

INORGANIC CHEMISTRY DIVISION (II)

Report to Montreal Bureau Meeting – April 2016 about ongoing and planned activities in the current biennium and some strategic outlooks

a. Memberhips (2016-7)

- President: J. Reedijk (The Netherlands); Vice President: L. Öhrström (Sweden),
- Secretary: M. Leskela (Finland),
- Titular Members: L. Armelao (Italy), T. Ding (China), P. Karen (Norway), R. D. Loss (Australia), D. Rabinovich (USA), T. Walczyk (Singapore/Switzerland), M. Wieser (Canada)
- Associate Members: Y. Abdul Aziz (Malaysia), J. Colon (Puerto Rico), M. Drabik (Slovakia), L. Meesuk (Thailand), K. Sakai (Japan), N. Trendafilova (Bulgaria).
- National Representatives: J. Darkwa (South Africa), M. Diop (Senegal), L. Galamba-Correia (Portugal), M. Hasekawa (Japan), S. Kalmyakov (Russia), A. Kiliç (Turkey), P. Knauth (France), G. J. Leigh (UK), S. Mathur (Germany), B.B. Yoon (South Korea).

Female members are marked in blue print.

During the GA in Busan, the presence of again a number of young observers was very much enjoyed and appreciated. Some of them, including the previous GA, have been elected as new members (2016-2017). The Division is happy with the new, faster election process for Division Members.

b. Division and Interdivision (sub)committees:

- * Commission on Isotopic Abundances and Atomic Weights (II.1), Chairman: J. Meija
- * Subcommittee on Isotopic Abundance Measurements, Chairperson: J. Irrgeher
- * Subcommittee on Stable Isotope Reference Material Assessment, Chairman W. Brand
- * Subcommittee on Natural Assessment of Fundamental Understanding of Isotopes: Chairperson: N. Holden
- * Interdivisional Subcommittee on Materials Chemistry, Chairman: C. Ober,

The Division currently sees no need to add new, or abandon existing (sub)committees.

I. Highlights and Executive Summary

Division II deals primarily with three subfields, seen as belonging to the “Inorganic Chemistry” area, as well as with the name-giving process of newly discovered chemical elements.

The three subfields are mentioned first, followed by a section on new elements.

I.1 Atom: Isotopic Abundances and Atomic Weights:

The “Atom” members in our Division have continued to be highly active and productive both inside and outside of IUPAC. These members are closely associated with the Commission on Isotopic Abundances and Atomic Weights, and the Subcommittee on Isotopic Abundance Measurements, and most of them are involved in IUPAC projects. This Commission has a primary role to publish evaluated isotopic compositions of the elements and their atomic weights. Steady improvements in isotopic measurement technologies and techniques have resulted in increasing numbers of publications of higher resolution isotopic composition data. Four place Atomic Weights tables without uncertainties, as most recently published in 2013 and 2015 (*Atomic weight of Yttrium*), will continue to be published for general educational and commercial use. Subcommittee chair Meija recently published an account in

Chemistry World (J. Meija, *Weighty decisions*, in Chemistry World, 22 January 2016). A new project, following a discussion in *Nature*, has started on group 3 of the Periodic Table, dealing with the question whether or not La/Lu and Am/Lr belong to this group. See also CI March 2016, 22-3.

1.2 Molecular Inorganic Chemistry:

A significant fraction of Division members belongs to the “molecules” area, including coordination chemistry, organometallic chemistry, bioinorganic chemistry, transition metal catalysis and main group chemistry. Nomenclature of inorganic chemistry is now covered in Division VIII, although terminology of new classes of compounds has a particular interest from our Division, as illustrated by some recent projects. Important and highly cited recommendations and technical reports are published, like on Coordination Polymers/Metal-Organic Frameworks (the paper by Öhrström et al. *Pure and Applied Chemistry* (2013) **85**, 1715-1724 has been already cited over 100 times). Another well cited report, dealing with a project on oxidation state definition, has appeared: Karen et al., *Pure and Applied Chemistry* (2014), **86**, 1017–1081. To generate further responses and prepare for the three focused write-ups, the project convener Pavel Karen published an Essay entitled "Oxidation State, A Long-Standing Issue" *Angew. Chem. Int. Ed.*, 2015, **54**, 4716 – 4726. The final project report manuscript on this topic is with ICTNS and PAC editor for review.

1.3 Solid State Inorganic and Materials Chemistry.

The members of this group are associated with the activity of Subcommittee on Materials Chemistry, and with contribution from Solid State High-temperature Materials Chemistry. The composition was renewed at the Istanbul GA. The Subcommittee on Materials Chemistry is exploring together with Division I ways of expanding the significance of Materials Chemistry with IUPAC and increasing the interaction between IUPAC and the Materials Chemistry user communities. A project to develop pedagogic material to teach technical material sciences is in preparation.

1.4 New Element News

At the end of 2014 Div II received the final report of the Joint Working Party (IUPAP/IUPAC) dealing with the verification and ratification of 4 new elements, i.e. 113, 115, 117 and 118. This news has been publicly announced on December 30, 2015 using an IUPAC Press Release. It was echoed by similar releases by some NAOs. Given the fact that elements 117 and 118 would fall in the columns of the halides and inert gases, at the Busan meeting the Division had started working on an update of a 2002 recommendation on how to name new elements. The resulting paper, after having been for 5 months provisional, had become final on February 29, and will appear in the April Issue of PAC. Meanwhile the discoverers laboratories have been invited to propose names and symbols for the new element, taking into consideration the updated recommendations. The proposed names and symbols are expected in early April, and will then be discussed within Division II – using correspondence – and if possible finalized at the off-year July meeting of the Division. After acceptance of names and symbols by the Division a provisional publication will be made for PAC; after 5 months the Bureau can decide on publication, even before the Council will ratify the names at the Brazil 2017 meeting.

The above-mentioned IUPAC press release has resulted in an overwhelming publicity, worldwide, in newspapers, magazines, television and websites, which is seen as a good sign of making IUPAC more visible. It also has resulted in many serious (and less serious) proposals for naming these new elements, even with internet petitions of over 150000 voters from 67 countries for a certain name. All writers with proposals for new names have been informed that only the discover laboratories can propose new names and symbols. Many articles in magazines have appeared describing the discoveries and presenting speculation on new elements beyond 118.

An updated summary of the procedures for the naming of new elements has been prepared by John Corish, i.e. both for validating and naming, and also how about appointing the joint Committee Members. This article has appeared in CI, 2016 March issue, pages: 9-11.

II. Overall Report of Division II activities and achievements from 2014-present

II.1 *Projects (Summary; details are in section IV)*. As of mid March 2016, the Division has 24 active projects on its project list, 5 of which are new since Busan. Some of the project activities have been mentioned above, or will be referred to below. An updated list is presented in section IV.

II.2. *Division Newsletter*: The Inorganic Division has developed a regularly appearing Newsletter since 2008 (about 2 times a year; the most recent one was published in December 2015). In addition to the members of Division II, this Newsletter has been sent to all IUPAC Division Presidents and the Executive Committee. This meanwhile popular and informative newsletter has also been used by some National Chemical Societies for subsequent redistribution. All previous ones are and remain available at the IUPAC Website.

II.3. *Welcome pack for new Division members*: The division continues to provide its new members with a welcome package dealing with the Division and IUPAC structure and protocols for e.g. project handling. This introduction to the Division and its work is highly appreciated, especially by the newest members, entering the Division for the first time, such as NRs. The package has also been made (and still is) available to other Divisions.

II.4. *IUPAC visibility in the outside world*: Just one example of a successful project: The output of the completed project (2009-012-2-200) on naming of coordination polymers and MOFs, see item I.2, was recently highlighted in Chem. Eng. News, a weekly magazine of the ACS (over 135000 subscribers). See details at: <http://cen.acs.org/articles/92/i6/Confusion-Over-Scientific-Nomenclature-Par.html> This article makes a general plea for the need of proper terminology and nomenclature, recognizing the role of IUPAC. The most recent, and very strong visibility of IUPAC and Division II has been realized through the press release and follow-ups around the four newly validated chemical elements.

II.5. *Periodic Table naming*

1. The DP and VP have served in an ad-hoc committee of the Bureau on a possible naming of the IUPAC Periodic Table : Mendeleev Periodic Table. In a brief report to the Executive Committee it was recommended not to do this. The full text of the recommendation. The ad-hoc group presented the following 2 recommendations to IUPAC.

a. The ad hoc task group recommends to IUPAC not to accept the suggested change in naming of the IUPAC Periodic Table. Such a change would definitely not be in accordance with the spirit and formalities of the IUPAC strategic plan, statutes, bylaws and general practice in nomenclature and terminology creation.

b. The task group, therefore also recommends not to develop criteria for any process that would be used to decide on priority, or naming of a chemical discovery, or an invention for either an individual or a group.

II.6 *Operations of the Division: seen from the perspective of the 6 IUPAC long-range term goals and the Strategic Plan 2015*

1. *IUPAC will provide leadership as a worldwide scientific organization that objectively addresses global issues involving the chemical sciences.*

The Division's operations are in the areas of Inorganic Chemistry covering the broad areas of Atoms, Molecules and Materials with the former being effectively subsets of the latter. "Atoms" covers areas such as the name giving process of new elements, and atomic weights and isotopes of the elements. Molecules cover that broad area of inorganic chemistry between atoms and materials chemistry, while Materials Chemistry deals with any inorganic material. In practice the boundary between organic and inorganic materials can be difficult to determine, and therefore the existence of the interdivisional

Subcommittee on Materials chemistry, which includes members of both Division II and Division V (Polymers) can be understood. All three areas do address global chemical community needs, as will also be clear from the following sections.

2. IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion.

The Division supports fundamental data evaluation projects that are vital to long term research in the chemical and other sciences. An ongoing major effort in this regard is the work done on Atomic Weights and increasingly also on Isotopic Abundances, both of which comprise fundamental data used by the entire chemical community. These data are also critical in international commerce and trade of chemicals and chemical products. Projects 2009-027-1-200 and 2013-032-1-200 are examples of successful IUPAC efforts towards international standardization of chemical measurements in this area. Project 2009-027-1-200 has been set out to establish a list of primary international standards in isotope ratio measurements. The resulting IUPAC Technical Report remains the most downloaded article from *Pure and Applied Chemistry* and its recommendations were officially endorsed by the International Committee of Weights and Measures in March 2015. The Division believes that IUPAC plays an important role in this ever-increasing need from the chemical community. The danger of this not being taken up by an international organization like IUPAC, is a burgeoning number of in-house standards for isotope ratio measurements that - as well as creating additional expense for the chemical community - also reduces standardization and unnecessarily complicates communication and chemical understanding.

Uncertainty of measurements plays an important role in the way chemists interpret and disseminate their results. Evaluation of uncertainty is a complex task and international guidelines such as the "Guide to the Expression of Uncertainty in Measurement", which is co-authored by IUPAC, go a long way to ensure uniform scientific discussion. Although atomic weights form the basis for nearly all chemical measurements, the atomic weight uncertainties still lack uniform interpretation. Project 2013-032-1-200 is an example of international collaboration between IUPAC and the Joint Committee for Guides in Metrology to establish a set of coherent guidelines on formal interpretation of standard atomic weight uncertainties.

3. IUPAC will assist chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement in the quality of life.

The same fundamental data that the Division provides for international standardization is also used by commerce and industry. The most significant examples of this are the above-mentioned latest atomic weights and isotope abundances. Isotopic abundances, which are becoming increasingly important in areas, in particular for legal and provenance cases and also in medicinal chemistry.

4. IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.

The Division reviews relevant IUPAC sponsored international conferences on the chemical sciences. Through the IUPAC project system the Division strongly supports the inclusion of chemists from as wide a range of countries as possible on project task groups. The Division also publishes a biannual newsletter of its activities, which are also distributed to all member country societies and are readily available on the IUPAC website. For the most recent one, see:

http://www.iupac.org/fileadmin/user_upload/divisions/II/Div_II_newsletter2015.pdf

5. IUPAC will utilize its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.

The Division has reported earlier on a project with CCE on the extension of a major project involving the Period Table of the Isotopes for the educational community. (Project number 2007-038-3-200) This project was very successful, and explored also ways to present this critical chemical representation of

real world chemistry and the resulting wealth of applications it provides to many areas of chemistry. A follow-up project, i.e. 2014-024-1-200 is to result in the creation an interactive, electronic version of the IUPAC Periodic Table of the Isotopes. In 2013, Division's Commission on Isotopic Abundances and Atomic Weights launched a redesigned website (see: <http://ciaaw.org>) featuring a wealth of information of its products and activities. This site functions as the authoritative online platform for the Commission's products. During the first three months of 2015, this website has been accessed from over 100 countries worldwide.

Wikipedia: On the suggestion of profs. Weiser and Öhrström all division members have been stimulated to read and also edit relevant pages in Wikipedia, in English or other languages. Currently entries such as the following may be interesting to refer to: <https://en.wikipedia.org/wiki/IUPAC>
https://en.wikipedia.org/wiki/IUPAC_Inorganic_Chemistry_Division
https://en.wikipedia.org/wiki/Commission_on_Isotopic_Abundances_and_Atomic_Weights

6. *IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender, and age.*

The Division actively pursues new members to participate in divisional elections based on merit and diversity, through existing membership and connections, young observer program, and through their national adhering organizations. Divisional projects are also reviewed for general diversity of the project task group.

III. Plans and Priorities for the 2016-2017 biennium and beyond

III.1. Significant and Planned Projects and Related Issues

- a. The role of IUPAC in Isotope Sciences Terminology will remain very important. Any terminology for the isotopic sciences should be managed by, or have a very significant input from Division II, where the primary IUPAC expertise in this field resides. A project on Global dissemination of an interactive isotopic periodic table is already in preparation. Also a project dealing with a fundamental understanding of isotopic abundance is in progress of submitting.
- b. Possible other new projects under consideration for submission are:
 - A Periodic Table of Life and other periodic tables, like a Periodic Table of allotropy of elements. These are planned to be ready at the centennial Paris 2019 meeting.
 - Terminology of Nanomaterials
 - Definition of Valence
 - Spotting errors in Wikipedia related to inorganic chemistry and nomenclature and submit corrections to Wikipedia
- c. The team of the Oxidation State Project that formally ended Dec. 31, 2015, has obtained an extension till Dec 31, 2016, in order to be able to deal with follow-up tasks on its agenda: 1) Discussion and finalizing the IUPAC Recommendation on the topic (provisional draft has been posted and awaits comment by May 31, 2016), 2) Suggestion how to modify the Gold-Book entries for Oxidation Number and Oxidation State (details of the wording are currently being discussed at the task group), 3) possibly a paper on *oxidation state in teaching* for the Journal of Chemical Education.
- d. The CIAAW has also new or updated projects in its planning, like updating atomic weights.

III.2 Revised Atomic Weights Projects

The most recent biennial review of atomic-weight determinations and other cognate data by the Commission on Isotopic Abundances and Atomic Weights (CIAAW) has resulted in changes for the standard atomic weights of cadmium, molybdenum, selenium, and thorium based on recent determinations of terrestrial isotopic abundances. In addition, the standard atomic weights of 15 elements have been revised based on the new assessment of their atomic masses by International Union of Pure and Applied Physics. The IUPAC Press Release of 24 Sep 2013 resulted in a significant amount of media enquiries and resulted in wide spread of articles in the global media, including the

Huffington Post, Telegraph, Yahoo! News, Chemical and Engineering News and Popular Science, to name a few. Work continues in this area in collaboration with the International Bureau of Weights and Measures (BIPM) in projects related to explaining the significance of, and how to work with these atomic weight intervals to the wider chemical community. The most recent atomic weight correction dealt with Yttrium (2015).

III.3 *Membership of the Division*

The Division will remain eager to continuously renew its membership and also recruit new members from the pool of young observers to the council meetings.

III-4. *General Divisional Operations*

Since some years within the Division we have a scheme available for each of the members and their duties within the division. The Division considers it of great importance that member have chances to become and remain active e.g. in projects. Therefore annual meetings of TMs, and if possible more members (AM. NR) have been and will be organized. The 2014 meeting, had a very good attendance (see below).

III-5. *Off year Meetings – 2014 and 2016*

Singapore off-year meeting (2014): The division's off-year meeting took place during 1½ day at National University of Singapore, kindly hosted and exemplary organized by Thomas Walczyk. Among notable items were a number of reports from IUPAC committees and affiliated organizations, discussions on sponsorship of conferences and the generation of new projects. The minutes have been distributed to the members.

For 2016 the off-year meeting is scheduled for France (Brest) on July 7-8.

III.6 *Interdivisional Subcommittee on Materials Chemistry*

The Division has substantial representation on the Interdivisional Subcommittee on Materials Chemistry (Current chair is C. Ober, also PP of Polymer Division) which together with Divisions I and IV is exploring ways of expanding the significance of Materials Chemistry with IUPAC and increasing the interaction between IUPAC and the Materials Chemistry user communities. Several ideas for projects were developed including a new project on development of a Materials Chemistry Education Website, now: 2013-037-1-200.

IV. **State of Projects – as of April 1, 2016**

The Division currently has 24 items on its Project List (up from 20 in June 2015), including three projects co-funded with other divisions, marked **in blue** in the Table below. Since early 2015, five new projects have been funded, as evident by their project code number (starting with 2015-). Projects administrated by other Divisions, but with Div II involved, are not listed here.

Some proposed projects are in the pipeline and close to submission, under evaluation or under revision, such as a project on a Periodic Table of Life, and project to showcase how to use Wikipedia to promote IUPAC activities and to inform about our division activities.

List of Division II-related active projects as of April 1, 2016

| | |
|----------------|--|
| 2008-040-1-200 | Towards a Comprehensive Definition of Oxidation State |
| 2009-023-1-200 | Evaluation of Radiogenic Abundance Variations in Selected Elements |

| | |
|--------------------------------|--|
| 2009-026-2-200 | Online Evaluated Isotope Ratio Database for User Communities |
| 2009-027-1-200 | Assessment of Stable Isotopic Reference and Inter-Comparison Materials |
| 2009-045-1-200 | Guidelines for Measurement of Luminescence Spectra and Quantum Yields of Inorganic Compounds, Metal Complexes and Materials |
| 2009-046-2-200 | Terminology and Definition of Quantities Related to the Isotope Distribution in Elements with More than Two Stable Isotopes |
| 2011-026-1-200 | Full Calibration of a New Molybdenum Isotopic Reference Material |
| 2011-027-1-200 | Evaluated Published Isotope Ratio Data (2011-2013) |
| 2011-028-1-200 | Evaluation of Published Lead Isotopic Data (1950-2013) for a New Standard Atomic Weight of Lead |
| 2011-040-2-200 | Developing of a Procedure for Using Intervals Instead of Fixed Values for Atomic Weights |
| 2012-036-2-200 | Recommendations for Isotope Data in the Geosciences II |
| 2012-045-1-800 | Nomenclature for Polyhedral Boranes and Related Compounds |
| 2012-046-2-800 | Handling of Inorganic compounds for InChI V2 |
| 2013-030-1-800 | Nomenclature for Metallacycles containing Transition Metals |
| 2013-032-1-200 | Guidelines for the Derivation of Values and Uncertainties from Standard Atomic Weight Intervals |
| 2013-037-1-200 | Creating an Educational Website for Materials Chemistry |
| 2014-001-2-200 | Terminology Guidelines and Database Issues for Topology Representations in Coordination Networks, Metal-Organic Frameworks and Other Crystalline Materials |
| 2014-002-1-200 | Assessment of Stable Isotopic Reference Materials [Follow-up to project 2009-027-1-200 (TGC: Willi Brand, CIAAW)]. |
| 2014-016-2-200 | Compilation of the Variation of the Isotopic Composition of the Elements via Crowd sourcing |
| 2015-030-2-200 | Assessment of Fundamental Understanding of Isotopic Abundances and Atomic Weights of the Chemical Elements (2016-2017) |
| 2015-037-2-200 | IUPAC Molecular Weight Calculator |
| 2015-053-1-200 | Survey of Definitions and Use of Common Solid-State Chemistry Terminology |
| 2015-031-1-200 | Revision of PAC 2002 paper: "How to name New elements" |
| 2015-039-2-200 | The constitution of group 3 of the Periodic Table. |