

## INORGANIC CHEMISTRY DIVISION (II) Report to the 48<sup>th</sup> GA Council, Busan,– August 2015

### Members (2014-2015)

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#### *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,

### I. Divisional Highlights

The Division is currently directly involved with over 20 ongoing projects, part of these jointly with other Divisions. A number of projects were completed during the last two years, and some of these are highlighted below.

The first of these is the project **Coordination polymers and metal organic frameworks: terminology and nomenclature guidelines**. Published as: IUPAC Recommendations 2013 Batten, Stuart R. et al., "Terminology of metal-organic frameworks and coordination polymers) Authors: in Pure and Applied Chemistry (2013) **85**, 1715-1724. As per July 1, 2015, this report has been cited already 65 times (22 times in period January-June 2015). A prepublication in CrystEngComm in 2012, inviting comments and suggestions, was already cited over 100 times.

The **Oxidation State Project** 2008-040-1-200, "Towards a comprehensive definition of oxidation state" has accomplished its first major goal by publishing in 2014 a IUPAC Technical Report on the subject: Pavel Karen, Patrick McArdle and Josef Takats, Pure and Applied Chemistry (2014), **86**, 1017–1081; (see: <http://dx.doi.org/10.1515/pac-2013-0505>). The Report introduces several novel approaches to oxidation state. Instead of definitory algorithm, there is one single generic definition based on ionic approximation of heteroatomic bonds. For the latter, the team has tested three alternative interpretations: bond polarity, average valence-orbital energy of the isolated atom, and the atom's contribution to the bonding MO. The Report provides a clear set of rules for determination of oxidation state, illustrated with numerous examples. It has been implemented in the Wikipedia page on Oxidation State. The Project, currently valid to Dec. 31, 2015, has three more planned tasks on its agenda: 1) Discussion and finalizing the IUPAC Recommendation on the topic (a first draft is ready), 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) a paper on oxidation state in teaching for Journal of Chemical Education (in discussion prior drafting). 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 (see: <http://dx.doi.org/10.1002/anie.201407561>)

A joint IUPAC/IUPAP Working Party continues to consider **claims for new elements with atomic numbers in the range 113 to 118** - see IUPAC project 2012-047-1-200. This project is expected to lead to clarification for claims to elements numbered 113, 115, 117 and 118. The joint IUPAC – IUPAP Joint Working Party was expected to report on its deliberations by the end of 2013, but this did not take place and we are now expecting the report by the end of 2015. The Division would like to acknowledge to contribution of IUPAC Treasurer, Prof John Corish, for his assistance with this important work. Even though these new elements have little current applicability, the approval of the naming of new elements is a high visibility activity for IUPAC that attracts significant public attention to the Periodic Table of the Elements and in general for IUPAC.

**Revised Atomic Weights Project** 2011-027-1-200, "Evaluated Published Isotope Ratio Data (2011-2013)" 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.

Finally, it is with pleasure to note that among the 10 most downloaded articles from PAC (as per end of 2014) several of them have an origin in our division. To be mentioned are:

- #1. Assessment of international reference materials for isotope-ratio analysis (IUPAC Technical Report) by W.A. Brand et al.
- #4. Atomic weights of the elements 2011 (IUPAC Technical Report) by M.E. Wieser et al.
- #5. Toward a comprehensive definition of oxidation state (IUPAC Technical Report) by Pavel; Karen et al.
- #8. Terminology of metal–organic frameworks and coordination polymers (IUPAC recommendations 2013) by S.R. Batten et al.

## **II. Operations of the Division: seen from the perspective of the 6 IUPAC long-range term goals**

*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\\_newsletter2014\\_1.pdf](http://www.iupac.org/fileadmin/user_upload/divisions/II/Div_II_newsletter2014_1.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/IUPAC_Inorganic_Chemistry_Division)

[https://en.wikipedia.org/wiki/Commission\\_on\\_Isotopic\\_Abundances\\_and\\_Atomic\\_Weights](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.

### **3) State of Projects – as of July 1, 2015**

The Division currently has 20 active projects (slightly up from 18 in 2014) on its project list.

In 2014 4 new projects have been funded, as visible by their project code numbers below.

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

In addition there are a few Projects co-funded with other divisions, visible in red color marks, in the Table below.

## List of Division-connected active projects as per July 1 2015

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 (2011-2014)
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 (2012-2013)
2011-028-1-200:	Evaluation of published lead isotopic data (1950 - 2013) for a new standard atomic weight of lead
2011-035-1-800:	Terminology and Nomenclature of Inorganic and Coordination Polymer
2011-040-2-200:	Developing a procedure for using intervals instead of fixed values for atomic weights
2012-036-2-200	Recommendations for Isotope Data in the Geosciences II
2012-044-1-100	Basic Terminology of Crystal Engineering
2012-045-1-800	Nomenclature for Polyhedral Boranes and Related Compounds
2012-046-2-800	Handling of Inorganic compounds for InChI V2
2012-047-1-200:	Discovery of Elements with Atomic Numbers greater than 113
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
2014-024-1-200	Development and Global Dissemination of an IUPAC Interactive Electronic Isotopic Periodic Table and Supporting Resources for the Education Community

### 4) Other Additional Information

#### *Divisional Election of 2016-17 members*

The Division is pleased to report the completion of its election for membership for the 2016-17 biennium. I would like to especially thank VP Öhrström and the nomination panel for pushing the elections through using the new, tight time schedule for these elections. The candidates elected need approval or Council.

### *General Divisional Operations*

Since a few 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 members 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).

### *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.

### *Off year Meeting – National University of Singapore – July 2014*

Singapore off-year meeting: The division's off-year meeting took place during 1½ day at National University of Singapore, kindly hosted and exemplary organised 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.

## **6. Other Significant Issues relevant to mention**

- The DP and VP 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. Full text of the recommendation: The ad-hoc group presents the following 2 recommendations to IUPAC.
- *1. 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.*
- *2. 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.*
- Division II members work closely with representatives from Division I and V towards the IUPAC Technical Project on the redefinition of the mole.
- A paper in Nature (Sato et al. Nature 520, 209-211; April 2015) and an accompanying commentary on the Ionisation Potential of Lawrencium has raised the question: would perhaps Lu and Lr better belong to the d block. On requests of Nature and Science the DP has responded that Div II will discuss the issue, and may invite project proposals on fine-tuning group-3 elements in the Periodic Table.