# INORGANIC CHEMISTRY DIVISION OF IUPAC

Minutes of Meeting at Brest 7 and 8 July 2016

## TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Introductions and announcements</td>
</tr>
<tr>
<td>2</td>
<td>Presentation and discussion of the Agenda</td>
</tr>
<tr>
<td>3</td>
<td>Approval of Minutes and action items from Division Meeting in Busan</td>
</tr>
<tr>
<td>4</td>
<td>Division Membership Updates</td>
</tr>
<tr>
<td>5</td>
<td>Reports of IUPAC Bureau and Executive Committee actions</td>
</tr>
<tr>
<td>6</td>
<td>Report from other IUPAC bodies and Affiliated Organizations</td>
</tr>
<tr>
<td>7</td>
<td>Report from Commission of Isotopic Abundances and Atomic Weights</td>
</tr>
<tr>
<td>8</td>
<td>Division Newsletter status and planning</td>
</tr>
<tr>
<td>9</td>
<td>Review of Division budget allocations and expenditures</td>
</tr>
<tr>
<td>10</td>
<td>Reports on recent, planned and proposed Division-sponsored conferences</td>
</tr>
<tr>
<td>11</td>
<td>Discussion on names and symbols of elements 113, 115, 117 and 118 proposed by the discoverers</td>
</tr>
<tr>
<td>12</td>
<td>Project-by-project review of Project status</td>
</tr>
<tr>
<td>13</td>
<td>Review of new project proposals</td>
</tr>
<tr>
<td>14</td>
<td>Discussion on the generation of other future projects</td>
</tr>
<tr>
<td>15</td>
<td>Status of the Information Package for new Division members</td>
</tr>
<tr>
<td>16</td>
<td>Planning elections for next biennium</td>
</tr>
<tr>
<td>17</td>
<td>Duties of Division members</td>
</tr>
<tr>
<td>18</td>
<td>Review of Action Item list of this meeting</td>
</tr>
<tr>
<td>19</td>
<td>Status of next Division meeting in Sao Paolo</td>
</tr>
<tr>
<td>20</td>
<td>Any other Businesses</td>
</tr>
<tr>
<td>21</td>
<td>Thanks and adjourn</td>
</tr>
</tbody>
</table>

Appendix 1 – Action items from Brest meeting
Appendix 2 – President’s report for Bureau meeting
Appendix 3 – Highlights of the COCI focus for 2016-2017
Appendix 4 – Interdivisional Committee on Terminology, Nomenclature, and Symbols
Appendix 5 – Report from Commission on Isotope Abundances and Atomic Weights
Appendix 6 – Status of the projects of Division II
INORGANIC CHEMISTRY DIVISION OF IUPAC
Meeting at Brest, July 7-8, 2016, Faculty of Letters, room “Yves Moreau”

DRAFT MINUTES

Attendance: Present were for part or all President, Jan Reedijk (Netherlands); Vice President, Lars Öhrström (Sweden), Secretary, Markku Leskelä (Finland); Titular Members: Lidia Armelao (Italy), Tiping Ding (China), Pavel Karen (Norway), Daniel Rabinovich (USA), Thomas Walczyk (Singapore), Associate Members: Jorge Colon (Puerto Rico), Ken Sakai (Japan), and National representatives: Mayoro Diop (Senegal), Philippe Knauth (France), Miki Hasegawa (Japan), IUPAC secretary general Richard Harsthorn (New Zealand)

Apologies were received from Titular Member Robert Loss (Australia), Michael Wieser (Canada), Associate member Milan Drabik (Slovakia) 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 11:30 a.m. on Thursday, July 7, 2016. Div. President Reedijk welcomed the members, especially new members, and also thanked the AM and NR 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 Busan (Leskelä) and status of the Action Items from the Busan meeting (Reedijk)

Minutes of the Busan (2015) 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. The final copy is available on the IUPAC Division II web page.

The action items from the Busan meeting were included in the Minutes of that meeting as Appendix 1. All of these items had been addressed by the designated individuals.
4- Division Membership Updates (Reedijk)

Jan Reedijk presented the Division members name by name and their terms. The important role of NAOs in making proposals for AMs and NRs well in time was pointed out.

5- Reports of IUPAC Bureau Meeting and Executive Committee actions (Reedijk)

The Bureau and Division Presidents had the meeting in Montreal Canada April 2016. Reedijk told the general news from IUPAC and showed the report he presented in the Bureau meeting from Division II. The main report from Division II this time was dealing with the naming of the four new elements.

A summarizing copy of the Report on Division II that Div. President Reedijk presented in the Bureau meeting is attached as Appendix 2.

6- Reports from other IUPAC bodies and Affiliated Organizations

Committee on Chemistry Education
No report was given due to the absence of previous AM Javier Garcia. Philippe Knauth volunteered to be the Division representative in CCE till and at in the next GA meeting in Sao Paulo 2017.

Chemical Nomenclature and Structure Representation Division (Division VIII)
No report was given. Nomination of a representative is needed. Dan Rabinovich told about the Div VIII projects he has been involved.

Committee on Chemical Industry (Leskelä)
No information from the activities of COCI was available to present. After the meeting Dr. Carolyn Ribes sent the COCI report to Bureau and highlights of the recent COCI activities are presented in Appendix 3.

Interdivisional Committee on Terminology, Nomenclature, and Symbols (Drabik)
The report on the activity of Milan Drabik in the Committee was presented and discussed and is attached as Appendix 4.

Systeme International d'Unites, SI – redefinition of mole
No report from the work in SI but there is an IUPAC project on redefinition of mole. The Task Group has produced the second draft of the manuscript.

Cross division activities (Öhrström)
There have been discussions for making plans how to activate cross divisional awareness. In next GA meeting we probably have a new procedure how to visits and reports between different divisions and commissions will take place.
7 - Report from Commission on Isotopic Abundances and Atomic Weights (CIAAW) and its Subcommittees, including the relevant Project Reports (Ding, Walczyk)

The report made by Juris Meija (Appendix 5) was discussed in detail. Two reports “Standard Atomic Weights of Elements 2013” and “Isotope Compositions of the Elements 2013” where published in 2013 and no separate report was made in 2015 because two years cycle was considered too short. There was a little concern if updates on atomic weights would be only after long intervals and only at the website. For the visibility of IUPAC publishing a paper every 3-4 years could be optimum. Discussions after the meeting clarified the situation and there are no reasons to be worried.

8 - Division newsletter status and planning (Öhrström)

Appearance frequency of the newsletter is one year and that is sufficient. Members were asked to contribute to the newsletter from their IUPAC related activities. Because the newsletter has great importance both internal in the division and external inside IUPAC and NAOs, the members were reminded to distribute the newsletter to their NAOs. Next issue will appear after this meeting and deadline for submitting material is the end of September.

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

Jan Reedijk presented the budget allocation during this biennium. The rule is to use maximum 30 % for meetings and rest for the projects. Division budget fulfills that balance requirement. JR showed the budget balances of the projects and as conclusion all the projects are well within the budget.

10 - Reports on recent, planned and proposed Division sponsored conferences

High Temperature Materials Conferences: HTMC-XV, was held in Orleans, France, March 29-April 1, 2016.

5th International Solvothermal and hydrothermal association conference, was held in NCKU Tainan, Taiwan, January 17-20, 2016. The time of the 6th conference is not known.

12th Solid State Chemistry conference (SSC 2016), will be held in Prague, Czech Republik, September 18-23, 2016 (Drabik)

Conference web site is http://www.ssc-conference.com/home Preliminary program http://www.ssc-conference.com/admin/scripts/source/programme_preliminary_SSC%202016.pdf). 150 – 200 scientists are expected to participate. The main topics of conference are: Preparation and synthesis; Phase and properties characterization; Nanomaterials, nanocomposites and catalysis; Magnetic, metal and alloy materials; Optical and photovoltaic materials; Theoretical approaches to solid-state chemistry. As an IUPAC delegate to the conference Milan Drabik will give information on the
IUPAC mission and activities and also the invited lecture “Notes on the challenge of methods of thermal analysis in solid state chemistry”. As part of the IUPAC sponsorship, papers based on the plenary lectures and selected presentations will be published in Pure and Applied Chemistry.

11 - Discussion on names and symbols of elements 113, 115, 117 and 118 proposed by the discoverers (Reedijk). Status reports, formal decisions by the Division, and follow-up planning

Jan Reedijk presented the slides on the new elements he showed in the Bureau meeting and also the protocol for naming of the elements.

Nobel symposium NS 160 on Chemistry and Physics of Heavy and Superheavy Elements was held in Lund Sweden May 29-June 3, 2016. The new elements were discussed in the Symposium and Jan Reedijk showed the slides he presented in the Symposium. The roles of IUPAC and IUPAP in the naming process of the new elements were discussed and situation is now clearer. There was also lively scientific discussion on reliability of the discoveries.

A press release on the names of the new elements 113 Nihonium (Nh), 115 Moscovium (Mo), 117 Tennessine (Ts), and 118 Oganesson (Og) was given by IUPAC June 8, 2016. More than 50 comments were thus far sent by the public to Jan Reedijk. Many of the comments were dealing with the translations (conversions) of the names to different languages. The problem concerns mostly tennessine and the advice could be: follow the protocol use for naming of astatine in that language. The comments need to be answered (will or has been be done by the chair).

The names of the new elements and their symbols were already discussed and commented by the Division members before the meeting. The symbol of tennessine was changed according to the comments given. The Division could unanimously accept the proposed names and the symbols and recommend the acceptance for Bureau and General Assembly.

Meeting was closed 16.30

Friday July 8

12 –Project-by-project review of project status (Rabinovich)

Dan Rabinovich presented the project-by-project review. Two projects have been completed during the last 12 months, namely: 2009-027-1-200 Assessment of Stable Isotopic Reference and Inter-Comparison Materials and 2015-031-1-200 How to Name New Chemical Elements.

Division II has 20 primary active projects 20 (16 continuing and 4 new projects), and 3 secondary active projects (projects in which Div II is participating). See for details in Appendix 6. Most of the projects are running well, only from projects of Kaiser and Villa no updates were available and the task group chairs need to be contacted again. Action by: Dan Rabinovich.
There are two projects where Division II members are in the task group but no funding is coming from our Division. The projects are:

2012-044-1-100 Basic terminology of crystal engineering (Öhrström)
2014-031-1-600 The environmental and health challenges of e-waste and its management: an emerging 21st century global concern (Armelao)

The project proposal on Diffusion in nanoporous solid by Rustem Valiullin discussed in Busan meeting is now running (2015-002-100) under Division I.

13 – Review of new project proposals (Rabinovich)

There are no pending projects (= reviewed projects waiting for funding).

The following projects are under preparation:

2017-xxx-1-xxx by Daniel Rabinovich (UNC Charlotte) on The Periodic Table of Life.

2017-xxx-1-xxx by Pavel Karen (University of Oslo) entitled Towards a Comprehensive Definition of Valence.

14 – Discussion on the generation of other future projects

Ken Sakai remained the project topic raised by Claudio Verani in Busan on Understanding of TOF and TON in catalysis. Ken Sakai will take the lead and put the proposal forward.

Lars Öhrström raised discussion on 2019 Periodic Table project. This should fit to IUPAC 100 years and coinciding Period Table 150 year jubilee. Lars will contact the IUPAC jubilee committee if a separate project on renewal of Periodic Table and history of Period Table is needed.

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

Current Present Division members are happy with content of the Information package. The package is now distributed to new members and also to young observers who attended the recent meetings.

16 - Planning elections for next biennium: appointment of Nomination Committee

The composition of nomination committee was discussed. The members are asked to send names and comments for the nomination committee to the planned chairman Lars Öhrström.
17 – 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 after that distributed separately.

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

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

19 - Status of the next year Division meeting in Sao Paolo July 7-8, 2017 and off year meeting 2018

General Assembly will be organized in Sao Paolo July 6-15, 2017. The division and committee meetings will be organized in a usual manner, probably on July 7 and 8.

Lars Öhrström discussed about a possible off year meeting in Africa 2018. Only 6 out of 53 African countries are IUPAC members. To make IUPAC more visible a meeting in Africa could be useful, maybe in connection with Federation of African Chemical Societies. The effort could be common with other divisions/committees (CCE, COCI) in order to be more convincing. At the same time Lars was asked to also prepare a backup plan, in case Africa would not materialize.

20 – Any other businesses

There were no other businesses.

21. Thanks and adjourn

Jan Reedijk closed the general meeting at 11.45 and thanked the participants for an active meeting.
Appendix 1

Action Items from IUPAC Inorganic Chemistry Division Committee
Brest, July 7 - 8, 2016

1. News items to Lars Öhrström for the newsletter before 1st October

2. Africa project Jan Reedijk discuss with appropriate DP:s (chemical industry, education, human health) Lars Öhrström to Mark Cesa, Mayoro Diop checks African chemistry conferences that could potentially be piggy-backed.

3. Projects:
   - 2014-024-1-200 Tiping Ding division monitor
   - 2015-030-2-200 Thomas Walczyk division monitor
   - 2015-037-2-200 Thomas Walczyk division monitor
   - 2015-039-2-200 Daniel Rabinovich division monitor
   - 2015-053-1-200 Jorge Colón division monitor

4. Add projects where we have an interest but no money invested: Daniel Rabinovich, updates from Lidia Armelao, (electronic waste), Lars Öhrström (crystal engineering)

5. New Projects:
   - Valence: Pavel Karen, look for task group members also outside the division (Committee on Chemical Education, Organic and Biomolecular Chemistry Div., Physical Chemistry Div.).
   - The periodic table of life: Daniel Rabinovich contact Human Health Div., Div. of Nomenclature Div., International Council for Science
   - Periodic Table printout formats & History of the IUPAC periodic table. Lars Öhrström contacts Lynn Soby and Juris Meija.
   - Turnover Numbers & Electro Catalysis: Ken Sakai proceeds.

6.Nomination committee suggestions: Risto Laitinen, Oulu, Finland, Lars Öhrström collects other potential names for the nomination committee.
Appendix 2

Appendix 2

Nobel Symposium
Discoveries of New Elements
May 31-June 3, 2016

IUPAC MISSION

The International Union of Pure and Applied Chemistry is the global organization that provides objective scientific expertise and develops the essential tools for the application and communication of chemical knowledge for the benefit of humankind and the world.

IUPAC MISSION

The International Union of Pure and Applied Chemistry accomplishes its mission by
- Fostering sustainable development
- Providing a common language for chemistry
- Advocating the free exchange of scientific information

IUPAC CORE VALUES

- We serve humankind by advancing chemistry worldwide.
- Scientific excellence and objectivity are the cornerstones of all our work.
- We value collaboration and communication among all our stakeholders.
- We strive for diversity and inclusiveness.
- We respect each other and the Union.
- We uphold the highest standards of transparency, responsibility and ethical behavior.

IUPAC

IUPAC’s unique role in the world chemistry community

- A focus on those aspects of chemistry where global consensus is essential for progress in research, commerce and policy.
- Respect for its objectivity and scientific excellence, providing access to the highest levels in the scientific, industrial, and policy communities to represent global chemistry.
- A worldwide base of volunteers with the best skills and background, recruited by transparent and well-understood processes.

IUPAC

Divisions and Standing Committees—
IUPAC’s Scientific Work

- Physical & Biophysical Chemistry
- Inorganic Chemistry
- Organic & Biomolecular Chemistry
- Physical Chemistry
- Analytical Chemistry
- Chemistry & the Environment
- Chemistry & Human Health
- Chemical Metrology & Standardization
- Committee on Chemistry & Industry (CCI)
- Committee on Chemistry Education (CCE)
- ChemAPM Committee
- Committee on Publications and Documentation (CPD)
- International Committee on Terminology, Nomenclature and Standards (ICTN)
Primary IUPAC Activities

Development of the Language of Chemistry
- Nomenclature, Symbols, Terminology
Standardization of Chemistry Methods
- Data Presentation
- Study of Analytical Methods
Critical Evaluation of Physico-Chemical Data
- Atomic Weights
- Thermodynamic Data
- Kinetic Data

Primary IUPAC Activities (Cont.)

- Data Exchange Standards for Computers and Instruments
- Endorsement of International Conferences
- Biennial IUPAC Congress
- More than 30 Specialized Symposia each Year
- Chemistry Education
- Industrial Safety and Environmental Programs
- CHEMRAWN Conferences addressing Chemistry and World Needs

Proposals for Projects

Anyone with a good idea can submit a proposal. IUPAC projects address issues of significance to the general chemistry community:
- Nomenclature, terminology, and symbols
- Validated and compiled data
- Standard methods and procedures
- Education and public understanding of chemistry
- Any subject that requires development of consensus among chemists worldwide

More information: www.iupac.org

IUPAC’s Color Books

- Chemical Terminology: Gold Book
- Quantities Units and Symbols in Physical Chemistry: Green Book
- Nomenclature in Organic Chemistry: Blue Book
- Compendium of Polymer Terminology and Nomenclature: Purple Book
- Analytical Terminology: Orange Book
- Biochemical Terminology: White Book
- Nomenclature in Inorganic Chemistry: Red Book
- Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Science: Silver Book

Individuals may become affiliated with IUPAC through the Affiliate Membership Program (AMP). Benefits include:
- Subscription to bimonthly magazine, Chemistry International
- Discounts on IUPAC Books and Pure and Applied Chemistry
- Registration discounts (10%) for most IUPAC-Endorsed Conferences
- Access to an international network of Chemists
A few interesting examples of our work

Current Projects
- Chemistry beyond Chlorine (Tundo)
- Healthy Life – Functional Food Ingredients (Rauter)
- Nomenclature of Cyclic Peptides (Reaney)
- Computational Chemistry – a workshop for sub-Saharan scientists (Whitehead)
- Network for Heterocyclic Chemistry within Mediterranean/North Africa (Floiró)
- Nuclear Magnetic Resonance (Garson)

IUPAC Richter Prize in Medicinal Chemistry
- Established in 2006. Acknowledges the key role that medicinal chemistry plays toward improving human health
- $10,000 awarded every two years to an internationally recognized scientist whose accomplishments demonstrate an outstanding level of contribution to the practice of medicinal chemistry or drug discovery.
- 2010 Prize was awarded to Arun Ghosh, Purdue University, for his use of “backbone binding” in the discovery of the HIV-1 protease inhibitor darunavir, for treating multidrug-resistant HIV.

The Periodic Table of Today (and Tomorrow?)

Wikipedia Correctness

The IUPAC-Solvay Award for Young Chemists
- Established to encourage young research scientists at the beginning of their careers.
- Awarded for the most outstanding Ph.D. theses in the general area of the chemical sciences.
- Next Deadline: 31 January 2016
1. Summary of Protocol
2. Status report of the four names and symbols

Stages in recognition/validation of new elements and their name-giving
1. IUPAC and IUPAP generate a 10-member expert panel (5-10 years).
2. A Chair for a Joint Working Group generated is selected from the panel, when a claim for (a) new element(s) is expected.
3. This chair will propose four additional JWG members, from different – non-involved – institutions, at least 2 from each Union.
4. This Panel decides on the validations and IUPAC secretariat publishes its decisions (December 2015 press release; PAC January 2016).
5. President of Division II invites discoverers to propose name/symbol (February 2016), asking them to consider the PAC paper in press (“How to name…”), and report by April 1.

Status as per APRIL 10, 2016
1. The four proposals were received in time (March 31).
2. Division II decides on acceptance, if needed after correspondence with discoverers. It is needed this time....
3. Division II has the proposals refereed by 12 experts (hopefully in May), and by the general public (5 months starting June 1).
4. Division II publishes the Names and Symbols in PAC end of 2016 or early 2017.
5. Bureau decides on final acceptance, and Council ratifies at its next meeting.

Four New Elements being named
(Confidential till Provisional Document)
113: Suggested as nihonium, Nh
115: Suggested as moscovium, Mc
117: Suggested tennesine, Tn*
118: Suggested oganesson, Og

* Tn was first used in 1923 for Thoron = 220Radon; and is still used in recent literature.
IUPAC Division II - Inorganic Chemistry
Brief Review for Bureau; Jan Reedijk

1. Projects: summary status
2. Special case: publicity about a project (outside world)
3. Elections and Process & Timing
4. Young Observers; Newsletter and Welcome Pack
5. Future

Montreal: April 2016

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Recently (or almost)
Completed Projects,

Selection only:
Successful one and a fast one.
A full listing is separately available

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- **2009-012-2-200 (ended in time 2012)**
  - TGC: Lars Öhrström
  - TG: Batten, Champness, Chen, Garcia-Martinez, Kitagawa, O’Keeke, Reedijk & Suh
- **Coordination polymers and metal organic frameworks: terminology and nomenclature guidelines**
  - Budget: USD 11,500; spent: USD 11,500;
  - The final recommendation was published in: *Pure Appl. Chem. 2013, 85, 1715-1724*. This manuscript was cited already over 100 times by March 2016.

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- **2008-040-1-200**
  - TGC: Pavel Karen
  - TG: Mc Ardle, Takats & Tatsumi
- **Towards a comprehensive definition of oxidation state**
  - Budget: USD 4,200; spent: USD 0; balance: USD 4,200.
  - This project work was mainly done by email exchanges and meetings at conferences.
  - A report of the project is available as a technical report: PAC, 89, Issue 6, pp: 1477-1501. The project has been extended till the end of 2016, to allow:
  1) Discuss and finalize the IUPAC Recommendation (provisional draft posted waiting comments by May, 2016),
  2) Suggest how to modify the Gold-Book entries for Oxidation Number and Oxidation State (details of the wording are being discussed at the task group),
  3) possibly a paper on oxidation state in teaching for the Journal of Chemical Education.

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**Interdivisional Project**

- **2013-037-1-200**
  - TGC: Christopher Ober
  - TG: Garcia-Martinez, Jones, Mathur, Wilson & Zharov
- **Creating Educational Website for Materials Chemistry**
- **Requested budget: USD 6,000 ($1,000 from Div. II)**
- **Div. II monitor: Mathur**
- **NB: Original proposal submitted to Div. I, II & IV**

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**Example of a fast project to update an older recommendation**

- **TGC: Jan Reedijk (Leiden University)**
  - TG: Corish, Garcia-Martinez, Koppenol & Meijs
- **How to Name New Chemical Elements**
- **Requested budget: USD 0**
  - Update to the 2002 IUPAC recommendations on how to name newly discovered chemical elements ([Pure Appl. Chem. 2002, 74, 787-791](http://dx.doi.org/10.1351/pac200274050787)).
  - Start date: 1 August, 2015 (at the Busan meeting)
  - Materialized end date: February 29, 2016
  - Now in press, PAC.
Selection of some New Proposals

A proposal started by a young observer

- **2015-053-1-200**
  - TGC: Robin T. Macaluso (University of Texas at Arlington)
  - TG: Milan Drabik, Melanie Kirkham, Cora Lind-Kovacs, Emma McCabe & Leopoldo Suescun.
  - Survey of Definitions and Use of Common Solid-State Chemistry Terminology
  - Requested budget: USD 9,000

Submitted: 17 November 2015
Start date: 31 December 2015
Planned end date: 31 December 2016

- **2015-039-2-xxx**
  - TGC: Eric Scerri (Dept. of Chemistry & Biochemistry, UCLA)
  - TG: Jensen, Öhrström, Ball, Restrepo & Lavelle
  - The Constitution of Group 3 of the Periodic Table
  - Requested budget: USD 5,815

Submitted: 9 November 2015
Start date: January 1, 2016
Planned end date: 2016

Projects plans to submit in next period or that have just been submitted

- Pedagogic material to teach technical material sciences
- A Periodic Table of Life
- Terminology of Nanomaterials
- Comprehensive Definition of Valence
- Develop a Periodic Table of allotropy of elements.
- Spotting errors in Wikipedia related to inorganic chemistry and nomenclature and submit corrections to Wikipedia.
Young Observers

• The Division actively wants to involve young scientists to take part in Division activities and projects, and plans to continue recruiting new Div. Committee members from them.
• At the last 2 GA meetings 8 YOs were present and we meanwhile 4 of them have joined our (Div.) activities (NR+projects).

Successful internal Division activities

• Since 2006 the Division has published about 2 Newsletters each year. In addition to the members of Division II, this Newsletter was sent to all IUPAC Division Presidents and the Executive Committee. This newsletter has also been used by some National Chemical Societies for redistribution. Previous ones are available at the IUPAC Website.
• For newly entering Division members a Welcome pack is made available introducing the Division activities and IUPAC structure and protocols for e.g. project handling. This has also been made available to other Divisions.

Elections for Division Members

• The proposals made to shorten these processes have been carried out, and have been well received by the division.
• Ready to go on next elections; thinking on how to activate NAOs to come up with good candidates; Division Nomination Committee plans to be more pro-active.

IUPAC visibility in the outside world:

• The output of the completed project on naming of coordination polymers and MOFs and its publicity (mentioned above). This article also makes a general plea for the need of proper terminology and nomenclature, recognizing IUPAC.
• The ongoing process of recognition and naming of newly discovered elements (see below).
• (Also petitions of groups of people to coin a new name should be mentioned; e.g. 160 000 people made a plea for the use of “Lemmium”)

Other current activities

• A set of procedures for the naming of new chemical elements is being performed (started Dec 30, 2015 with a press release).
• The PAC papers on the valorisation of the four new elements have appeared (January 2016).
• The discovery laboratories have been invited to propose names and symbols.
• New names and symbols are expected to be ready for public review this summer.
Appendix 3

**Highlights of the COCI Focus for the 2016-2017 Biennium**

1. Regional Workshop in China supported by SINOPEC; theme: Chemical Industry and Sustainable Development (Sept 2016).

2. ThalesNano Prize for Flow Chemistry: Biennial award to be presented at IMRET 14 meeting in Beijing. (Sept 2016)


4. Regional Safety Training Programs. Currently 1-2 Fellows from developing countries are trained to deliver improved Environmental, Health, and Safety programs to their institution. An extended program in Uruguay will create a center for learning with a 400-800% increase in participation.

5. Responsible Care linkage with the International Council of Chemical Associations [ICCA].

Appendix 4

Interdivisional Committee on Terminology, Nomenclature, and Symbols (Drabik)

My present position in this committee is Associate Member (one of two AMs of the committee), originally nominated by the division II. I am not (at present) Member / representative of the division II to the committee. Anyway; some aspects of my communications, activities and work within the ICTNS during the period 2015 – 2016 should be quoted, these relevant of division II are as follows:

a) Extensive series of referee reports done on request of the Editor of PAC. The types of referred manuscripts (and papers published) cover IUPAC Recommendations and Technical reports, incl. numerous ones resulting from activities and projects of the division II.

b) Special attention has been devoted to referee reports of the issues of discovery, terminology and symbols of four new elements, including proposals of discoverers on naming these new elements (as press releases so IUPAC Recommendation, jointly by division II and ICTNS).

c) The entire activities have been completely accomplished by electronic correspondence with Prof. R. Weir - Chair of ICTNS, Prof. H. Burrows and/or with the editorial office of PAC.
Appendix 5

Summary of CIAAW activities for 2016

This report provides a summary of CIAAW activities since its 2015 Vienna meeting.

Core business

The Commission has published the “Atomic Weights of the Elements 2013 (IUPAC Technical Report)” and “Isotopic Compositions of the Elements 2013 (IUPAC Technical Report)” in *Pure and Applied Chemistry*. During the review of these two publications, CIAAW has collaborated closely with ICTNS and has received several substantive comments aimed at improving its work. While not all of these could be addressed immediately, CIAAW is committed to addressing many of the comments raised by the ICTNS in the near future. To this end CIAAW commends the quality and the rigor of ICTNS reviews which help to improve the long-term quality and consistency of its work.

The Chairman and the Secretary have decided that CIAAW will not publish the Atomic Weights Report for 2015. The 2015 updates have already been announced by IUPAC and international media (American Chemical Society, Royal Society of Chemistry) and they have been posted on ciaaw.org. Given the time it took to produce the 2013 report (over two years), it was determined that two-year cycle for standard atomic weight reports is too short.

General data reduction framework

During the 2015 meeting, CIAAW Chairman gave a presentation before SIAM about the data reduction methods. It was noted that, unlike other similar organizations such as CODATA or AME, CIAAW does not employ formal statistical tools for data reduction of various published results. Currently, CIAAW Chairman is working closely with A. Possolo, Chief Statistician (NIST) and Associate member of CIAAW, to develop modern statistical tools that can be applicable to the work of CIAAW. This will also address the issue in regards to the coverage probability of the quoted confidence intervals.

Atomic Weight Uncertainty Guidelines

[2013-032-1-200] In order to resolve issues about the interpretation of standard atomic weight uncertainties, the Task Group has submitted two manuscripts to *Pure and Applied Chemistry*. The Provisional Recommendation was posted on iupac.org with comments requested by 31 August
2016. Task Group has received the first round of comments from ICTNS and is currently working on addressing them. [2015-037-2-200] CIAAW chairman has prepared necessary codes for online calculator of molecular weights and their uncertainties to be placed on ciaaw.org. A draft calculator (v.0.2) is currently running in a test mode on http://ciaaw.shinyapps.io/App-2.

Redefinition of the mole

[2013-048-1-100] CIAAW is involved in the IUPAC Project on the redefinition of the mole through its Chairman. The Task Group has produced the second draft of the manuscript and R. Marquardt, Past President of IUPAC Div I, attended the meeting of the CIPM Consultative Committee for Units (CCU) in June 2016.

SNIF diagrams

CIAAW has received requests in the past to make available the tabular versions of its SNIF diagrams detailing the natural variations of atomic weights of the twelve interval elements. As a consequence, Dr. Coplen has submitted a manuscript to Pure and Applied Chemistry that details the numerical values of CIAAW atomic weight diagrams showing natural variations. These diagrams will soon be available on ciaaw.org in a tabular fashion. Chairman has already prepared the necessary web infrastructure for these tables which are currently available in attest mode at http://ciaaw.org/temp-natural-variations.htm

Other business

Two emeritus members of CIAAW, Dr. Coplen and Dr. Holden have submitted manuscript to Pure and Applied Chemistry outlining the history of the footnotes for standard atomic weights. Work is currently underway to implement further updates to the ciaaw.org following the 2015 meeting and to disseminate the draft CIAAW charter to Division II for comments. This activity is relevant to project 2011-040-2-200.

IUPAC Project 2009-027-1-200 has been closed. CIAAW would appreciate if Div. II could transfer the remaining balance to the successor project 2014-002-1-200. Within the framework of IUPAC Project 2014-002-1-200, CIAAW and its Subcommittee on Stable Isotope Reference Material Assessment (Chairman Groening, IAEA) has recently been involved in the data analysis of recent suite of international isotopic reference materials [reported in Analytical Chemistry, 10.1021/acs.analchem.5b04392] before CIAAW can recommend these values in its Isotope Reference Material Report.

The Chair of CIAAW has been appointed IUPAC representative to Joint Committee for Guides in Metrology Working Group 1: GUM (JCGM-WG1:GUM).

Juris Meija, Chair CIAAW

July-4, 2016
Appendix 6

Status of the projects of Division II

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, Brest
7-8 July 2016

Outline

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

(August 2015 – July 2016)

- **2009-027-1-200**
- TGC: Willi Brand (Max Planck Institute for Biogeochemistry)
- TG: Böhlke, Coplen, 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:


  **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:

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

7 July 2016 (Juris Meija):
Project is COMPLETE. Request will be made to transfer (if possible) remaining funds (USD 1,443) to the successor Project No. 2014-002-1-200.

COMPLETE

• 2015-031-1-200
• TGC: Jan Reedijk (Leiden University)
• TG: Corish, Garcia-Martínez, Koppenol & Meija
• How to Name New Chemical Elements
• No requested budget.
• Div. II monitor: n/a.
• Updates:
  • Project was approved and started on 1 August 2015.

October 2015:
Provisional Recommendation entitled “How to Name New Chemical Elements” is made available for public review until 29 February 2016.

May 2016:
IUPAC Recommendations

Willem H. Koppenol, John Corish, Javier Garcia-Martinez, Juris Meija and Jan Reedijk*

How to name new chemical elements (IUPAC Recommendations 2016)

DOI 10.1515/pac-2015-0802
Received August 20, 2015; accepted March 1, 2016

Status Report on Active Projects
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

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...)
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).

7 March 2016 (Pavel Karen):
A manuscript with the Provisional IUPAC Recommendation has been drafted and is open for discussion at the www.iupac.org website (commenting period ends on 31 May 2016). Similarly for the Gold Book entries for both "oxidation number" and "oxidation state." One last extension until the end of the year was requested and granted.

Start date: 1 January 2009
Planned end date: 31 December 2016

- **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 5,643; balance: USD 2,857.
- 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):

Variation in the terrestrial isotopic composition and atomic weight of argon (IUPAC Technical Report)

(cont…)

4 August 2015 (Wieser):
Three TG members (de Laeter, Hirata & Schönberg) are no longer active. A request to add three new TG members (Zhu, Irgeher & 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.

No updates to report

Planned end date: 31 December 2016
• 2009-026-2-200
• 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, CIIAW):
Due to the inactivity of key TG members, and in consultation with the current TGC, the Commission on Isotopic Abundances and Atomic Weights (CIIAW) 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 CIIAW 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 CIIAW.

(cont...)

November 2014
The task group will produce a prototype online database by 2015 CIIAW 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 CIIAW members for entry of the 2017 TSIW 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, TGC):
An electronic database hosted by CIIAW and a prototype web interface were set up in early 2015 (www.ciaaw.org/database).

7 July 2016 (Meija, TGC):
Project is progressing well. Database infrastructure has already been setup on ciaaw.org and during the 2015 meeting a new data analysis framework, in conjunction with the scope of Project No. 2011-027-1-200, was presented.

Start date: 1 April 2011
Planned end date: 1 April 2016
• 2009-045-1-200
• TGC: Hitoshi Ishida (Kitasato University)
• TG: Beeby, Bunzli, Campagna, De Cola, Ford, Gordon, Hasegawa, Katoh, Keene, McCusker, Nozaki, Sakai, Tobita, Vloek & 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 (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 Pacificchem 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.

9 August 2015 (Ken Sakai):
Manuscript was submitted to Pure and Applied Chemistry in October ’14. A no-cost extension will be requested soon.

(cont…)
Decision Letter (PAC-REP-14-07-06.R1)

From: weir@rmc.ca
To: ishida@sci.kitasato-u.ac.jp
CC: cwurzbacher@verizon.net

Subject: Pure and Applied Chemistry - Decision on Manuscript ID PAC-REP-14-07-06.R1

Body: Dear Prof. Ishida:

I am pleased to inform you that your manuscript ID PAC-REP-14-07-06.R1 entitled "Guidelines for Measurement of Luminescence Spectra and Quantum Yields of Inorganic and Organometallic Compounds in Solution and Solid State" has been recommended for publication in Pure and Applied Chemistry, subject to minor revision suggested by the reviewer(s). Relevant comments and recommendations are summarized in the attached extracts from reports.

6 July 2016 (Ishida, TGC):

Revised manuscript (R2) was submitted on 12 June 2016. Workshop planned if funds are still available.

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 613; balance: USD 5,387.
- Div. II monitor: Rabinovich
- Updates:


- 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.

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

- 2011-026-1-200
- TGC: Michael Wieser (U. of Calgary)
- TG: Schönbarg, Zhu, Gröning & Meiia
- 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.
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:


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 (Irgeher) and a no cost extension (until Dec. ’17) have been requested.

Start date: 1 December 2012
Planned end date: 31 August 2017

- 2011-027-1-200
- TGC: Ronny Schönberg (Institute for Geosciences, U. of Tübingen)
- 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 19,287; balance: USD 113.
- 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.

11 August 2015 (Ty Coplen):
Manuscript ("Isotopic Compositions of the Elements 2013") was submitted to PAC in May 2015. Resubmitted after responding to reviewer comments in late July 2015.

7 July 2016 (Juris Meija):
CIAAW revised the Table of Isotopic Compositions of the Elements (TICE) in February 2016. The update involved a critical evaluation of the recent published data. The new TICE 2013 includes evaluated data from the "best measurement" of the isotopic abundances in a single sample, along with a set of representative isotopic abundances and uncertainties that accommodate known variations in normal terrestrial materials. The corresponding Technical Report has been published in PAC.

(cont…)

7 July 2016 (Norman Holden):

DE GRUYTER

IUPAC Technical Report

Juris Meija*, Tyler B. Coplen, Michael Berglund, Willi A. Brand, Paul De Bièvre, Manfred Gröning, Norman E. Holden, Johanna Irgeher, Robert D. Loss, Thomas Walczyk and Thomas Prohaska

Isotopic compositions of the elements 2013 (IUPAC Technical Report)

Start date: 3 January 2012
Planned end date: 31 December 2015
• 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 2,976; balance: USD 3,424.
  • Div. II monitor: Ding
  • Updates:

8 August 2013 (Juris Mejja):
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 Mejja & 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 Mejja & 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 Mejja & 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 be described in a publication.

6 July 2016 (Juris Mejja, CIAAW):
Dr. Zhu presented the extensive work on lead isotope data during the 2015 CIAAW meeting and CIAAW discussed this in regards to the standard atomic weight of lead. It is expected that Dr. Zhu will finish writing up this work and make a recommendation before CIAAW in 2017.

Start date: 1 April 2012
Planned end date: 1 March 2016
• **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 6,629; balance: USD 771.
  • 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):**

**6 July 2016 (Juris Meija, CIAAW):**
Dr. Coplen has submitted a manuscript to PAC that details the numerical values of CIAAW atomic weight diagrams showing natural variations. These diagrams will soon be available on ciaaw.org in a tabular fashion. TGC has already prepared the necessary web infrastructure for this which is currently available at http://ciaaw.org/temp-natural-variations.htm. Project to be COMPLETE soon.

Start date: 1 April 2012
Planned end date: 1 September 2016
**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 Divisions II and V and from the Project Committee and was approved shortly thereafter.

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

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**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)*


1School of Chemistry, Bangor University, UK; 2BfH, Germany; 3INEOS, Russian Academy of Sciences, Moscow, Russia; 4NanoGermes AS; Begevendi, Denmark, 5School of Chemistry, Leeds University, Leeds, UK; 6University of Leeds, UK and the Institute of Inorganic Chemistry of the Czech Academy of Sciences, Bohu u Prahy, The Czech Republic; 7Qubit University, Finland; 8Columbus, USA; 9Charotta, NC, USA; 10Instituto de Ciencia de Materiales de Aragon (ICMA), Zaragoza, Spain; 11Advanced Chemistry Development, Moscow, Russia.

July 2016 (Rabinovich):
Revisions of the draft Technical Report continue.

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: Druckendorf, 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 (Köl) representative from Div. II and TG member
- $1,500 co-funding from Div. II

9 August 2015:
Dr. Rey (TGC) has withdrawn from the project and no other updates are available.

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 Metallacyles Containing d-Block Elements

(IUPAC Recommendation)

Alan T. Hutton1, Edwin C. Constable2, Risto Laitinen3, Ebbe Nordlander4, Warren H. Powell5, Daniel Rabinovich6

1Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa; 2Department of Chemistry, University of Basel, Spitalstrasse 51, CH-4056 Basel, Switzerland; 3University of Oulu, PO Box 3000, FIN-90014, Finland; 4Centre for Chemistry and Chemical Engineering, Lund University, Box 124, SE-22100, Sweden; 51436 Haven Crest Court, Columbus, OH 43220-3841, USA; 6University of North Carolina, Charlotte, NC, USA.

*E-mail: inorganic.nomenclature@iupac.org. Sponsoring body: IUPAC Division of Chemical Nomenclature and Structure Representation.

July 2016 (Rabinovich):
Revisions of the draft Technical Report continue.

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

(cont...)

6 July 2016 (Juris Meija, CIAAW):

In order to resolve issues about the interpretation of standard atomic weight uncertainties, the Task Group has submitted two manuscripts to PAC. The Provisional Recommendation was posted on lupac.org with comments requested by 31 August 2016.

Submitted: 1 July 2013
Start date: 1 September 2013
Planned end date: 1 September 2016
• **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 545; balance: USD 5,455.
• 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 has been funded by Divisions II and IV.

**12 August 2015 (Ober, TGC):**
The preliminary website is up and feedback and suggestions are welcomed:
http://iupac-materials.chem.utah.edu/?page_id=52

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

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• **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 4,440; balance: USD 4,560.
• 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.

**9 August 2015:**
Poster presented at the 45th IUPAC World Chemistry Congress in Busan, South Korea (poster NM-P0558-MON).
15 October 2015 (Öhrström, TGC):
Progress report made (poster presentation) at the EuroMOF conference in Berlin (11-14 October 2015).

7 July 2016 (Öhrström, TGC):
A "discussion" paper is currently drafted highlighting the scientific questions of the project. The steering committee for the Reticular Chemistry Structure Resource (RCSR) is in place: http://rcsr.anu.edu.au/about

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, CIAW)].
• 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.

(cont...)
6 July 2016 (Juris Meija, CIAAW):

CIAAW has recently been involved in the data analysis of a recent suite of international reference materials that were published in Analytical Chemistry [Anal. Chem. 2016, 88, 4294-4302] before CIAAW can recommend these values in its Isotope Reference Material Report. The work on this project is ongoing.

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: Irregeher, 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: Ding
- 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).

(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.

No updates to report

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 (The King's University College, Edmonton, Canada)
- TG: Apotheke, Coplen, Hoffman, Martin, Tarbox, Walczyk & Wieser
- Assessment of 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 11,000; balance: USD 3,000.
- Div. II monitor: Ding
- Updates:

No updates to report

Submitted: 28 September 2015
Start date: 1 October 2014
Planned end date: 1 September 2017
**2015-030-2-200**
- TGC: Norman Holden (Brookhaven National Laboratory)
- TG: Coplen, de Bièvre, Wieser & Böhlke
- **Assessment of Fundamental Understanding of Isotopic Abundances and Atomic Weights of the Chemical Elements (2016—2017)**
- Budget: USD 5,000; spent: USD 0; balance: USD 5,000.
- Div. II monitor: Walczyk
- Updates:
  - Resubmission of 2015-030-1-xxx after peer-reviewing (comments were provided by Div. II & CCE)
  - Approved on 2 December 2015: USD 4,000 from Div II & USD 1,000 from CCE

*7 July 2016 (Norman Holden):*
Task group member Paul de Bièvre passed away on 11 April 2016 at the age of 82; remaining TG members are planning a meeting for early 2017.

Submitted: 28 September 2015  
Start date: 2 December 2015  
Planned end date: 31 December 2017

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**2015-037-2-200**
- TGC: Juris Meija (National Research Council Canada)
- TG: Possolo & Prohaska
- **IUPAC Molecular Weight Calculator**
- Budget: USD 2,000; spent: USD 0; balance: USD 2,000.
- Div. II monitor: Walczyk
- Updates:
  - Initially submitted to Divisions I & II, the Committee on Chemistry and Industry (COCl), and the Committee on Publications and Cheminformatics Data Standards (CPCDS)
  - After initial screening of potentially interested parties, suggestions for a revised proposal were provided to the TGC for a resubmission.

*6 July 2016 (Meija, TGC):*
CIAAW Chair has already prepared necessary code for online calculator of molecular weights and their uncertainties to be placed on ciaaw.org. A draft calculator (v.0.2) is currently running in a testing mode at:
http://ciaaw.shinyapps.io/App-2

Submitted: 5 November 2015  
Start date: 30 November 2015  
Planned end date: 31 December 2017
• **2015-039-2-200**
  • TGC: Eric Scerri (Dept. of Chemistry & Biochemistry, UCLA)
  • TG: Jensen, Öhrström, Ball, Restrepo & Lavelle
  • The Constitution of Group 3 of the Periodic Table
  • Budget: USD 5,800; spent: USD 0; balance: USD 5,800.
  • Div. II monitor: Rabinovich
  • Updates:
    • Comments from peer-reviewers sent to TGC on 21 October 2015
    • Proposal resubmitted on 9 November 2015

**7 July 2016 (Scerri, TGC):**
A meeting of the Task Group is being planned for the Spring 2017 National ACS Meeting in San Francisco, California.

Submitted: 9 November 2015
Start date: 18 December 2015
Planned end date: ???

• **2015-053-1-200**
  • TGC: Robin T. Macaluso (University of Texas at Arlington)
  • TG: Milan Drabik (Slovak Academy of Sciences), Melanie Kirkham (ORNL), Cora Lind-Kovacs (U. of Toledo), Emma McCabe (U. of Kent) & Leopoldo Suescun (U. of the Republic, Uruguay)
  • Survey of Definitions and Use of Common Solid-State Chemistry Terminology
  • Budget: USD 9,500; spent: USD 0; balance: USD 9,500.
  • Div. II monitor: Colón
  • Updates:
    • Submitted to Divisions II & VIII and CCE
    • Approved on 31 December 2015: USD 5,700 from Div II, USD 2,800 from Div VIII and USD 1,000 from CCE

**June 2016 (Macaluso, TGC):**
Survey of the scientific literature dealing with the definitions of alloy, intermetallic, crystal, liquid crystal, ionic crystal, etc. was initiated in January 2016 and Task Group members met via Skype in June 2016 to communicate progress reports.

Submitted: 17 November 2015
Start date: 31 December 2015
Planned end date: 31 December 2017
Update on **Pending** Proposals: 
**Undergoing Peer-Review**

- **2015-042-1-xxx**
- TGC: Norman Holden (National Nuclear Data Center, Brookhaven National Laboratory, NY, USA) & Peter Mahaffy (The King's University College, Edmonton, Canada)
- TG: Apotheke, Coplen, Hoffman, Martin, Tarbox, Walczyk & Wieser
- *Development and Global Dissemination of an IUPAC Interactive Electronic Isotopic Periodic Table. Recommendation of Feasibility of a 100th Anniversary IUPAC Periodic Table of the Elements and Isotopes.*
- Requested budget: USD 14,000
- Div. II monitor: Rabinovich
- Updates:
  - Original proposal submitted to **Div. II** and **CCE**
  - Revised version of 2012-016-1
  - Revised scope of 2014-024-1-200
  - Proposal **declined** due to conflict with another Division II project (No. 2014-024-1-200) and thus re-submission is not planned.

Submitted: 2 October 2015
Start date: xxx yyyy zzzz
Planned end date: ???
Update on Proposals in Preparation

- **2017-xxx-1-xxx**
- TGC: Pavel Karen (University of Oslo)
- TG: Rabinovich, Leskelä,... others?
- **Toward a Comprehensive Definition of Valence**
- Requested budget: USD 5,000
- Div. II monitor: ???
- Updates:
  - To be submitted to Division II

Proposal in preparation

Submitted: xx yyyy 2017 (?)
Start date: xx yyyy 2019 (?)
Planned end date: ???
2016-xxx-1-xxx
TGC: Daniel Rabinovich (UNC Charlotte)
TG: Verani (Wayne State U.), Lim (UNIST), Jorge Colón (UPR), 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 2017 (?)
Start date: 1 September 2017 (?)
Planned end date: xx yyyyyy 2019 (?)

Project Expenses vs Budget (as of 6 May 2016)

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<th>Project Numbers</th>
<th>Total Project Budget</th>
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<th>Remaining Funds</th>
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$167,250.00 $108,414.55 $2,302.58 $102,056.97

Completed projects (8/2015–7/2016): 2
Primary active projects: 20 (16 continuing, 4 new)
Secondary active projects: 3