically and expertly assess them. The Inorganic Division houses classic IUPAC expertise in the assessment and determination of Atomic Weights and in a broad range of topics in Inorganic Nomenclature (Commissions II.1 and II.2 respectively). In addition the importance of modern Inorganic Materials and of Materials Chemistry was recognised some time ago and Commission II.3 has over recent years, through a policy of active recruitment, built up impressive expertise in materials. Our fourth Commission, which started life as a limited lifetime Commission, is specialised in Isotope Specific Measurements as References and has quickly established itself as a key player in the operation of International Measurement Evaluation Programmes (IMEPs).

The Division was represented at the meetings of the IUPAC Committee on Biomolecular chemistry by Prof. G. J. Leigh (Geneva Aug. 24th 1997) and by Prof. N. G. Connelly (London Feb. 14th 1998) as reported by its Chairman Prof. U. K. Pandit. Commission II.2 will continue to provide representation for the Division at this Committee.

2. THE NAMING OF NEW ELEMENTS

The Division has proposed to the President and Officers a procedure to be followed in the naming of elements 110 to 112 that would ensure that the kind of difficulties that arose in the naming of elements 103 to 109 could not reoccur. This proposal has been well accepted by the relevant communities. The first stage of the procedure, which is the assignment of priorities to claims by a joint IUPAC/IUPAP Working Party, is now almost completed. Provided that the timetable can be adhered to the report of this Working Party will be available at Berlin. The next stage, that of seeking suggestions for names from the Laboratories to which the priorities have been assigned, can then commence. This will be followed by the formal proposal of names by the Commission for Inorganic Nomenclature (CNIC) and the review and approval procedures. Because the preparation of element 114 and more recently of elements 116 and 118 have now been reported, the need for a well-established and accepted naming procedure is very obvious.

3. REPORTS FROM THE COMMISSIONS

Commission II.1 *Commission on Atomic Weights and Isotopic Abundances.*

The principal function of this Commission is to provide the worldwide chemical and scientific communities with accurate data on atomic weights and isotopic abundances of the chemical elements. The rapid development of mass spectrometric methods has led to

more and more precise isotopic measurements in various materials and has made it possible to recognise small isotopic variations in many elements due to chemical or physical effects. These isotopic variations have assumed considerable importance in many areas of endeavour and measurements of them are indispensable in both technological and scientific applications.

Three subcommittees optimise the Commission's efforts to collect, interpret, summarise and define the increasing amount of new data. These are the Subcommittee for Isotopic Abundance Measurements; the Subcommittee for Natural Isotopic Fractionation and the Subcommittee for Non-Terrestrial Isotopic Abundance Data. All these subcommittees met at Kloster Seeon (Germany) 20-21 August 1997 and reported to the Commission at Geneva.

Publications

'Isotopic Composition of the Elements 1997'. *Pure and Appl. Chem.* 70 (1998) 217-235. This is a completely revised version of a report first published in 1991.

'History of the Recommended Atomic Weight Values from 1882 to 1997: a Comparison of Differences from Current Values to the Estimated Uncertainties of Earlier Values', *Pure and Appl. Chem.* 70 (1998) 237-257.

In preparation

'Atomic Weights of the Elements 1997'. This publication appears from the Commission every two years and the 1997 version, which will appear in PAC, is currently in the final proof stage. For the first time ever no changes in atomic weights will be reported but the paper will contain important information from the subcommittees.

'Natural Isotopic Fractionation of Selected Elements'. This paper, currently in circulation, is a summary paper on the observed fractionation of some thirteen elements.

'Reporting of Relative Lithium Isotopic Abundance Ratio Data'. This paper is also currently in circulation within the Commission prior to publication.

Future Activities

In addition to its commitment to continue to provide the standard values for atomic weights of the elements and on isotopic compositions the Commission has initiated a project on an '*The Year 2000 Element by Element Review of the Atomic Weights*'. This will be a major publication and will update an earlier 1984 edition. An expert group met in Hiroshima in November 1998 and a draft has been prepared for the Berlin General Assembly. The volume will contain a review of the 20th century effort and a forecast into the 21st century. Several themes will be addressed including the move from chemical to

physical methods of calculating atomic weights, the rise of metrology and the evolution of the concept of constant atomic weights in nature to that of variability in nature. The Subcommittee for Non-Terrestrial Isotopic Abundance Data is preparing a summary of isotopic variations in all non-terrestrial matter and a new edition of 'The Technical Booklet' is also in preparation.

The Commission has now also established a Web page containing documents and reports but with access confined to Commission members during its trial period.

Commission II.2 *Commission on Nomenclature of Inorganic Chemistry*

The main elements in the work programme of this Commission have continued to be in the core activity of defining inorganic nomenclature. Particular emphasis has recently been placed on the Second Volume of the Red Book, on a revision of its First Volume and on the emerging development of Computer Assisted Nomenclature. The Commission met at Delaware (July 25 - 27th, 1998) with the meeting being supported by Montell and DuPont.

Red Book Volume II

This major project is very close to publication. Chapter 8, which describes the nomenclature for *Inorganic Radicals* was reviewed in detail at Delaware and has undergone some major changes. It will need to be resubmitted to IDCNS for approval. It is planned separately to submit the revised chapter for publication in , *Pure and Appl. Chem.* parallel to its inclusion in Red Book Vol. II

Revision of Red Book Volume I

This project has now been externally reviewed and accepted under the new procedures and is our first Divisional project. It is led by Professor N.G. Connelly and was thoroughly considered at Delaware by a Working Group of the Commission. Particular attention will be paid to monitoring, insofar as is possible, consistency with the current Red Book I, Red Book II, the Blue Book and the Guide (1993). Each chapter of the current version was reviewed, the necessary revisions were outlined and agreed and responsibility for each was assigned to a member of the Working Group.

Computer Assisted Nomenclature

This project, which is being driven by a Working Part of the Commission led by Professor A. Dress, was also extensively discussed at Delaware. The estimated time required for software development for this very major change in nomenclature practice was 10 man-years and the Working Party envisaged a realistic perspective for IUPAC nomenclature work in that decade as having parallel efforts within local and global nomenclature systems. Local nomenclature is concerned with naming in the traditional sense of the word within restricted classes of compounds whereas global nomenclature is ambitiously

viewed as a universally (or almost universally) applicable method for computer encoding of chemical structures. The Commission will make detailed suggestions that IUPAC set up a task force which should be able to attract external support and funding e.g., from the EU and/or commercial sources. A work programme for such a Task Force has also been drawn up. The area of Computer Assisted Nomenclature is clearly of very major interest to IUPAC with considerable commercial potential.

Transfermium Elements Nomenclature

The Commission reviewed the rules and boundary conditions for the naming of transfermium elements with particular reference to the principles to be followed in the naming of elements 110-112 (cf. Section 2 above).

Publication in Nomenclature

'Principles of Chemical Nomenclature – A Guide to IUPAC Recommendations' by G. J. Leigh, H. A. Favre and W. V. Metanowski and edited by G .J. Leigh (Blackwell Science, Oxford, 1998)

Other Projects

The Commission also considered at Delaware and has reported progress on the *Metallacycles* project and the *Muonium* paper. The problems arising in the usage of *Ligand Abbreviations* were discussed and a revised document will be circulated.

Commission II.3 *Commission on High Temperature Materials and Solid State Chemistry*

This Commission works primarily on focused international projects concerned with inorganic materials. A Web page is in place describing its current projects and it has provided a further listing of potential Materials projects for the IUPAC strategic initiative in this area. The Commission met at Ljubljana (June 12/13th 1998) where considerable progress was reported in its work programme.

Technical and Educational Projects

A report entitled '*Chemical Research Needed to Improve High Temperature Processing of Advanced Ceramic Materials*' was reviewed at Ljubljana and is currently being amended in preparation for publication.

Also reviewed was a major report on '*High Temperature Mass Spectrometry Ionisation Cross Sections*' which has now been distributed to experts. A final version will be reconsidered by the Commission at Berlin.

Another Commission-sponsored article for *Pure and Appl. Chem.* will describe the 'Calculation of Equilibrium Thermodynamic Properties of High Temperature Superconductors.' Its value will be to inform on the existence of collected data and on a new tool for their interpretation.

A report giving details of twenty-one 'Teaching Experiments in Solid State Chemistry' each of which has been tested and evaluated by Commission members will shortly be made available to interested users on the Web through the IUPAC Website.

Other ongoing projects in the ceramics area concern the 'Surface Analysis of Ceramics' and 'The Structure and Properties of Ceramic Fibres'.

Terminology Projects

An manuscript entitled 'Terminology for Diffusion in the Solid State' and containing in excess of 100 terms has now completed the review process, has been approved by IDCNS and is in course of publication in *Pure and Appl. Chem.*

A paper containing proposed 'Terminology of Silicon Nitride based Ceramics' has been published in *J. Eur. Ceram. Soc.* and *Bull. Amer. Ceram. Soc.* for comment. It will now be sent to additional expert reviewers before publication.

A Pool Project with Commission IV.1 has now produced an extensive list of abbreviations and terms and the resulting manuscript 'Terminology Used in Sol-Gel Processing of Advanced ceramics and Inorganic/Organic Polymers' has been discussed by both Commissions. A complete and corrected draft document will be ready for Berlin.

'Terminology of Vapour Deposition.' Six experts are each contributing a section to a draft document which will be considered by the Commission at Berlin.

Sub-committee on the Characterisation of Carbonaceous materials and New Carbons

The objective of this sub-committee is to assemble the various national standards for this most important and widely used material and to publish a comparative listing of those standards that are considered to be critical. This project is now nearing completion and the resulting report will replace an earlier and by now almost obsolete listing (*Pure and Appl. Chem.*, 51 (1976) 1561). The sub-committee has also identified a need for clear terminology for carbon nanotube materials.

Conference Series on High Temperature Materials Chemistry

The plans for the Tenth conference in this series to be held at Julich on April 10th -14th 2000 are now well advanced. Approval for its sponsorship has now been received from IUPAC and the panel of invited speakers has been announced.

Professor Karl E. Spear

It is with the greatest of regret that I have accepted the resignation of Karl Spear from the chair of Commission II.3. He has, over many years given outstanding service and effective leadership including the hosting of the highly successful ninth in the Conference Series on High Temperature Materials Chemistry at Penn State in 1997. He is a great colleague and will be sorely missed.

Commission II.4 *Commission on Isotope Specific Measurements as Traceable References*

This Commission is promoting international traceability of measurements using primarily isotope dilution mass spectrometry (IDMS) to establish the reference values. In conjunction with the International Measurement Evaluation Program (IMEP) organised by the Institute for Reference Materials and Measurements (IRMM),EU, the Commission has made a very significant contribution by providing the IDMS data to the determination of the reference values and to the evaluation of accuracy of analytical methods used in the IMEPs.

The Commission has changed membership in the current biennium to become more international, with members from Japan, USA, Switzerland, China, Belgium, Germany and Korea. To give the new members the opportunity to fully participate in the planning and execution of the new activities, the Commission will meet on October 12 and 13, 1998, at the National Institute of Materials and Chemical Research, Tsukuba, Japan.

This meeting will review the status of the ongoing IMEPs (described briefly below) and will also discuss future programmes. The agenda will include: promotion of the on-going IMEPs; preparation of new types of reference materials (considering cost and labour) required for the future IMEP studies; increasing the number of participating certifying laboratories and evaluation of traceability of IDMS for the determination of trace elements in more complicated natural matrices such as soil and sediment These discussions are definitely needed to establish IDMS for various types of materials as a traceable reference in chemical measurements and to evaluate accuracy of other analytical methods used in the analysis of complex real-world samples.

Current Programmes

International Measurement Evaluation Programmes(IMEP-6): Trace Elements in Natural Water

This was the largest project undertaken by the Commission with more than 250 participants. All data have been received and have been statistically analysed . Reference values for 14 elements in natural and artificial water have been established by the co-operation of 4 national laboratories in 3 countries. Full publication appeared in *Accreditation and Quality Assurance*, 3 (1998) 56-68.

International Measurement Evaluation Programme(IMEP-7): Trace Elements in Human Serum

Certification was finished, with more than 300 participating laboratories. A participant report is in progress and will be published in September, 1998.

International Measurement Evaluation Programme(IMEP-9): Trace Elements in Natural Water

Samples have already been distributed and certification is in progress. A participant report will appear in early 1999. This round is also running as the CCQM-9 study (part of it, namely Cd and Pb) .

International Measurement Evaluation Programme(IMEP-10): Trace Elements in Plastics

Samples have been obtained and some certification measurements have been completed. The samples have been distributed to 35 participants. A participant report is pending and will be ready by end of 1998.

International Measurement Evaluation Programme(IMEP-11): Automobile Catalysts

Samples have been prepared and distributed. Participants have been identified. Metals (Pt, Zr, Hf, Ce) have been certified. A participant report will appear in early 1999.

4. FUTURE PLANS OF THE DIVISION

The Division Committee met, hosted and assisted by the Executive Director Dr. John Jost, at the IUPAC Secretariat at NC on December 12th and 13th 1998 to plan for its future within the proposed new structures. The Committee identified two serious concerns for the future. The first was the fact that the apprentice/peerage slow but reliable development of Commission personnel may no longer be available. The second was their belief that the new Division Committee might not be able to cover the very broad range of topics necessary to adequately represent modern Inorganic Chemistry. They also expressed deep concern that the question of the electorates after 2001 for the Division Committees that

are destined to be the kernel of the future scientific work of the Union had not even been addressed. Setting aside these serious reservations the future plan developed for the Division within the framework of the proposed changes is set out below.

The Division Committee

In line with recommended procedures a Nominating Committee was chosen to select a slate of candidates for the election of the new Division Committee at Berlin. Its external members were: J. M. Thomas (U.K.), I. Bertini (Italy) and F. G. Hawthorne (U.S.A.) while D. H. Busch (Secretary) and L. Schultz (Chair II.1) will serve from the current Committee. This Nominating Committee, which represents the very wide range of interests of the Division, is currently working to produce a list of candidates that will present the electors with real choices. The Division decided to continue for the next biennium its practice of including its Commission Chairs, as members of the Division Committee but will elect five new TMs at Berlin to bring the strength of the Committee up to ten. In the interests of continuity the Division decided that four Commission chairs should become TMs of the Division committee in 2001: in addition two new TMs should be elected. This would bring the total number of TMs on the Division Committee to 12, which exceeds the suggested limit of 10. However the Division Committee believed that because of the breadth of the field it might be necessary to request further expansion of the Division Committee in the future.

The Division Structure in the Immediate Future.

After a detailed review of its current activities and of its future needs the Committee decided that the work of the Division could be most effectively managed in the new structure by organising its projects under three Co-ordinating Groups. These would seek to reflect the scope of modern Inorganic Chemistry and would be in the broad subject areas of 'Elements', 'Molecular Species' and 'Materials'. They would be small, consist typically of 4-5 project leaders and their memberships would be subject to change being determined at any time by the Division's funded projects. The Committee believes that in common with industry and other research institutions who manage in project-based environments these Co-ordinating Groups would provide the knowledgeable leadership vital to advance the various separate areas. It will be obvious from the responses of the individual Commissions briefly reported below that they did not all accept that their work could be continued under the proposed project-driven system. However they did accept that the Co-ordinating Groups presented a possible way forward and it is intended that exploratory inaugural meetings of these groups will be held at Berlin.

The Responses of the Commissions.

Commission II.1 *Commission on Atomic Weights and Isotopic Abundances*

The work of this Commission is unique and needs to continue because of its great benefit to society at large. Clearly some adjustments are possible and the work on isotopic abundances should be emphasised because of its importance in areas such as medicine and forensics. The problem identified here was how to handle under the new structures a project that was truly on going. The Chair stressed the crucial role of the Commission as a rallying point about which the various sub-committees could operate and will discuss with his Commission members as to whether they should request the Commission to be continued after 2001.

Commission II.2 *Commission on Nomenclature of Inorganic Chemistry*

The imposition of precise timelines on volunteers was seen as an added burden and it was considered unlikely that the necessary larger fraction of a volunteer's discretionary time needed would be forthcoming. The need for historical continuity and the training of new members is vital in the work of this Commission and is a problem with which II-1 is already struggling. Although it found it difficult to envisage how the new system would work the Commission regarded the retention of a core of informed and experienced individuals in the Co-ordinating Groups as being a possible way forward.

Commission II.3 *Commission on High Temperature Materials and Solid State Chemistry*

The proposed changes in IUPAC should cause no special problems since they would represent only minor changes from present practice. The major problems that worry the Commission were (i) recruitment of effective project members and (ii) initiation of suitable IUPAC projects. The effectiveness of the Co-ordinating Groups in addressing these problems could not be predicted.

Commission II.4 *Commission on Isotope Specific Measurements as Traceable References*

Geographical dispersion and internationalisation of the Commission's tasks have been proceeding since the GA at Geneva with affiliation to and sponsorship by IUPAC being essential for the level of co-operation achieved. The Chair stressed that the activities were large multinational co-ordinated studies with timelines of 4-6 years with an expectation of two to four such projects running simultaneously. The work did not fall easily into the types of projects envisioned in the new structures for the Union.

SUMMARY

The commissions of Division II cover very diverse areas of modern inorganic chemistry. They provide unique fundamental and essential core information and standards on the atomic weights of the elements, on their terrestrial and non-terrestrial isotopic abundances, on isotope specific measurements as traceable references, on inorganic nomenclature, and

on inorganic and high-temperature materials and solid-state chemistry. These are very well established functions that rely not only on the established expertise of the Commission members but on carefully built up networks of complementary expertise that rely on the Commissions for their direction. The value of their output far exceeds the IUPAC funding that they receive. The expertise in Commission II.3 is primarily in the area of materials chemistry and is capable of a major contribution to the Union's effort in this area.

The Division has welcomed the opportunity of the proposed restructuring of the Union to examine its own ongoing activities in depth. It has responded immediately to the proposed new procedures for the selection of the Division Committee and believes that project-driven funding with the attendant evaluation procedures will ensure the best use of the Union's resources. The Division Committee has produced a plan for its future that is in line with the proposed changes but serious reservations remain as to the ability of the new Division Committee to manage the scientific work of the Division as well as has been done by the existing Commissions. In the main these stem from the breadth of our activities and the pivotal role of the Commissions in providing a focus for and directing the enormous amount of voluntary work undertaken by our extensive networks of dedicated scientists.

John Corish
June 15th 1999