Item 10: Report of Inorganic Division (II)

International Union of Pure and Applied Chemistry

Inorganic Division

Report to Council

Brisbane – July 2001

1. Executive Summary

The Division has embraced the restructuring of the Union and has striven to effectively implement the changes necessary following the decisions of Council at Berlin. As reported at that time to the Bureau and Council this Division carried through the new election procedure for the Division Committee for the current biennium and five members, four of whom were completely new to IUPAC, were elected at our Open Meeting at Berlin. This has been very beneficial and has extended the expertise available to the Division to additional central areas of Inorganic chemistry. Because these actions made this a period of rapid change an extraordinary meeting of the Division Committee, at which both former and the new members attended, was held in December 1999 at Berkeley. This was a constructive and wide-ranging meeting devoted in the main to deciding our strategy and priorities for the future and to planning how the Division would operate after the demise of the Commissions. During the past biennium, the Division Committee met again in Dublin (August 11^{th} /12^{th}). The Commissions have continued to produce excellent work over a very broad remit and in line with the strategic goals of the Union and. This is evidenced by their outputs listed in Section 4 below. Commission II.2 met also in Dublin (August 19^{th} /21^{st}), Commission II.3 met in Ankara (September 18^{th} /19^{th}), Commission II.4 met in London (November 15^{th} /16^{th}) and Commission II.1, has, as usual continued to do its work by correspondence. It will meet, together with its network of sub-committees that are essential for its work, just prior to the General Assembly in Brisbane. In addition, there were many informal contacts and discussions, particularly between the officers of Commissions II.1 and II.4, to discuss how best to ensure that the very important work on isotope abundances and atomic weights could be most effectively continued and extended.

2. Activities and Strategic Plan of the Division

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The Division Committee has given a great deal of careful thought to the changes and opportunities resulting from the discontinuation of the present Commissions and the transition to the project-driven system. It has analysed the activities that are and will remain important to the Division and has determined how best to contribute to the IUPAC mission by continuing to serve the international chemistry community and the other scientists who have relied on its output. The Division has requested that a new 'Commission on Isotopic Abundances and Atomic Weights' be established. This it sees as imperative to maintain IUPAC's leadership in the area of atomic weight evaluation and of mass spectroscopic measurements and for the IMEP programmes to continue to be recognised as a truly international effort guaranteed by IUPAC expertise. The Committee firmly believes that the very major and unique resources represented by the large number of experts in all aspects of isotopic measurements associated with the current Commission II.1 and the substantial network of laboratories brought together under the umbrella of the IMEP programmes of Commission II.4 can survive only under the auspices of an IUPAC Commission. The Division is also of the opinion that these activities in the areas of isotope measurements and atomic weights are one of the premier and highly visible products of the Union in addressing its objectives. The proposed new Commission will have a new remit, with both fundamental and applied aspects. It will do some of the core work of the Union and its programme will be exactly in harmony with the objective as stated in the Strategic Plan of serving as a scientific international non-governmental body in objectively addressing global issues. It will also be providing tools (standardised methods) to help advance international research and will be assisting chemical industry to attain new standards in chemical metrology: two more goals set by the IUPAC Strategic Plan. The large network of teams associated with the activities of determining atomic weights and the very many laboratories that take part in the IMEP programmes is a clear demonstration of IUPAC leading an international effort and so obtaining maximum value for the funds invested in it (Strategic Goal No. 10).

The Division Committee will manage its other diverse activities and the projects through which these will be implemented through three co-ordinating groups. These will be dedicated with 'elements', 'compounds' and 'materials' and will be comprised of the Division leadership working with other experts as appropriate. They will provide the basis for the generation, assessment and, most importantly, the management of projects and will be responsible for the provision of strong, viable and relevant programmes in each of these areas.

The focus of current work on molecules and nomenclature lies in the extension of systematic Inorganic nomenclature to a range of new classes of compounds in Red Book II and the complete revision of Red Book I. Another emphasis is the computer generation of nomenclature. A last emphasis in the ongoing work is the integration and interaction with organic nomenclature including organometallic nomenclature. These objectives are again in accordance with the stated objective of the Strategic Plan to develop standardised nomenclature. However, the Division has two concerns in this area. The first is to ensure that the needs of inorganic chemists are met by IUPAC nomenclature recommendations and that the current emphasis on preferred names does not result in the recommendation of ridiculous names that will never see general use for inorganic compounds. The second is finding a mechanism to maintain IUPAC's considerable current expertise in inorganic nomenclature. The Division believes that IUPAC

contributions to inorganic nomenclature will require close interaction between the proposed new Nomenclature Division and area experts in the Inorganic Division and does not at this time see how the continuity of the essential expertise can be maintained.

The Division's oversight of the naming process of new elements is well advanced for elements 110-112. An independent joint IUPAC-IUPAP expert Working Party (JWP99) has produced a report establishing priorities (cf. Publications below) that has been approved by IUPAC and IUPAP. Commission II.2 has written to GSI, the accepted discoverers of element 110, requesting their suggestion of a name for the element so that the remaining steps in the process can be followed through. A joint expert Working Party will shortly be established to consider claims for the confirmed discovery of elements 111, 112, 114, 116, 118 and perhaps others. A further publication that will lay down the procedures to be followed in the naming of new elements in the future is in the final stage of review.

A last direction in the area of molecules and compounds is the exploration of ways to initiate projects in important topics of international concern in molecular and biological chemistry, areas not recently covered within IUPAC. A first step in this direction has been the expansion of the Division Committee to include expertise in these areas and this broadening process will be continued with the second election to the Division Committee to be carried out under the new procedures at Brisbane.

The current focus of the work in materials, in solid-state and in high temperature chemistry is of three types. Projects in progress will clarify and standardise terminology in materials areas, particularly in interdisciplinary areas involving chemistry but not exclusive to chemists. Other projects summarise current understanding or status of a subject, pointing out deficiencies that need to be addressed. A third series of projects provide material, subjects, experiments or references for covering these subjects in chemistry and materials science curricula. This work will contribute to the strategic goal of the Union to contribute toward the enhancement of education. It will be a direct response to a need identified at the World Conference on Science (Budapest, June 1999) for more access from less-developed countries to education in materials science, which is widely recognised as a key enabler of the new technologies. The Division intends to continue as the central focus for IUPAC's work on inorganic materials and to maintain an active interaction with the 'materials science' community. The extensive work of the Division in the area of materials chemistry, as represented in the main in the work programme of Commission II.3, will be selectively continued. A number of Projects have been approved and funded under the new system (cf. the list below). It is hoped that this momentum built up by past Commission-led activities can be maintained in the project-driven system but the Committee is concerned that about the loss of projects in Inorganic Materials under the new system as, up to now, these projects have depended upon being nurtured by a focused Commission.

The Division will certainly continue to provide the backing necessary for the series of International Conferences on High-Temperature Materials Chemistry of which the next Conference will take place in Tokyo in 2003 (cf. list below). This is now the recognised

world forum in high temperature materials chemistry and as such serves the two Strategic Goals of organising forums to help advance international research and encouraging projects of an interdisciplinary nature.

The Division also organised in conjunction with UNESCO a symposium 'Science and new Materials' at the World conference on Science (Budapest , June 1999)

3. The Future

Despite the very strong performance of the Division during the current biennium (cf. Section 4 below) there is considerable concern in the Division for its future. The establishment of the new Commission will ensure that IUPAC continues the work started prior to the foundation of the Union to define accurate atomic weights for the world scientific community and further develops the IMEP programmes as an accepted guaranteed international standard for a range of applied academic and commercial measurements. In addition to the specific concerns expressed in the foregoing section regarding our nomenclature and materials chemistry activities, there is a general concern arising from the response to date to the new project-driven system. The only projects that the Division has received, and it has received and processed a good number, are those that are a direct outgrowth of Commission activities and interactions and we see no evidence so far that other proposals will be forthcoming after the Commissions disappear.

4. Inorganic Chemistry Division (II): Outputs

(i)Publications since July 1999.

Names for muonium atoms and ions (II.2)
Pure Appl. Chem., 73(2), pp. 377-380, 2001

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

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Thermodynamic characterization of high-temperature superconductors in the yttrium-barium-copper-oxygen system. The Y123 solid solution.(II.3)
Pure Appl. Chem., 72(3), pp. 463-477, 2000

Names for inorganic radicals (II.2)
Pure Appl. Chem., 72(3), pp. 437-446, 2000

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)
Accred Qual Assur 4 (1999) 11, 463-472

In press
Red Book II, to be published this year by the Royal Society of Chemistry

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

In review

On the discovery of the elements 110-112, by P.J. Karol

An overview of the atomic weights during the twentieth century: Part 1. Their ongoing conceptual significance; Part 2. The evolution of their values and uncertainties, by J.R. deLaeter, J.K. Bokle, P. DeBievre, H. Hidaka, H.S. Peiser, K.J.R. Rosman, and P.D.P. Taylor

(ii)Projects initiated and funded since previous GA

Thermodynamic Characterization of High-Temperature Superconductors in the Yttrium-Barium-Copper-Oxygen System
Task Group Chairman: G.F. Voronin

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Standardization of Methods for the Characterization of Inorganic Membranes
(Part of the Strategic Initiative on Materials)
Task Group Chairman: Ed Yi Hua Ma

Collecting, Testing and Dissemination of Experiments in Solid State and Materials Chemistry
Task Group Chairman: M. Kizilyalli

Characterization of Carbon Materials
Task Group Chairman: H.P. Boehm

Glossary of terms relating to polymeric gels and networks, hybrid inorganic polymeric materials and the processing thereof
Task Group Chairman: R.G. Jones *(in collaboration with Division IV)*

Element by Element Review of Atomic Weights to the Year 2000
Task Group Chairman: J.R. de Laeter

(iii) Projects completed in this biennium.

230/24/93 - Chemical Research Needed to Improve High Temperature Processing of Advanced Ceramics
230/28/95 - Terminology of Silicon Nitride Based Ceramics and Related Materials
240/7/95 - Automobile Catalysts
240/11/97 - Trace Elements in Natural Water
240/12/98 - Carbon Isotope in CO_2
240/13/98 - Trace Elements in Polyethylene
240/14/98 - Trace Elements in Sediment
(The last five projects are part of the IMEP Programme)

For a complete list of current projects see
< http://www.iupac.org/divisions/II/cp2.html>

(iv) Conferences

Commission II.3 organised the Tenth IUPAC-sponsored International Conference on High-Temperature Materials Chemistry in Juelich (April 10th /14^{th}, 2000) during which the Commission met informally. HTMC-X had a record attendance in excess of 250 and a very full programme of plenary, keynote and contributed papers and posters. The Conference was highly successful and the series is now established as the premier international forum for exploring the combination of chemistry and materials science as these affect understanding, production and use of high-temperature materials.

John Corish

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Dublin, May 6th 2001.