



IUPAC

International Union of Pure and Applied Chemistry

Inorganic Chemistry Division (II) Newsletter 2012_2

Editors Note: Below you will find the 2012-2 Newsletter; it was compiled thanks to your kindness to send materials. So keep sending your items, including pictures, or suggested topics for future issues, preferable via email to Reedijk@chem.leidenuniv.nl. I can handle most formats of attachments.

Kindest regards, Jan Reedijk.

Division II Members 2012-2013 (*pictures and short descriptions of member activities: see last 2 pages*)

President: [Loss, Robert D.](#), **Vice President:** [Reedijk, Jan](#); **Secretary:** [Leskelä, Markku](#);

Titular members: [Mathur, Sanjay](#); [Drabik, Milan](#); [Sakai, Ken](#); [Holden, Norman E.](#); [Öhrström, Lars R.](#); [Karen, Pavel](#); [Tshuva, Edit Y.](#)

Associate members: [Ding, Tiping](#), [Garcia-Martinez, Javier](#), [Buchweishaija, Joseph](#); [Rabinovich, Daniel](#); [Vannier, Rose-Noelle](#); [Kiliç, Adem](#);

National representatives: [Abdul Aziz, Farina](#); [Trendafilova, Natasha](#); [Prugovečki, Biserka](#); [Chandrasekhar, V.](#); [Youngme, Sujittra](#); [Toma, Henrique](#); [Ali Saqib](#).

Division II Subcommittees and Commissions currently in operation are the following:

[Subcommittee on Isotopic Abundance Measurements](#)

[Interdivisional Subcommittee on Materials Chemistry](#)

[Commission on Isotopic Abundance and Atomic Weights](#)

[Stable Isotope Reference Material Assessment](#)

Off-year Division Activities

The so-called **off-year meeting of Division II** was held in 2012 at the University of Cologne (Host-organizer has been prof. Sanjay Mathur and his team), from Sept. 6 (arrival in pm), 7, and 8 (Departure day).

Attendance was very good with 14 delegates (3 officers, 5 TM, 5 AM and 1 NR); only 2 TMs and 1 AM were unable to attend. Project updates and new projects plans were discussed in detail, and summarized below.

A group picture of the 14 delegates is below.



From left to right: Sanjay Mathur, Markku Leskelä, Rose-Noelle Vannier, Tiping Ding, Javier Garcia, Robert Loss, Edit Tshuva, Daniel Rabinovich, Henrique Toma, Norman Holden, Adem Kiliç, Pavel Karen, Jan Reedijk

Project Planning and Progress News:

A recent project, joint with Divisions VIII and IV, proposing the **revision and extension of the 1984 recommendations of (single-stranded) metal-based coordination polymers** had been granted in 2011. The group had a first meeting, in the end of February 2012 in Leiden, NL, followed by an informal meeting in Cologne, Sept. 7, 2012 of a subgroup, consisting of Lars Öhrström, Richard Jones and Jan Reedijk. The convenor of the group is prof. Richard Jones from Division IV. The final report is expected during 2013 or early 2014.

The MOF project (convenor prof. Lars Öhrström: <http://www.iupac.org/web/ins/2009-012-2-200>) can report as follows:

The IUPAC task group on "Coordination polymers and metal organic frameworks: terminology and nomenclature guidelines" met for a final one-day meeting at the University of Stockholm, 24th May to draft new recommendations. In collaboration with the Swedish Chemical Society we benefited from this occasion by also arranging a one-day Trends in Inorganic Chemistry symposium, with the theme *Metal-Organic Frameworks, Porous Coordination Polymers and Zeolites*. This meeting took place on the 23rd May and also featured talks by local host Xiaodong Zou,

Univ. of Oslo's Unni Olsbye and Tina Düren from the Univ. of Edinburgh. See www.tinc.nu.

The preliminary conclusions from the project were also presented at the International Conference on Coordination Chemistry in Valencia, Spain (poster, Jan Reedijk) and at the 3rd Metal-Organic Framework meeting in Edinburgh, UK (invited talk, Lars Öhrström & Neil Champness). At the latter meeting we also had the opportunity to promote IUPAC organization and projects.



Left to right: Xiao-Ming Chen, PR China, Neil Champness, UK, Javier Garcia Martinez, Spain & Div. II, Lars Öhrström, Sweden & Div. II, Stuart Batten, Australia, Susumu Kitagawa, Japan, Michael O'Keeffe, USA, Jan Reedijk, the Netherlands & Div. II.

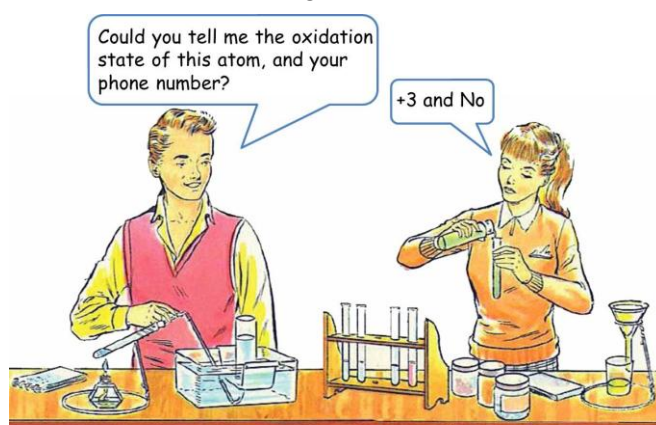
Pavel Karen report as follows on the [Oxidation State Project](#).

The project 2008-040-1-200 "Towards a comprehensive definition of oxidation state" is nearing completion. The task-group members are chemists involved in complexes, in organometallic chemistry and in solid state and molecular chemistry: Josef Takats (University of Alberta, Edmonton, Canada), Patrick McArdle (NUI Galway, Galway, Ireland) and Pavel Karen (University of Oslo, Oslo, Norway; the task-group chairman). After the start in March 2009, the project went through following milestones: 1: Anamnesis (2009); 2: Case studies (January 2010–June 2011); 3: Write-up (from July 2011).

The anamnesis explored the history and present state of the oxidation state via drafting and commenting five internal documents: 1 IUPAC definitions, 2 Textbook definitions, 3 Difference oxidation state versus number, 4 Purpose and all uses of oxidation state (see figure), 5 List of telling examples. In the historical excursion, we encountered an oxidation grade in a textbook by Wöhler from 1835 (recovered from a depository in Oslo), which is based on the number of oxygen

equivalents an atom can bond to. Many textbooks stick to this simple principle. Other textbooks adopt a more flexible algorithmic definition based on moving bonds onto the electronegative partner. IUPAC's Gold Book lists one definition for oxidation state of the former type, and another definition for the oxidation number, of the latter type; based on atom's charge after ligands are removed together with their electrons.

For the case studies, we selected 75 molecules and 25 solids, on which we tested several alternative definitions and algorithms via Power Point files subsequently commented by the two task-group members. It soon turned out that entire groups of compounds need special attention: Haptocomplexes. Molecular $H_2 \cdots 2H^-$ complexes. Non-innocent ligands (prone to oxidation-state changes a chemist might wrongly blame on the central atom). Oxidation-state tautomerism (a dichotomous oxidation-state combination that tilts over when thermal energy is supplied). Electronegative Lewis-acid ligands. Oxidation state in Lewis acid–base adducts in general.



The extent of relevant examples led us to a decision to write a Technical Report first, which will later be extracted into an eventual much shorter Recommendation. We had originally planned to write also an article for JCE on oxidation state in chemical education, but this activity still lies well ahead.

The Technical Report introduces several novel approaches to oxidation state: Instead of definitory algorithms, there is one single generic definition based on ionic approximation of bonds. For the latter, we have tested three alternative interpretations: bond polarity, average valence-orbital energy of the isolated atom, and the atom's contribution to the bonding MO. We have developed several algorithms on how to calculate oxidation state, suited for both molecules and extended solid structures. These algorithms are either

bondless, or bond based. The latter consist of an algorithm of moving bonds and an algorithm of summing bond orders.

The project's outlook is to finish early in 2013 the remaining subsections in the Technical Report, of so far 59 pages. Before submission, it will be made available in the Division II web-discussion forum. Then it will go through the IUPAC peer review process and PAC editorial treatment. In the meantime, a short recommendation set will be drafted and discussed; eventually world-wide on the IUPAC website, as all Recommendations now are.

Meetings, Events and IUPAC Sponsored Conferences

ICCC, Valencia, 2012

From Sept. 9-13, the 40th ICCC conference was held in Valencia, Spain. International Conferences of Coordination Chemistry have been held since 1950; it is the oldest existing series of specialized conferences. The meeting attracted some 900 delegates from over 50 countries, and took place in the Convention Center Valencia. The meeting was addressed at the opening by prof. Luis Oro, on behalf of IUPAC. At the end of the meeting, the post of Executive Secretary was - after 24 years - taken over from prof. Jan Reedijk, by prof. Chris Orvig (Vancouver).

Major Conference Highlights the Importance of Research, Best Practices, and New Technologies in Chemistry Education

For the first time, the two major international conferences on chemical education, the 22nd International Conference on Chemistry Education and the 11th European Conference on Research in Chemical Education, joined in Rome in **July 2012** to present and discuss the most significant developments in Chemistry Education.

As a prelude to this international conference that convened hundreds of chemistry practitioners and educators at the University of Rome "La Sapienza" the [Virtual Colloquium to Sustain and Celebrate IYC 2011 Initiatives in Global Chemical Education](#) was held from May to June 2012. This initiative allowed global participants to discuss a total of thirteen papers in an online environment. The Virtual Colloquium served as an excellent pre-conference activity and as an excellent example of the increasing importance of online tools in education.

As in previous editions of the International Conference on Chemistry

Education, the Distinguished Contribution to Chemistry Education Award was presented to those individuals who during their careers done outstanding contributions to the field. On this occasion, this prestigious award was given to Prof Robert (Bob) Bucat from Western Australia University and Prof Peter Mahaffy from the King's University College, Edmonton, Canada



Prof. Robert Bucat and Prof. Peter Mahaffy (third and fifth from the left on the picture, respectively) received the Distinguished Contribution to Chemistry Education Award at the 22nd International Conference on Chemistry Education in Rome.

Division II Associate Member Javier Garcia-Martinez, who served as a jury member of the Distinguished Contribution to Chemistry Education Award, representing the IUPAC Bureau, organized the symposium "Chemistry 2.0: creating on-line communities" where the use of online educational tools was discussed. Specific examples of applets, websites and on-line tools, many developed for the International Year of Chemistry, were presented by international experts on new technologies and chemistry education.

●9th Japan-China Joint Symposium on Metal Cluster Compounds in Fukuoka, Japan

The 9th Japan-China Joint Symposium on Metal Cluster Compounds was held in Fukuoka, Japan during **August 13-16, 2012**, with prof. Ken Sakai as symposium chairman. This symposium was initiated in the Institute for Molecular Science, Okazaki, Japan, by Prof. Kazuo Saito and Prof. Jiayi Lu many years ago. This event series has been providing great opportunities for the coordination chemistry societies of Japan and China to promote exchange and collaborative activities. The symposium was co-organized by one of the governmentally funded projects of Japan, called "Coordination Programming" Project leader Prof. Hiroshi Nishihara, University of Tokyo. The co-chairman of the symposium

from the Chinese side was Prof. Rong Cao, Fujian Institute of Research on the Structure of Matter Fujian. Several important Chinese professors were also attending.



Extremely high level scientific topics especially focused on coordination chemistry were reported and discussed, which made the 9th joint symposium truly successful. All the delegates also enjoyed having deeper discussion over the joint meals and social events throughout the symposium period.

The two countries agreed to hold the 10th joint symposium in 2015 in Fuzhou, China. It is planned in that year to celebrate the 100th birthday of one of the most important persons correlated with this joint symposium, i.e. Prof. Prof. Jiayi Lu.

Two new elements: Flerovium (114) and Livermorium (116). Report by Robert Loss.

Following an extensive period of, investigation and confirmation of the discovery, internal and external review, and public consultation, the approval process for these two new elements; flerovium with the symbol **Fl** for the element with $Z = 114$ and livermorium with the symbol **Lv** for the element with $Z = 116$; was completed with their official adoption on 23 May 2012 by the IUPAC Bureau as delegated to act by the IUPAC Council meeting on 3–4 August 2011. The recommendation was then published in *Pure Appl. Chem.*, **84** (2012) 1669–72. The Division would like in particular to thank all those involved in this process

A new IUPAC/IUPAC working party has been convened to consider evidence for new elements with Atomic Numbers 113, 115, 117 and 118. The working party is expected to report by the end of 2012 and hopefully the Division will have something to report on the matter in the next newsletter.

Conference announcement: The XXIVth International conference on Coordination and Bioinorganic chemistry: Recent Developments In Coordination, Bioinorganic And Applied Inorganic Chemistry, Smolenice, Slovakia, June 2 – 7, 2013

The XXIV. ICCBIC is organized in the Congress Centre of the Slovak Academy of Sciences in Smolenice Castle by the: Slovak Chemical Society, Slovak Technical University in Bratislava, University of Alexander Dubček in Trenčín and Slovak Academy of Sciences. The conferences on coordination chemistry held regularly in Slovakia (Central Europe), have a long tradition. The First Conference of this kind was organized in 1964. Many top coordination chemists, Nobel prize winners including, from all over the world have attended the Conferences till now and Smolenice Castle became the place where many new scientific and personal contacts were established. More information on the conference you can find at the website www.iccbic.stuba.sk

Contacts via e-mail are possible at the address: iccbic@stuba.sk

Duties of Division Members

Starting 2012 all division member duties (TM&AM) have been made visible in a matrix table. This was prepared on the request of the newly elected members. A [welcome package](#) for the new members has been updated and was distributed to all newly elected members (2012-2013). (*Copies are still available for others, if wished so*).

Call for new project interest: Definition of valence.



At the 2012 division meeting in Cologne a project on the definition of valence was suggested by Pavel Karen. It could include the etymology of valence. Is it a power or ability of an element to bond? Or perhaps an extent to which an atom bonds or can bond to other atoms? Can it be quantified? The following definitory algorithms are known:

- 1) Number of electrons that an atom uses in bonding
- 2) Number of two-electron bonds or its equivalents an atom forms
- 3) Absolute value of the atom's oxidation state
- 4) The Gold-book definition

Members and other readers are encouraged to deliver input and examples of conflicting numerical results for valence with any of the above definitions, and perhaps propose a new definition. Pavel invites comments at: pavel.karen@kjemi.uio.no In early 2013 he will decide to submit an IUPAC proposal.

Project overviews in a (clickable) Table are available on the next page.

Recently started and ongoing Divisional projects (titles & hyperlinks)
Status project Division as per September 2012

Running Project of Division II	Clickable weblink
Recommendations for Isotope Data in Geosciences	http://www.iupac.org/web/ins/2006-016-1-200
Priority claims for the discovery of elements with atomic number greater than 111	http://www.iupac.org/web/ins/2006-046-1-200
Evaluation of Isotopic Abundance Variations in Selected Heavier Elements	http://www.iupac.org/web/ins/2007-029-1-200
Evaluated Compilation of International Reference Materials for Isotope Abundance Measurements	http://www.iupac.org/web/ins/2007-031-1-200
Development of an Isotopic Periodic Table for the Educational Community	http://www.iupac.org/web/ins/2007-038-3-200
Towards a comprehensive definition of oxidation state	http://www.iupac.org/web/ins/2008-040-1-200
Coordination polymers and metal organic frameworks: nomenclature guidelines	http://www.iupac.org/web/ins/2009-012-2-200
Evaluation of Radiogenic Abundance Variations in Selected Elements	http://www.iupac.org/web/ins/2009-023-1-200
Technical Guidelines for Isotope Abundances and Atomic Weight Measurements	http://www.iupac.org/web/ins/2009-025-1-200
Assessment of Stable Isotopic Reference and Inter-Comparison Materials	http://www.iupac.org/web/ins/2009-027-1-200
Online evaluated isotope ratio database for use communities (2011-2014)	http://www.iupac.org/web/ins/2009-026-2-200
Evaluated Published Isotope Ratio Data (2010-2011)	http://www.iupac.org/web/ins/2009-029-1-200
Guidelines for Measurement of Luminescence Spectra and Quantum Yields of Inorganic Compounds, Metal Complexes and Materials	http://www.iupac.org/web/ins/2009-045-1-200
Terminology and definition of quantities related to the isotope distribution in elements with more than two stable isotopes	http://www.iupac.org/web/ins/2009-046-2-200
Evaluated published isotope ratio data (2011-2013)	http://www.iupac.org/web/ins/2011-027-1-200
Evaluation of published lead isotopic data (1950-2013) for a new standard atomic weight of lead	http://www.iupac.org/web/ins/2011-028-1-200
Development a procedure for using intervals instead of fixed values for atomic weights: an educational exercise	http://www.iupac.org/web/ins/2011-040-2-200

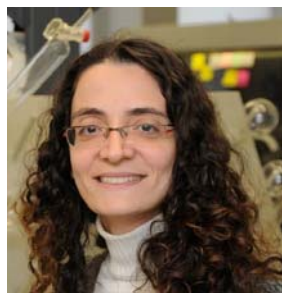
Compiled by Daniel Rabinovich, October 2012

[Appendix on next pages:](#)
[Members of the Division](#)

Addendum to the Newsletter 2012-2

Members of the Division Committee!

Titular members 2012-2013:



Prof. Edit Y. Tshuva, Hebrew University, Jerusalem. She has research interests and expertise in the field of molecular bioinorganic chemistry.

Milan Drabik works on chemistry aspects of cements and ceramics with a focus on studies of Macro Defect Free Materials (*MDF*) in Comenius University and Slovak Academy of Sciences, Bratislava, Slovakia.



Norman Holden is a specialist in radioactive isotopic half lives and decay constants, and also atomic weights and isotopic composition of the chemical elements. He has served IUPAC since 1971.

Pavel Karen is from the University Oslo. He is an inorganic chemist interested in transition-metal oxides with strongly-correlated electrons and properties such as superconductivity or valence mixing/ordering.



Markku Leskelä, Professor of Inorganic Chemistry, University of Helsinki, Finland.



His research deals with synthesis of metal-organic compounds and their use in making of thin films – especially by atomic layer deposition nanostructures and use in catalytic activation of small molecules. He has been Secretary of the Division since early 2012.



Robert D. Loss: President of the Division. His research interests are in Isotope Science and its applications in nuclear science and technology. Working in the Physics Department of Curtin University of Technology, Perth Australia, he has been a Member of Division

II since 2006, and a member of the Commission on Isotope Abundances and Atomic Weights since 1992.

Sanjay Mathur is a materials inorganic chemist at the University of Cologne. His research centers around various facets of Nanochemistry. He has been active in the Division since 2003.



Lars Öhrström, is Professor of Inorganic Chemistry at Chalmers Tekniska Högskola, Göteborg, Sweden. His main interests are in coordination polymers and metal-organic frameworks and the analysis and understanding of molecular crystal structures, in particular by using network topology analysis.

Jan Reedijk, is a Molecular Inorganic Chemist from Leiden University (Coordination and Bioinorganic Chemistry). He has been in Division 2 since 2006, and is currently vice-president.



Ken Sakai is a molecular inorganic chemist with a strong interest in photochemistry from Kyushu University, Fukuoka. He has been on the division since 2007.

Current Associate Members of the Inorganic Division Committee:

Members for the period 2012-2013 are:

Rose-Noelle Vannier, from Lille, France. She has expertise in the field of solid state chemistry and materials.



Joseph Buchweishaija, from Dar-es-salaam, Tanzania; his research interest is the area of materials.

Daniel Rabinovich, from Charlotte, North Carolina USA. Daniel, who is a synthetic bioinorganic chemist; he has taken over the Division II project administration in 2012.



Adem Kiliç, Gebze Institute of Technology, Kocaeli, Turkey. His expertise is in the area of molecular inorganic chemistry (Phosphazene Chemistry).

Javier Garcia-Martinez, is from the university of Alicante, Spain, and is a Materials Inorganic Chemist. He is also a member of the Bureau.



Tiping Ding is an isotope chemist from the Laboratory of Isotope Geology, the Institute of Mineral Resources, Chinese Academy of Geological Sciences.

National Representatives for 2012-2013 with their main scientific interests and expertise, and a picture, are presented below:

Yang Farina Abdul Aziz, from Bangi Selangor, Malaysia. She has expertise in the field of molecular inorganic chemistry.



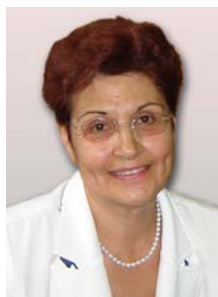
Biserka Prugovečki, from Zagreb, Croatia. She has expertise in crystallography.

Sujittra Youngme from Khon Kaen University, Thailand, has expertise in molecular inorganic chemistry.

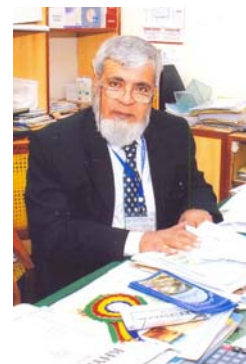


Henrique Eisi Toma, from Sao Paulo, Brasil; his expertise is in molecular materials.

V. Chandrasekhar, Indian Institute of Technology, Kanpur; he has expertise in the field of molecular inorganic chemistry.



Natasha Trendafilova from Sofia, Bulgaria; she has expertise in theoretical chemistry.



Ali Saqib from Quaid-i-Azam University, Islamabad, Pakistan; his expertise is in coordination chemistry and main group chemistry.