**INORGANIC CHEMISTRY DIVISION OF IUPAC**

**Minutes of Meeting at Busan 8 and 9 August 2015**

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**INORGANIC CHEMISTRY DIVISION OF IUPAC**
**Meeting at Busan, August 8-9, 2015**

**DRAFT MINUTES**

**Attendance:** Present were for part or all *President*, Jan Reedijk (Netherlands); *Vice President*, Lars Öhrström (Sweden), *Secretary*, Markku Leskelä (Finland); *Titular Members*: Tiping Ding (China), Milan Drabik (Slovakia), Daniel Rabinovich (USA), *Associate Members*: Joseph Buchweishaija (Tanzania), Javier Garcia-Martinez (Spain), Ken Sakai (Japan), and *National representatives:* Yang F. Abdul Aziz (Malesia), *Young observers*: Guillermo Ahumada (Chile), James Darkwa (South Africa), Miki Hasegawa (Japan), Claudio Verani (USA), Luisa Whittaker-Brooks (USA), *IUPAC past president, Division adjugated emeritius* Kaz Tatsumi (Japan), *IUPAC treasurer* John Corish (Ireland) and Ehud Keinan (Israel)

**Apologies** were received from *Titular Member* Robert Loss (Australia), Edit Tsuva (Israel), Thomas Walczyk (Singapore), Michael Wieser (Canada), *Associate members* Paul Karen (Norway), Adem Kilic (Turkey), *National representative* Biserka Prugovecki (Croatia), *Young observer* Brian Korgel who could not attend.

Paragraphs in the minutes have been written in the order they were presented in the agenda. Discussions were carried out in a few cases in slightly different order.

**1 – Introductions and announcements (J. Reedijk)**

The meeting commenced at 9:30 a.m. on Saturday, August 8, 2015. Div. President Reedijk welcomed the members, and also thanked the AM members for attending on other funding. Those present introduced themselves and described their professional affiliations and areas of expertise.

**2 – Presentation and discussion of the Agenda (Reedijk)**

The previously distributed Agenda was accepted by the meeting. Lars Öhrström volunteered to collect the "Action Items" for this meeting which are added in these Minutes as **Appendix 1**.

**3 – Approval of Minutes from Division Meeting in Singapore (Leskelä) and status of the action items from the Singapore meeting (Reedijk)**

Minutes of the Singapore (2014) meeting had been distributed in draft form previously and amended according to corrections and comments received from the Division members and distributed by email to the Division members during Spring. The final version of the Minutes was approved without further change and thanks were given to the Division Secretary. The final copy will also be available on the IUPAC Division II web page. Unfortunately, there has been a delay in

putting the minutes of the previous meetings on the web page due to the changes of responsive persons and reorganizations in IUPAC office.

The action items from the Singapore meeting were included in the Minutes of that meeting as Appendix 1. All of these items had been addressed by the designated individuals.

**4- Reports of IUPAC Bureau and Executive Committee actions (Reedijk)**

The Bureau and Division Presidents did not have a separate meeting in 2015 but the meeting is now in Busan. Reedijk told the general news from IUPAC and they were dealing restructuring of the IUPAC office, renewing the web-site and financial issues. Economic situation of IUPAC is tight but John Corish told that it seems that the budget for next biennium (2016-17) should remain the same as in this biennium (2014-15).

A copy of the Report on Division II that Div. President Reedijk will present in the Bureau meeting is attached to these Minutes as **Appendix 2.**

**5 - Report from IUPAC Officers**

No report from IUPAC officers.

**6- Reports from other IUPAC bodies and Affiliated Organizations**

Jan Apotheker from Committee on Chemistry Education (CCE) told about the recent activities. Interactive Educational Periodic Table is an important part of the activities and it is common with Div II. Norman Holden sent a report on the status of the project "Development and Global Dissemination of IUPAC Interactive Periodic Table" (IPTI-2). The project is a follow-up to the project "Development an Isotopic Periodic table for Chemistry Education (2007-038-3-200).

The activity of Javier Garcia as editor of a book on Chemistry Education (Wiley-VCH) was again appreciated. The situation of Javier was discussed because he has been an important link between Div II and CCE. If Spain will be taken back to IUPAC in council meeting, Javier can continue as NR. Dan Rabinovich is teaching chemistry in stamps – that could also be of interest of CCE.

Dan Rabinovich reported his activities with Div VIIII (Chemical Nomenclature and Structure Representation Division). More discussions on common interests were planned for the interdivisional meeting on Sunday, but this meeting did not take place.

**7 - Report from the 2015 elections; current and future list of Division Members (Öhrström)**

Earlier the election of new member for IUPAC bodies was a slow process. The new model to speed up the process was taken in use this year. Election is prepared in a committee where the division's representative is the vice-chairman. Voting is made electronically and taken care by the secretariat.

The final results of the elections were presented.

A few things concerning the elections were discussed. The NAOs are suggesting candidates but based on those it is difficult select people so that we can fulfill the requirements of different expertise (atoms, molecules, materials), geography and gender. The election committee could be more active and propose candidates to fill the missing representation. The other issue is that it is unclear who will inform the people elected. Because secretariat is taking care of the voting process it was felt that they should do the information. After that the Division representatives (president, vice-president, secretary) can send their congratulations (before end of the year 2015).

**8 - Division newsletter status and planning (Öhrström)**

Appearance frequency of the newsletter was discussed. Once in a year is usually enough. Next issue will appear after this meeting and deadline for submitting material is end of September. The newsletter has great importance both internal in the division and external inside IUPAC and NAOs. The feedback from newsletters has always been positive. The members were reminded to distribute the newsletter to their NAOs.

**9. - Review of Division budget allocations and expenditures (Reedijk)**

Jan Reedijk presented the budget allocation during this biennium. 30.6 % was used for meetings which exceeds the guideline 30 %. The exceeding was because of the off-year meeting in Singapore which was a bit expensive, and endorsed by the treasurer. All the projects are well in the budget.

If the budget will remain the same Div. II will have USD 48 000 for 2016-17.

**10 - Report from Commission on Isotopic Abundances and Atomic Weights (CIAAW) and its Subcommittees, including the relevant Project Reports (Ding)**

Tiping Ding went through the report made by Juris Meija and Thomas Prohaska. The core activities include submission of two reports “Standard Atomic Weights of Elements 2013” and “Isotope Compositions of the Elements 2013”. International Committee of Weight and Measures (CIPM) has adopted the work of CIAAW on use of delta value isotope ratio measurements for traceability. CIAAW recognized that Theodore W. Richards received 100 years ago Nobel prize for his accurate determinations of atomic weights and he was that time member of CIAAW.

CIAAW has renewed the web-site. It receives plenty of visits all over the world (people from 130 countries recently visited the site). CIAAW has been active in project on uncertainties in standard atomic weights. The Commission recommends new standard atomic weight for Yb 173.045(10). CIAAW has also participated in the project on Redefinition of mole.

Report of CIAAW is in **Appendix 3.**

**11 - Preliminary discussion on group 3 of periodic Table in view of a recent paper in Nature, and commentaries.**

The position of Lawrencium in Periodic Table has been questioned because of the paper of Sato *et al.* (Nature 520 (2015) 209.) where they report its ionization potential. In a comment paper William Jensen proposed that Lr and accordingly Lu should be put on Group 3 below yttrium and La and Ac should be on the f-element side row. The paper of Bernard Schaeffer (J. Mod. Phys. 5 (2014) 117) supports this claim. After discussion the recommendation is that a project should be created and Jensen should be involved in the task group. Prof. Scerri will be invited to submit a project. Lars Öhrström is willing to join such a project.

**12 – Reports from other IUPAC bodies and Affiliated Organizations**

Markku Leskelä described the highlights on Committee on Chemical Industry (COCI). The representative of COCI was expected to visit the Division on Sunday but did not show up.

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) is represented by Milan Drabik. He gave a short report on the activities during last 12 months. ICTNS checks all the IUPAC documents for the correct terminology. Jan Reedijk suggested that ICTNS should discuss the decimal numbering style used in documents (allowed or not?).

ICNTS had meeting during Sunday and Monday and Milan made a report after that.

Norman Holden has sent a report from the collaboration with International Union of Geological Sciences (IUGS). One important activity has dealt with the isotopic Periodic Table. The Div II is very grateful to Norman Holden for his excellent work in this and other projects. Report is in **Appendix 4**.

The Interdivisional Subcommittee on Materials Chemistry (ISMC) has it meeting on Monday and it was participated by Milan and Markku. The Materials Chemistry educational web-site which has been created by Ilya Zharov (University of Utah) (http://iupac-materials.chem.utah.edu/) was discussed and a lot of feedback was given to Ilya. The other main discussion topic was creation of new projects. Minutes of that meeting are in **Appendix 5**.

**13 - Reports on recent, planned and proposed Division sponsored conferences**

Div II has had in the past supported the conference series: High Temperature Materials Conference. This triennial Conference was last held in 2012 in Beijing, China. There is no information wheter or not this conference series is continued.

Milan Drabik told about IUPAC endorsed 25th International Conference on Coordination and Bioinorganic Chemistry held in Smolenice (Slovakia) in June 2015. The conference was chaired by prof. Milan Melnik. The conference was very successful. This time no IUPAC young scientist awards were given.

Brian Korgel has applied IUPAC sponsorship for the 4th International Solvothermal hydrothermal association conference held in France Oct. 2014 but was too late in the application for IUPAC endorsement.

ICCC conferences have for long time has had an IUPAC label, and so will the next conference to be held in Brest (France) in 2016 have. After 2018 the IUPAC – ICCC association will be discontinued. Asian coordination chemistry conference to be held in Malaysia will also ask the IUPAC endorsement.

Meeting was closed 16.00

Division had a common dinner in restaurant Ming-Ju – 8 delegates could attend.

**Sunday August 9**

**14 –Project-by-project review of project status (Rabinovich)**

Dan Rabinovich presented an introduction to projects: what they are, project process flow, and application forms. **Appendix 6.**

Dan made the project-by-project review. No projects have been completed during the last 12 months. Division II has 17 primary active projects 17 (14 continuing, 3 new), 5 secondary active projects 5 (projects in which Div II is participating). See for details in **Appendix 7.**

**15 –Review of new project proposals (Rabinovich)**

There are no pending projects (= reviewed projects waiting for funding) and one project which is under review.

2015-002-1-xxx is by Rustem Valiullin (Faculty of Physics and Earth Sciences, University of Leipzig, Germany) on Diffusion in Nanoporous Solids. It is also considered by Div I and Div V.

The following projects are under preparation:

2015-xxx-1-xxx by Norman Holden (Brookhaven National Laboratory) on Assessment of Fundamental Understanding of Isotopic Abundances and Atomic Weights of the Chemical Elements (2016—2017).

2016-xxx-1-xxx by Daniel Rabinovich (UNC Charlotte) on The Periodic Table of Life.

2016-xxx-1-xxx by Pavel Karen (University of Oslo) entitled Towards a Comprehensive Definition of Valence.

2016-xxx-1-xxx by Robin Macaluso (University of Texas at Arlington) on Classification of Solid State Compounds by chemical bonding

From the new projects discussed in 2014 Terminology of Nanomaterials and Nanotechnology in Materials Chemistry has not progressed to a proposal. The proposal for Magnetic Information file for Magnetochemistry was submitted but received negative review. The future of this project is open.

**16 – Discussion on the generation of other future projects**

Claudio Verani made a suggestion for a project on Understanding of TOF and TON in electrocatalytic water splitting and perhaps even wider. The topic created live discussion.

**17 – Status of the Information Package for new Division members (Öhrström)**

Division members are happy with content of the Information package. The package is now distributed to new members but from now on it should be sent also to young observers who attended the meeting.

**18 – Duties of Division members (Reedijk)**

Jan Reedijk presented the list of members and their current duties. The list will be completed after this meeting and updated January 1 2016, and after that distributed.

**19 - New Elements: status report and naming procedures; 112-118 (Loss/Reedijk/Corish)**

John Corish explained the process of naming new elements and the different steps are listed in **Appendix 8**. The division members are asked to go through the procedure and look at the papers from the naming of Cn, Fl and Lv.

There are four claims at the table: elements 113, 115, 117, 118. The working group has worked for years and given two reports – one for elements 113, 115, 117 and the other for 118. Before publishing in PAC the reports are carefully reviewed and sent back to the laboratories for checking. Reports are rewritten after comments and they are soon ready for publishing. IUPAC executive committee will designate the discovering laboratories for each element. After publishing the naming process is in hands of Div II. We have to check the proposed names and symbols. (The book of Lost Elements can be useful in checking). Final decision of the names is usually made by Council but because the next meeting is only after 2 years it is suggested that duty is delegated to Bureau.

After the meeting it was realized that the 2002 rules for naming elements could be too restrictive, for especially elements 117 and 118. So a request to ICNTS was made August 12 - the draft of which was circulated to all members after the meeting – and all responded positive – to change the rigid rule to a more flexible one.

**20 – Review of Action Item list from this meeting (Öhrström)**

The review of Action Items was made (**Appendix 1**).

**21 - Status of planning of the next year Division meeting in South Korea General Assembly**

Off-year meeting 2016 was discussed and general opinion was that a meeting would be useful. One option is to have it in connection to 42th ICCC Conference in Brest (France). The ICCC conference is held July 3-8. Just after the meeting all members were consulted about this venue. All those who responded were positive, so the president will explore thin in the coming months.

**22 – Publicity Issues: Periodic Table; Oxidation State Definition (Karen)**

Periodic table is the visible "business card" of IUPAC. The Russian proposal to change the name to Mendelejev Periodic table was handled in a small project headed by Div II people and it was proposed to the Executive committee that no changes should be made.

The oxidation project of Pavel Karen has gained a lot of visibility both the massive article in PAC and essay in Angewandte Chemie have already collected high number of citations.

**23 – Any other businesses**

There were no other businesses.

**24. Thanks and adjourn**

Jan Reedijk closed the general meeting at 12.00 and thanked the participants for an active meeting.

**Interdivisional meetings**

Sunday: 14.00-14.45 Div II – Div VIII in 214
15.00-15.45 Div II – Div I – Div V in 213 (part of Div II) discussion on mole
15.00-15-45 Div II – CCE in 214 (part of Div II):

The meeting with CCE did not happen. Short notes from the second meeting are in **Appendix 9**.

## Appendix 1

### Action Items from IUPAC Inorganic Chemistry Division Committee
### Busan, August 8 - 9, 2015

1. Send items for the division newsletter to Lars Öhrström, ohrstrom@chalmers.se. [all]
2. Make the division newsletter available to respective NAO. The pdf can be uploaded and advertised on any website related to an NAO or close affiliate.[all]
3. http://www.ciaaw.org needs to mention IUPAC not just the logo. [Ding] FIXED!
4. Prepare for new element name and symbol proposals. [all]
5. Contact Brian Korgel about 4th & 5th International Solvothermal and Hydrothermal Association Conference. [Leskelä]
6. New member Information Package update for new members and Young Observers. [Öhrström]

# Appendix 2

## Report on Division II for Bureau by Div. President Reedijk

**INORGANIC CHEMISTRY DIVISION (II)**
**Report to the 48th GA Council, Busan,– August 2015**
**Members (2014-2015)**
**President:** J. Reedijk (The Netherlands)
**Past President :** R. D. Loss (Australia)
**Vice President:** L. Öhrström (Sweden),
**Secretary:** M. Leskela (Finland),
**Titular Members:** T. Ding (China), M. Drabik (Slovakia), D. Rabinovich (USA), E. Tshuva (Israel), T. Walczyk (Singapore), M. Wieser (Canada)
**Associate Members:** J. Buchweishaija (Tanzania), P. Karen (Norway), J. Garcia Martinez (Spain), A. Kiliç (Turkey), K. Sakai (Japan), R-N. Vannier (France),
**National Representatives:** Y. Abdul Aziz (Malaysia), A. Badsha (Pakistan), L. Armelado (Italy), V Chandrasekhar (India), L. Galamba-Correia (Portugal), S. Kalmyakov (Russia), B. Prugovečki, Biserka (Croatia), N. Trendafilova (Bulgaria), L. Meesuk (Thailand). S. Mathur (Germany),

*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 P. 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 abovementioned 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

*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.

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

The Division currently has 23 items on its Project List (up from 18 in 2014), including a few Projects co-funded with other divisions, marked in red in the Table below. In 2014-15, four new projects have been funded, as evident by their project code number below.

Some 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 blue color marks, in the Table below.

**List of Division II-related active projects as of 1 July 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 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).

*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 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.

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

*1.* 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 is was recommended not do this. Full text of the recommendation: The adhoc group presents 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.*

2. Division II members work closely with representatives from Division I and V towards the IUPAC Technical Project on the redefinition of the mole.

3. 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 be placed in 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.

# Appendix 3

**Report for the IUPAC Inorganic Chemistry Division**
**Commission on Isotopic Abundances and Atomic Weights**

**Report for 2015**

Juris Meija, Chair
Thomas Prohaska, Secretary

From July 31 to August 4, CIAAW met in University of Natural Resources and Life Sciences, Vienna (Vienna, Austria) under the Chairmanship of Dr. Juris Meija.
The following were present in the 2015 CIAAW meeting: Juris Meija (Canada), Thomas Prohaska (Austria), Manfred Gröning (Austria), Xiang-Kun Zhang (China), Tiping Ding (China), Johanna Irrgeher (Austria), Jochen Vogl (Germany), Antonio Possolo (USA), Harro Meijer (The Netherlands), Lesley Chesson (USA), Norman Holden (USA), Michael Wieser (Canada), and Thomas Walczyk (Singapore)

This report provides a summary of the Commission activities for 2015 and summarizes the 2015 meeting.

## 1. Core activities

After lengthy review and discussions, “Standard Atomic Weights of Elements 2013” has been submitted to *Pure and Applied Chemistry* on 26 March 2015 and will be published shortly. The Commission has also submitted “Isotopic Compositions of the elements 2013”. TICE-2013 report

has been revised and updated extensively from the previous TICE-2009 report. In particular, care has been taken to ensure the compatibility between the standard atomic weights and the corresponding isotopic compositions, especially when it comes to the uncertainties. In addition, all data present in this publication have been verified and recalculated afresh to eliminate dormant errors which can occur in datasets that have been compiled over such a long period of time. All original documents that have been used in this publication have been deposited in the CIAAW database (database of IUPAC best measurements).

In March of 2015, the International Committee of Weights and Measures (CIPM) decided (decision CIPM/104-26) to adopt the traceability exception related to delta value isotope ratio measurements based on the recent work published by CIAAW by brand et al (Pure Appl. Chem. 2014; 86(3): 425–467). This is an important recognition of the work of CIAAW and highlights the continued relevance of the work of the CIAAW.

**2. Web presence**

In June 2014, the Commission unveiled a new design for its website at ciaaw.org. The new site employs responsive design aimed at enhanced visibility on mobile devices and at enhanced user interactivity. The new website displays significantly more content than previously, and the Commission has plans to further revitalize the site by adding popular electronic calculators such as the molecular weight uncertainty calculator, the isotopic pattern calculator and other graphical data displays, and further historical information about CIAAW.

Based on the Google Analytics data of the ciaaw.org traffic, the number of ciaaw.org users has doubled in 2015 as compared to Jan-Jun 2014 and the number of tablet and mobile users has also tripled. In 2015, ciaaw.org has been visited from 130+ countries which is an indication of the global outreach of the CIAAW.

**3. Uncertainties of standard atomic weights**

Following the 2009 CIAAW meeting in Vienna, a request was sent to the Joint Committee for Guides in Metrology (JCGM) of BIPM for advice on the uncertainty evaluation of standard atomic weights. A reply was received in June-2013 and, subsequently, a IUPAC Project was launched during the 2013 IUPAC General Assembly. This project aims to produce formal guidelines on the said matter. In particular, this project will provide much needed clarity on the matter of interpreting atomic weights – an issue that became apparent only after the introduction of the interval notation.

The Task Group met in June 2014 (Delft, Netherlands) under the Chairmanship of Dr. Adriaan van der Veen. Two reports are well-underway, both to be published in PAC: (1) IUPAC Recommendation on the use of atomic weights and (2) the accompanying IUPAC Technical Report with in-depth technical discussions. The draft of the former manuscript which outlines the basic philosophy of the Task Group has been circulated to CIAAW and JCGM.

Over the last year, CIAAW chairman has received several requests to explain the uncertainty calculation of molecular weights by mail. It has become clear that CIAAW has to inform the public on the matter in its 2015 meeting. In addition, CIAAW chairman has prepared necessary codes for online calculators of molecular weights and their uncertainties to be placed on ciaaw.org. These issues were discussed at length during the CIAAW 2015 meeting in Vienna and the Commission resolved to endorse probabilistic interpretation of standard atomic weights using various probability density functions, including the rectangular distribution.

**4. New standard atomic weights**

In its 2015 meeting, CIAAW recommended to revise the standard atomic weight of ytterbium to 173.045(10) from 173.054(5) based on the work of Jun Wang et al from the National Metrology Institute China.

**5. Interval notation**

In its 2015 meeting, CIAAW discussed at-length the format of its *Atomic Weights* report and the comments it has received in regards to the interval notation.

Recognizing that the Table of Standard Atomic Weights should be as simple, informative, and convenient to use as possible, recognizing the need to provide with a single atomic-weight values to the users in the educational institutions and science communities alike, and recognizing the continued value of the standard atomic-weight intervals in conveying the fact that atomic-weight values are not constants of nature, CIAAW decided to issue only one Table in its publication *Atomic Weights of the Elements* (IUPAC Technical Report). In addition to the standard atomic weights, this table will also provide single abridged atomic-weight value for each element.

**6. Redefinition of the mole**

CIAAW is involved in the IUPAC Project on the redefinition of the mole through its Chairman. The Task Group on the redefinition of the mole met in Zurich (July 2014), and had its last meeting in

January 2015 in Ottawa and are currently preparing the report to the IUPAC Bureau. The minutes of the meetings are deposited to iupac.org. The Task Group approved the proposed definition of the mole as it appears in the Draft 9th SI Brochure (16 Dec 2013)* only “in principle” because several additions are warranted. First, the Task Group members agreed to recommend changing the quantity name “amount of substance” to “chemical amount”. In addition, the Task Group drafted an informative paragraph explaining the nature of the quantity which is currently known by the name “amount of substance” and its relationship with the Avogadro number, the Avogadro constant, and the number of entities. This informative paragraph will be sent to the drafting committee working on the 9th edition of the SI Brochure in order to better complement the normative definition of the mole. In reaching the decision, the Task Group conducted a survey among IUPAC NAOs and a large number of replies from NAOs were received.

**7. CIAAW Charter**

During its 2015 meeting, CIAAW circulated a draft Charter which aims to record and codify the practices and responsibilities of the CIAAW members. The Charter will be circulated to Division II and IUPAC Secretariat for comments and will be formally adopted by CIAAW in 2017.

**8. Members of CIAAW for 2016-2017**

The Commission coopted the following members for the 2016-2017:
*Chair*: Juris Meija (Canada)
*Secretary*: Thomas Prohaska (Austria)
*Titular members*: Manfred Gröning (Austria), Xiang-Kun Zhang (China), Johanna Irrgeher (Austria), Jochen Vogl (Germany)
*Associate members*: Antonio Possolo (USA), Harro Meijer (The Netherlands), Lesley Chesson (USA)
*National Representatives*: Paul de Bievre (Belgium)

**9. Members of Subcommittee for Isotopic Abundance Measurements (SIAM) for 2016-2017**

*Chair*: Johanna Irrgeher (Austria)
*Secretary*: Jochen Vogl (Germany)
Paul De Bièvre (Belgium)
John-Karl Böhlke (USA)
Willi A. Brand (Germany)
Lesley Chesson (USA)

Tyler Coplen (USA)
Tiping Ding (China)
Manfred Gröning (Austria)
Norman Holden (USA)
Harro Meijer (The Netherlands)
Juris Meija (Canada)
Thomas Prohaska (Austria)
Thomas Walczyk (Singapore)
Michael Wieser (Canada)
Shigekazu Yoneda (Japan)
Xiang-Kun Zhu (China)

**10. Subcommittee on Stable Isotope Reference Material Assessment for 2016-2017**

*Chair*: Manfred Gröning (Austria)
John-Karl Böhlke (USA)
Willi A. Brand (Germany)
Tyler Coplen (USA)
Tiping Ding (China)
Thomas Prohaska (Austria)
Robert D. Vocke (USA)
Jochen Vogl (Germany)
Thomas Walczyk (Singapore)

**11. Subcommittee on Natural Assessment of Fundamental Understanding of Isotopes for 2016-2017**

*Chair*: Norman Holden (USA)
Secretary: Tyler Coplen (USA)
John-Karl Böhlke (USA)
Paul De Bièvre (Belgium)
Michael Wieser (Canada)

**Appendix 4**

# Status Report on the IUGS/IUPAC Project

Norman E. Holden, Task Group member

The joint Task Group of Unions includes members of the International Union of Geological Sciences (IUGS) and members of the International Union of Pure and Applied Chemistry's (IUPAC) Inorganic Chemistry Division Committee and the Analytical Chemistry Division Committee. This Task Group recommends isotope data in the geosciences. It deals with the evaluation of radioactive half-life data for long-lived nuclides that are used for the geological dating of materials. It will also resolve issues dealing with the definition of the year with representatives of the BIPM, IUPAP and the IAU.

The Task Group has completed a paper on the half-life (decay constant) of Rb-87, which has been published in the Geochimica et Cosmochimica Acta journal, volume 164 (2015) 382-385. Work is presently underway on a paper on the status report on the three uranium half-lives, U-234, U-235, and U-238 for eventual submission to Geochimica et Cosmochimica Acta.

There was a previous publication in Pure Applied Chemistry (2001) vol. 83, No. 5, pp 1159-1162; http//dx.doi.org/10.1351/PAC-REC-09-01-22) on the definition of the year, which raised issues with some other international organizations. There will be continuing discussions (which had begun some time ago) with representatives of the BIPM, IUPAP and the IAU later this year to try to resolve the various issues related to this matter, perhaps resulting with a future joint publication.

# Appendix 5

**Report from ISMC, Interdivisional Subcommittee on Materials Chemistry**

Notes of the meeting held during the 45th IUPAC G.A., 10/08/2015, Busan, BEXCO, Room 217

**Attendees:** Milan Drabik (II), Markku Leskela (II), Savio Moniz (YO), Elizabeth Mansfield (YO), Shelley Claridge (YO), Rai Kookana (VI), Frank van Veggel (I), Jeanne Bolliger (YO), Natalie Stingelin (IV), Christopher Ober (IV), Vladimir Gubala (VII), Linda Johnston (VII), Clara Majalhas (V), Ilya Zharov (ISMC)

**Executive Summary:**

1) There was agreement that there will be a rotation of chairs at the next GA and a representative of Division I (Physical and Biophysical Chemistry), one of the founding divisions, will take on a 4-year term.
2) The ISMC will serve not only to foster materials chemistry within IUPAC but will also act to catalyse interdivisional activities.
3) The MC education website will receive input from all present at the ISMC meeting and update the content before the next meeting of the ISMC.
4) The ISMC meeting will be held once at the GA and 3 times electronically (e.g. Skype) during the next biennium.
5) All present will be solicited for interdivisional terminology and other projects during the next 2 months
6) One or more interdivisional workshops will be planned for the next GA/WCC to foster a better understanding of the activities between divisions that might cooperate on ISMC projects.

Ober welcomed all attendees and after a brief period for introductions, gave his personal view of the history of ISMC. It was founded by division I (Physical and Biophysical Chemistry), II (Inorganic Chemistry) and IV (Polymers) to look for areas of interdivisional cooperation. The first chair, Len Interrante, also pushed for an independent budget but was unsuccessful. As an interdivisional sub-committee, ISMC has no budget and instead depends on 1) occasional project related funding from the founding divisions and 2) funding that can be provided by the projects committee for project proposals. At the moment, ISMC only has support for one funded project, the Materials Chemistry Education Website.

Ober presented a proposed agenda for the meeting. (See meeting slides)

The last meeting of ISMC was arranged for the 2014 San Francisco ACS meeting based on interest by those in attendance at the GA held in Istanbul 2013. Unfortunately, only attendees from Divisions I and IV were present. For this reason it was proposed that the meeting schedule be changed in future (see later in the minutes). Items discussed in San Francisco included the lack of diversity among speakers at the Busan WCC, the need for new projects, progress on the ISMC Educational website, participation from other divisions and better reporting to interested divisions, and better engagement of Young Observers.

In response to the lack of diversity in the preliminary program (many American and Korean men), the organizer of the Materials Chemistry session at the Busan WCC was contacted and a list of 20

potential women speakers from a diverse set of countries was provided. A number of these people were eventually added to the final scientific program at Busan.

Division presidents outside the 3 founding organizations were contacted and representatives from 8 divisions (I, II, III (YO), IV, V, VI, VII, VIII (YO)) attended the IMC meeting as a result. In addition, a general invitation to Young Observers was made and 5 were in attendance.

Ober also pointed out that the IUPAC Centenary (2019). The IUPAC 100 Committee met for the first time in Busan and will work on establishing a set of goals and actions for IUPAC. Possible goals that ISMC might focus on in its future activities include:

- Creating a common language of chemistry
- Better reaching the developing world
- Exciting the public about chemistry and its benefit to society (materials chemistry in particular is excellent for that)
- Use the Centenary to grow resources for ISMC

**ISMC Materials Chemistry website** (Project No. 2013-037-1-200):

The website project was funded as special project with modest contributions by divisions. A dummy website is up and running thanks to Ilya Zharov and his students. Ilya Zharov was unable to attend in person and was brought in to the meeting using Skype. The website is populated with areas where materials chemistry is important. This project is looking for new content and input on how it is organized. All attendees will be contacted and asked to provide input. It is our expectation that this website will go live before the next GA.

The current website address is: http://iupac-materials.chem.utah.edu

Discussion covered organization of the way materials are divided into several categories and subcategories, by now not a part of IUPAC website. Initial thoughts were that there needs to be traditional materials (ceramics, metals, semiconductors and polymers) health needs to be increased in content, catalysts and other categories need more prominence.

A suggestion for new links to the materials chemistry series of articles in PAC (Milan Drabik) could be included and new books should be added.

What videos should this website link to?

And importantly, what should the website NOT do?

All attendees will be contacted for input on the website.

**New projects:**
In order to move forward, the ISMC needs new projects. They should involve 2 or more divisions. Topics suggested at the last meeting of ISMC at the ACS meeting in San Francisco include: energy, sustainability, health, electronics or nanotechnology

Ideas put up for discussions include:

i. ionic liquids – it was noted that similar project already exists
ii. polymer inorganic devices (II,IV)

iii. Biomedical materials (IV, VII)
iv. Nanocomposites and hybrids (I,II, IV)
v. Time release materials
vi. Toxicology, nano and health effects
vii. Div. VIII: mentioned projects on nomenclature project of basic terminology of materials such as carbon nanotubes (ongoing)
viii. Organization of materials according to their "service properties/functions/applications" – proposed
ix. An important question is: How to manage a project proposal?

Concrete proposals included: 1) workshops to be held between divisions to improve an understanding between divisions on areas of interest and cooperation and 2) scientific workshops/symposia on of topics common interest. A goal will be to hold this in Brasil in two years. Ober and Gubala will work on this.

An important discussion was held to include short guides and terminologies of i) polymers (published), ii) inorganic materials - "small red book" about to appear, and iii) to grow the languages available on the educational website. For the short term any website will likely be in English but in the long term the project should be expanded to involve a choice of other languages. Ober will contact all attendees to get additional thoughts on possible projects and to foster several new proposals.

**Staying in contact:**
Ober proposed that given the poor attendance at the last ISMC meeting that in future, face to face meetings would take place at the GA, and that "WebEx" be used for off GA meetings going forward. ISMC would meet twice per year (once at GA and 3 times until following GA via electronic means)
A likely time for these electronic meeting would be during the July-August period and the January-February period each year. Those present agreed to this.

**Rotation in leadership:**
When founded, the chair was Len Interrante (Division II). Subsequently, Ober (Division IV) was elected. Ober suggested that ISMC establish a period of 4 years for ISMC chair and that initially the next chair come from the 3$^{rd}$ founding division, Division I. This was agreed to by those present. Therefore Ober will continue as chair until the Brasil GA in 2017 and will arrange for an election to take place prior to the 2017 meeting.

**Appendix 6**

# An Introduction to IUPAC Projects

Dan Rabinovich
Department of Chemistry
The University of North Carolina at Charlotte

UNC CHARLOTTE

## *IUPAC Projects*

- IUPAC operates using a project-driven system that encourages participation by the worldwide chemistry community:


E.D. Becker *Chem. Internat.* **2001**, *23*, 12.

- Projects should address one of the goals listed in the *IUPAC Strategic Plan*:
  - Related to the needs of the chemists in the *world* (not a country or region).
  - Should be related to the role of chemistry for the needs of mankind.
  - Carried out by an international team of experts (*i.e.*, the Task Group).

# Project Submission and Approval Process

- Anyone or any group may submit a project (4-6 people per Task Group).
- Length: 1-3 years.
- Total budget: $5-9K.
- Use of funds: meetings of the task group (*i.e.*, travel), administrative costs, generation of products (publications, online resources, etc.).
- Submission form and guidelines are available online.
- Project proposal submitted by e-mail to the Secretariat.
- Forwarded to the appropriate Division for peer-reviewing (~4 months).
- Suitable topics:
  - International standardization of nomenclature and terminology
  - Publication of glossaries in particular fields
  - Setting standards for spectral and other data
  - Forging agreement on analytical methods
  - Compilation and evaluation of quantitative data (thermodynamics, kinetics, etc.).

# Project Submission Form

- Project title
- Task group Chair
- Task group members
- Objective and rationale (< 100 words)
- Intended stakeholders
- Dissemination plan
- Intended publications (*e.g.*, PAC)
- Project description (~250 words)
- Time frame
- Milestones
- Criteria for evaluation of outcomes
- Relevant IUPAC bodies
- Suggested referees

*International Union of Pure and Applied Chemistry*

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**PROJECT SUBMISSION FORM**

v. 12/2010

Any individual or group can submit a project, with or without current affiliation with an IUPAC body. Projects can be submitted at any time. For detailed information, see the additional *Guidelines for Completion of the Project Submission Form*. Frequently Asked Questions on *Project Submission and Approval Process* are also available on the Union's web site at <http://www.iupac.org/projects/>.

This form should be completed with a word processor and returned to the IUPAC Secretariat, preferably as an e-mail attachment to <secretariat@iupac.org>. Please do not remove section headers and answer all questions; indicate NA when a question does not apply to the proposal.

| *for administrative use only* | *Submitted* _____ ; # _____ |
|---|---|
| **Date** | |
| **Project Title** | |
| Series Title (*if applicable*) | |
| **Task Group Chair** | (include address and e-mail) |
| **Task Group Members** | (include address and e-mail) |
| **Name of the person submitting this form** (*if not the proposed Task Group Chair*) | (include address and e-mail) |
| **Objectives and Rationale** (This should summarize the principal objectives and rationale, and the intended outcomes.) (*see Guidelines*) | (<100 words) |
| **Intended Stakeholders:** (Give details of the intended stakeholders and interest groups, and how they will benefit from your Project Objectives.) (*see Guidelines*) | (<100 words) |
| **Dissemination Plan** (Indicate how the results of this Project will be communicated to target stakeholders and, if relevant (e.g. for IUPAC Recommendations), how the Task Group will involve stakeholders in the refinement of Project outcomes.) (*see Guidelines*) | |
| **Intended Publication:** (please tick boxes) (*see Guidelines*) | IUPAC Recommendation ☐<br>IUPAC Technical Report ☐<br>Other type of manuscript to be published in a journal other than *Pure and Applied Chemistry* ☐ |

**Appendix 7**

# IUPAC Division II - Inorganic Chemistry Review of Projects

Dan Rabinovich

Department of Chemistry
The University of North Carolina at Charlotte, USA


IUPAC Division II meeting, Busan
9 August 2015

## Outline

- **Completed** Projects
- Status Report on **Active** Projects (*Continuing* and *New*)
- Update on **Pending** Proposals: *Peer-Reviewed* (Awaiting Funding)
- Update on **Pending** Proposals: Undergoing Peer-Review
- Update on Proposals in **Preparation**

# **Completed** Projects

(August 2014 – July 2015)

No projects were *completed* during this period

# Status Report on **Active** Projects

- **2008-040-1-200**
- TGC: Pavel Karen (University of Oslo)
- TG: McArdle, Takats & Tatsumi
- Towards a Comprehensive Definition of Oxidation State
- Budget: USD 4,200; spent: USD 0; balance: USD 4,200.
- Div. II monitor: Holden
- Updates:

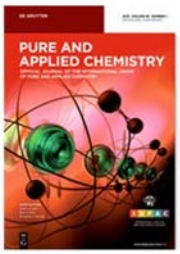
**September 2011**
The experimental part of the project is finished (the research, analysis, data gathering, calculations, and discussions of about 100 examples among 3 task group members). The write-up of the Technical Report (TR) is currently almost complete and being refined. Write-up of a Recommendation will be started soon. Write-up of a pedagogical summary for *Journal of Chemical Education will be commenced soon.*

**June 2013**
The intended new TR sections were written and the TR manuscript was published on April 24 at the IUPAC discussion forum. Some aspects were discussed with two division members and the Division VIII Chair, R. Hartshorn. On May 31, the TR manuscript was submitted to PAC. A no-cost extension was requested on 6 June 2013 (new expected end date: 1 March 2014).

*(cont…)*

**March 2014**

A revised manuscript of the Technical Report was submitted to PAC on 24 September 2013. On 7 January 2014 the manuscript was accepted for publication and is currently *in press* [to be published probably in volume 86, issue no. 4, April 2014].




**June 2014**

Technical Report published (*Pure Appl. Chem.* **2014**, *86*, 1017-81) and key concepts added to the Wikipedia entry for *oxidation state*.

DE GRUYTER DOI 10.1515/pac-2013-0505 — Pure Appl. Chem. 2014; 86(6): 1017–1081

IUPAC Technical Report

Pavel Karen*, Patrick McArdle and Josef Takats

**Toward a comprehensive definition of oxidation state (IUPAC Technical Report)**

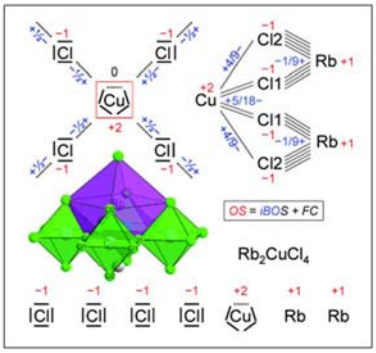
**29 July 2014**

Remaining tasks include making changes to the IUPAC entries in the Gold Book, the publication of recommendations in *PAC*, and writing an article about oxidation state in teaching for the *Journal of Chemical Education*. An additional extension until the end of 2015 will most likely be requested.

*(cont…)*

**10 March 2015**

Invited essay ("Oxidation State, a Long-Standing Issue!") published in *Angew. Chem. Int. Ed.* **2015**, *54*, 4716-4726.
*[open access]*




**27 July 2015** *(Pavel Karen)*:

A final 6-month extension will probably be required (and requested) for the conclusion of the proposed outcomes (e.g., Gold Book entries, JCE article).

Start date: 1 January 2009
Planned end date: 31 December 2015

- **2009-023-1-200**
- TGC: Michael Wieser (U. of Calgary)
- TG: de Laeter, Hirata & Schönberg
- Evaluation of Radiogenic Abundance Variations in Selected Elements
- Budget: USD 8,500; spent: USD 3,340; balance: USD 5,160.
- Div. II monitor: Loss
- Updates:

**September 8, 2012:**

The isotopic abundance variations of the radiogenic elements Re, Os, Rb, Sr, K, Nd, Sm, Hf, Lu, and Ar are being evaluated to determine the variability of the atomic weight. These data will be incorporated in the Commission's Technical Report of the Table of Standard Atomic Weights. The evaluation of Ar is complete and was approved by the Commission at the Calgary meeting in 2011 for incorporation in the Table of Standard Atomic Weights 2011, to be published this year. The reports on the remaining elements are still in progress and will be presented to the Commission for approval at the upcoming Commission meeting in 2013.

*(cont…)*

**July 2014** (*Juris Meija & Thomas Prohaska, CIAAW*)**:**

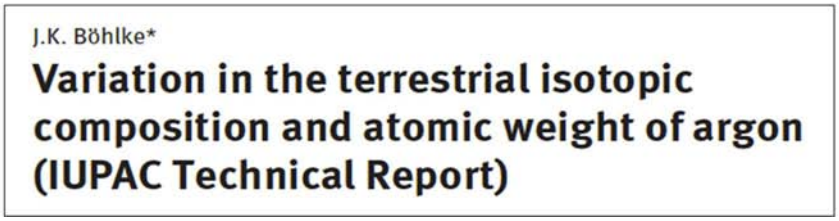
Commission on Isotopic Abundances and Atomic Weights (CIAAW) will request a no-cost extension and strive to complete the project during its next annual meeting.

**24 July 2014** (*Michael Wieser, TGC*)**:**

J.K. Böhlke has authored a report on Ar. The manuscript was submitted to *PAC* and is *in press*. Literature reviews are complete for Sr and a report is in preparation. Literature reviews for the remaining elements (Re, Os, Rb, K, Nd, Sm, HF, and Lu) are in progress. The goal is to have this work complete for the next CIAAW meeting and incorporate it in TSAW2015.

**4 August 2015** (*Wieser*)**:**

J.K. Böhlke's IUPAC Technical Report was published in: *Pure Appl. Chem.* **2014**, *86*, 1421-1432.



**4 August 2015** (*Wieser*)**:**

Three TG members (de Laeter, Hirata & Schönberg) are no longer active. A request to add three new TG members (Zhu, Irrgeher & Walczyk) has been made.

**6 August 2015** (*Meija & Prohaska*)**:**

A set of elements that need further investigation was identified and current work is undertaken to review the radiogenic variation on a number of elements such as Ar, He, Sr, Rb, Hf and Pb; a no-cost extension will be requested in the near future.

## Planned end date: 31 December 2015

- **2009-026-2-200**
- (new)TGC: Juris Meija (National Research Council Canada)
- TG: Böhlke, Gröning, Loss, Wieser & Prohaska
- Online Evaluated Isotope Ratio Database for User Communities
- Budget: USD 6,000; spent: USD 0; balance: USD 6,000.
- Div. II monitor: Loss
- Updates:

**August 2013** (*Bob Loss*):
The TGC and a TG member are no longer involved in the project; alternative contributors are currently being sought and will hopefully allow completion of the project in a timely fashion.

**July 2014** (*Juris Meija & Thomas Prohaska, CIAAW*)**:**
Due to the inactivity of key TG members, and in consultation with the current TGC, the Commission on Isotopic Abundances and Atomic Weights (CIAAW) would like to request to: (1) change the TG Chairmanship to J. Meija, (2) remove R. Kessel from the TG, and (3) add T. Prohaska to the TG. The CIAAW has discussed the project and is prepared to deliver the project by its next annual meeting. It would also like to request a no-cost extension of the project deadline.

**November 2014**
A new task group has been established and a timeline revised.
Key aim: to establish a database for the CIAAW.

*(cont…)*

**November 2014**
The task group will produce a prototype online database by 2015 CIAAW meeting and be trialed by the other task group members shortly afterwards. The initial prototype will focus on data entry, retrieval, access control, archiving and version control. In 2016, prototype output filters will be developed and tested by TG members. For example, users will be able to specify whether they would like specific isotope data for many elements or all accessible data for a single element.

Following testing the task group will make the necessary changes and adjustments as required and make it available for use by CIAAW members for entry of the 2017 TSAW and TICE data. It is anticipated that new online database will be approved and recommended for open use by the wider community in the summer of 2016 and publicized via the IUPAC website.

**6 August 2015** (*Meija*)**:**
An electronic database hosted by CIAAW and a prototype web interface were set up in early 2015 (www.ciaaw.org/database).

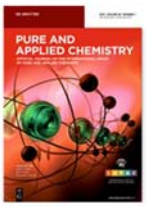
Start date: 1 April 2011
Planned end date: 1 April 2016

- **2009-027-1-200**
- TGC: Willi Brand (Max Planck Institute for Biogeochemistry)
- TG: Böhlke, Coplen, Brand, Gonfiantini, Gröning, Qi & Vocke
- Assessment of Stable Isotopic Reference and Inter-Comparison Materials
- Budget: USD 9,600; spent: USD 8,157; balance: USD 1,443.
- Div. II monitor: Loss
- Updates:

September 2010 – project announcement published in *Chem. Int.* Sep-Oct, p. 23

**8 August 2013** (*Juris Meija*):
Draft manuscript was circulated to all members of the Subcommission in July 2013. Task group members met during the CIAAW meeting in Aug. 2013 and made considerable progress towards the completion of the project. Completion of the project and publication in PAC is expected shortly.

**20 March 2014**:
Technical report published:
Brand, W. A.; Coplen, T. B.; Vogl, J.; Rosner, M.; Prohaska, T. *Pure Appl. Chem.* **2014**, *86*, 425-467.




*(cont…)*

**16 May 2014**:
Request from TGC for a no-cost extension to pay the cost of attendance of Haiping Qi (USGS) to a meeting on new stable isotope reference materials at the IAEA headquarters in September, 2014.

**July 2014** (*Juris Meija & Thomas Prohaska, CIAAW*):

The TG is meeting in September 2014 at the IAEA (Vienna) for closing of the project.

*No updates to report*

Planned end date: 30 September 2014

- **2009-045-1-200**
- TGC: Hitoshi Ishida (Kitasato University)
- TG: Beeby, Bunzli, Campagna, De Cola, Ford, Gordon, Hasegawa, Hasegawa, Katoh, Keene, McCusker, Nozaki, Sakai, Tobita, Vlcek & Yam
- Guidelines for Measurement of Luminescence Spectra and Quantum Yields of Inorganic Compounds, Metal Complexes and Materials
- Budget: USD 8,000; spent: USD 0; balance: USD 8,000.
- Div. II monitor: Sakai
- Updates:

**July 2010 - project announcement published in** *Chem. Int.* Jul-Aug, p. 21

- A draft of the report has not been prepared yet but hopefully will within the next 2 months (Beeby, Bunzli & Ishida).
- Workshop at an international photochemistry conference such as the International Symposium on the Photochemistry and Photophysics of Coordination Compounds (ISPPCC) is being planned.

*(cont…)*

- Updates:

**Ishida e-mail message** (9 August 2013):

Re: IUPAC Div II project 2009-045-1-200

ishida@sci.kitasato-u.ac.jp

To: Rabinovich, Dan

Cc: ishida@sci.kitasato-u.ac.jp

Dear Don:

I am so sorry that I have not sent any report and updated information. We actually had stopped the project work, but we have recently discussed on the work and we again recognize it as an important work for the inorganic chemists who measure the emission spectra and quantum yields of inorganic compounds. Actually, I was consulted by such inorganic chemists in the USA, and I and my coworker measured their samples.

I hope we will continue the project, or restart it in near future. Anyway, I will report the update informational.

Best regards.

Hitoshi

*(cont…)*

- Updates:

**Ishida e-mail message** (11 March 2014):

- A draft of the report on guidelines for the measurement of luminescent spectra and quantum yields has been written by Beeby, Bunzli & Ishida and will be circulated among Task Group members in April 2014, then forwarded to all the Division II members.
- Request to hold workshop at the Pacifichem 2015 conference (Dec. 2015) was declined and TGC was urged to complete submission of manuscript as soon as possible (by July 1st?).

**July 2014** (*Ken Sakai*)**:**

The manuscript has been completed and will soon be submitted to *Pure and Applied Chemistry*. One (last?) no-cost extension will be requested soon.

*No updates to report*

Start date: 1 May 2010
Planned end date: 31 December 2011

- **2009-046-2-200**
- TGC: Jan Kaiser (University of East Anglia)
- TG: Angert, Berquist, Brand, Ono, Röckmann & Savarino
- Terminology and Definition of Quantities Related to the Isotope Distribution in Elements with More than Two Stable Isotopes
- Budget: USD 6,000; spent: USD 188; balance: USD 5,812.
- Div. II monitor: Rabinovich
- Updates:

**September 2010 - project announcement published in Chem. Int. Sep-Oct, p. 23**

- Poster presented at the General Assembly of the European Geosciences Union in Vienna (April 2012).
- Talk on the project presented to a meeting of Ph.D. students and supervisors at the Marie Curie Initial Training Network (INTRMIF).

**11 August 2013** (*Dan Rabinovich*)**:**

The TG will have another informal meeting during the Goldschmidt Conference in Florence (25-30 August 2013) with the goal of agreeing on a definition of the triple isotope excess.

*(cont…)*

**May 2014** (*Juris Meija*)**:**

A (preliminary) project report was published online:
http://adsabs.harvard.edu/abs/2014EGUGA..1616810K

**24 July 2014** (*Dan Rabinovich*)**:**

The TGC gave a presentation on the project at the European Geosciences Union (EGU) meeting in Vienna in 2014, and continued to discuss the draft definition with colleagues and TG members at an isotope meeting in Tokyo in July 2014. A no-cost extension will be requested in due course.

*No updates to report*

Start date: 1 July 2010
Planned end date: 30 June 2016

- **2011-026-1-200**
- TGC: Michael Wieser (U. of Calgary)
- TG: Schönberg, Zhu, Gröning & Meija
- Full Calibration of a New Molybdenum Isotopic Reference Material
- Requested budget: USD 10,200; spent: USD 0; balance: USD 10,200.
- Div. II monitor: Loss
- Updates:

**24 July 2014** (*Michael Wieser, TGC*)**:**

An isotopic composition and atomic weight analysis of Mo in the NIST standard solution SRM 3134 was completed and published in the *Journal of Analytical Atomic Spectrometry* (DOI: 10.1039/C3JA50164G). This report was evaluated by the CIAAW in 2013 and is the basis for the new recommended atomic weight of Mo. In addition, the relative isotopic composition of a laboratory Mo solution and Johnson-Matthey metal rod were also reported. Work is now ongoing to incorporate similar determinations in two additional laboratories, as described in the project proposal.

*(cont…)*

**4 August 2015** (*Michael Wieser, TGC*)**:**

Members of TG evaluated two very important publications reporting on the calibration of the isotopic composition of the atomic weights and isotopic compositions of molybdenum reference materials, specifically:

> Mayer, A.J.; Wieser, M.E. The absolute isotopic composition and atomic weight of molybdenum in SRM 3134 using an isotopic double spike. *J. Anal. At. Spectrom.* **2014**, *29*, 85.
>
> Malinovsky, D.; Dunn, P.J.; Petrov, P.; Goenagga-Infante, H. Investigation of mass dependence effects for the accurate determination of molybdenum isotope amount ratios by MCICPMS using synthetic isotope mixtures. *Anal. Bioanal. Chem.* **2014**, *407*, 869.

Results to date indicate that the NIST SRM 3134 now has a reliable absolute isotopic composition and atomic weight and demonstrate that, for the materials investigated so far, isotopic variability is the result of mass dependent fractionation processes.

Since one of the TG members (Schönberg) is no longer able to participate, the addition of a new TG member (Irrgeher) and a no cost extension (until Dec. '17) have been requested.

Start date: 1 December 2012
Planned end date: 31 December 2015

- **2011-027-1-200**
- TGC: Ronny Schönberg (Institute for Geosciences, U. of Tübingen)
- TG: Böhlke, Brand, Berglund, Coplen, De Bievre, Ding, Gröning, Hirata, Holden, Loss, Meija, Prohaska, Singleton, Walczyk, Wieser, Yoneda & Zhu
- Evaluated Published Isotope Ratio Data (2011-2013)
- Budget: USD 19,400 (USD 6,695 from Division II; USD 12,705 from Project Committee); spent: USD 10,130; balance: USD 9,270.
- Div. II monitor: Walczyk
- Updates:

**8 August 2013** (*Juris Meija*):
The Subcommission on Isotopic Abundance Measurements (SIAM) met in Gebze, Turkey, on August 4-5, and evaluated published isotope ratio data. SIAM made the recommendations to the CIAAW, which were accepted during the 2013 CIAAW meeting. The IUPAC Table of Isotopic Composition of the Elements 2013 will be published in *Pure and Applied Chemistry* in 2014.

**July 2014** (*Juris Meija & Thomas Prohaska, CIAAW*):
Production of TICE-2013 is well-underway and the project is expected to be completed shortly; a no-cost extension will be requested.

*(cont…)*

**28 July 2015** (*Ty Coplen*):

An IUPAC Technical Report ("Isotopic Compositions of the Elements 2013") has been submitted to PAC and will be accepted for publication after a few corrections are made based on referees' comments and suggestions.

Start date: 3 January 2012
Planned end date: 31 December 2014

- **2011-028-1-200**
- TGC: Xiang-Kun Zhu (Chinese Academy of Geological Sciences)
- TG: Holden, Hirata & Prohaska
- Evaluation of Published Lead Isotopic Data (1950-2013) for a New Standard Atomic Weight of Lead
- Budget: USD 6,400; spent: USD 0; balance: USD 6,400.
- Div. II monitor: Ding
- Updates:

**8 August 2013** (*Juris Meija*):
The task group chairman presented the draft report to the CIAAW members during the 2011 Calgary meeting. Significant progress has been made in this project and the follow-up progress report was expected during the 2013 CIAAW meeting, however, the task group Chairman was unable to attend the meeting due to visa problems.

**July 2014** (*Juris Meija & Thomas Prohaska, CIAAW*):
No updates available due to communication problems. Division II monitor (Tiping Ding) will contact TGC for updates and to ask him to request a no-cost extension.

*(cont…)*

**July 2014** (*Juris Meija & Thomas Prohaska, CIAAW*):
No updates available due to communication problems. Division II monitor (Tiping Ding) will contact TGC for updates and to ask him to request a no-cost extension.

**6 August 2015** (*Juris Meija & Thomas Prohaska, CIAAW*):
Almost 6,000 data entries have been evaluated so far; the compiled data was discussed during the 2015 CIAAW meeting. Based on the results (and those of Project 2009-023-1-200, TGC: Wieser), a discussion on how to implement the large variation and time shift of radiogenic isotopes in the consideration of standard atomic weights will de described in a publication.

Start date: 1 April 2012
Planned end date: 1 Mar 2014

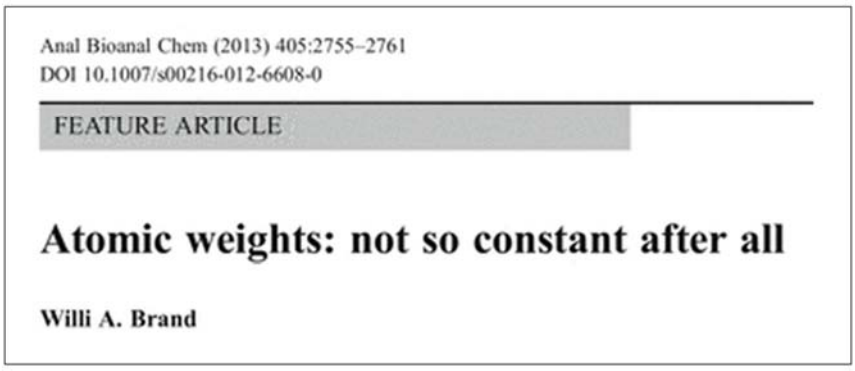
- **2011-040-2-200**
- TGC: Willi A. Brand (Max Planck Institute for Biogeochemistry)
- TG: Meija, Milton & Wieser
- Development a Procedure for Using Intervals Instead of Fixed Values for Atomic Weights; an Educational Exercise
- Budget: USD 7,400; spent: USD 1,300; balance: USD 6,100.
- Div. II monitor: Holden
- Updates:

**8 August 2013** (*Juris Meija*):
The task group members have been working to solicit the wider opinion of the scientific community, in particular, the opinion of several ISO Technical Committees, and that of the JCGM WG-1 (BIPM). Position paper will be formulated after careful consideration of the presented advice and opinions.

**July 2014** (*Juris Meija & Thomas Prohaska, CIAAW*):
The project has been delayed to ensure concerted efforts with Project 2013-032-1-200 (TGC: van der Veen). Together with BIPM and JCGM, work is well-underway to generate a manuscript by the end of 2014; a no-cost extension will be requested.

*(cont…)*

**6 August 2015** (*Juris Meija & Thomas Prohaska, CIAAW*):
A feature article ["Atomic Weights: Not So Constant After All"] was published in *Anal. Bioanal. Chem.* **2013**, *405*, 2755-2761.


Anal Bioanal Chem (2013) 405:2755–2761
DOI 10.1007/s00216-012-6608-0

FEATURE ARTICLE

**Atomic weights: not so constant after all**

**Willi A. Brand**

Start date: 1 April 2012
Planned end date: 1 March 2015

- **2012-036-2-200**
- TGC: Igor M. Villa (Institut für Geologie, Bern, Switzerland)
- TG: De Bievre, Holden & Renne
- Recommendations for Isotope Data in the Geosciences II
- Focus on four nuclides used in geochronology: $^{40}K$, $^{87}Rb$, $^{176}Lu$ and $^{187}Re$.
- Requested budget: USD 9,000; balance: USD 9,000.
- Div. II monitor: Walczyk
- Updates:

**September 2013** (*Fabienne Meyers, IUPAC*)**:**
The proposal gained support from Divisons II and V and from the Project Committee and was approved shortly thereafter.

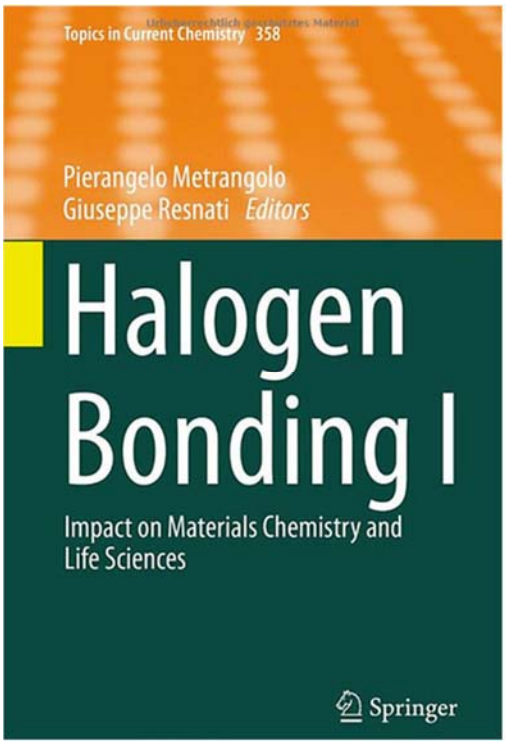
*No updates to report*

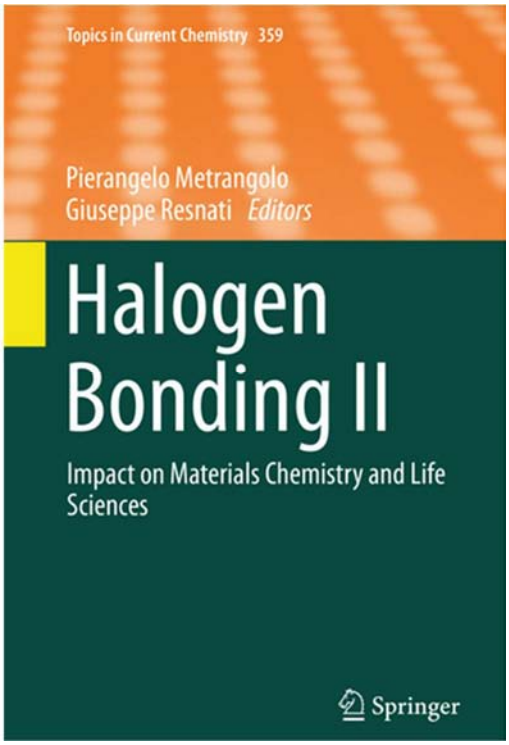
Submitted: 12 July 2013
Start date: 1 October 2013
Planned end date: 31 December 2016

- **2012-044-1-100**
- TGC: Pierangelo Metrangolo & Giuseppe Resnati (NFMLab, Milano)
- TG: Aakeröy, Gao, Barbour, Nangia, Ogawa, Öhrström, Guru Row, Rogers, Zaworotko, Bernstein, Hosseini, Seddon, Desiraju, Bacchi, Rissanen & Reutzel-Edens
- Basic Terminology of Crystal Engineering
- Div. II monitor: Öhrström
- Updates:
  - Original proposal submitted to Div. II, III & VIII
  - Approved and funded by **Div. I** (USD 10,000)
  - Div. II is interested in contributing to the project *[action item from Istanbul meeting]* → *???*

*No updates to report*

Submitted: 1 November 2012
Start date: 1 February 2013
Planned end date: 31 December 2014




- **2012-045-1-800**
- TGC: Michael A. Beckett (Bangor University, UK)
- TG: Brellochs, Chizhevsky, Damhus, Kennedy, Laitinen, Powell, Rabinovich, Viñas & Yerin
- Nomenclature for polyhedral boranes and related compounds
- Budget: USD 7,205; spent: USD 3,009; balance: USD 4,196.
- Div. II monitor: Rabinovich
- Updates:
  - Original proposal submitted to Div. VIII (Chemical Nomenclature and Structure Representation)
  - USD 1,000 contribution from Div. II *[31 January 2013]*
  - Funded by **Project Committee**
  - Dan Rabinovich (USA) representative from Div. II and TG member

**April-May 2014** (*Beckett, TGC*):
A preliminary Technical Report has been drafted and TG members have been charged with investigating the more challenging aspects of the project. The TG will will during the Imeboron 15 meeting in Prague (24-28 August 2014) and the TGC will present a poster with highlights of the project.

**May-August 2015** (*Rabinovich*):
Draft of Technical Report continues to be revised; most recent version will be discussed during the IUPAC General Assembly in Busan.

**(Complete draft 210715) Nomenclature for boron hydride and related species. (IUPAC Recommendations)***

Michael A Beckett[1,*], Bernd Brellochs[2], Igor T Chizhevsky[3], Ture Damhus[4], John D Kennedy[5], Risto Laitinen[6], Warren H Powell[7], Daniel Rabinovich[8], Clara Viñas[9], Andrey Yerin[10].

*[1]School of Chemistry, Bangor University, UK; [2]BHH, Germany; [3]INEOS, Russian Academy of Sciences, Moscow, Russia; [4]NovoZymes A/S, Bagsvaerd, Denmark; [5]School of Chemistry, Leeds University, Leeds, UK University of Leeds, UK and the Institute of Inorganic Chemistry of the Czech Academy of Sciences, Řež u Prahy, The Czech Republic; [6]Oulu University, Finland; [7]Columbus, USA; [8]Charlotte, NC, USA, [9]Institut de Ciencia de Materials de Barcelona (CSIC), Bellaterra, Spain; [10]Advanced Chemistry Development, Moscow, Russia.*

Submitted: 5 November 2012
Start date: 1 February 2013
Planned end date: 31 December 2015

- **2012-046-2-800**
- TGC: Hinnerk Rey (Elsevier Information Systems GmbH, Frankfurt am Main, Germany)
- TG: Druckenbrodt, Hartshorn, Damhus, Schenk & Sitzmann
- Handling of Inorganic compounds for InChI V2
- Requested budget: USD 10,000; approved for USD 5,000
- Div. II monitor: Mathur
- Updates:
  - Original proposal submitted to Div. VIII (Chemical Nomenclature and Structure Representation)
  - Recommended for funding by the **Project Committee**
  - Sanjay Mathur (Köln) representative from Div. II and TG member
  - $1,500 co-funding from Div. II

*No updates to report*

Submitted: 15 November 2012
Start date: 1 March 2013
Planned end date: 30 June 2015

- **2013-030-1-800**
- TGC: Alan T. Hutton (U. of Cape Town)
- TG: Constable, Laitinen, Nordlander, Powell & Rabinovich
- Nomenclature for metallacycles containing transition metals
- Budget: USD 13,720; spent: USD 1,520; balance: USD 12,200.
- Div. II monitor: Rabinovich
- Updates:
  - Original proposal submitted to Div. VIII (Chemical Nomenclature and Structure Representation)
  - Funded by **Project Committee**
  - Dan Rabinovich (USA) representative from Div. II and TG member
  - Contribution of USD 1,000 from Div. II

**June 2014** (*Hutton, TGC*):
TG will meet and discuss the project during the Div. VIII "off-year" meeting, to take place in Bangor, Wales, UK, on 3-4 August 2014.

**8 August 2015** (*Rabinovich*):
TG met during the General Assembly in Busan (South Korea) to discuss and update the latest version of a manuscript to be submitted to PAC:

*(cont…)*

# Nomenclature for Metallacycles Containing d-Block Elements

# (IUPAC Recommendation)

Alan T. Hutton*[1], Edwin C. Constable[2], Risto Laitinen[3], Ebbe Nordlander[4], Warren H. Powell[5], Daniel Rabinovich[6]

*[1]Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa; [2]Department of Chemistry, University of Basel, Spitalstrasse 51, CH-4056 Basel, Switzerland; [3]University of Oulu, PO Box 3000, FIN-90014, Finland; [4]Centre for Chemistry and Chemical Engineering, Lund University, Box 124,SE-22100, Sweden; [5]1436 Havencrest Court, Columbus, OH 43220-3841, USA; [6]University of North Carolina, Charlotte, NC, USA.*
**E-mail: inorganic.nomenclature@iupac.org. Sponsoring body: IUPAC Division of Chemical Nomenclature and Structure Representation.*

Submitted: 5 June 2013
Start date: 1 July 2013
Planned end date: 31 December 2015

*(cont…)*

- **2013-032-1-200**
- TGC: Adriaan van der Veen (VSL = Dutch Metrology Institute)
- TG: Possolo, Meija & Hibbert
- Guidelines for the Derivation of Values and Uncertainties from Standard Atomic Weight Intervals
- Budget: USD 5,000; spent: USD 1,849; balance: USD 3,151.
- Div. II monitor: Wieser
- Updates:
  - Original proposal submitted to **Div. II**
  - Complementary to 2011-040-2-200 (TGC = W. A. Brand)
  - Interest from Commission I.1 *[Kaoru Yamanouchi]*
  - 4 favorable reviews [Rev1,V,VIII,Rev2] & 1 unfavorable review [Rev3]
  - No interest from CCE *[Mustafa Sözbilir, 8 July 2013]*

**6 August 2015** (*Juris Meija & Thomas Prohaska, CIAAW*):
Two publications are currently under review by the TG members and associated experts.

Submitted: 1 July 2013
Start date: 1 September 2013
Planned end date: 1 October 2015

- **2013-037-1-200**
- TGC: Christopher Ober (Cornell University, Ithaca, NY, USA)
- TG: García-Martínez, Jones, Mathur, Wilson & Zharov
- Creating Educational Website for Materials Chemistry
- Budget: USD 6,000 ($1,000 from Div. II); spent: USD 0; balance: USD 6,000.
- Div. II monitor: Mathur
- Updates:
  - Original proposal submitted to Div. I, II & IV
  - Very good internal reviews.
  - External reviews needed/required.
  - 25-July-2014 *(Singapore meeting)*: project was been funded.

*No updates to report*

Submitted: 22 July 2013
Start date: 1 October 2013
Planned end date: 1 October 2016

- **2014-001-2-200**
- TGC: Lars Öhrström (Chalmers U. of Technology, Sweden)
- TG: O'Keefe, Bourne, Proserpio, Blatov, Lah, Eon, García-Martínez, Batten, Hyde & Wiggin
- Terminology Guidelines and Database Issues for Topology Representations in Coordination Networks, Metal-Organic Frameworks and Other Crystalline Materials
- Budget: USD 9,000; spent: USD 0; balance: USD 9,000.
- Div. II monitor: Sakai
- Updates:
  - 25-July-2014 *(Singapore meeting)*: project was been funded.
  - Funding: USD 2,000 ea. from Divisions I (Physical and Biophysical Chemistry) and VIII (Chemical Nomenclature and Structure Representation); USD 5,000 from Division II.
  - USD 6,000 also provided by the Samara Center for Theoretical Material Science.

Submitted: 2 February 2014
Start date: 12 June 2014
Planned end date: 31 December 2016


- **2014-002-1-200**
- TGC: Manfred Gröning (IAEA, Vienna, Austria)
- TG: Brand, Coplen, Irrgeher, Prohaska, Vogl, Wang & Wieser
- Assessment of Stable Isotopic Reference Materials *[Follow-up to project 2009-027-1-200 (TGC: Willi Brand, CIAAW)]*.
- Budget: USD 7,100; spent: USD 0; balance: USD 7,100.
- Div. II monitor: Loss
- Updates:
  - Original proposal submitted to Div. II
  - 7 favorable reviews received from Div. II and Div. V (Anal. Chemistry)
  - TGC provided detailed response to minor issues raised by reviewers
  - Co-funded by the Divisions of Analytical Chemistry (Division V) and Chemistry and the Environment (Division VI).

**6 August 2015** (*Juris Meija & Thomas Prohaska, CIAAW*):
As a follow-up to Project 2009-027-1-200, a first round of compilation of new data has been obtained and should be complete by the end of the year; additional reference materials were identified during the 2015 CIAAW meeting.

Submitted: 10 January 2014
Start date: 1 August 2014
Planned end date: 31 July 2016

- **2014-016-2-200**
- TGC: Thomas Prohaska (University of Natural Resources and Life Sciences, Vienna)
- TG: Irrgeher, Coplen, Wieser & Vogl
- Compilation of the Variation of the Isotopic Composition of the Elements via Crowdsourcing
- Budget: USD 9,150; spent: USD 0; balance: USD 9,150.
- Div. II monitor: ???
- Updates:
  - Original proposal submitted to **Div. II**
  - 7 favorable reviews received from Div. II and Div. V (Anal. Chemistry)
  - TGC provided detailed response to minor issues raised by reviewers
  - Approved on **15 December 2014**
  - Co-funded by the Divisions of Analytical Chemistry (Division V) and Chemistry and the Environment (Division VI).

NEW

*(cont…)*

**6 August 2015** (*Juris Meija & Thomas Prohaska, CIAAW*)**:**

As a follow-up to Project 2009-027-1-200, a first round of compilation of new data has been obtained and should be complete by the end of the year; additional reference materials were identified during the 2015 CIAAW meeting.

The TG will collaborate closely with Project 2009-026-2-200 (TGC: Meija) in order to install a proper database.

Submitted: 13 May 2014
Start date: 15 December 2014
Planned end date: 31 December 2016

- **2014-024-1-200**
- TGC: Norman Holden (National Nuclear Data Center, Brookhaven National Laboratory, NY, USA) & Peter Mahaffy (King's University College, Edmonton, Canada)
- TG: Apotheker, Coplen, Hoffman, Martin, Tarbox, Walczyk & Wieser
- Development and Global Dissemination of an IUPAC Interactive Electronic Isotopic Periodic Table and Supporting Resources for the Education Community
- Budget: USD 14,000; spent: USD 0; balance: USD 14,000.
- Div. II monitor: Rabinovich
- Updates:
  - Original proposal submitted to **Div. II** and **CCE**
  - Revised version of 2012-016-1
  - Co-funded by Division II (USD 4,000), CCE (USD 4,000), and the Project Committee (USD 6,000)

NEW

*(cont…)*

**6 August 2015** (*Juris Meija & Thomas Prohaska, CIAAW*)**:**

The work on the IPTI-2 started on 14 May 2015 with a conference call between the TGCs, TG member Coplen, and two students of TGC Mahaffy to review the objectives of the project.

Submitted: 27 June 2014
Start date: 1 October 2014
Planned end date: 1 September 2017

## Update on **Pending** Proposals: Peer-Reviewed (Awaiting Funding)

(August 2014 – July 2015)

No projects in this category during this period

## Update on **Pending** Proposals: Undergoing Peer-Review

- **2015-002-1-xxx**
- TGC: Rustem Valiullin (Faculty of Physics and Earth Sciences, University of Leipzig, Germany)
- TG: Kärger, Ruthven, Jobic, LeVan, Brandani, Coppens, Farooq, Stepanov & Ravikovitch
- Diffusion in Nanoporous Solids
- Requested budget: USD 10,000
- Div. II monitor: ???
- Updates:
  - For consideration by the Divisions of Physical and Biophysical Chemistry (Div. I), Inorganic Chemistry (Div. II) and Analytical Chemistry (Div. V).

NEW

*Proposal under review*

Submitted: 26 January 2015
Start date: xx yyyy zzzz
Planned end date: ???

## Update on Proposals **in Preparation**

- **2015-xxx-1-xxx**
- TGC: Norman Holden (Brookhaven National Laboratory)
- TG: Coplen, de Bievre, Wieser & Böhlke
- Assessment of Fundamental Understanding of Isotopic Abundances and Atomic Weights of the Chemical Elements (2016—2017)
- Requested budget: USD 5,000
- Div. II monitor: ???
- Updates:
  - Proposal draft completed, to be submitted to Div. II

Review fundamental issues and concerns that have been raised by members of the Commission on Isotopic Abundances and Atomic Weights (CIAAW). Discuss the issues and present the recommendations to CIAAW to help provide a future direction for work on isotopic abundances and atomic weights of the chemical elements.

*Proposal in preparation*

Submitted: xx yyyy 2015
Start date: xx yyyy zzzz
Planned end date: ???

- **2014-xxx-1-xxx**
- TGC (?): Christopher Ober (Cornell University, Ithaca, NY, USA)
- TG (?): xxxx
- Terminology of Nanomaterials and Nanotechnology in Materials Chemistry
- Requested budget: USD xxxx
- Div. II monitor: ???
- Updates:
  - To be submitted to Divisions II and V (?)

*Proposal in preparation (?)*

Submitted: xx yyyy zzzz
Start date: xx yyyy zzzz
Planned end date: ???

- **2014-xxx-1-xxx**
- TGC (?): Roman Boca (Slovak University of Technology, Bratislava, Slovakia) and Javier García-Martínez (U. of Alicante)
- TG (?): Dunbar, Gómez-García, Clerac & Herchel
- Magnetic Information File for Magnetochemistry
- Requested budget: USD xxxx
- Div. II monitor: ???
- Updates:
  - To be submitted to Divisions II and V (?)

*Proposal in preparation (?)*

Submitted: xx yyyy zzzz
Start date: xx yyyy zzzz
Planned end date: ???

- **2016-xxx-1-xxx**
- TGC: Daniel Rabinovich (UNC Charlotte)
- TG: Verani (Wayne State U.), Lim (UNIST), García-Martínez (?), others…
- The Periodic Table of Life
- Requested budget: USD xxxx
- Div. II monitor: ???
- Updates:
  - To be submitted to Division II & CCE

*Proposal in preparation*

Submitted: xx January 2016 (?)
Start date: 1 July 2016 (?)
Planned end date: xx yyyyyyy zzzz(?)

- **2016-xxx-1-xxx**
- TGC: Pavel Karen (University of Oslo)
- TG: Rabinovich, García-Martínez (?), Tshuva (?), Leskelä (?), others...???
- Towards a Comprehensive Definition of Valence
- Requested budget: USD xxxx
- Div. II monitor: ???
- Updates:
  - To be submitted to Division II

*Proposal in preparation*

Submitted: xx January 2016 (?)
Start date: 1 July 2016 (?)
Planned end date: 31 December 2019 (?)

- **2016-xxx-1-xxx**
- TGC: Robin Macaluso (University of Texas at Arlington)
- TG: Melanie Kirkham (ORNL), Cora Lind-Kovacs (Toledo), Leopoldo Suescun (U. of the Republic, Uruguay), Rabinovich (?), García-Martínez (?), others...???
- Classification of Solid State Compounds
- Classification of solid state materials based on chemical bonding (rather than physical behavior…)
- Requested budget: USD xxxx
- Div. II monitor: ???
- Updates:
  - To be submitted to Divisions II & VIII

*Proposal in preparation*

Submitted: xx January 2016 (?)
Start date: 1 July 2016 (?)
Planned end date: 31 December 2019 (?)

# Project Expenses *vs* Budget (as of 11 June 2015)

| Project Numbers | Total Project Budget | 2015 Starting Balance | 2015 Spent | Remaining Funds | Planned End Date |
|---|---|---|---|---|---|
| 2008-040-1-200 Karen | $4,200.00 | $4,200.00 | | $4,200.00 | 31-Dec-15 |
| 2009-023-1-200 Wieser | $8,500.00 | $5,160.00 | - | $5,160.00 | 31-Dec-15 |
| 2009-026-2-200 Meija | $6,000.00 | $6,000.00 | - | $6,000.00 | 1-Apr-16 |
| 2009-027-1-200 Brand | $9,600.00 | $1,443.00 | - | $1,443.00 | 30-Sep-14 |
| 2009-045-1-200 Ishida | $8,000.00 | $8,000.00 | - | $8,000.00 | 31-Dec-11 |
| 2009-046-2-200 Kaiser | $6,000.00 | $5,812.00 | $424.58 | $5,387.42 | 30-Jun-16 |
| 2011-026-1-200 Wieser | $10,200.00 | $10,200.00 | - | $10,200.00 | 31-Dec-15 |
| 2011-027-1-200 Schonberg | $19,400.00 | $9,270.00 | - | $9,270.00 | 31-Dec-14 |
| 2011-028-1-200 Zhu | $6,400.00 | $6,400.00 | - | $6,400.00 | 1-Mar-14 |
| 2011-040-2-200 Brand | $7,400.00 | $6,100.00 | - | $6,100.00 | 1-Mar-15 |
| 2012-036-2-200 Villa | $9,000.00 | $9,000.00 | - | $9,000.00 | 31-Dec-16 |
| 2012-047-1-200 Karol | - | - | - | - | 1-Jul-15 |
| 2013-032-1-200 van der Veen | $5,000.00 | $3,151.00 | - | $3,151.00 | 1-Oct-15 |
| 2013-037-1-200 Ober | $6,000.00 | $6,000.00 | - | $6,000.00 | 1-Oct-16 |
| 2014-001-2-200 Ohrstrom | $9,000.00 | $9,000.00 | $1,140.54 | $7,859.46 | 31-Dec-16 |
| 2014-002-1-200 Groening | $7,100.00 | $7,100.00 | - | $7,100.00 | 31-Jul-16 |
| 2014-016-2-200 Prohaska | $9,150.00 | $9,150.00 | - | $9,150.00 | 31-Dec-16 |
| 2014-024-1-200 Holden/Mahaffy | $14,000.00 | $14,000.00 | - | $14,000.00 | 1-Sep-17 |
| | | | | | |

Completed projects (9/2014–7/2015): 0
**Primary** active projects: 17 (14 *continuing*, 3 *new*)
**Secondary** active projects: 5

## Appendix 8

**Procedure for naming new elements**

1. Claim check by referees
2. IUPAC/IUPAP accept (Exec Comm. secretariats)
3. Designation of the discovery PAC
4. Name and symbol proposal asked from lab to Div. II
5. Div II: first check on “forbidden”name and/or symbol
6. Article with provisionial Recommendation in PAC (if more than one, in one article); 15 referees check name and symbol (nominated by Div Pres)
7. Simultaneous Public review for 5 months (via website IUPAC)
8. Council approves name and symbols (Bureau may have a mandate)

# Appendix 9

**Report on Cross-over meeting of Divisions II and VIII**

Attendees:

- Division II: Jan Reedijk (JR, The Netherlands), Lars Öhrström (LÖ, Sweden), Markku Leskelä (ML, Finland), Tiping Ding (TD, China), Ken Sakai (KS, Japan), Yang F. Abdul Aziz (YA, Malesia), Guillermo Ahumada (GA, Chile)
- Division VIII: Alan T. Hutton (ATH, South Africa), Richard M. Hartshorn (RMH, New Zealand), Risto S. Laitinen (RSL, Finland)

1. Organizational matters:

   a. There was some confusion in the relationship between the projects 2011-035-1-800 and 2011-028-1-200. It was concluded that there was a system error, since the number code and the title do not indicate that they are Division VIII projects.

   b. DR is a member of both boron and metallacycle task groups, but he couldn't participate because of the lack of Div. II funds. JR said that he needs to know well in advance with a proper request if funding is needed.

2. A report on InChI for inorganic compounds was presented in Istanbul. Since then there has been no progress. The task group leader has withdrawn from the project and a new task group chair is being searched.
   RMH reported that the descriptive character string of InChI is being converted to QR codes (analogous to the bar code but can be used as a link to web page). There is a possibility to include also additional information of the compounds, such as catalogue numbers, batch numbers, web pages, health and safety aspects etc. The chemical manufactures would place the QR code in the containers from where it can be read when needed.
   It is imperative to conduct a survey with users to establish what kind of information is needed. There will be a worksho during the General Assembly in Busan, and another one during the ACS National week in Boston. A third workshop was being planned to be held in Brussels by the end of the year 2015. RMH is the IUPAC representative in the InChI trust.
   ML noted that the EU chemical office in Helsinki should be interested in the development of InChI.
   It was also reported that a future project will be concerned with InChIs of mixtures. The funding will be provided by chemical companies or regulatory bodies.
3. Report of Division II:
   The following projects which were in preparing stage were presented
   a. The constitution of group 3 of the periodic table.
      In the project it is proposed that IUPAC should make an official recommendation in favor of the composition of group 3 of the periodic table as consisting either of
      (1) the elements Sc, Y, Lu and Lr, or
      (2) the elements Sc, Y, La and Ac.

   b. Periodic Table of life
      The aim in the project is to show via Periodic Table the importance and role of different elements to life
   c. Survey of Definitions and Use of Common Solid-State Chemistry Terminology

Project's goal is to propose definitions of selected solid-state terms such as intermetallic, liquid crystal, semi-crystal, ionic crystal, molecular crystal, covalent crystal etc. None of these has an entry in the IUPAC Gold Book, a Google search of these terms reveals an acceptable definition for all of them.

d. Toward a comprehensive definition of valence
At present, term valence is used in connotations that imply several somewhat differing definitions. This project will research the history and current use of valence, analyze a series of examples, and consider whether a comprehensive definition of valence for atoms in compounds can be formulated.

4. Report of Div VIII:

a. TINCOP: Document of inorganic single-strand polymers is 60 % ready. However, there are some interferences with the kappa rules that need to be sorted out.

b. Kappa (RMH): Draft document has been completed. The meeting of the task group appended by some other Division VIII members decided that the exemption convention will be removed from the document and the examples will be modified accordingly. TinCops can use the existing draft discrecarding the exemption convention. The concept of uncertainty-kappa is being debated and might be needed for single-strand polymers.

c. ATH reported that the Brief guide to inorganic chemistry (essentials in inorganic chemistry) has been published as an asap publication (no page numbers in PAC, yet). The four-page format is planned as an appendix. The PAC publication is in September and the future CI will have the four-page version as a centerfold. The analogous essentials of organic essentials is 80-90 % ready.

d. It was discussed how the use of chemical nomenclature nomenclature in wikipedia should be handled. There is a need to get the nomenclature information fixed in wikipedia without having random changes taking place. The copyright agreement of the Brief Guides allows the reproduction of the document in any format provided it is reproduced in its entirety and unchanged. One way is to have a reference with a hyperlink.

e. ATH described two projects in progress: A document on kappa-convention and that of the selection of central atoms. Div VIII is organizing workshops (ACS and RSC) to explore, how PINs are used by industry. In early 2015 there was also a scoping meeting between ISO/Div VIII on how to name nanoparticles. The role of Division II could be in the identification of suitable persons for such a project.

f. There is a need for a project for standardising the use of terms such as "acceptable", "preferred", "recommended", etc. At the moment the terminology is confusing and does not assist clarity.