IUPAC
International Union of Pure and Applied Chemistry

Inorganic Chemistry Division (II) Newsletter 2009

Editors Note: Following on from last year's successful newsletter I am pleased to present you with the second of the Division II newsletter for the 2008-9 biennium. This edition features news and activities from past and present members - I hope you find these useful and/or interesting. Many thanks to those who have provided photos and news items. If you have an item or images about any of the Division members or associated activities, please forward these to me, preferable via email. (r.loss@curtin.edu.au). All the best from Bob Loss.

Division II People

President: Tatsumi, Kazuyuki, **Vice President:** Loss, Robert D., **Secretary:** Interrante, Leonard V.
Past President: West, Anthony R.
Titular members: Coplen, Tyler B., Ding, Tiping, Garcia-Martinez, Javier, Leskelä, Markku, Oro, Luis A., Reedijk, Jan, Suh, Myunghyun Paik
Associate members: Chadwick, Alan V., Drabik, Milan, Holden, Norman E., Mathur, Sanjay, Sakai, Ken, Takats, Josef
National representatives: Basova, Tamara V., Bologna Alles, Aldo, Gonfiantini, Roberto
Karen, Pavel, Liu, Ling-Kang, Öhrström, Lars R.

Division II Subcommittees and Commissions
Subcommittee on Isotopic Abundance Measurements
Subcommittee on Characterization of Carbonaceous Materials and New Carbons
Interdivisional Subcommittee on Materials Chemistry
Commission on Isotopic Abundance and Atomic Weights

Meetings and conferences

Commission on Isotopic Abundances and Atomic Weights workshops and Related Project Meetings 2009

All over the period 22 – 29 July 2008, all at IAEA Vienna.

Educational Periodic Table Workshop (Project number 2007-038-3-200) , Together with CCE - July 21 July 22.

SIAM: (Subcommittee on Isotopic Abundance measurements), July 23-24 and July 27.

CIAAW: July 28-29. For further details contact CIAAW secretary, Michael Wieser, mwieser@ucalgary.ca,

IUPAC 45th General Assembly

Commences August 1 2009, Glasgow UK

Division II , General Assembly meeting: July 31 - August 1, 2009, Glasgow

Obituaries

The past Month has seen the very sad passing of two long serving former Division II members.

Prof Etienne Roth, passed away on Thursday, March 19th. Etienne served formally on CIAAW from 1967 until 1979 including 4 years as Chairman of CIAAW, and continued as an active contributor to Commission until just a few weeks before he passed away. Divisional member, long time colleague and friend, Norman Holden said, "Etienne's death brings an end to a long and successful scientific career and an equally long period of major contributions to our Commission. Etienne's thoughtful comments on the issues and questions before the Commission will be sorely missed."

Professor Kevin Rosman passed away on Monday, March 22 2009. Kevin served as formal Member of CIAAW from 1983 to 1995 including a period as Chair of SIAM, and continued to make many contributions to the work of the Commission until several years ago. He was a major author on the 1997 “Isotopic Composition of the Elements”, and a member of the team that produced the major “2000 Review of the Elements” publication.

Kevin was one of my [Editor] PhD supervisors and had retired from full time teaching duties only some 7 months earlier. As well as an outstanding contribution to the world of isotope science, Kevin’s contribution in building CIAAW’s understanding of the need for applying rigorous uncertainty protocols in isotopic abundance and atomic weight evaluations will be long remembered.

News From the World of Metrology

Submitted by Paul De Bièvre
IUPAC delegate to the JCGM at the BIPM in Paris-Sèvres, “Focus on Metrology” and member of the Analytical Chemistry Division V Committee

The new “International Vocabulary of Metrology”, as unanimously voted into existence by eight international organizations (BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, OIML) is now freely available -since 2008-06-14- from:
http://www.bipm.org/en/publications/guides/vim.html

The newest documents related to the Guide for Expression of Uncertainty in Measurements, as unanimously voted into existence by eight international organizations (BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, OIML) is now (status 2009) freely available from:
http://bipm.org/en/publications/guides/gum.html

The next revision of the VIM may be decided by the JCGM (Joint Committee on Guides for Metrology) in Dec 2009 (to be finished by 2014/2015).

Article to watch out for

Chemistry International will feature an article in the 2009 May-June Issue on, “What is Materials Chemistry”, by Peter Day and Divisional Secretary, Len Interrante, and Past President Anthony West.

What Is “Materials Chemistry?”

by Peter Day, Leonard Interrante, and Anthony West

The words “materials” and “chemistry” have only been linked relatively recently, yet “materials chemistry” now accounts for a significant fraction of chemical science. The phrase has often been used quite indiscriminately, so IUPAC launched a project to try to define it. This article presents some of the background and conclusions to the study.

The Rise of Materials Chemistry

What do the following topics in contemporary chemistry have in common? (1) Using NH_3 incorporated in simple inorganic solids as a medium for storing hydrogen; (2) designing and assembling chemically patterned or anisotropically shaped colloidal particles into arrays with predefined geometries; (3) predicting the structures of molecular and hybrid crystals through computer simulations; (4) creating porous crystals of metal oxides templated by mesoporous silica cages. The answer is that all were the subjects of recent articles published in one of the main international journals devoted to materials chemistry.[1] In view of this ubiquity, it is surprising that as recently as 20 years ago, the words “materials” and “chemistry” were rarely linked together. Now, in 2009, “materials chemistry” represents one of the major growth sectors in pure and applied chemistry and accounts for a significant fraction of all publications in the chemical sciences.

Several straightforward measures verify these assertions. As an indication of its broad global outreach, entering the phrase “materials chemistry” into the Google search engine results in a number of hits comparable to those of traditional chemistry disciplines, such as “physical chemistry,” “organic chemistry,” “inorganic chemistry,” or “macromolecular chemistry.”

Figures for citations covering these major subdisciplines in the journals of one leading chemical society are as follows (2006 figures):

Organic chemistry	115 968
Physical chemistry	108 742
Macromolecular chemistry	76 448
Inorganic chemistry	58 002
Materials chemistry	38 890

The figure for materials chemistry is especially impressive, because it has risen from nearly zero in just a short period of time.

The number of articles submitted to *Chemistry of Materials*, one of the major journals in the field, increased 18-fold over the first 19 years of its existence. Similar increases in submissions over the last decade have been noted in other journals that focus partly or entirely on materials-related chemistry, such as the *Journal of Materials Chemistry* (RSC), *Advanced Materials* and *Advanced Functional Materials* (Wiley), *Nature Materials* (NPG), *Journal of Solid State Chemistry* (Elsevier), and many others dealing with more specialized areas of materials chemistry and materials science. The number of citations of papers from these materials chemistry journals, and their corresponding “Impact Factors,” has also increased enormously.

Increasingly, however, the phrase “materials chemistry” is being bandied about indiscriminately, often by those merely in search of a buzzword. What does it really mean?

Defining Materials Chemistry

Given that the phrase “materials chemistry,” although coined only recently, has become so popular within the chemical community, it is pertinent to ask how materials chemistry should be defined—what it is and (perhaps more importantly) what it is not. Because one of IUPAC’s roles is to provide internationally agreed-upon definitions and standards, it was reasonable to take up this question; a project was launched in 2005 with this goal:

To assemble, collate, and disseminate information about the scope of the newly emerging discipline of materials chemistry, leading to an authoritative definition of the subject within the family of chemical sciences.

The objective was not so much to produce lists of specific topics or categories of compounds and phenomena, which would quickly become out of date, but to establish some principles that could be deployed by IUPAC and the chemical community at large to help structure this new discipline within the broad family of chemical sciences.

The Origins of Materials Chemistry

Chemistry began, and largely continues today, to be inextricably associated with preparing, processing, and utilizing “materials,” both natural and synthetic. Early examples include tanning and dying skins and

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In this article, the authors discuss the recent linking of the terms “materials” and “chemistry”, which now accounts for a significant fraction of chemical science. The phrase “materials chemistry” has often been used quite indiscriminately, so IUPAC launched a project to try to define it. This article presents some of the background and outcomes to the study, including an operational definition of “Materials Chemistry”.

Titular Member Award

Javier Garcia Martinez, named a Young Global Leader

The World Economic Forum (WEF) has recognized Titular Member, Javier Garcia Martinez, as one the 2009 Young Global Leaders for his pioneering work in nanotechnology and energy, his leadership, and his commitment to shaping a more sustainable global future.

WEF each year recognizes distinguished young leaders below the age of 40 from around the world. This year, 230 individuals, including Javier Garcia Martinez, were selected from a

pool of almost 5,000 candidates. Other members of the class of 2009 are: Chad Hurley, co-founder & CEO of YouTube, Josh Sliverman, CEO of Skype, Mark Zuckerburg, founder & CEO of Facebook, Chris Martin, lead singer of Coldplay, and Tiger Woods.

Javier is 4th from the left.

In 2005, Javier co-founded Rive Technology, Inc., to commercialize the technology that he developed during his post-doctoral stay at MIT. The technology is a proprietary method of modifying the pore structure of a zeolite, making it more accessible to larger molecules in a feedstock. Rive selectively introduces mesopores (pores nearly four nanometers in diameter) into a zeolite, allowing larger molecules to access the zeolite and get "cracked" into valuable products. As a result, petroleum refiners obtain a higher yield of desirable products such as gasoline, diesel fuel, and propylene, and less of undesirable products like heavy cycle oil and coke.

Rive's new catalyst fits readily into existing refineries and enables refiners to increase throughput and profitability with minimal capital investment. Rive Technology has raised over $22 million in venture capital and recently opened a extensive R&D facility in Princeton, NJ.

More information is available at http://www.weforum.org/ and http://www.rivetechnology.com/

Nomenclature Issues

Submitted by Jan Reedijk, Leiden University, NL;

Many authors are aware that in (additive) coordination nomenclature anionic ligands obtain the name of the anion in names of compounds, with the last letter changing in –o.

So acetate becomes acetato, nitrate becomes nitrato, azide becomes azido, catecholate becomes catecholato, etc. upon coordination. Till recently, the older nomenclature was still used and allowed, like "chloro" to indicate chloride as a ligand. However, chloro is also used as a substitutive prefix in organic compounds, e.g. chlorobenzene, or tetrachloromethane. These substituted prefixes, like in chlorobenzene, cyanobenzene, dibromomethane, tetrachloromethane, etc. remain unchanged. To avoid confusion and aid in teaching, the most recent IUPAC rules (2005) have harmonized this issue now, so that ALL anionic ligands, upon coordination to a metal, have the simple change in the ending from –e to –o.

Coordinated halides in additive nomenclature are now all consistently used in names. with the anionic ending –e being changed to –o. So: fluorido, chlorido, bromido, cyanido, thiocyanido, hydrido, hydroxido, nitrito-N, nitrito-O, peroxido, oxido (and not oxo, fluoro, chloro, bromo, nitro, peroxo, etc., anymore). The BF4- anion will have the formal name tetrafluoridoborate (when coordinated: tetrafluoridoborato). This is very helpful indeed, especially in teaching; however, it will have consequences on the formal names of well-known compounds, which will initially appear a bit unusual to the non-inorganic chemists. Like for cisplatin: cis-diamminedichloridoplatinum(II), or:μ-oxido-bis[trichloridoiron(III)].

Compare coordination and organic nomenclature in: tetrachloridotin, and tetrachlorostannane, respectively. (Tetrachlorotin is therefore a misnomer).

Full details are in: Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005; Edited by N.G. Connelly, T. Damhus, R.M. Hartshorn and A.T. Hutton; The Royal Society of Chemistry, 2005 [ISBN 0 85404 438 8].

Small Table of anionic ligands:

Anion name	Name when coordinated to a metal and in a coordination name	Old, trivial, and non-IUPAC recomd. name in coordination nomenclature
acetate	acetato	(no change)
azide	azido	(no change)
chloride	chlorido	chloro
cyanide	cyanido	cyano
hydroxide	hydroxido	hydroxo
hydrogenperoxide	hydrogenperoxido	hydroperoxo
nitrate	nitrato	(no change)
oxide	oxido	oxo
peroxide	peroxido	peroxo
phenoxide	phenoxido	phenoxo
tetrafluoridoborate	tetrafluoridoborato	tetrafluo(ro)borato
thiocyanate	thiocyanato	(no change)
sulfide	sulfido	(no change)

For commonly used group names, e.g. polyoxometallates, oxoacids, there is of course no change.

Project News

Submitted by Dr Ty Coplen USGS

New Division II Project

2008-040-1-200 Prof. P. Karen,
Towards a comprehensive definition of oxidation state

The current IUPAC definition of oxidation state appears to be circular. The objective of this project is to obtain a comprehensive definition of the term "oxidation state" for an atom in a molecular entity or extended structure, and to suggest an algorithm to evaluate its numerical value in an unambiguous manner. A glossary of terms related to oxidation and reduction will be created.

Presentation at EGU 2009

"How, when, and why to submit an IUPAC (International Union of Pure and Applied Chemistry) project proposal"

Tyler Coplen is presenting a 30-minute workshop at the European Geosciences Union, General Assembly, meeting in Vienna in April about how, why and when to prepare an IUPAC project proposal.

Most Atomic Weights are not Constants of Nature

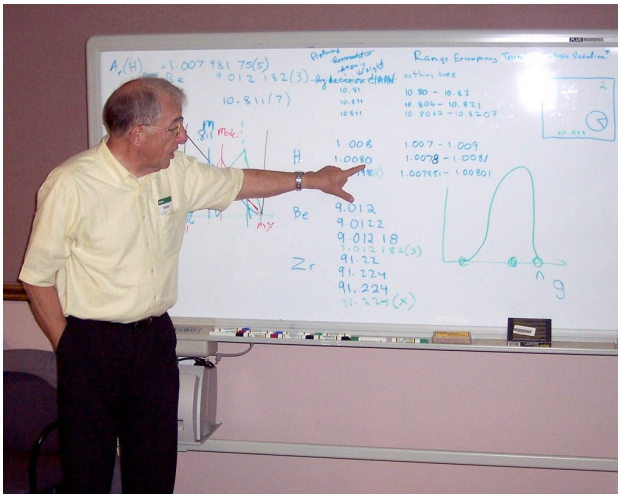
One of the fundamental problems in chemistry recognized by workers in Division II is that teachers commonly lead students to believe that all atomic weights are constants of nature.

More than half of the chemical elements have 2 or more stable isotopes and about 20 of these elements have measurable variations in relative amounts of the these isotopes that cause a measurable variation in atomic weight eg, the atomic weight of boron in naturally occurring specimens ranges between 10.8062 and 10.8207. On a 5-place table we would write 10.806 to 10.821. Two IUPAC projects are discussing how IUPAC can provide better education to the public. These are;

1. Project 2006-025-1-200 (Dr. N. Holden, "Assessment of fundamental understanding of isotopic abundances and atomic weights of the chemical elements")
2. Project 2007-038-3-200 (Dr. N. Holden, "Development of an Isotopic Periodic Table for the Educational Community")

One possibility under consideration is that where appropriate, current values in the IUPAC Periodic Table be replaced by a range. For example, the current value for boron of 10.811(7) might be replaced by 10.806—10.821.

In the photo below Paul De Bièvre discusses the merits of various options at a meeting of these two projects in Reston, Virginia.



New method for IUPAC Project

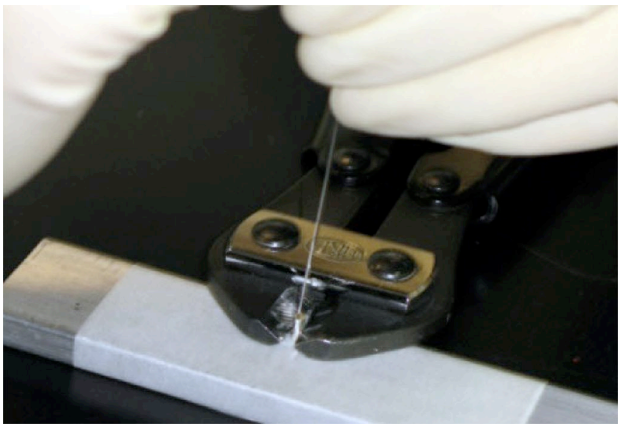
IUPAC project 2005-022-1, Brand and Coplen, "Calibration of Organic and Inorganic Oxygen-bearing Isotopic Reference Materials"

The Problem

Solid oxygen isotopic reference materials are anchored by two isotopic reference waters distributed by both the International Atomic Energy Agency in Vienna and the U.S. National Institute of Standards and Technology in Gaithersburg, Maryland, USA. Thus, to calibrate these solid materials we must also introduce liquid water into the same analyzer. About 25 µL of this reference water must be introduced into a silver capsule and seal before there is measurable oxygen isotopic fractionation, which occurs with any evaporation of the water. With this small amount of water it is a challenge to seal a sample with minimal isotopic fraction.

The Solution

An improved loading and sealing method for sealing small amounts of water in silver capsules was developed for this project, see below.



EuCheMS News

By EuCheMS President Luis Oro,

Europe is growing together, but the European research landscape is changing, with growing socio-economic challenges and the impact of globalisation on science and technology requiring policy responses. In this context, in recent years, the European Association for Chemical and Molecular Sciences, EuCheMS, legally established in March 2006, has made significant progress. Nowadays, the organisation gathers 50 member societies, which in total represent some 150,000 individual chemists in academia, industry and government in over 35 countries across Europe.

We should like to continue the efforts to create a European identity among the chemical societies, to increase the visibility of chemistry at the European level, and very specially to act as political voice towards European and international organizations. With the actual enlarged EU is very important that EuCheMS provides a point for discussion in order to influence EU government and politicians on the development of the European Research Area and the key role of Chemistry as a central science. We should be able to show that Chemistry has the tools and concepts to help answer some of the frontier questions arising in other disciplines. In other words, Chemistry is the science of creativity, making able to set goals of as type most other sciences cannot hope to attain.

The EuCheMS chemistry congresses, held in Budapest (2006) and Torino (2008), the future Nuremberg congress, to be held in 2010, and the numerous European scientific meetings, sponsored events and development of initiatives in specific areas carried out by Divisions and Working Parties are important catalysts for promoting European chemistry, that merit all our support. In this context we should welcomed the recent creation of the Division of Inorganic Chemistry, chaired by Prof. Nikos Katsaros. In particular, EuCheMS is sponsoring the 10th FIGIPAS meeting in Inorganic Chemistry, to be held in Palermo, Italy, on 1-4 July 2009.

On the other hand, EuCheMS should continue to promote educational, professional and ethical matters, and attracting chemists in the early stages of their careers through the very successful European Young Chemists network. We should be able to attract the most talented young people to the important chemistry research problems, such as those related to energy and /or environmental issues. However we should be aware of the risk of loosing core chemistry by supporting only interdisciplinary major challenges, and therefore we should advocate chemist as providers of solutions and this require core competences, and, without any doubt inorganic chemistry is a key area for this purpose.

Recent and ongoing Divisional projects

The Development of an Isotopic Periodic Table for the Educational Community (2007-038-3-200)
Analysis of the usage of nanoscience and technology in chemistry (2007-040-2-200)
Evaluated published isotope ratio data (2007-2009) (2007-028-1-200)
Evaluated compilation of int. reference materials for isotope abundance measurements (2007-031-1-200)
Recommendations for isotope data in geosciences (2006-016-1-200)
Assessment of fundamental understanding of isotopic abundances and atomic weights of the chemical elements (2006-025-1-200)
Terminology for conducting, electroactive and field-responsive polymers (2006-028-1-400)
Terminology for self-assembly and aggregation of polymers (2005-043-2-400)
Priority claims for the discovery of elements with atomic number greater than 111 (2006-046-1-200)
Evaluated published isotope ratio data (2005-2007) (2005-027-1-200)
Calibration of organic and inorganic oxygen-bearing isotopic reference materials (2005-022-1-200)

Chemical Synthesis of Functional Nanostructures

By Sanjay Mathur
Institute for Inorganic Chemistry, University of Cologne

Sangay is the only one without a costume and the glass in his hand!

Sangay's research group is involved with the synthesis and characterization of inorganic nanostructures by different chemical routes involving liquid (sol-gel, hydrothermal) or vapor phase (thermal and plasma CVD) processing of chemical precursors. The emphasis of the on-going projects spans from fundamental to applied aspects of innovative chemical procedures for materials synthesis. The group has developed new concepts for the molecule-based growth of nanoparticles, nanowires and nanostructured coatings for applications targeting bio-medical (drug delivery, implant integration), sensors (gas, opticsa and humidity), protective (barrier and corrosion-resistant coatings) and functional surfaces (photo-catalytic, hydrophobic, hydrophilic).

Details of Sangay's group and its research is available at http://www.mathur.uni-koeln.de/news.html?&L=1