CHEMISTRY International

The News Magazine of IUPAC





Progress of Chemistry in South Korea ►

Medicinal Chemistry in IUPAC ►



Chemistry International

CHEMISTRY International

The News Magazine of the International Union of Pure and Applied Chemistry (IUPAC)

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Cover: An Aerial view of the open space in Chamchuri Square Shopping Mall in Bangkok with some of the participating students and teachers of the Young Ambassadors for Chemistry program, Page 32

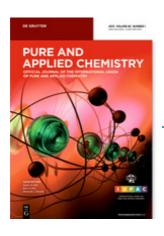


50

Contents









Stamps	international	, page 3
--------	---------------	----------

Treasurer's Column Ringing the Changes—For the Future by John Corish	2
Stamps International Dreams Make Good Stories	3
Progress of Chemistry in South Korea by Choon H. Do Meeting the Google Expectation for Chemical Safety Information by Leah McEwen and Ralph Stuart Medicinal Chemistry in IUPAC by Robin Ganellin Youth Views on Sustainability by David Yafté Díaz-Sánchez	4 12 17 21
Thieme-IUPAC Prize 2016 Call for Nominations IUPAC-SOLVAY International Award for Young Chemists IUPAC-ThalesNano Prize in Flow Chemistry Call for Nominations CHEMRAWN VII Prize for Green Chemistry Call for Nominations Standard Atomic Weight of Ytterbium Revised De Gruyter to Launch Chemistry Standards Database Solubility Data Series Books Now Available on Web L'Oréal-UNESCO Awards for Women in Science 2015 Announced Berhanu Abegaz Heads the UNESCO International Basic Sciences Programme (IBSP) Scientific Board Christo Balarew Receives Presidential Honors In memoriam: Nikola Kallay (1942-2015)	24 24 25 25 26 27 27 28 28 29
Project Place Storing Energy: with special reference to renewable energy sources Nomenclature for Polymeric Carriers Bearing Chemical Entities with Specific Activities and Names Measurement of Photoluminescence Quantum Yields Young Ambassadors for Chemistry (YAC)	30 30 31 32
Making an ImPACt Latest Updates from PAC Conferences Brief Guide to the Nomenclature of Inorganic Chemistry IUPAC Glossary of Terms Used in Neurotoxicology	36 37 37
IUPAC Provisional Recommendations Source-Based Nomenclature for Single-Strand Homopolymers and Copolymers Glossary of Terms Used in Extraction	38 38
Bookworm Ionic Polymerization, Part I & II Polymers and Organic Chemistry Macromolecular Complexes	39 39 40
Conference Call POLYCHAR 23 World Forum Advanced Materials Science Assessments and Research Integrity	42 44
Where 2B & Y	46
Mark Your Calendar	49
Index 2015	50

Treasurer's Column



Ringing the Changes— For the Future

by John Corish

s the world economy continues to return, if somewhat haltingly, to a more vibrant state, it is good to be able to report that during the past twelve months there have been significant and beneficial

changes in all aspects of the financial management and operation of the Union. It goes without saying that it has not been possible for IUPAC to emerge completely unscathed from the very difficult financial conditions that have prevailed during and since the recession, but we have come through these circumstances very well. More importantly, we have now set the foundations in our revenue generation and financial management information systems and expenditure controls that will enable us to progress and prosper in the future. The Executive Director and Secretary General have worked this year to bring the management accounting for all operations in-house and the Secretariat is now using new GAAP-compliant software. The recent appointment of a financial controller will ensure that our management accounting is undertaken in a much more timely manner.

Our three principal income streams remain the National subscriptions paid by our member countries, the income from our investment portfolio, and the profits from our publications and I will report on these in reverse order. The year that has just passed, 2014, was the first in our new collaborative publication venture with De Gruyter. The result has been very encouraging. The net profits from our publications—the subscriptions to Pure and Applied Chemistry, less its publication and distribution costs, and those of Chemistry International—had been steadily declining during the years prior to 2014, but this decline has now been turned around and we are likely to see instead an increase in this income in the future as the new arrangements settle down. Important decisions still remain to be made in respect of Chemistry International, and new income-earning possibilities have also been opened up by a new value-added database for IUPAC standards and recommendations.

At its meeting in February 2014 the Finance Committee, after a thorough review of our Investment Portfolio carried out in the light of the then-prevailing

market conditions, advised that the Union should move to more proactive management of its resources while maintaining its prudent approach to ensure the safe preservation of our capital. Tenders for the management of the portfolio were solicited from financial management companies and, following interviews, the Finance Committee advised that the portfolio be managed by BB&T and Scott and Stringfellow. These new arrangements were negotiated by the Executive Director and the Treasurer and implemented in November 2014 with a new Investment policy statement being put in place to govern their operation.

The national subscriptions of our National Adhering Organisations provide the mainstay of the funding that is used to operate the Union and to finance our various programmes. The proportion to be paid by each member has been decided for many years using a model based on the values of the chemical production of each country as reported annually by Cefic. To avoid abrupt changes in these subscriptions the relevant Cefic data were averaged over the five most recent years for which they were available. Countries were also offered the option to pay in U.S. dollars or in their national currencies. In the latter case the exchange rates used were averaged over the four quarters of the year prior to a Council meeting—again to minimise abrupt changes in the subscription for any member. Unfortunately, the algorithm developed and used over the years in this model failed when used to calculate the national subscriptions for the upcoming biennium (2016-17). A significant number of countries were assigned very large and unacceptable percentage increases in their subscriptions. This failure was due in part to changes in the pattern of distribution of the manufacture of chemicals across the world but with this effect being greatly aggravated by the steady and large increase in the value of the U.S. dollar relative to most other currencies, particularly during the past two years. These exchange rate changes have also rendered the value of the payments being made in National currencies in the current biennium quite considerably smaller than was calculated at the time that they had been budgeted, thus reducing the real income of the Union. To overcome these difficulties an interim model to apply for the next biennium only was proposed, in consultation with the Officers and with the approval of the Bureau, to the recent Council meeting at Busan. The basic tenet of this model is to equally share the current financial burdens by setting the same percentage increase, five percent year on year, for all members on their current subscriptions. The budgets proposed

also carried manageable deficits and the recovery was thereby moderated so that it will be gradual. In addition to accepting this interim arrangement, the Council also agreed to the setting up of a task force which will, in the immediate future, consult with all stakeholders, especially the National Adhering Organisations, to establish a new model on which to base the calculations of national subscriptions in the future. This new model is scheduled to be ready next year and will be sent for approval to the next Council meeting in Brazil in 2017.

As the end of my service as Treasurer of IUPAC approaches, I wish to thank my fellow Officers and the

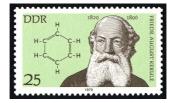
professional staff at the Secretariat for their unstinting support and help throughout. I am confident that all of the measures that have been put in place to improve and maintain our financial wellbeing will ensure that the Union can move on with confidence to celebrate its Centenary in 2019 and to continue for many years thereafter.

John Corish <i corish@tcd.ie> has been treasurer of IUPAC since January 2008. He has served IUPAC at many levels since 1979, including chair of the Subcommittee on Materials Chemistry, president of the Inorganic Chemistry Division, and member of the Finance Committee.



Dreams Make Good Stories

It is impossible to know with certainty whether Dmitri Mendeleev envisioned the first draft of the periodic table while snoozing, or if Paul McCartney was actually inspired by Morpheus to compose "Yesterday", the iconic Beatles song. Otto Loewi (1873-1961), the German pharmacologist who discovered the role of acetylcholine in the transmission of nerve impulses, claimed that he first dreamed the critical experiments that eventually led to his Nobel Prize in Physiology or Medicine in 1936. Would any of these creative accomplishments be less significant had they not been concocted when their authors were asleep?



The case of the hexagonal structure of benzene, first proposed by the eminent German organic chemist August Kekulé (1829-1896) in a paper published in 1865

in the *Bulletin de la Société Chimique de Paris*, is perhaps a little more peculiar. It was only 25 years later that Kekulé, speaking about his seminal contributions to structural organic chemistry at the legendary Benzolfest held in Berlin, disclosed publicly that the original idea for the cyclic structure of benzene was derived from a reverie he experienced in which a snake was biting its own tail (i.e., a vision of the mythical ouroboros). It doesn't really matter if Kekulé's belated revelation was completely accurate, or if the story was

embellished over time to enhance its pedagogical value. The fact is that Kekulé's chemical intuition and insightful work in the second half of the 20th century has had a profound effect in the development of modern organic chemistry, including the highly scrutinized concept of aromaticity.



Kekulé, who was a chemistry professor at the University of Ghent (1858-1867) when he suggested the correct molecular structure of benzene 150 years ago, was honored with a postage stamp issued in Belgium in 1966. The sesquicentennial of Kekulé's birth in the city of Darmstadt was similarly commemorated by the German Democratic Republic in 1979. Interestingly, both stamps feature the classic structural representation of benzene as cyclohexatriene, with alternating single and double bonds, but unfortunately depict some incorrect interatomic angles for the prototypical aromatic molecule.

In closing, I must confess that I don't know what I will be writing about in my next *Stamps International* note. I am always looking for interesting stories to illustrate with postage stamps so, in my quest for inspiration, perhaps all I need to do is relax and take a nap!

For a brief description of Kekulé's purported dream, see: A.J. Rocke, Angew. *Chem. Int. Ed.* 2015, **54**:46-50.

Written by Daniel Rabinovich <drabinov@uncc.edu>

by Choon H. Do

The Lamp of the East

In the golden age of Asia Korea was one of its lamp-bearers And that lamp is waiting to be lighted once again For the illumination in the East.

-Rabindranath Tagore (1861-1941)

t was an historic event for the Korean Chemical Society (KCS) to host the 45th IUPAC World Chemistry Congress (WCC) and the 48th IUPAC General Assembly (GA) in August 2015. It was the first time that the WCC and GA have been hosted in Korea since KCS became a member in the early 1960s. KCS applied for membership in 1961 and the application was approved the following year. Dr. Dong Il Kim and Prof. Sun Kyung Kim attended the 22nd GA in London in 1963 as the first KCS delegates.

Several international conferences sponsored by IUPAC have been held in Korea: Chemrawn IX on the Role of Advanced Materials in Sustainable Development was held in Seoul in September 1996, the 36th International Symposium on Macromolecules (MAC-RO) was held in Seoul in August 1996, and the 19th International Conference on Chemical Education (ICCE) was held in Seoul in August 2006.

To mark this year's special occasion, when the IUPAC WCC and GA are held in Busan, Korea, CI invited Choon H. Do to describe the history and the future prospects of chemistry in Korea.

Ancient Chemistry in Korea

According to a legend on the establishment of Korea, the Korean people are descendants of Dangun, the son of a Heavenly God who came down to Korea with

"rain, cloud, and wind" and married a woman transformed from a bear by taking garlic and mugwort for three weeks. In BC 2333 they set up a kingdom named Gojoseon (Old Joseon). Interestingly, this legend tells us that Koreans recognized from a long time ago the importance of the environment and chemistry to sustaining human life. Rain, cloud, and wind are important factors for agriculture, and garlic and mugwort were used as medicines in ancient Korea. It also depicts the Korean endurance for hardship.

According to unearthed remains, Koreans have inhabited the Korean peninsula from the Paleolithic period. A petroglyph at Daegok-ri, Ulsan, probably carved in the Bronze or Iron Age, shows several types of whales, animals, and tools for hunting (Fig. 1). Among other things, these early inhabitants knew how to hunt giant whales and record these events on the stone wall in an artistic manner.

After Gojoseon, some of the northern territory of Korea was occupied by China's Han Dynasty and was renamed Hansagun. In the meantime, three kingdoms-Silla, Goguryeo, and Baekje-were established in BC 54, BC 37, and BC 18, respectively. From the period of these three kingdoms, the history of Korea is relatively well documented. The three kingdoms were unified by Silla in AD 668 and the Silla Dynasty lasted until AD 935. Gun Wang set up the Goryo Dynasty in AD 918 and overthrew Silla in AD 935 to rule Korea. The Koryo Dynasty lasted until 1393, when General Sung-gye Lee, the leader of a military coup in 1392, set up the Joseon Dynasty and became a King himself. The Joseon Dynasty was merged into Japan and dissolved in 1910. Japan occupied and ruled Korea from 1910 until 1945. Korea became independent from Japanese rule on 15 August 1945 at the end of World War II. The Korean peninsula was divided in two, with the northern part ruled by the Soviet Union and the southern part by the United States from 1945 to 1948. South Korea

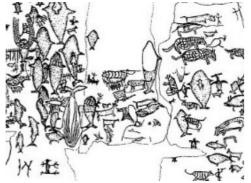


Fig. 1: Petroglyph in Daegok-ri, Ulsan, Korea. Fig. 2: Gold crown in Silla Lines were redrawn for emphasis.



Dynasty



Fig. 3: Glassware imported from Persian region

Period	Names of Nations
Ancient Korea	Gojoseon (BC 2333-BC 108)
	Hansagun (BC 108 -AD 314)
Three Kingdoms	Silla Dynasty (BC 57-AD 935)
Period and Unified	Goguryeo Dynasty (BC 34-AD 668)
Silla Kingdom	Baekje Dynasty (BC 18-AD 660)
Medieval and early	Goryo Dynasty (AD 918-1392)
modern Korea	Joseon Dynasty (AD 1392-1910)
Occupation period by	
Japan (1910-1945)	
Independence (1945)	
Modern Korea, Korean	South Korea (1948-present)
War (1950-1953)	North Korea (1948-present)

Table 1: A Brief History of Korea

was formally established 15 August 1948 with observation by UN Temporary Commission on Korea, and North Korea was established 9 September 1948. The Korean War erupted 25 June 1950 and lasted until a cease-fire was declared 27 July 1953. This cease-fire remains in place today. The history of Korea is briefly outlined in Table 1.

Chemistry in the Three Kingdoms Period

We can guess the state of chemistry in the Three Kingdoms Period through the archaeological remains of the Silla Dynasty. These survived at a relatively higher rate than those of the Goguryeo and Baekje Kingdoms. Of these remains, gold crowns, steel lumps, and glassware are notable for chemists. Figure 2 shows a gold crown excavated from a tomb of the Silla Dynasty period. Many other remains were also made of gold. Silla produced significant gold and knew how to handle it. Iron lumps in shallow sheet shapes were also found in tombs. These iron lumps were first produced as a sponge iron form and then hammered into wrought iron. These iron lumps were used as basic materials for

Fig. 4: A stone soldier statue in front of the 38th ruler, King Wonseong's tomb (reign period: AD 785-798)



tools such as armor, helmets, and agricultural implements, and were exported to Japan and China according to written documents.

From the Three Kingdoms Period Korea was an open society and traded with foreign countries freely. Glassware shown in Figure 3, for example, might come from the Persian region. Another very interesting example is a stone soldier standing in front of the tomb of King Wonseong (reign period AD 785-798), 38th King of the Silla Kingdom (Fig. 4). The figure of the stone soldier is similar to western figures, and indicates that foreigners lived in Korea from ancient times. According to legend, Queen Hwangok Huh came from India in AD 48 and married Suro Kim, the founding King of the Garak Kingdom, a small kingdom between Silla and Baekje that was later merged into Silla. She became the progenitor of the Korean surname 'Huh'.

Chemistry in Medieval and Early Modern Korea

During the period between the 10th and early 20th centuries AD, two dynasties, the Koryo (918-1392) and Chosun (1392-1910), rose and fell in Korea. Because the society of these two dynasties was disrupted for long times by invasions from Mongolian and Chinese forces from the north, and by Japanese forces from the south, Koreans had difficulties developing new sciences and technologies. Nevertheless, a few noticeable developments were made.

Invention of metallic type and printing

A Buddhist book, 'Jikji', printed in 1377 in Goryeo Dynasty using metallic type, is stored in the Manuscrits Orientaux division of the National Library of France (Fig. 5). This book was confirmed as the world's oldest extant book printed with movable metal type by UNESCO in September 2001 and is included in their Memory of the World Programme. It shows that Koreans continuously improved science and technology not only for sustenance, but also for spiritual progress.

Compilation of medical knowledge

Medical and medicinal information is always very important to human life. In 1613, the Korean court physician Jun Huh and his colleagues compiled a book, 'Dongeuibogam' (Principles and Practice of Eastern Medicine), an encyclopedia of medical knowledge and treatment techniques. Many prescriptions are still applied today and are sources of research in herbal medicine. The book also describes the ideals of preventive





Fig. 5: 'Jikji' (left), the oldest extant book printed with movable metalloid type; and the medical books Dongeuibogam (right), part of the UNESCO "Memory of the World" Programme.

medicine and public health care by the state, ideals that are very advanced even from the modern point of view. Dongeuibogam was added to the Memory of the UNESCO World Programme in 2009 (Fig 5).

Invention of Korean alphabet, 'Hangeul'

The invention of Korean alphabet, "Hangeul", in 1446 by a group of scholars designated by King Sejong (Fig. 6), is worth mentioning. It was easy for Koreans to learn, and consequently became an excellent tool for learning and communication. The Korean alphabet is composed of 14 consonants and 10 vowels. The shapes of the consonants and vowels are shown in Table 2. One will notice that the shapes are simple, geometrical, and symmetrical. Ordinary people can learn this system in a short time, and it can describe foreign languages without difficulty. It is also a very good fit for modern computer tasks. Needless to say, the invention of the Korean alphabet contributed greatly to the development of science and technology in Korea.

'Hermit nation' and 'Morning calm'

Evidence shows that Koreans did not actively make contact with foreign countries between the 10th and 20th centuries, except for China and Japan. Korea remained unknown in western countries for a long time. Then, in 1668, a Dutch sailor named Hendrick Hamel wrote a report, "Hamel's Journal and a description of the Kingdom of Korea (1653-1666)", after escaping from Korea. In 1653 Hamel and other sailors had landed in Korea after their Dutch merchant ship was wrecked. They were held for 13 years. Hamel's journal was edited into a book and Korea became known to westerners. At this time, Korea became known as the 'Hermit nation' and the 'Morning calm' country.

It's is not known precisely why Koreans didn't continue contact with westerners during these long periods. However, the leaders and scholars of those periods failed to match the progress of the modern civilizations of the world. One theory, although it is not proven, is that recovery from the invasion and oppression by outsiders took a long time. Some leaders tried to establish contact with western civilization in the 19th century, but their impacts were weak. At the start of the 20th

century, Korea lost its opportunity to catch up by itself and came under Japanese occupation when the Joseon Dynasty was merged with Japan in 1910.

Table 2: Korean alphabet, "Hangeul"

Consonants (14 characters)	ヿ
Vowels (10 characters)	Ͱ ╞┤╡⊥ ╨⊤╥−┃

Fig. 6: The Great King Sejong, who invented 'Hangeul', the Korean alphabet, is shown on the 10,000 Won Korean banknote.



Independence and Post-Korean War Reconstruction

As a result of the conclusion of World War II, Korea gained its independence 15 August 1945. Living under the oppression of other countries had been difficult, and the oppressed society lacked human rights, as well as the structures required to develop proper

education, science, and creative minds. Korea had one misfortune on the top of another. Koreans experienced the tragedy of fratricidal war between 1950 and 1953. Some of the remaining resources left after independence were reduced to ashes by the war.

Immediately following independence, only a few Koreans obtained a Ph.D. degree and the number of graduates majoring in engineering and sciences at Korea's universities and technical high schools were mere hundreds. To change this, the Korean Chemical Society (KCS) was established 7 July 1946. The specialties of the 36 charter members included chemistry, chemical engineering, agriculture, and medicine.

During and after the war, many foreign countries helped to reconstruct Korea. They supplied not only food and clothes but also construction materials for housing and schools for education. They helped to set up factories and to build roads. Some of this foreign aid came from the United Nations Korean Reconstruction Agency (UNKRA), created by the United Nations to help economic reconstruction in 1950 and focused on aiding war refugees and the homeless. The United Nations Development Programme (UNDP) aided Korea from 1963, while the Development Assistance Committee (DAC) of the Organisation for Economic Co-operation and Development (OECD) also helped to rebuild Korea's economy. The U.S. Agency for International Development (USAID) also assisted South Korea in building its agricultural, educational, and industrial sectors. According to DAC data, the total foreign assistance to Korea was USD 13 billion. This foreign assistance was used to overcome poverty and achieve economic development-in 2000 the UNDP reclassified South Korea from recipient of aid to a donor. During this period, many elements of western culture

and institutions were introduced into Korea. Commodities such as coffee, penicillin, canned food, and nylon socks were imported. 'Jeep', 'three-quarter' and 'GMC' became common names for small passenger cars and medium and large trucks at the time.

Policy makers recognized what should be done to reconstruct the country, to eliminate hunger and poverty, and to provide shelters for people suffering from war, and executed their plans. With the assistance of various international organizations and foreign countries, the Korean government and the country's private sectors began to help themselves. Mungyung Cement Co., Gyungbuk, was established in October 1957 with Dutch technologies. Sheet Glass Manufacturing Plant in Inchon was built in 1957 through the aid of UNK-RA. An automatic glass bottle factory was set up with help from the United States. A fertilizer plant was built in Chungju, Chungbuk in 1959. It produced urea fertilizer and was the first chemical plant in South Korea. The plant not only produced fertilizer, but also had a role in educating many chemical engineers and scientists who later became leaders in the chemical industries. Inchon Iron factory started to produce steel from open-hearth furnaces in 1956. Polyurethane slabstock foam was produced in 1957 by importing technology and raw materials from Bayer, of Germany. South Korea began to have some basic industries and plans for further development by late 1950.

Current Status of Chemical Industries

Today, the production of Korean chemical industries is about EUR 132.1 billion and ranked 5th in the world (Fig. 7). In 2013, the total exports of these industries were USD 83,535 million, while the imports were USD

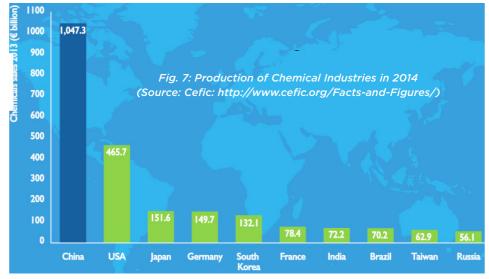




Fig. 8: Commemorative stamp for the set-up of an oil refinery as one of 5-year economic development plan (1964).



Fig. 9: Ulsan Petrochemicals complex

60,014 million. (2014 Annals of Science and Technology, Ministry of Science, ICT & Future Planning, S. Korea). This includes petrochemicals, fine chemicals, fertilizers, ceramics, paper and its raw materials, abrasion products, plastics, and rubber products. The total balance of Korea's chemical industries trade is in the black, but shows deficits of USD 9,180 million in the trade of fine chemicals, USD 2,184 million in industrial chemicals, and USD 2,998 million in ceramics. These data indicate that chemical industries in Korea are still behind in fine chemicals and specialty chemicals and need to invest and develop these fields.

Petrochemicals

As initial reconstructions commenced after the Korean War, a military coup arose in 1961. The new government executed a series of economic development plans. Ulsan Petrochemical Complex was established between 1968 and 1973. An Oil refinery producing 35,000 bbl/day was built in 1964 in a joint venture with Gulf Oil (Figs. 8 & 9)—many companies were established either through a joint venture or independently. The first naphtha cracking facility, needed for the production of polymers and petrochemicals, was set up in 1973, and



Fig. 10: Location of Ulsan, Yosu, and Daesan petrochemicals complexes.

Nylon 6 was produced by Hankook Nylon Co. in 1963. The production of PE, PP, PS, PVC, PET, BR, SBR and acrylic fiber started. Ulsan became the largest city for petrochemical production in Korea. Currently they are focusing on the bio-, nano-, and fine-chemicals fields.

After Ulsan Petrochemicals Complex, Petrochemical complexes were set up at Yosu in 1976-79 and at Daesan in the 1990s (Fig. 10). Global chemical companies such as BASF, BP, Solvay, S-Oil, Mitsui, Eastman Chemical, Rhodia, DuPont, Mobil, Total, and Dow are now operating in Korea.



Fig. 11: Stamp commemorating the construction of POSCO (1973)

Iron and Nonferrous metals

Pohang Iron & Steel Company (POSCO) was set up by a joint venture between Korean and Japanese companies in 1968 and begun production of steel in 1972 (Fig. 11). POSCO built a 2nd mill in Gwangyang in 1988. Onsan Industrial Complex in Ulsan was planned in 1974 for the production of nonferrous metals, aluminum, copper, zinc, nickel, and lead, and completed in 2000. Through the production of plastics, steel and nonferrous

metals, they were able to supply basic materials for the automobile, shipbuilding, and electronics industries.

Government and National Research Institutes

The Korean government eagerly supports the progress of economic development and science and engineering. The Ministry of Education; the Ministry of Science, ICT & Future Planning; and the Ministry of Trade, Industry & Energy are the main engines to propel the policy of the Korean government supporting education, research, innovation, science, and technology. They have set up many national research institutes

and organizations. Some important institutes are described below:

Central Industry Research Institute: This institute, established under the Ministry of Commerce & Industry in 1949, was the first governmental agency for science and technology. As the only place where most scientists and engineers could work after independence, they shaped the first community of science, technology, and industry.

Korea Atomic Energy Research Institute (KAERI): At the time that nuclear power was emerging, and as people witnessed the nuclear power of the bombs dropped on Japan, the newly born Korean government focused on catching up with contemporary nuclear science and technology. The Korean government initiated KAERI and imported a research reactor, the Triga Mark II from General Atomics in 1962 for peaceful use agriculture, industry, medicine, science, and engineering. Using this research reactor, they trained not only nuclear scientists and engineers but also pure scientists and engineers. They have also recruited scientists and engineers from abroad. Currently, South Korea is operating 23 nuclear power reactors, producing 20.7 billion watts and supplying 35% of the country's total electricity.

Korea Institute of Science and Technology (KIST):

During summit talks in 1965, Korean President Chunghee Park and U.S. President Lyndon B. Johnson agreed to establish a research and development institute in Korea. A deal to establish KIST was signed in 1966 and the Institute was completed in 1969. It was the first multi-disciplinary scientific research institute in Korea and has since contributed significantly to the development of the Korean sciences in many areas. As scientists and engineers joined KIST, the research positions there created the first major "reverse brain-drain" from overseas.

Korea Research Institute of Chemical Technology (KRICT): KRICT was established in 1978 with the aim of applying chemistry research to strengthen the Korean chemical industry's international competitiveness.

There are many other institutes established by the Korean government or with governmental support. Some of these related to chemistry are the Institute for Basic Science (IBS), Korea Research Institute of Bioscience and Biotechnology (KRIBB), Korea Basic Science Institute (KBSI), Electronics and Telecommunications

Research Institute (ETRI), Korea Testing & Research Institute (KTR), Small & Medium Business Administration (SMBA), Korea Textile Development Institute (KTDI), and Korea Institute of Footwear & Leather Technology (KIFLT).

Chemical Education and Universities

Before independence, there was one university, and few private technical colleges and technical or agricultural high schools. Following independence, the Korean people quickly re-established the national education system using a small reservoir of human resources in education. National Universities were established in each province. Many private universities were also established with influential support.

Seoul National University was established in 1946 by combining Kyungsung Imperial University and other technical colleges that existed before independence. Other national universities were established at Busan, Kyungbook, Chonnam, Chonbuk, Chungbuk, Chungnam, Gangwon, and Jeju.

The private universities have diverse foundation origins. Yonsei University, with roots from 1885, became a college in 1915 and university in 1957. Its beginnings come from a hospital founded by American protestant missionaries of the Presbyterian Church. Korea University was established in 1946 by renaming Bosung Technical College, which was established in 1905 by a private supporter. Sungkyunkwan University traces its roots to the Korean Confucian educational system and rituals of the Chosun Dynasty. It was founded in 1398, although its current university system was enacted in 1946. Inha University was established in 1954 through donations by Korean emigrants living in Hawaii in the hope of assisting development in Korea through education. Ewha Womans University is the first women's university in Korea. It was founded in 1886 by the American Methodist Episcopal mission, and the current university form was established in 1945. Sookmyung Women's University was established in 1906 as the first royal private educational institution for women.

The number of universities and colleges increased very quickly following independence and through the modern era due to "education fever". Currently there are 190 4-year universities and 140 2-year colleges in Korea. More than 80% of high school graduates register at college or university.

After the Korean War, the education system followed that of the United States. One notable program during this time was the Minnesota Project by USAID.

	Journals	Magazines
KCS	Bull. Kor. Chem. Soc. (in English), J. Kor. Chem. Soc. (in Korean)	ChemWorld
KIChE	Kor. J. Chem. Eng. (in English), Kor. J. Chem. Res. (in Korean).	News & Info. For Chem. Eng.
PSK	Macromol. Res. (in English), Polymer (in Korean)	Polym. Sci. & Tech.
KSICE	J. Ind. Eng. Chem. (in English), Ind. Chem. (in Korean)	Prospectives of Ind. Chem.
CerS	J. Kor. Ceram. Soc. (in Eng. & Korean)	Ceramist
KSBMB	Exp. Mol. Medicine (in English), BMB Reports (on-line J.)	KSBMB News (on-line only)

Table 3. Some key Societies and their publications

This program provided universities in Korea with staff improvement and equipment in engineering, medicine, agriculture, and public administration. Through this program, faculty members visited the United States to obtain a degree and to catch up with the development of modern science and technology. Many scholars also went to Germany, France, and other European countries.

At most universities, the chemistry departments were placed in the college of liberal sciences, while chemical engineering departments were set up in the college of engineering. Departments of applied chemistry, industrial chemistry, fiber technology and polymer were also established in the college of engineering. The chemists and chemical engineers trained in all of these departments became the workhorses of the chemical industry in Korea.

Relatively recently, several notable national and private universities were established. Postech (former Pohang Institute of Technology) was established in 1986 by the support of POSCO, while Korea Advanced Institute of Science and Technology (KAIST) was established in 1971. Following the model of KAIST, regional universities with the same purposes have been established: Gwangju Institute of Science and Technology (GIST) in 1993, Ulsan National Institute of Science and Technology (UNIST) in 2009, and Daegu Gyeongbuk Institute of Science and Technology (DGIST) in 2011.

Chemical Scientific Societies and Associations

Many chemists and chemical engineers are active in research and in presenting their works through various

domestic and international scientific societies. Chemists and chemical engineers organized many societies according to their scientific interests and disciplines. Each society actively holds meetings, conferences, and forums and publishes journals, magazines, and newsletters. Because most scientific terms and definitions came from abroad, many scientific societies translated English terms they used into Korean terms. To this end, the Korean Union of Chemical Science and Technology Societies (KUCST) published "Terminologies of Chemical Science & Engineering" including chemistry, chemical engineering, and polymer and industrial chemistry.

Scientific societies related to chemistry and chemical engineering are as follows (year of establishment in parentheses): Korean Chemical Society (KCS) (1946), Korean Institute of Chemical Engineers (KIChE) (1962), Polymer Society of Korea (PSK) (1976), Korean Society of Industrial and Chemical Engineering (KSIEC) (1990), Korean Ceramic Society (CerS) (1957), Korean Society of Biochemistry and Molecular Biology (KSBMB) (1948), Korean Society for Biomaterials (KSB) (1996), The Rubber Society of Korea (RSK) (1966), and Korean Electrochemical Society (1983)

Small specialty societies are also emerging: Korea Polyurethane Society (2004), Korean Hydrogen and New Energy Society (2005), Korean Silicon Society (2011). Further, chapters of many international chemical societies are active in South Korea, including the American Chemical Society, The Royal Society of Chemistry, and the Society of Plastics Engineers.

Many different sections of chemical industries, such as textiles, rubber, plastics, electronics, steel, automobile, fertilizer, construction materials, cosmetics, and medicine, etc., form professional associations to

The Korean Journal of Chemical Engineering

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share information on new technologies, environmental effects, and safety. They have contributed to the development of Korean chemical industries greatly. Some examples are Korea Chemical Industry Council (KOCIC) and Korea Petrochemical Industry Association (KPIS). KOCIC's purpose is to promote the exchange of information and cooperation with various organizations from the global chemical industry, such

as the International Council of Chemical Associations (ICCA). KPIS was created for the development of the petrochemical industry and to facilitate international cooperation.

Future and Challenges

2015 is the 70th year after Independence and comes over 60 years after the Korean War. Currently active chemists and chemical engineers are therefore the 3rd and 4th generations after independence and modern chemistry were introduced to Korea. They are a

very talented group and expect to lead the current and next generations in contributing to the state of the art of global chemical science. Many of them are world class chemists and chemical engineers. (see Chemists and Chemical Engineers in S. Korea, published online at www.chemistryculture.org/en-chemculture/en-koreanchemistandengineer.htm)

Some problems may arise in the future, such as the reduction in population and downsizing of the economy. As in other developed countries, Koreans are also facing challenges relating to the environment, sustainability, and the need to increase the public understanding of chemistry. We have to plan for the future. It is less than 20 years since Korean society began to heavily invest in research science and technology. We spent a long time laying the foundation. Now we expect the ability of chemical talents. With open-minded sprit of inquiry and curiosity toward chemistry and education, Korean chemical scientists will research and cooperation with scientists of overseas.

Scientists couldn't show their talents under the oppression and the restriction of opportunities that existed under the feudal social system and in the colonial period. Progress is hardly made under war and disorder, or in an uneasy society where human beings suffer from poverty and hunger. The development of the Korean chemical industries is an example of the progress that can be made in a peaceful and free society.

Epilogue—Busan harbor, gateway for connection with overseas

Busan is the 2nd largest city in S. Korea and its population is about 3.5 million. The city was a temporary capital for the Republic of Korea during the Korean War. Busan port was the place where relief goods and war supplies were unloaded during the war, but now it

is the largest container port in Korea, and the 5th largest in the world.

Busan exhibits the prosperity of the Korean people after overcoming the difficulties, hunger, and poverty caused by the war and the colonial period. Busan has many stories. A documentary film by R. J. McHatton, "Ship of Miracles" tells the story of the rescue of over 14 thousand refugees by a single ship, the SS Meredith Victory. It is the largest rescue operation in the history of mankind. The refugees landed safely in the southern part of Busan, where they became Busan citizens. A UN Memorial Cemetery com-

memorates the soldiers of 16 nations who participated in the war on the side of South Korea.

I trust the meeting of IUPAC General Assembly and World Chemical Congress in Busan has been an opportunity not only for chemists and chemical engineers to discuss chemical issues and present their research, but also for IUPAC to show to the world that chemists and chemical engineers change and improve human life for the better. This occasion was also a fresh opportunity to upgrade the level of chemistry in Korea.

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Meeting the Google Expectation for Chemical Safety Information

Chemical Risk Assessment in Academic Research and Teaching

by Leah McEwen and Ralph Stuart

magine a scenario in an academic research lab: you are working on a chemical system that has not yet been well characterized, perhaps looking at new catalysts, trying new reagent combinations, or scaling up a new reaction for more sample. How might you gauge the reactivity potential against the equipment and procedures in place to ensure control is maintained? How do you identify critical points in the system where subtle or even inadvertent changes in condition or operation could send things awry, possibly becoming dangerous? How do you assess the potential hazards of untried chemistry? Is there any helpful information readily available at your fingertips? Would a search engine as accessible as Google be able to turn up appropriate data for such scenarios?

Understanding this situation for research chemists has taken increased prominence over the last five years following a series of highly publicized incidents in academic laboratories in the United States and elsewhere.

Government [1], scientific [2], professional [3], and academic [4] organizations have raised concerns about the planning and oversight of chemical laboratory operations in the academic setting. Academic institutions and individual chemists

What new ideas might an intersection of chemistry service professionals—educators, hygiene officers, health and safety directors, librarians, information scientists—bring to bear on this conundrum?

have been subject to criminal prosecution in response to specific incidents where the primary consideration was adequacy of planning and supervision of the work being conducted in the laboratories.

The immediate impact of these events has been a rapid increase in the level of documentation expected to support chemistry research in the academic setting. For example, following the death of a researcher in the University of California system [5], principle investigators of chemistry research laboratories on all 10 campuses are now required to identify which of 45 different hazards are associated with the work in their laboratories, so that the appropriate Personal Protective Equipment (PPE) can be issued to lab workers [6]. However, this approach does not address the broader

range of issues that chemists face when planning experiments and managing labs that may contribute to hazardous situations.

Studying lesser-characterized chemistry is a prime focus in chemistry research and all chemical reactions involve energy changes. If too much energy is released too quickly for the immediate environment to absorb it, material damage and dangerous circumstances can result. Known reactivity and interactions of materials as well as documented hazards and handling protocols can help inform prevention and mitigation planning for runaway and even unanticipated reactions. Incident investigations also indicate that many additional factors may be involved in the escalation of adverse chemical lab events, including process conditions, equipment limitations, laboratory setup, and training of operators, among others. There is an increasing focus on assessing risks against a range of considerations in local context. It can be a significant challenge to identify and locate the relevant data and information needed to inform these analyses.

Potentially useful information is widely dispersed across a spectrum of scholarly, supplier, agency, and other institutional data collection, reporting, and publication venues. The most readily available data collec-

tions focus on a small number of well-characterized compounds and involve significant time and expense to maintain. Other initiatives, aimed more broadly, are hampered by ambiguous data provenance. The diversity of data formats in-

tended for different audiences and applications often means that the quality of the information is difficult to evaluate, organize, and apply in assessing risks associated with using reactive chemicals. The challenge is particularly pressing in the highly decentralized academic sector, characterized by novel chemistry, novice researchers, and very little consistency of practice and resources within and among institutions. How would a research lab manager working with a new protocol apply the exposure control information on Safety Data Sheets (SDS) that was intended for large-scale hazmat clean-up situations? How would a chemistry student in a teaching lab discern the hazards associated with different physical forms of a compound, perhaps in a variety of dilutions?

What new ideas might an intersection of chemistry service professionals—educators, hygiene officers, health and safety directors, librarians, information scientists—bring to bear on this conundrum?

Braving a record snowstorm and sustained by a small exploratory grant, 25 members of the Chemical Health and Safety (CHAS), Chemical information (CINF), and Chemical Education (CHED) Divisions of the American Chemical Society (ACS) and the ACS Committee on Chemical Safety, Environmental Health and Safety Task Force teamed up at Cornell University in Ithaca, NY in the winter of 2014 to pool their expertise and characterize the opportunities and challenges facing chemical safety information in the academic context. The primary goal of this initial meeting was to identify an overarching paradigm within the chemistry domain that could provide a framework for describing the lab safety process.

The education community provided a model for risk assessment and management in the academic laboratory characterized by a series of tasks necessary to work towards a safety culture: Recognize the hazards, Assess the risks, Manage the hazards, and Prepare for emergencies (RAMP, Figure 1). The group added, "Protect the environment" and the initiative was dubbed "iRAMP" to reflect the iterative nature of both the RAMP process and the project [7].



Figure 1: The iRAMP paradigm for managing chemical safety in the laboratory. Reprinted by the authors from http://www.irampp.org/blog.

To support this process, the workshop identified emerging tools from the safety profession and regulatory agencies that can be deployed to support a range of safety planning and management activities. These include the Global Harmonization System of Hazard Classification (GHS) [8], Safety Data Sheets (formerly 'Material' SDS) [9], systems of exposure controls [10], research scale laboratory standards [11], prudent practice guidance for academic research labs [12], and a variety of risk assessment methods [13]. Librarians can support this process by focusing on the scholarly processes for critical inquiry, information evaluation techniques, and documentation best practices. Similarly, information scientists are developing new technologies for structuring and interlinking data across sources.

Late in the winter of 2014, another diverse group of chemical professionals from the education, laboratory safety, academic librarianship, and information science sectors convened at the offices of the Royal Society of Chemistry in Cambridge, UK. They reviewed information sources and specific environmental health and safety field cases in the context of current information management technologies. The field cases considered a variety of applications, including Lessons Learned-type factor analyses based on reported laboratory incidents, control banding of laboratory ventilation rates, and risk assessment of common higher education teaching laboratory processes. The discussion re-emphasized the need to consider both hazard potential and exposure potential when assessing risk. Hazards associated with chemical research involve process conditions as well as chemical reactivity potential. These considerations can help inform local decisions for integrating hazard controls and prudent laboratory management practices.

Could a collective approach be developed that would support the use of these varied tools and information sources, connecting relevant data and official guidance into varied local management systems and planning workflows?

From these meetings we were able to take away a set of general goals for the project. The diversity of academic science and laboratory settings argues for a safety culture of prudent practices where not all scenarios can be anticipated, planned for, or addressed in established policies. Such dynamic systems suggest that a formulaic risk management "wizard" is not appropriate; assessing risk is site specific and involves educated judgment. How can we support iterative information discovery and reuse for a range of use-cases in a sustainable, transferable, and scalable manner? Laboratory work evolves in a variety of local contexts under diverse regulatory requirements using loosely determined types of information management systems.

Meeting the Google Expectation for Chemical Safety Information

This situation calls for a flexibly structured ecosystem of data, domain expertise, and workflow tools mapped to essential commonalities of chemistry research and safety planning processes. A functioning information ecosystem relies on strong data management practices, including robust description of relevant chemistry research processes; collation and indexing of currently published data; organization and visualization tools for evaluation and use of data in risk assessment; codification of output formats; cross-walks for incorporation into local systems; and archiving and markup of method and analysis documentation for future reference.

What are the opportunities for amalgamating and opening up chemical data and information relevant to hazard recognition and safety planning and connecting them to create a flexible and functional information ecosystem?

A key challenge for connecting the relationships between multiple types of factors is the predominant organization of chemical information by chemical entity. The safety literature is no exception, focusing on the hazard-related properties of individual chemicals or substances without reference to specific experimental context or to the surrounding laboratory conditions. Scale, concentration, temperature, pressure, flow rate, and many other chemical, process, operator, and envi-

ronmental factors have the potential to trigger a runaway hazardous situation. The presence of other compounds in the experiment or immediate vicinity must also be considered. A more complete risk assessment process, as described by the RAMP model, involves a holistic, laboratory level

approach to managing risks beyond hazard identification. Complementing the "object-based" focus on specific chemical entities with "process-based" indexing could better identify information and data buried in the published literature on how these chemicals are being used under various conditions and combinations and the potential for subsequent unintentional interactions to arise.

There are currently a number of exploratory efforts to develop semantic description for indexing and linking disparate information for a variety of scientific, management, and educational applications. Semantic description of data elements such as the Resource Description Framework (RDF) [14] can support flexible

querying across a variety of information types. These technologies are just recently moving beyond describing the basic bibliographic information types into developing approaches for more specified domain data types [15]. Chemical health and safety management is traditionally an information-intensive discipline and has created many data structures for supporting safe practices and incident analysis in chemical laboratories. Looking across the domain reveals many information management practices to build on, including the SDS format and GHS labeling system, clearinghouses of reviewed chemical hazard data such as the European Committee Agency portal, and information exchange formats and algorithms such as the International Uniform Chemical Information Database protocol (IUCLID) [16] and the IUPAC International Chemical Identifier (InChI) [17].

Developing safety management tools and models useful for the academic sector will necessitate tapping into digitally curated data in ways that are relevant to the decision-making processes of research chemists, safety professionals, institutional administration, and other stakeholders. For example, a researcher might be looking at two known chemicals in a proposed reaction scheme and want to know of any conditions that might trigger an adverse outcome, if there are

any known procedures for minimizing the likelihood of these conditions, and how to mitigate potential harm if something untoward did occur. The relevant data and information may come from a diverse set of sources covering physical properties, synthesis protocols, and previously re-

viewed incidents. However, these sources vary widely, and much of the data is available only in text format, often not parsed with the necessary granularity and not recognized by computers in the implied scientific context. This "text-locked" state of the data limits the options for searching, analysis, tagging, and linking into information management systems such as electronic laboratory notebooks (ELNs). Similarly, institutional Environmental Health and Safety staff need to collect information about different chemical properties to support campus-wide laboratory operations, including coordinating emergency response planning, addressing ventilation needs, and providing waste disposal services.

This situation calls for a flexibly structured ecosystem of data, domain expertise, and workflow tools mapped to essential commonalities of chemistry research and safety planning processes.

Chemical Risk Assessment in Academic Research and Teaching

How do we better identify and organize chemical hazard and risk management concepts to facilitate the discovery and use of what has been reported? Can we classify and define chemical reactivity in the context of hazard identification, evaluation, and exposure control? The iRAMP project is currently collaborating with the PubChem program at the US National Library of Medicine to explore opportunities and challenges on a practical level. Objectives include connecting the broad range of information sources relevant to chemical safety planning, applying vocabularies of relevant concepts to index and annotate reports, and analyzing indicators to extend classification of potential hazards across lesser-characterized chemical interactions. The approach is to develop a data stream based on the community standard format of the Laboratory Chemical Safety Summary (LCSS) [18] described by the National Research Council in Prudent Practices [19]. This data stream consolidates the safety and health-related data reported in open, authoritative literature, and can be downloaded or hyperlinked into institutional systems to augment local chemical information, such as chemical inventories, lab-specific personal protective equipment assessments, or ELNs. The project is not aimed at developing local chemical management systems or interfaces, but to facilitate management of the data stream through user manuals and examples of use in risk assessment protocols.

A critical component that has been identified for scalability and sustainability is the use of robust chemical identifiers to allow linking and validation of the information collected. The familiar CAS Registry Number is ubiquitous across many chemical safety information sources, but is not designed for linking and does not include important chemical designations related to concentration and purity. IUPAC projects are underway to extend the InChI algorithm to incorporate the GHS designations and support better linking and access to documentation of chemicals from manufacture through waste disposal and emergency response. In response to community input, we are also investigating the development of a chemical incompatibility classification that will group potentially similar hazardous interactions, extending the functionality of the chemical reactivity worksheets available in CAMEO [20].

Next steps include extending the LCSS profiles beyond hazard information about specific chemicals to include additional relevant data such as process variables and to support further annotation of reactivity hazards. It will be possible to leverage domain terminology to more systematically analyze the reported

data and construct specific process scenarios, such as "chemical A + chemical B under X condition could lead to Y type of adverse event". An ongoing effort is the development of a Chemical Safety Ontology (CSO) that establishes the relationships among chemical safety concepts, such as hazard classification and exposure control, and maps these to the semantic information structures used by computers for indexing, classification, and further organization through knowledge graphs. These approaches will rely on terminology and descriptions developed for use in the chemistry enterprise.

The chemistry domain boasts myriad glossaries and regulatory terminology developed for a wide range of chemical research and applied subdisciplines, including those represented in the IUPAC color books [21]. Ascertaining the applicability and interconnectivity of the available vocabularies to the questions around chemical hazard management and safety planning will require a process of review and curation by chemistry research support professionals, including environmental safety officers and chemistry librarians in collaboration with domain information scientists. A successful model that interlinks and semantically enables a range of authoritative vocabularies is the AGROVOC thesaurus, a project of the Agriculture Information Management Standards (AIMS) initiative under the auspices of the Food and Agriculture Organization of the United Nations [22]. Could such a work model be developed in the chemistry domain to integrate chemistry vocabularies more systematically into chemical information management systems, building on the efforts of the current IUPAC Color Book Data Management project [23]?

Everyone we have connected with in the chemical safety, chemical information, and chemical education communities has appreciated the complex nature of the challenge and the potential for a multi-faceted community approach. Safety is a global concern for our discipline and we welcome ideas and contributions from all stakeholders and locations interested in moving this



Meeting the Google Expectation for Chemical Safety Information

effort forward. The laboratory safety data stream provided through the PubChem database is an ideal proof-of-concept to support community engagement in managing information relevant to chemical safety planning; large scale, government-based, and open to use. The initial word from the academic chemical safety community is that this approach will add much needed value to the prominent electronic information search scenario for researchers via Google. Stay tuned for the next chapter of this compelling exploration.

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Medicinal Chemistry in IUPAC

Analogue-based

Drug Discovery

Accomplishments During the Last Decade

by Robin Ganellin

previously reported on Medicinal Chemistry in IUPAC, its accomplishments during the previous decade from 1992 to 2002, and its relationships with industry, in an article in *Chemistry International* [1]. Medicinal Chemistry is a key topic for the Subcommittee on Drug Discovery and Development (SC-D3) of the IUPAC Chemistry and Human Health Division (Div VII).

In mid 2002, the Subcommittee was renamed the Subcommittee on Medicinal Chemistry and Drug Development because many medicinal chemists expressed concern about the loss of the subject name. Yet, to be more inclusive and recognizing that drug discovery involves the application of other scientific

disciplines in addition to medicinal chemistry, the Subcommittee has recently reverted to its original name. Furthermore, the subject has broadened: drug discovery and development now has to include biological, as well as small-molecule drugs [2].

Members of the SC-D3 have been drawn mainly from the pharmaceutical industry and academia, and generally met twice a year, usually alternating between North America and Europe. The membership is truly international, in scope and diversity. The SC meetings provide the opportunity for invaluable discussions that generate and develop project ideas. The SC output has included publication of books, glossaries, and articles; establishment and operation of the IUPAC-Richter Prize in Medicinal Chemistry; and organization of educational schools in medicinal chemistry and international meetings.

Books

Analogue-based Drug Discovery

A member of our Subcommittee, Dr. Janos Fischer, read in SCRIP that out of the 35 new substances marketed in Germany in 1998, 12 were classified as "novel", 9 as "improvements on existing therapeutic principles", and 14 as "me-toos" [3]. The description "me-too" is generally used pejoratively to denigrate pharmaceutical companies for not doing "real research". The implication is that discovery of only novel (*i.e.* first in class) medicines

represent "real research". The "me-toos" are considered copies made in order to share commercial success. This is not a reasonable view, however. Generally, these "metoos" are analogues that improve upon properties of the "novel" (pioneer) medicines. The design and discovery of such analogues is actually the historical means by which a particular drug therapy becomes optimized for the benefit of the patients. This derogatory description of drug research inspired the SC-D3 to initiate a project documenting the valuable properties of analogue drugs. Articles on analogue drugs were compiled in a series of

books published by Wiley-VCH in 2006 [4], followed in 2010 and 2013 by two more books [5,6].



Practical Studies for Medicinal Chemistry

This textbook produced with Latin America and other less developed regions in mind, contains 41 practical experiments in medicinal chemistry that do not

require expensive starting materials or reagents and that only depend on low-cost instrumentation and techniques [7]. All experimental details are provided in English; most are also presented in Spanish or Portuguese. The book aims to assist in the post-graduate training of medicinal chemists and to better prepare them to conduct research into the discovery and development of new drugs to treat diseases indigenous to their own countries. The interdisciplinary laboratory exercises are representative of the field of medicinal chemistry and are easy to reproduce. The book is freely available online (see URL in ref. 7) and open to all interested teachers and students. A paper edition was published by the Universidad Nacional de Rio Cuarto, Argentina.

Glossaries

Terms Related to Pharmaceutics

The terms used in pharmaceutics are rarely covered by existing glossaries, and when they are, their definitions are often inappropriate and require new or modified definitions to better fit the new context. In the **Glossary of Terms Related to Pharmaceutics** [8], pharmaceutics is defined as the science of preparation of drugs, dosage forms, and drug delivery systems, taking into account the pharmacokinetics and pharmacodynamics of the drug as well as its physical and chemical properties. Thus, many branches of chemistry, such as organic, inorganic,

Medicinal Chemistry in IUPAC

physical, solid-state, colloid, and surface chemistry, as well as nanotechnology and others, play roles in pharmaceutics. Even biopharmaceutics, the more biologically oriented branch of pharmaceutics, draws on chemical concepts such as (pharmaco)kinetics, absorption, dissolution, diffusion, and others.

Terms Used in Biomolecular Screening

Biomolecular screening has become a critical part of the drug discovery process. The **Glossary of Terms Used in Biomolecular Screening** [9] contains approximately 175 definitions related to various aspects of the screening process, such as assay types, data handling, and relevant technologies. The field of biomolecular screening is multidisciplinary in nature, and this glossary, which was compiled by a task force that included members of the Society for Biomolecular Screening and Professor Larry Walker, editor of *J. Biomolecular Screening*, contains authoritative definitions.

Terms Used in Medicinal Chemistry

A Glossary of Terms Used in Medicinal Chemistry was published by the Subcommittee in 1998 [10]. The web version clearly demonstrated the interest and value of such a tool, and between 1999 and 2007, the total usage based on a log of IP addresses was over 200 thousand. There were 25 countries that exceeded 500 uses, led by the USA, which had 73 700. It was appropriate, therefore, that we compiled a substantial list of 150 new entries to provide an update 10 years later. Part II of A Glossary of Terms used in Medicinal Chemistry was published in 2013 [11].

Terms Used in Computational Drug Design

A Glossary of Terms Used in Computational Drug Design was produced by the Subcommittee in 1997 [12]. Since then, the subject has undergone considerable change, particularly because new high-throughput technologies and the genomics revolution have fueled a need for novel computational methods to handle the resulting deluge of data. In addition, simple computational tools are now available for use by medicinal chemists. The update—or Part II—of this glossary will provide intellectual support for conversations between laboratory and computational chemists, and for the interpretation of calculations that a bench chemist or student might perform. Currently under preparation, it will add 210 new or revised terms that, inter alia, describe methods used in virtual screening, data mining, and cheminformatics (see IUPAC project 2010-057-3-700).

Other Glossaries under preparation

About 170 terms directly related to the **field of drug metabolism** have been compiled and defined under IUPAC project 2000-009-1-700. These represent just those terms that are considered to be most relevant for medicinal chemistry out of a list of some 600 that were originally compiled. The glossary has been reviewed publically, revised, and is soon ready for submission as IUPAC recommendations. A project to revise the 1990 **Glossary of Terms Used in Combinatorial Chemistry** [13] was initiated in 2004. Since, however, the scope encompassed by the name "combinatorial chemistry" has evolved and so the project is still in progress (IUPAC project 2003-044-1-700).

Analysis of Glossary Terms to Establish Biological Context by Text Data Mining

This project sought to extend the usefulness and applicability of the glossaries in general, by exploring methods for identifying the various contexts in which the terms appear in the scientific literature. The study concentrated on Bioinformation in Drug Development. With the ongoing changes in the field, the glossary-based approach did not seem to adapt in concert with the evolution of terms and their use in the field. An alternative approach, using an ontology-based methodology, was adopted that was based, not on specific terms, but rather on concepts and relationships. This provided a computational platform that can be applied to a range of problems in pharmaceutical R&D. An example is summarized in a 2011 publication [14].

Articles

Stand-alone Drugs

The top 100 most frequently used drugs, which accounted for 56% of total sales based on their sales data in 2006, were analysed for their analogue basis. This led to the identification of nine "stand-alone drugs", i.e. drugs which analogues that improve upon them have not yet been discovered. Examples of such "stand-alone drugs" are acetylsalicylic acid (aspirin), diltiazem (an L-type calcium antagonist), levodopa (dopamine pro-drug), acetaminophen (or paracetamol, antipyretic and analgesic), aripiprazole (dopamine partial agonist), metformin (oral hypoglycemic), and lamotrigine (anti-convulsant).

Rather than publishing an article, a chapter in the book series *Analogue-based Drug Discovery* compiles these data [15].

Accomplishments During the Last Decade

New Drugs for Neglected Tropical Diseases

In Latin America and the Caribbean regions, at least 210 million people live below the poverty line. This is approximately 40% of the population. These impoverished and marginalized populations are heavily burdened with neglected tropical diseases (NTD's). Based on their prevalence and the healthy life years lost from disability, hookworm infection, other soil-transmitted helminth infections, and Chagas disease are the most important NTD's in Latin America and the Caribbean, followed by dengue, schistosomiasis, leishmaniasis, trachoma, leprosy, and lymphatic filariasis.

The solutions to this situation do not depend on simply having appropriate drugs, but are complex and involve public health, disease control, education, and political will. That said, having appropriate drugs would be very helpful. A project (IUPAC project 2009-033-1-700) aims to identify chemistry researchers and testing laboratories, and their equipment and facilities, in Latin America who are currently working to discover new drugs to treat NTD's. The survey data have been combined and published [16].

A networking workshop aimed at the currently identified researchers in Latin America is being planned. The next stage will be to stimulate other medicinal chemists in Latin America to also conduct research in this area, and to make contacts between them and the testing laboratories, promoting self-help.

Natural and Synthetic Substances Related to Human Health

There is a widespread belief on the part of the general public that natural substances are inherently superior to synthetic substances with regard to efficacy and safety in matters related to human health. This question was examined by reviewing the therapeutic use of drugs and herbal medicine preparations, the role of vitamins and nutrients, and the effects of toxic substances. A comparison of the characteristics of natural and synthetic substances within these categories shows a similar range of favourable and unfavourable effects. It is clear that molecular structure and dose determine the effect of substances on human health, not whether they are of natural or synthetic origin.

An IUPAC Technical Report has been published which purpose was to explore the subject by reviewing, in an illustrative manner, drug substances, herbal medicinal preparations, vitamins and nutrients, and toxic substances, with a view to providing an informed, rational perspective [17]. An abbreviated summary was released by Eurekalert in April 2003 [18].

IUPAC-Richter Prize in Medicinal Chemistry

This Prize was arranged through Dr. Janos Fischer to improve the general awareness of IUPAC among medicinal chemists. It was established by a generous gift from the Hungarian Pharmaceutical Company Gedeon Richter, PLC (Budapest, Hungary) to acknowledge the key role that medicinal chemistry plays toward improving human health. The prize of \$10,000 is awarded every two years to a scientist whose activities or published accounts have made an outstanding contribution to the practice of medicinal chemistry, or to an outstanding example of new drug discovery. This prize has been presented five times between 2006 and 2014. The prize recipients have lectured at the ACS National Medicinal Chemistry Symposium in the USA and at the EFMC International Symposium on Medicinal Chemistry (ISMC) in Europe. Contact with the medicinal chemistry community has been outstanding. Past awardees: Prof. Malcolm F.G. Stevens. Nottingham Univ., UK (2006), Small molecule anticancer drugs, including temozolomide, lectured at Istanbul, Turkey, and Turin, Italy; Dr. Jan Heeres, Janssen Pharmaceutica, Belgium (2008), Ketoconazole and related heterocyclic antimycotics, lectured at Pittsburgh, PA, USA and Torquay, UK; Prof. Arun K. Ghosh, Purdue Univ., USA (2010), Use of backbone binding in discovery of HIV-1 protease inhibitor darunavir. lectured at Minneapolis, MN, USA and Brussels, Belgium; Prof. Stephen Hanessian, Montreal Univ., Canada (2012), For considerable synthesis contributions to medicinal chemistry, lectured at Tucson, AZ, USA and Berlin, Germany; and Dr. Helmut Buschman, ex Grünenthal, Aachen, Germany (2014), Novel analgesic, tapentadol, lectured at Charleston, SC, USA and Lisbon, Portugal.

The prize has been truly international in that seven different countries are represented overall, either for the place of work or for the original nationality of the recipient.

Training of Medicinal Chemists

SC-D3 published a series of papers on the formal training of medicinal chemists, aiming to circumvent the more haphazard learning that occurs when chemists are left to teach themselves "on the job". A summary was published in 2005 [19].

Research and Training in Latin America

This past decade, Prof. Antonio Monge has been very active in arranging for courses and symposia in various

Medicinal Chemistry in IUPAC

countries in Latin America: short courses were established in Montevideo, Uruguay (September 1999); Rio de Janeiro, Brazil (August 2001); Peru (May 2003); Columbia (May 2003); Bolivia (June 2003); Lima, Peru (October 2004); Montevideo, Uruguay (December 2004); Havana, Cuba (November 2006); Reynosa and Monterrey, Mexico (March 2007); Istmo, Guatemala (August 2007); Huancayo, Peru (October 2007); Buenos Aires, Argentina (May 2010); and Lima, Peru (October 2010).

The Subcommittee also held meeting in Rio de Janeiro, Brazil (February 2005) .The meeting also to coincide with the XI Summer School in Pharmaceutical and Medicinal Chemistry at the Laboratory of the Federal University of Rio de Janeiro and where seven SC-D3 members lectured at a short 4-day course entitled "Highlights in Medicinal Chemistry" [20].

Training in the Indian Subcontinent

Increased medicinal chemistry employment in Asian pharmaceutical companies and Contract Research Organizations collaborating with US and European companies have created a need for chemists with state of the art knowledge of medicinal chemistry. Dr. M. Chorghade has convinced the Indian Council of Scientific & Industrial Research (CSIR) to run courses in different cities. Two symposia were held in Rajkot and Nagpur (February 2011), at which five members of the Subcommittee gave lectures. An MCI course (Medicinal Chemistry in India) based on the successful Drew University Residential School on Medicinal Chemistry, was thought on 11-15 February 2013, at Sri Ramachandran University in Chennai. (The original course is taught annually since 1986 on the Drew University campus in Madison, New Jersey; www.drew.edu/ resmed). The course was a resounding success: a total of 112 participants from industry (90) and academia attended this short course while industry and academic experts from USA participated in the interactive teaching sessions and discussions.

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www.iupac.org/body/703

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Youth Views on Sustainability



Chemical Waste Management at Clinical Laboratories

From lab curiosity to suitable environment—healthcare for the world and human beings.

by David Yafté Díaz-Sánchez

aste, a very popular word these days, commonly refers to a human-made product with no significant value, which must be eliminated. When I was younger, I studied at a technical college in the south of Mexico City. I used to ask my teachers what happens to chemical waste generated at the clinical laboratory. Today, I study metallurgical chemical engineering, but I cannot forget my old questions about chemical waste, because some chemical waste has properties that make it hazardous to health and the environment.

When working in a clinical laboratory, hazardous waste is often produced. It must be reduced and, where it cannot be, its potential risk or impact to the environment and our health should be minimized. There are, principally, two kinds of dangerous waste at clinical laboratories: chemical waste and biological waste. This article focuses on chemical waste.

Chemical waste may be hazardous in several different ways [1,2]. It could be corrosive, like HNO $_3$, or toxic, like NaCN, or could be hazardous to the environment, like CuSO $_4$. There are different types of chemical waste, and we must learn how to treat them properly. Sometimes a neutralization reaction is enough to make waste less dangerous, but at times more is necessary.

Some examples:

Example 1: Spectrophotometric determination of chloride ion in blood

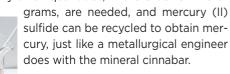
The principle of this method is the quantitative displacement of thiocyanate by chloride from mercuric thiocyanate. The subsequent formation of a red ferric thiocyanate complex is measured colorimetrically. Here the intensity of the colour formed is proportional to the chloride ion concentration in the sample:

$$\begin{array}{l} 2Cl^{\text{-}}_{(aq)} + Hg(SCN)_{2(aq)} \to HgCl_{2(aq)} + 2SCN^{\text{-}}_{(aq)} \\ SCN^{\text{-}}_{(aq)} + Fe^{3+}_{(aq)} \to FeSCN^{2+}_{(aq)} \end{array}$$

In this case the reagent used to measure the chloride ion in blood contains mercury compounds, which are highly toxic and can be accumulated in the human body. The mercury concentration in this reagent is 6 mmol L⁻¹, and usually about 0.250 L is used. This makes treating this waste properly a necessity. One possible treatment is to add thioacetamide, which releases hydrogen sulfide while heating in aqueous solution, permitting the precipitation of the very insoluble mercury (II) sulfide without noxious odors.

$$\begin{split} &C_2 H_5 NS_{(aq)} + H_2 O_{(l)} \rightarrow H_2 S_{(aq)} + C_2 H_5 NO_{(aq)} \\ &HgCl_{2(aq)} + H_2 S_{(aq)} \rightarrow HgS_{(s)} + 2HCl_{(aq)} \\ &K_{sp(HgS)} = 4.0 \times 10^{-54} \end{split}$$

Although both thioacetamide and hydrogen sulfide are toxic, only small quantities, in the order of micro-



$$HgS_{\scriptscriptstyle(s)} + \mathrm{O}_{\scriptscriptstyle 2(g)} {\:\rightarrow\:} Hg_{\scriptscriptstyle(l)} + \mathrm{SO}_{\scriptscriptstyle 2(g)}$$



The Youth Views on Sustainability series is a joint project with YourFormula.eu, the online platform and multimedia magazine powered by Cefic (The European Chemical Industry Council). It highlights the views of the younger generations on sustainability matters and features in print in *Chemistry International* some blog posts from the YourFormula site. Such features have been published in *Chem Int* in July 2014 (p.11), Nov 2014 (p.14), and May 2015 (p.18).

Youth Views on Sustainability

Going beyond mercury, in an industrial scale, this can be used to obtain the always useful $\rm H_2SO_4$ from the $\rm SO_2$.

$$\begin{split} 2\mathrm{SO}_{2(\mathrm{g})} + \mathrm{O}_{2(\mathrm{g})} &\to +2\mathrm{SO}_{3(\mathrm{g})} \\ \mathrm{SO}_{3(\mathrm{g})} + \mathrm{H}_2\mathrm{SO}_{4(\mathrm{l})} &\to +\mathrm{H}_2\mathrm{S}_2\mathrm{O}_{7(\mathrm{l})} \\ \mathrm{H}_2\mathrm{S}_2\mathrm{O}_{7(\mathrm{l})} + \mathrm{H}_2\mathrm{O}_{(\mathrm{l})} &\to +2\mathrm{H}_2\mathrm{SO}_{4(\mathrm{l})} \end{split}$$

Example 2: Hemoglobin determination by Drabkin's reagent

Hemoglobin, the oxygen-carrying protein of erythrocytes (red blood cells), is oxidized by hexacyanoferrate (III) ion to methemoglobin and cyanide complex to get cyanmethemoglobin:

$$\begin{array}{l} Hb(Fe^{II})_{(aq)} + Fe[(CN)_{6}]^{3} \cdot_{(aq)} \to Hb(Fe^{III})_{(aq)} + Fe[(CN)_{6}]^{4} \cdot_{(aq)} \\ Hb(Fe^{III})_{(aq)} + CN \cdot_{(aq)} \to HbCN(Fe^{III})_{(aq)} \end{array}$$

Drabkin's reagent contains cyanide ions, which are extremely poisonous. This time, cyanide concentration in the reagent is 77 mmol L⁻¹. As in the first example, usually about 0.250 L is used. Fortunately, we can find a few different ways to treat this waste. One of them is the destruction of cyanide by oxidation with H_2O_2 using $CuSO_4$ as a catalyst [3]:

$$CN_{(aq)}^{-} + H_2O_{2(aq)} \rightarrow CNO_{(aq)}^{-} + H_2O_{(1)}$$

The cyanate produced reacts with water at pH<7 to produce ammonium and carbonate ions:

$${\rm CNO^{\text{-}}_{(aq)}} + 2{\rm H_2O_{(l)}} {\to} {\rm CO_3^{\,2\text{-}}_{(aq)}} + {\rm NH_4^{\,+}_{(aq)}}$$

It is essential to make this treatment "one step at a time". If we attempt to make these reactions in just one step, adding $\rm H_2O_2$ and $\rm CuSO_4$ to cyanide and immediately adding an acid to push down the pH, we could die, because cyanide reacts with acids to produce the even more poisonous gas hydrogen cyanide.

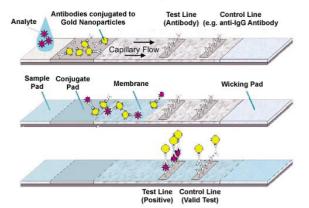
However, not all is bad news—we can even find gold if we know where to look....

Example 3: Pregnancy tests and the rainbow's end

Most pregnancy tests are based on the detection of the human chorionic gonadotropin (hCG) in urine and serum. Because hCG is a hormone produced by the placenta and other tissues when a woman is pregnant, its presence in urine and serum is an early indicator of pregnancy. Commonly, a pregnancy test is a onestep lateral flow chromatographic immunoassay. The test strip in the device consists of a conjugate pad containing mouse monoclonal anti-hCG antibodies conjugated to colloidal gold and a nitrocellulose membrane strip containing two lines, a test line and a control line.

The magic word here is gold. Like with "e-waste", this is an example of urban mining, where we can find gold in higher concentrations than in the mined ores [4]. Contrary to e-waste, a pregnancy test only contains gold, and its extraction process can be hydrometallurgical or pyrometallurgical. In the hydrometallurgical method we could try to use an alternative lixiviant, such as amino acid- [5] or thiosulfate- [6] based solutions. Recently, these last systems have been identified as potential industrial competitors to cyanide based systems.

Lateral Flow Assay Architecture



But pregnancy tests are just an example. We can find gold and other precious metals in a large number of clinical tests and studies. A well-established source of silver (3-6 g m⁻²) is X-ray radiographs. Approximately 2 billion radiographs are taken around the world per year [7]. These are now collected to recover silver, which has an insufficient world production. Other tests contain precious metals, as well. For example, plasmonic ELISA tests contain colloidal gold, and surface plasmon resonance uses thin layers of gold or silver and is often used in immunology. We need only search in these and other tests to find the pot at the rainbow's end.

Technical and economic studies need to be done to determine the most inexpensive and least toxic methods to get precious metals from these sources efficiently and economically. This last example revolutionizes the way we see what we call "waste". Each day we can find that more and more things contain silver,

Chemical Waste Management at Clinical Laboratories

gold, palladium, and other useful materials.

Some reflections about waste management and treatment

I have been writing a Standard Operating Procedure (SOP) manual where I clearly record, step by step, the reactions needed to reduce the potential risk of chemical waste. My technical college has recently improved that manual, and together we are working to evaluate the document. While few people are interested in these types of projects, they are important in changing the way people think about waste. At school, in industry, or in research laboratories, everyone who produces chemical waste must know why and how to treat them. This is not just an issue for teachers, auxiliary laboratory workers and students have to learn about chemical waste management as well. Each action plan needs a person to supervise and ensure that everything is being done correctly. This person must know about chemistry, chemical waste, and health care and must be qualified to evaluate any method to minimize chemical waste, assisted in this by chemists, medical professionals, and biologists.

Safety data sheets are good resources to get information about the chemical wastes of chemical substances. Generally, a small number of substances of daily use have properties comparable to cyanide or mercury (II), but remember, waste can be reactive, corrosive, explosive, oxidant, toxic, poisonous, flammable and/or hazardous to the environment. Personnel must be constantly vigilant, taking discussion sessions with experts and caring about themselves and their safety.

Only if we are concerned about treating chemical clinical waste can we guarantee the well-being of every person who visits a clinical laboratory. Otherwise, we quickly shall see how the green hills around our technical college become grey, and the sown fields

near to us turn into sterile loads of soil. I am sure this is not only happening here in Mexico.

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IUPAC Wire

See also www.iupac.org

Thieme-IUPAC Prize 2016 Call for Nominations

hieme Chemistry, IUPAC, and the Editors of SYNTHESIS, SYNLETT, SYNFACTS, and Science of Synthesis announce the Thieme-IUPAC Prize for 2016. This award is presented every two years on the occasion of the International Union of Pure and Applied Chemistry – International Conference on Organic Synthesis (IUPAC-ICOS). The 2016 ICOS will be held at IIT Bombay in Mumbai, India, 11-16 December 2016. The prize is awarded to a scientist under 40 years of age whose research has had a major impact in synthetic organic chemistry.

The prize is given on the basis of scientific merit for independent research dealing with synthesis in the broadest context of organic chemistry, including organometallic chemistry, medicinal and biological chemistry, designed molecules, and materials. Candidates must be under 40 years of age as of 1 January of the year in which the prize is awarded.

The Thieme-IUPAC Prize has been awarded to Stuart L. Schreiber in 1992, Paul Knochel in 1994, Eric N. Jacobsen in 1996, Andrew G. Myers in 1998, Alois Fürstner in 2000, Erick M. Carreira in 2002, John F. Hartwig in 2004, David W. C. MacMillan in 2006, F. Dean Toste in 2008, Phil S. Baran in 2010, Melanie S. Sanford in 2012, and Martin D. Burke in 2014.

Nominations must be accompanied by a biographical sketch of the nominee, a list of the candidate's ten most significant publications, and a statement of how the candidate's research has had a major impact on the field of synthetic organic chemistry. The material will be confidentially forwarded to an independent selection committee. Nomination materials should be submitted by e-mail to marcus.white@thieme.de.

Deadline: **December 11, 2015** www.thieme.de/en/thieme-chemistry/thieme-iupac-prize-55182.htm

2016 IUPAC-SOLVAY International Award for Young Chemists announced

he 2016 IUPAC-SOLVAY International Award for Young Chemists is intended to encourage outstanding young research scientists at the beginning of their careers. The awards are given for the most outstanding Ph.D. theses in the general area of the chemical sciences, as described in a 1000-word essay. The award is generously sponsored by Solvay.

IUPAC will award up to five prizes in 2016. Each prize will consist of USD 1000 cash and travel expenses to the next IUPAC Congress. In keeping with IUPAC's status as a global organization, efforts will be made to assure fair geographic distribution of prizes.

The awards will be presented at the IUPAC Congress in Brazil in July 2017. Each awardee will be invited to present a poster on his/her research and to participate in a plenary award session, and is expected to submit a review article for possible publication in *Pure and Applied Chemistry*.

Applications may be submitted, as described below, to the IUPAC Secretariat. In addition, some IUPAC National Adhering Organizations are soliciting applications in their own countries, frequently in conjunction with a national award. In such cases, applications may be submitted to the NAO or to the Secretariat (not both). The list of NAOs is available.

Procedures for the 2016 Award

- Entrants must have received the Ph.D. (or equivalent) degree, or completed all Ph.D. requirements including successful defense of the doctoral thesis, during calendar 2015 in any of the countries that are members or associate members of IUPAC. Entrants need not be citizens or residents of one of these countries at the time the application is submitted.
- The research described in the entrant's thesis must be in the field of the chemical sciences, defined as "chemistry and those disciplines and technologies that make significant use of chemistry."
- The IUPAC-SOLVAY Award recognizes only work that was performed while the entrant was a graduate student.
- Application requires submission of a completed entry form, together with the material listed below.
- An essay must be submitted by the entrant that
 describes his or her thesis work and places it in
 perspective relative to current research in the
 chemical sciences. The essay must be written in
 English by the entrant and may not exceed 1000
 words. [For applications submitted through NAOs,
 a national language may be permissible, and the
 NAO will assist in translation to English. The announcement by the appropriate NAO should be
 consulted.]
- Two supporting letters are required, one from the thesis adviser and/or chair of the thesis committee and one from an additional faculty member who is familiar with the applicant's thesis work.

IUPAC Wire

These letters should comment on the qualifications and accomplishments of the applicant and the significance of the thesis work.

 Complete applications must be received at the IUPAC Secretariat by 1 February 2016.

For information, contact IUPAC Secretariat: secretariat@iupac.org

www.iupac.org/news/news-detail/article/2016-iupac-solvay -international-award-for-young-chemists-announced.html

2016 IUPAC-ThalesNano Prize in Flow Chemistry—Call for Nominations

he IUPAC-ThalesNano Prize was established in 2011. It will be awarded again in 2016 and will be presented at the 14th International Conference on MicroReaction Technology (IMRET) in September 2016 Beijing, China. A contribution to travel expenses will be provided.

The prize is to be awarded to an internationally recognized scientist, whose activities or published accounts have made an outstanding contribution in the field of flow chemistry in academia or industry.

The Prize—of a monetary value of USD 7500—has been established by a generous gift from the Hungarian Technology company ThalesNano Inc. to acknowledge the key role that flow chemistry plays towards the improvement of chemical processes.

Applicants should be received by nominations only, with just one person needing to serve in that capacity, although a total of five individuals should be listed as referees overall. The package must be submitted electronically and should contain a complete resume, a professional autobiography of not more than two pages, and a one-page summary of what the individual considers to be his/her activities, accomplishments and/or publications that have had the most significant impact upon the field of Flow Chemistry. The material will be forwarded confidentially to an independent selection committee appointed by the IUPAC Committee on Chemistry and Industry.

Nomination materials should be submitted by **31 January 2016** to the chair of the IUPAC Committee on Chemistry and Industry, Dr. Bernard West, by email at: bernard.west@sympatico.ca

www.iupac.org/news/news-detail/article/2016-iupac-thalesnano-prize -in-flow-chemistry.html

CHEMRAWN VII Prize for Green Chemistry—Call for Nominations

UPAC is now seeking nominations for the 2016 CHEMRAWN VII Prize for Green Chemistry. The CHEMRAWN VII Prize was first announced in August 2008* and since, has been awarded every two years at the IUPAC International Conference on Green Chemistry. The Prize of USD 5000 is granted to a young investigator (less than 45 years of age) from an emerging region who is actively contributing to research in Green Chemistry. The Prize was been awarded to Noureddine Yassaa (Algeria) in 2010, Rashimi Sanghi (India) in 2012 and Vânia G. Zuin (Brazil) in 2014.

Nominations for the 2016 Prize must be submitted by **25 March 2016**. Each nomination should include a CV and two letters of support, plus a brief summary of accomplishments illustrating the contributions of the applicant to research in Green Chemistry. Examples of research topics that are covered by the prize include:

- Atmospheric Chemistry
- Use of Alternative Feedstocks
- Use of Innocuous Reagents
- Employing Natural Processes
- Use of Alternative Solvents
- Design of Safer Chemicals
- Developing Alternative Reaction Conditions
- Minimizing Energy Consumption

Complete applications should be sent to the IUPAC Secretariat by e-mail to <secretariat@iupac.org> before the submission deadline.

The Selection Committee comprises the Chair of IUPAC Committee on Chemical Research Applied to World Needs, CHEMRAWN, the President of the Organic and Biomolecular Chemistry Division, and the Chair of the Subcommittee on Green Chemistry.

The next award will be presented at the 6th IUPAC International Conference on Green Chemistry, 4-8 September 2016, Venice, Italy <www.greeniupac2016.eu>

The winner will be asked to give a lecture on that Conference.

www.iupac.org/news/news-detail/article/chemrawn-vii-prize-for-green-chemistry-2016-call-for-nominations.html

Standard Atomic Weight of Ytterbium Revised

he IUPAC Commission on Isotopic Abundances and Atomic Weights (II.1) met under the chairmanship of Dr. Juris Meija, at the University of Natural Resources and Life Sciences Vienna, Austria, prior to the 48th IUPAC General Assembly in Busan, Korea, in August 2015. Following its meeting, the Commission recommended a change to the standard atomic weight of ytterbium. The IUPAC Bureau, at its meeting on 14 August, approved this change.

The standard atomic weight of ytterbium has been changed based on a recent measurement of terrestrial isotopic abundances from 173.054(5) to 173.045(10). For ytterbium, which was first obtained in a pure state some 50 years ago, only two calibrated measurements of its isotopic composition have been made. These measurements differ from one another. Ytterbium exemplifies a situation that is true for many other elements: well-documented isotope ratio measurements are still needed.

In addition to revising standard atomic weights, CIAAW discussed the uncertainty interpretation of standard atomic weights and resolved to endorse probabilistic interpretation of standard atomic weights using various probability density functions, including the uniform probability distribution as outlined in the Eurachem/CITAC Guide when no specific knowledge is available about the isotopic composition of a material of interest. In all cases, probability distributions describe the lack of knowledge about isotopic compositions of particular materials or classes of materials and not the actual distribution of natural abundances. These changes and considerations will be published in the upcoming release "Atomic Weights of the Elements 2015", which will appear in Pure and Applied Chemistry. The revised values can also be found online at the website of the commission (www.ciaaw.org).

The importance of determining precise atomic weights has long been recognized, resulting in the creation of the International Atomic Weights Committee in 1899. IUPAC has overseen the periodic evaluation and dissemination of standard atomic-weight values since its formation in 1919.

For further information, contact Dr. Juris Meija <juris.meija@nrc.ca>

www.iupac.org/news/news-detail/article/standard-atomic-weight-of--vtterbium-revised.html

De Gruyter to Launch Chemistry Standards Database

Available starting in 2016, the IUPAC Standards Online database will make standards and recommendations in the field of chemistry quickly and easily accessible to internet users. De Gruyter is developing the database together with the International Union of Pure and Applied Chemistry (IUPAC), the organization responsible for establishing internationally binding standards for scientists working in research and industry, for patent lawyers and other legal professionals, as well as for environmental scientists and toxicologists. A beta version of the database was presented at the 45th World Chemistry Congress in August in Busan. South Korea.

"The tremendous benefit of this database is that it will bring all standards and recommendations previously published in the journal of *Pure and Applied Chemistry* into the digital era, making it easily available from a central location," says Karin Sora, Senior Editorial Director for Science & Technology at De Gruyter.

With over 60 National Adhering Organizations, over 100 adhering organizations, and 5000 affiliate members, IUPAC is the world authority on chemical nomenclature, terminology, standardized methods for measurement, atomic weights, and many other critically evaluated data.

Dr. Mark Cesa, President of IUPAC, views the annual updating of the database as a particular strength: "In 2013 alone there were 1000 new standards. Having this information easily available from a central source will make the work of chemistry professionals around the world much easier."

http://www.degruyter.com/view/db/iupac

Solubility Data Series Books now Available on Web

n the 1970s, IUPAC's Solubility Data Commission (now the Subcommittee on Solubility and Equilibrium Data) embarked on a project to compile and critically evaluate experimental data for solubility in systems of scientific and practical interest. The first volume in the IUPAC Solubility Data Series, covering the solubility of helium and neon in liquid solvents, was published in 1979. Subsequent years saw many volumes on gas-liquid, liquid-liquid, and solid-liquid solubilities. These volumes are an invaluable scientific resource.

Now, thanks to an agreement between IUPAC (which holds the copyright to these volumes) and the National Institute of Standards and Technology (NIST), NIST has made the contents of these monographs (Volumes 1-65) freely available in digitized PDF form online at the website: http://srdata.nist.gov/solubility/IUPAC/iupac.aspx.

Some volumes on the site are broken into subsections with Table of Contents; this feature will be extended to the rest of the volumes as resources permit.

Beginning with Volume 66 in 1998, this series was renamed the IUPAC-NIST Solubility Data Series, with several volumes each year (up to Volume 103 so far) published in the Journal of Physical and Chemical Reference Data; see http://jpcrd.aip.org. Links to these publications are provided from the NIST site.

http://srdata.nist.gov/solubility

L'Oréal-UNESCO Awards for Women in Science 2015 Announced

ive exceptional women scientists from around the world received the 2015 L'ORÉAL-UNESCO Prize in Physical Sciences in an Awards Ceremony which took place on 18 March 2015 at the Grand Amphitheatre of the Sorbonne University (Paris, France). The Awards promote scientific excellence and the contribution of women to science, in particular in Life Sciences and the Physical Sciences, and in the service of advancement of knowledge, its impact on society, and sustainable development. By giving these female researchers increased visibility, the awards show the way for new generations, encouraging young women to follow their example.

Since the launch of the programme, 82 outstanding women researchers have received the L'Oréal-UNESCO For Women in Science Prize, two of whom have gone on to receive the Nobel Prize.

IUPAC congratulates all the Awardees. A special recognition goes this year to Professor Yi Xie, laureate Asia-Pacific, who was, in 2013, one of the Awardees of the IUPAC Distinguished Women in Chemistry or Chemical Engineering.

Asia-Pacific: Professor Yi Xie

Committed to preserving our planet, Prof.Yi Xie has dedicated her life to finding new and intelligent solutions to address the environmental challenge. She has been rewarded for her significant contributions to creating new nanomaterials with promising applications in the conversion of heat or sunlight into electricity. Her work will greatly contribute to lessening pollution and boosting energy efficiency, and will open promising prospects for the future



Yi Xie, photograph © Brgitte Lacombe

Europe: Profesor Dame Carol Robinson

A risk-taker, Prof. Robinson has always done things her way: she left school at 16, studied part-time while working, and then took an eight year career break to raise her children before returning to academia. Prof. Dame Carol Robinson has been honored for creating a revolutionary method for studying how proteins function, particularly membrane proteins, and establishing a whole new scientific field: gas phase structural biology. Her pioneering work could have a significant impact on medical research.

Latin America: Professor Thaisa Storchi Bergmann

Passionate and determined, Prof. Bergmann is convinced that education for all is the key to a better world and hopes to contribute to promoting science as a captivating and fun career path through her work. Prof. Thaisa Storchi Bergmann has been honored for her work leading to the understanding of massive black holes, one of the most enigmatic and complex phenomena of the universe: she was the first researcher to discover that matter could escape from black holes.

North America: Professor Molly S. Shoichet

A people person, Prof. Shoichet also participates in special athletic events for people with spinal cord injuries, is actively involved in human rights issues, and has contributed to launching a social media campaign designed to "connect today's research with tomorrow's reality." She has been rewarded for the development of new materials to regenerate damaged nerve tissue and for a new method that can deliver drugs directly to the spinal cord and brain. Her work is putting chemistry at the service of medicine in spectacular new ways.

Africa and the Arab States: Professor Rajaa Cherkaoui El Moursli

Nicknamed «research activist», Prof. El Moursli dedicates much of her time to raising the level of scientific research in her country, and has been instrumental in improving Moroccan healthcare by creating the 1st master's degree in medical physics. Prof. Rajaâ Cherkaoui El Moursli has been honored for her key contribution to one of the greatest discoveries in physics: proof of the existence of the Higgs Boson, the particle responsible for the creation of mass in the universe.

www.loreal.com/csr-commitments/foundation/science/ women-and-scientific-excellence

Berhanu Abegaz heads the **UNESCO International Basic** Sciences Programme (IBSP) scientific board

The African Academy of Sciences' executive director Berhanu Abegaz has been elected chair of the UNESCO International Basic Sciences Programme (IBSP) scientific board.

The United Nations Educational, Scientific and Cultural Organization established the multidisciplinary programme to strengthen national capacities in the basic sciences and in science education. Its scientific board advises UNESCO's leadership on basic science matters.

Abegaz, who was previously vice-chair of the board, was elected at the ninth meeting of the IBSP scientific board held in Paris, France, in May 2015. He will be deputised by Marina Bentivoglio, a professor of histology at the University of Verona in Italy, and Glacius Oliva, a professor of structural biology at the University of São Paulo in Brazil.

www.unesco.org/new/en/natural-sciences/science-technology/ basic-sciences/international-basic-sciences-programme/

Christo Balarew receives **Presidential Honors**

n 25 May 21015 Prof. Balarew was awarded the Order of Saints Cyril and Methodius 1st class the highest award for scientific achievements conferred by the President of Bulgaria. This prestigious honor adds to several national and international awards already conferred to Prof. Balarew for his scientific and applied achievements.

Professor Christo Balarew is a prominent Bulgarian scientist. During most of his professional career he has worked at the Institute of General and Inorganic Chemistry of the Bulgarian Academy of Sciences in Sofia. Some of his scientific achievements can be summarized by the following:

According to Balarew, inorganic salts are considered ionic coordination compounds. In their crystal structures the metal ions are coordinated by anions or water molecules and in this way coordination polyhedra are formed. They are linked with one another, with other ions, or with water molecules through ionic (electrostatic) or hydrogen bonds. To prognose the composition and structure of the most probable complexes, not only the geometrical factor (Pauling rules), but also Pearson's concept of hard and soft Lewis acids and bases (HSAB) and crystal field stabilization energy are involved. A procedure for predicting the complexes in the crystal structures was elaborated. On this basis double salts formation was explained and a theory for the isomorphous and isodimorphous co-crystallization was created. This allows theoretical calculations of the distribution coefficients of admixtures between

IUPAC Wire



Chris Balarew (right) receives Presidential Honors from President Rosen Plevneliev (left)

the crystals and the solution and of the free energy of phase transitions to be performed on the basis of solubility data.

Balarew also elaborated a model for explaining the nucleation and the kinetics of crystallization of highly soluble salts.. Nucleation starts when some of the complexes existing in the solution display high activity sufficient to reach and surpass the solubility product of the crystallizing salt. These complexes or some of their directly derivable forms (e.g. those obtained by condensation) together with other ions or molecules form the crystal structure. This means that the activity of definite species in the solution (complexes, molecules or simple hydrated ions) that are able to be incorporated directly or with minor changes into the crystal structure is of primary importance for the crystallization process. The lowest critical supersaturation needed for nucleation and the highest rate of crystallization are displayed by those salts whose complexes in the solution have analogues in the crystal structure of the crystallizing salt. The knowledge of the type and composition of the species in the solution is of crucial significance for the elucidation of the ability for supersaturation and for the crystallochemical explanation of the Ostwald step rule.

The experience accumulated during these scientific studies was applied by Prof. Balarew to the elaboration of technologies for producing reagent-grade chemicals, synthesizing new materials, and developing methods for hydrometallurgical extraction of useful components from natural raw materials or from industrial waste products, including technologies for utilization of marine chemical resources.

Prof. Balarew is an active IUPAC participant, and has been since 1979, mostly in the Analytical Chemistry Division. In 1999 he has been President of the National Committee of Chemistry of Bulgaria for IUPAC. Prof.

Balarew is coauthor of many publications in the field of Pure and Applied Chemistry. He was Chair of the 10th ISSP International Symposium on Solubility Phenomena, Varna, 22-26 July 2002. He is a member of the Editorial Boards of many IUPAC - Solubility Data Series Volumes since 1989.

In memoriam: Nikola Kallay (1942-2015)

n 20 April 2015, Professor Nikola Kallay passed away in his sleep, leaving a huge gap in his family, among his friends and colleagues, and in the chemical community as a whole.

He was a Titular Member of Commission I.1 from 1977 to 1985, Associate Member until 1989, and initiator of the project on the revision of the *IUPAC Green Book* which lead to its first edition in 1988, second edition in 1993, and third edition in 2007. Those of us who worked with him will remember the many discussions and fierce arguments we had as well as the charm with which he introduced "jokers" for each one of us, writing the text by which a particular formulation could be passed even if we were unable to reach a unanimous agreement on it.



The Working Party on the revision of the Green Book in Dubrovnik, Croatia, March 1986: from left Tom Cvitaš, Klaus Homann, Ian Mills, Kozo Kuchitsu and Niki Kallay.

Proiect Place

Storing Energy: with special reference to renewable energy sources

The intermittent nature of many renewable energy sources (such as wind, solar, tides or rainfall) makes it difficult to take full advantage of the potential of these sustainable and renewable forms of energy. The collection of chapters making up this book project shows the many ways and means of solving this problem by storing the energy. Written by international experts, the 26 chapters will present the latest developments in this fast moving field of energy storage. Most of the energy storing processes currently being researched or commercially developed are discussed, giving the reader the opportunity to compare the different processes and to decide which process is best suited for their resources, be it abundant sunshine, wind, tides, rivers, or mountain reservoirs, and whether it is for grid or even off-grid energy storage.

The book will be divided into 5 sections:

- 1. An Introduction on The Need of Energy Storage
- 2. Electrical Energy Storage Techniques (including mechanical/thermo-mechanical and gravitational; liquid air; compressed air; pumped hydro with compressed air; and advanced rail energy storage)
 - 2.1. Electrical (including batteries of all kinds; and super-capacitors)
 - 2.2. Thermal (phase changing materials; solar ponds; and sensible thermal energy storage)
 - 2.3. Chemical (hydrogen from water electrolysis; chemical reactions-zeolites/water/inorganic oxides; power to gas; traditional energy storage; large scale hydrogen storage caverns)
- 3. Emerging Concepts (superconducting magnetic storage)
- 4. Integration (grid and off-grid energy storage)
- 5. International Issues (Energy in China and the politics of introducing sustainable energy systems)

The options for gas (hydrogen or methane or air) storage (by Fritz Crotogino).



This book project came out of discussions linked to a previous book (www.iupac.org/project/2012-041-1-100) Future Energy, Second edition: Improved, Sustainable and Clean Options for our Planet, published in 2014.

For further information, contact the Task Group Chair Trevor Letcher <trevor@letcher.eclipse.co.uk>

www.iupac.org/project/2015-006-1-100

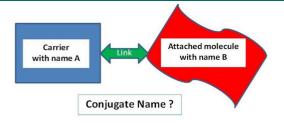
Nomenclature for polymeric carriers bearing chemical entities with specific activities and names

How to name a complex conjugate and allow easy identifications of the carrier, of the bound specific entity and of the link while respecting the established IUPAC rules as much as possible? This is the problem which this new project intends to solve.

In organic chemistry, the nomenclature allows the unequivocal drawing of the molecule structure. In polymer chemistry, the situation is more complex and one can use either the 'source-based' or the 'structure-based' systems of nomenclature to name a polymer. Source-based nomenclature leads to rather simple names, but it does not reflect the structure of the polymer it names. Information on the polymerization process is necessary to draw it. In contrast, structure-based nomenclature allows the drawing of the polymer structure directly from the name without requiring knowledge of the chemistry involved in the polymer formation. The strict rules of IUPAC organic nomenclature are adapted to the naming of the constitutional units of a polymer.

Recently, the members of the Subcommittee on Polymer Terminology (SPT) prepared a document for the "Nomenclature of Chemically Modified Polymers" (Pure Appl. Chem. 87(3), pp. 307-319 (2015)). This document revealed the need for a particular nomenclature system to deal with current, common structures of conjugates which combine macromolecular carriers and chemical entities.

The field of polymeric conjugates is rapidly growing. The development of conjugates depends on the collaboration of people from different disciplines and the name of a conjugate can be different depending on who generated it among the various specialists. The applications of conjugates require the permanent or temporary immobilization of complex chemical species chemically bound to a carrier that can be a macromolecule, a micelle, a microparticle, a nanoparticle, or a large solid support. These complex chemical species



are easily characterized and identified by functional names. In contrast, recognition and identification can be almost impossible if the strict structure-based naming of the conjugate is used, because both the carrier and the complex species are chemically modified. The binding function alters the names of the bound entity as well as that of the polymeric carrier. Sometime this binding function plays an important role, as in the case of specific chemical entities that are to be released by degradation under predefined physical or chemical conditions. In pharmacology, drugs or other bioactive species like peptides, proteins, polysaccharides, or polynucleotides are temporarily attached to polymeric systems for the purpose of being transported up to a targeted site in the human body and released there to exert their therapeutic action. In some applications, conjugates involve molecules with other specific activities, like dyes or radioactive labels, ligands to target receptors present in cell membranes, solubilizing species, stimuli-sensitive entities to make smart systems, or pesticides and insecticides for treatments in agriculture, etc. Some of the carriers of the bound entities can be so complex that they are named using letters like FGFs and VEGF growth factors, albumin and fibrinogen proteins, DNA, siRNA, etc.

IUPAC recommendations for the structure and source-based nomenclatures of polymers have clear limitations when dealing with complex conjugates. This new project aims to create rules that will allow unambiguous and facile naming of such modern complex conjugates together with easy recognition of the moieties introduced to take advantage of their specific activity.

The project is focused on macromolecules (organic or inorganic) suitable for attachment of (or to) complex chemical entities, including small molecules, macromolecules and biopolymers known and named in relation to their utility. However, the recommendations will be applicable to other kinds of carriers (small organic molecule to make prodrugs, inorganic supports, surface and porous systems, etc.) provided they bear identified chemical functions suitable for attachment.

For further information, contact the Task Group Chair Michel Vert <michel.vert@univ-montp1.fr> www.iupac.org/project/2014-034-2-400

Measurement of Photoluminescence Quantum Yields

Quantum yield (QY) is one of the most important quantitative properties of a luminescent sample and robust ways to measure it are essential in the application of luminescence techniques. In this project, the task group will perform an inter-laboratory comparison of the two main methods for QY measurements, the classical relative method based on standards, and the absolute method using integrating spheres which has recently gained popularity.

A previous IUPAC project (www.iupac.org/project/2004-021-1-300; see *Pure Appl. Chem.* 2011, 83, 2213-2228) has clearly shown a shortage of standards for relative QY measurements of solutions. Recently, absolute measurements have become more popular as a result of the wider availability of integrating sphere equipment, but their reliability is still to be established.

Further standards are needed to fully cover the wavelength range of interest, from ~250 to ~1000 nm. Preferred reference compounds have broad and featureless absorption spectra and have proven emission quantum yields independent of the excitation wavelength. The reference values should preferably be those of air-equilibrated samples. The second purpose of the project is to establish the variability of independent QY measurements in different laboratories. Therefore ten laboratories world-wide have been invited to take part in this test. The laboratories are well-equipped and experienced, but are not specialists or method developers in the field. We are interested in find out what is the current practice in a normal good laboratory.

Twenty-two samples have been selected in the first stage of the project. For eight of these samples, the quantum yields are considered very well established. The other samples have been measured against these eight standards, or were measured using integrating spheres. The results of the measurements are currently being collected.

The outcomes of this new project will provide insight into the reproducibility and inter-laboratory variability of QY measurements using the two methods and detail an extended set of standards and protocols for QY measurement.

For further information, contact the Task Group Chair Fred Brouwer <a.m.brouwer@uva.nl>

www.iupac.org/project/2013-040-1-300

Young Ambassadors for Chemistry (YAC) achievements in Thailand and Cambodia

by Lida Schoen and Mei-Hung Chiu

In November 2014, all our YAC dreams came true in Bangkok and Phnom Penh, where, following the initiative of Datuk Dr. Ting Kueh Soon (Institut Kemia Malaysia, and former President of the Federation of Asian Chemical Societies), we were able to hold the 39th and 40th Young Ambassadors of Chemistry (YAC) events.

For those unfamiliar with YAC, it is a project that trains teachers around the globe to help students communicate the benefits of chemistry. A typical YAC event encompasses two to three days of teacher workshops, followed by a one-day, public event where students—the Young Ambassadors for Chemistry—share their enthusiasm and interest with the public at large, either in a public square or as part of a science festival. That last day of the YAC event is usually a festive time and fun for everyone involved.

During YAC's lifetime, we have organized 40 events, both small and large, in 29 different countries. Thailand and Cambodia represent events number 39 and 40. Since 2004, 14 YAC events were facilitated by two projects supported by IUPAC and its Committee on Chemistry Education (CCE project 2007-005-2-050 and 2003-055-1-050), while 26 further events were supported by other organizations (Science Across the World programme, British Council, Life Long Learning projects of the European Union, National Chemistry Associations and National Science Foundations).

Train the trainers

During the course of each event, the YAC team aims to train the participating teachers (Thailand: 40, Cambodia: 36) to organize more YAC events with students after the YAC team has left.

We focus on the chemistry of local daily life products: their composition, production (techniques), and application in relationship to the curriculum. Although we all speak the universal language of chemistry, we try to avoid language problems with adapted methodology: teachers research the chemistry of a local product in a group of 4 to avoid language problems. They present drawings with their ideas and results. Teachers love this group work as they use their mobile phones to find information and discuss the results in the local language.

Next, we discuss how to organize this way of teaching and learning in classrooms with all local 'difficulties':

a strict curriculum, no time to prepare, and not all colleagues willing to change.



Teacher trainer Mr. Set Seng in Phnom Penh.

Augmented reality (AR)

Mei-Hung updates the participants on the possibilities of Augmented Reality (AR). As the number of smartphones and tablets dramatically increases across the world, the school science curriculum should embrace this new innovative technology for scaffolding students' learning of complicated chemistry concepts. In both countries participants were enthusiastic to use the app and to learn about the benefits of new technologies.

Practical work

During YAC training, we pay a lot of attention to the practical work the teachers will have to guide during the event. Teachers (and later the students) are asked to design, produce, and market an innovative local cosmetic line. They begin following instruction about possible pitfalls during the production and theories about suitable raw materials, such as polymers, detergents, oils, emulsifiers, colors, and perfumes. All necessary ingredients, packaging, and decoration materials needed for a TV promotion campaign are available. Teachers collaborate in groups of 4 and share the workload.

After 90 minutes hard work, each group presents their cosmetic lines in a 30 second TV spot. These spots show that teachers are a creative species, able to act, dance, and sing! Juries have a hard job choosing the winning groups after considering: (1) the outlook and quality of individual products, (2) cohesion in the line, (3) quality and originality of labels, and (4) originality of the TV commercials.

We end by reflecting on the expectations of the

Project Place



Prof. Boonnak Sukhummek in Bangkok.

participants that they wrote down at the start of the course. All teachers receive a certificate of attendance with the signature of the IUPAC President.

YAC event

On the last afternoon, the trained teachers guide the many students (70 in Bangkok, 50 expected, 120 in Phnom Penh, 50 expected), who love to participate in the YAC event. As the various roles are divided at the end of the training course, the teachers know exactly what to do, resulting in 'stations' for raw materials, colors and perfumes, packaging, and stationery.

In Thailand, the venue was an open space on the 1st floor of the Chamchuri Square Shopping Mall. In Cambodia, we worked in a covered open space in front of the Royal University of Phnom Penh, where soon three TV stations began recording the activities of 120 very enthusiastic students and 40 teachers!



All groups start designing and producing their innovative cosmetic lines by following instructions in the local language. Some students act as roving reporters. They ask the visiting public to fill in a questionnaire about their image of chemistry before and after other students in the group demonstrate their activities.

After the students finish their practical work, including their TV spot with accompanying promotion materials, we show the results to the audience. Most groups contain a number of great actors, so their performances generate great enthusiasm, as the audience cheers them on!

In Bangkok, two speakers, who were the best actors during their own presentations, did a great job warming up the audience.

The winning groups received presents from Taiwan and the Netherlands before a group picture with students and teachers was taken.







Media coverage

Dow Chemicals Thailand (cosponsor of YAC Thailand) helped to collect clippings of publicity around the 1st YAC Thailand. Between November 24 and December 29, 2014 Prof. Tantavanon received 17 clippings from 11 different media publications on paper, blogs, and websites with pictures, picture galleries, and a few videos, including an interview with Prof. Tantayanon.

YAC results in Taiwan

After YAC Cambodia we traveled to Taipei, YAC's place of birth in 2004. We visited a junior and a senior high school with teachers who took part in our first YAC course/event. In both classes we experienced dedicated teachers who apply many YAC ideas with their enthusiastic students, making. YAC activities sustainable events in those schools...

Evaluations: Positive public image of chemistry

Our roving student reporters managed to collect many completed questionnaires from the public: 85 in Thailand and 63 in Cambodia.

The audience during YAC events is most probably not representative of the general public. The image of chemistry is already quite positive (80% in Thailand, 75% in Cambodia), possibly because there are mainly relatives and friends of our enthusiastic teachers in the crowd.

The public in Thailand and Cambodia consider chemistry important in their daily life. They mention preparation and preservation of food, vitamins, medicines, and drinking water. The main channels of knowledge about chemistry are the internet and TV, with newspapers and radio occasionally mentioned. 30% think they would know more about chemistry if they could have done activities like the students experience through YAC! The public in both countries highly values this activity, and they also often mention the relation of chemistry to other subjects in daily life, such as art and marketing. Guiding people about the role of chemistry in daily life seems to be strengthened in school instruction

The general opinion is that the YAC event helps students understand chemistry, how to use it and how to connect theory and practice. It shows that chemical substances and products are useful. The presentations of the students' work are also appreciated as very cre-

Our questionnaire is about the image of chemistry:

Which one of the following pictures shows best what you think about chemistry? Number the pictures in your order of preference, with 1 under the picture that reminds you most of chemistry and a 5 under the picthat reminds you least of chemistry.



Results in Thailand and Cambodia show simlar results to those shown below the pictures, with luckily the picture showing blowing gases or an explosion least preferred. Participating students in Thailand and Cambodia choose more or less the same order of preference—they all prefer working alone like in the 3rd picture above!

Gap between school learning and contextualized learning

Students provide promising feedback to the YAC events. They write down their favorite new knowledge about products present or useful in daily life and ways to acquire new knowledge. They love to collaborate with other students. Last but not least, a lot of fun is often mentioned: 'I want have this event to be continued. Please often organize this event.'

Feedback from the teachers show the same picture: a lot of new knowledge and new skills learned, and exciting possibilities to teach students exciting chemistry related to their daily lives, e.g. the chance to use local herbs and extract local dyes.

Communication skills enhanced

Many teachers also mention improving their skills in communication, presentation, and using the internet. The teachers appreciate learning about international science projects and how to join and exchange experiments with students in other countries/cultures: 'Our new skills are not only important to chemistry teachers, but to all students and teachers in other subjects'.



New (Young) Ambassadors for Chemistry

A few teachers mentioned plans to study how to be an ambassador for chemistry and to acquire or share information related to our daily life and

how to persuade students who have the wrong image of chemistry.

Project Place

In Thailand a few language teachers also took part. They were positive about the course. As teaching and promoting chemistry concerns content and communication, they can be our best ambassadors!

Local organizers

All recommendations to local organizers and the YAC team are very clear: more frequent, longer courses with more practical work related to students' daily lives. Other recommendations are to include more examples of simple hands-on activities and new ways to teach. A longer course can offer more time to reflect, more time to train the teachers and develop activities, and more opportunities to practice English with the trainers.

Prof. Tantayanon will introduce the Thai report to the national meeting of Chemistry Department Heads and discuss possibilities for more YAC events. She will present the results of our evaluations with the public, the participating students (during the YAC event) and with the teachers (during the YAC event and the 1.5 day YAC course). Prof. Tantayanon managed to obtain substantial financial support for the course and event from Dow Chemical Thailand.

Dr. Huy Sieng will publish the Cambodian report in Cambodian Chemical Society' annual bulletin. The CCS staff will continue to share this knowledge with other teachers in the provinces through the CCS' training programme. She would like IUPAC, CCE to provide Cambodia with more practical work and handouts, as well as with materials and chemical substances. Moreover, she would like IUPAC, CCE to organize more (YAC) events for students, because Cambodia lacks laboratory equipment and chemicals for students' lab work.

Acknowledgments

- IUPAC for facilitating travel expenses of Mei-Hung Chiu and Lida Schoen;
- Barentz Pharma & Cosmetics, the Netherlands for donating the Chinese emulsifier Tinci (Guangzhou Tinci Materials Technology Co., Ltd.

- (www.tinci.com);
- Sasol Germany for donating the detergent for the shampoo (www.sasolgermany.de);
- Florale Haircare Group for donating professional 'cream' jars (www.floralehaircare.com).

Thailand

- Department of Chemistry, Chulalongkorn University, Bangkok for facilitating and organizing the YAC course and event;
- Chemical Society of Thailand (CST) for facilitating the YAC course and renting the venue;
- Dow Chemical Thailand for overall financial support;
- National Science Museum (NSM) for providing the training room;
- Prof. Tantayanon and her staff for perfect organization, Prof Sairoong Saowsupa for translation and analysis of the questionnaires.

Cambodia

- Royal Academy of Cambodia (RAC) and the Cambodian Chemical Society (CCS, H.E. Dr. Neth Barom, Chairman of CCS's board of directors) for facilitating and financing;
- Royal University of Phnom Penh (RUPP) for providing the venue;
- Provincial Department of Education, Youth and Sports, RAC and CCS for financial support;
- Dr. Huy Sieng and CCS's Executive Committee, including Dr. Sotha Chek for organization and Sotha also for translation and analysis of the questionnaires.

Special thanks to many helpers for corrections and translations from Thai/Khmer on the questionnaires, and Phana Cheng (Cambodia), for additional photos.

For more information and for links to recent YAC accounts online or in CI, see www.iupac.org/project/2007-005-2-050



All officials, organisers and participants in the National Science Museum in Bangkok.

Making an imPACt

Latest Updates from PAC Conferences

by Hugh D. Burrows, Scientific Editor, Pure and Applied Chemistry

In this section of CI, we keep you up to date on what is happening in Pure and Applied Chemistry (PAC). PAC is the official journal of IUPAC, and publishes IUPAC Technical Reports and Recommendations together with articles arising from IUPAC-endorsed conferences. Occasionally we also publish special issues containing selected, peer reviewed articles by experts in the field and concentrating on topics of current interest and relevance. As Scientific Editor, I look after the Conferences and special topics side, while Ron D. Weir and

Jürgen Stohner, respectively chair and secretary of the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS), are responsible for the publication of IUPAC Technical Reports and Recommendations.

The June and July 2015 PAC issues (issues 6 and 7) featured papers from the XXVth IUPAC Symposium in Photochemistry, which was organised by Dario M. Bassani in Bordeaux, France from 13-18 July 2014. This marks the 50th anniversary of a highly successful series of conferences. To celebrate, an article

by Silvia Braslavsky traced the history and evolution of these meetings from their start under the direction of George S. Hammond in Strasbourg, France, in 1964 (PAC 87(7), pp. 663-705). (A Brief History was published earlier in *Chem Int.* March 2014, pp. 12-13)

Nathan D. McClclenaghan (Université Bordeaux) was Conference Editor for these PAC issues, which contained the Porter Medal-winning prize lecture from Masahiro Irie on the discovery and development of photochromic diarylethenes, together with papers on topics as diverse as mechanistic photochemistry in photochemically induced radical reactions with furanones (Michael Oelgemöller and Norbert Hoffmann), singlet oxygen reactions with natural polyunsaturated substrates (Axel G. Griesbeck et al.), and artificial photosynthesis (Giuseppina La Gnnga and Fausto Puntoriero). In keeping with the interests of the organizers, papers were presented on azobenzene-based photochromism and its application in supramolecular devices from the groups of Jiro Abe and Alberto Credi. A detailed discussion was given by Chihaya Adachi et al. on how thermally activated delayed fluorescence

is leading to the development of highly efficient electroluminescent materials with potential applications in the third generation of organic light-emitting diodes (OLEDs).

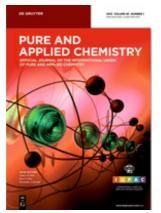
Other topics covered in these issues are novel push-pull fluorophores (William G. Skene), how ultrafast spectroscopy is challenging new empirical rules in molecular photophysics (Majed Chergui), enhanced light energy conversion using plasmons in gold nanostructured titanium dioxide semiconductor photoelectrodes (Hiroaki Misawa), and the use of titanium dioxide-based heterogeneous photocatalysis to remove heavy metals and arsenic from water (Marta I. Litter). These papers provide a fitting celebration to an excellent anniversary meeting.

> The August issue of PAC features articles based on Keynote lectures in the 2nd International Conference on Bioinspired and Biobased Chemistry & Materials. This has the acronym N.I.C.E. meaning "Nature Inspires Chemistry Engineers", and was organized by Frédéric Guittard with the assistance of Elena Celia and Jeanne Tarrade, in Nice, France, from 15 to 17 October 2014. The goal of this series is to share ideas in the growing fields of bioinspired chemistry and materials, to see how nature has developed solutions for many current

problems, and to envisage solutions for a sustainable future. Problems tackled include optimization of resources, energy efficiency, transport, and water and waste treatment.

The topics covered range from mimicking calcite-based functional material of the human body (Rüdiger Kniep) through a bioinspired approach to produce conducting polymer-based systems with parahydrophobic properties (Frédéric Guittard et al.) to using the inspiration of the structure of butterfly wings to produce porous carbon electrodes with ridge/pore array hierarchical architecture (Tongxiang Fan et al.). The new field of biofabrication uses 3D printing technologies with high spatial resolution for processing both cells and biomaterials into constructs suitable for tissue engineering. A comprehensive review is provided by the group of Thomas Scheibel, which includes a demonstration of how spider silk can be used as a cytocompatible and printable bioink.

Polymeric materials are discussed in articles from the groups of Shchipunov on self-organized chitosan bionanocomposites, and of Runguo Wang and Liqun



Zhang on biobased elastomers with tunable damping properties. Interfacial control is important for immobilising biomolecules onto nanostructured materials for various applications. Mikhael Bechelany and coworkers show how atomic layer deposition can be applied to this problem. Interfaces are also involved in the study by Kock-Lee Law, who presents a detailed discussion on water-surface interactions and considers the important practical problem of how the terms hydrophilicity, hydrophobicity, and superhydrophobicity can be defined in such cases.

Bioisnpired materials are also relevant to energy and electronic. Marsella, Berand, Vullev and coworkers report a molecular level approach for bioinspired electrets based on β -aminoacids. The electronic properties of these can be tuned by appropriate chemical substitution.

Finally, Yves Queneau and co-workers show how glucosyloxymethylfurfural, which is readily obtained from natural sources, can act as an excellent scaffold for developing molecular architectures based on carbohydrates, including some fairly elaborate targets.

The area of bioinspired chemistry is rapidly developing, and we look forward to publishing articles from future editions of this interesting series of Conferences.

www.degruyter.com/pac

Brief guide to the nomenclature of inorganic chemistry

Richard M. Hartshorn, et al

Pure and Applied Chemistry, ahead of print, online 29 July 2015

This IUPAC Technical Report is one of a series that seeks to distill the essentials of IUPAC nomenclature recommendations. The present report provides a succinct summary of Nomenclature of Inorganic Chemistry – IUPAC Recommendations 2005.

The content of this report is republished and disseminated as a four-sided lift-out document (see insert to this *CI* issue) and is available for inclusion in text-books and similar publications.

http://dx.doi.org/10.1515/pac-2014-0718

IUPAC Glossary of terms used in neurotoxicology (IUPAC Recommendations 2015)

Douglas M. Templeton, Michael Schwenk, and John H. Duffus

Pure and Applied Chemistry, 2015 Volume 87, Issue 8, pp. 841-927

A major goal of IUPAC is to promote "regulation, standardization, or codification" globally in relevant areas of chemistry. To this end, the Division of Chemistry and Human Health (Division VII), recognizing the importance of toxicology to chemists, produced the Glossary of Terms Used in Toxicology, 2nd ed., in 2007 [PAC 79, 1153 (2007)]. That glossary was intended to provide clear and concise definitions for a range of terms in toxicology and toxicokinetics, primarily for chemists who find themselves working in toxicology or requiring a working knowledge of the subject. It was also recognized that other scientists, regulators, and managers must from time to time interpret toxicological information, and it was hoped that the Glossary would also provide them with ready access to internationally accepted definitions of relevant terms. A number of subspecialties have broadened the scope of toxicology; in 2009 the Division expanded the collection of available definitions with publication of a Glossary of Terms Used in Ecotoxicology [PAC 81, 829 (2009)], and again in 2012 with a Glossary of Terms Used in Immunotoxicology [PAC 84, 1113 (2012)].

In the years since publication of the 2nd edition of the general glossary, we have recognized that a number of the terms continue to evolve and definitions need periodic refinement. It is also apparent that now a searchable, electronic database updating and combining entries from the previous glossaries is desirable, and achievable. A project to achieve this is underway, but at its inception we realized that some areas of toxicology had been under-represented, and addressing this deficit would enhance the usefulness of the database. One area felt to be under-represented was neurotoxicology, and the present document is an attempt to address this deficit.

The primary objective of this Glossary of Terms Used in Neurotoxicology is to give clear definitions for those who contribute to studies relevant to neurotoxicology, or must interpret them, but are not themselves neurotoxicologists, neuroscientists or physicians. This applies especially to chemists who need to understand

Making an imPACt

the literature of neurotoxic effects of substances without recourse to a multiplicity of other glossaries or dictionaries. The Glossary includes terms related to basic and clinical neurology insofar as they are necessary for a self-contained document, and particularly terms related to diagnosing, measuring, and understanding effects of substances on the central and peripheral nervous systems. The glossary consists of about 800 terms as primary alphabetical entries, and includes Annexes of common abbreviations, and examples of chemicals with known effects on the nervous system. Intended to stand alone as an IUPAC Recommendation

in the narrower field, it is also destined for integration into the revised, online Glossary of Terms Used in Toxicology, currently under construction.

The authors hope that among the groups who will find this glossary helpful, in addition to chemists, are toxicologists, pharmacologists, medical practitioners, risk assessors, and regulatory authorities. In particular, it should facilitate the worldwide use of chemistry in relation to occupational and environmental risk assessment.

http://dx.doi.org/10.1515/pac-2015-0103

IUPAC Provisional Recommendations

Provisional Recommendations are drafts of IUPAC recommendations on terminology, nomenclature, and symbols, made widely available to allow interested parties to comment before the recommendations are finally revised and published in IUPAC's journal *Pure and Applied Chemistry*. Full text is available online.

Source-Based Nomenclature for Single-Strand Homopolymers and Copolymers

IUPAC recommendations on source-based nomenclature for single-strand polymers have so far addressed its application mainly to copolymers, non-linear polymers and polymer assemblies, and within generic source-based nomenclature of polymers. In this document, rules are formulated for devising a satisfactory source-based name for a polymer, whether homopolymer or copolymer, which are as clear and rigorous as possible. Thus, the source-based system for naming polymers is presented in a totality that serves as a user-friendly alternative to the structure-based system of polymer nomenclature. In addition, because of their widespread and established use, recommendations for the use of traditional names of polymers are also elaborated.

Comments by 31 December 2015

Corresponding author: Richard G. Jones kapitimana@gmail.com www.iupac.org/project/2003-042-1-800

Glossary of Terms Used in Extraction

Approaches for analytical-scale extraction are developing rapidly as new strategies are implemented to improve sample throughput and to minimize material use in laboratory methods and to develop on-site capabilities. In this contribution, definitions and recommendation for symbols for the terms used in analytical extractions are presented. Exhaustive, microextraction, elevated temperature, microwave- and ultrasound-assisted, parallel batch, flow through systems, and membrane extraction approaches are discussed. An associated tutorial titled "Extraction" provides a detailed introduction to the topic.

Comments by 31 January 2016

Corresponding author: Janusz Pawliszyn <janusz@uwaterloo.ca> www.iupac.org/project/2011-063-1-500

Bookworm



Macoumolecoder Symposia 149 Ionic Polymerization, Tomic Polymerization Part | & ||

Macromolecular Symposia Vol. 349 and 350, March and April 2015

Editor: Tatsuki Kitayama, Sadahito Aoshima, and Masami Kamigaito

The Ionic Polymerization series of symposia have roots in the individually-held international symposia on cationic, anionic, and ring-opening polymerizations. In 1992, the European Polymer Federation Workshop on "Anionic Polymerization and Related Processes" was held in Mainz, Germany. Leading experts who attended the workshop recognized the closer relationship and interplay among these polymerization processes in view of precise control of polymer structures and macromolecular architectures. They prepared and distributed a circular letter through the international community to ask for opinions on the merger of these symposia. The decision to merge was made during the 11th International Symposium on Cationic Polymerization and Related Processes, held in Borovetz, Bulgaria, in 1993. The first "International Symposium on Ionic Polymerization" was held in Istanbul, Turkey, in 1995. Otto Vogl, a member of the International Advisory Committee of IP2013 who passed away on April 27, 2013, and Yusuf Yagci, the chair of the first IP, published the first conference report with a brief description of the history of the symposia [1]. After Istanbul, the IP series symposia have been held around the world in the following sequence:

Istanbul, Turkey (1995) \rightarrow Paris, France (1997) \rightarrow Kyoto, Japan (1999) \rightarrow Crete, Greece (2001) \rightarrow Boston, USA (2003) \rightarrow Goa, India (2005) \rightarrow Kloster Banz, Germany (2007) \rightarrow Krakow, Poland (2009) \rightarrow Akron, USA (2011) \rightarrow Awaji, Japan (2013)

The latest International Symposium on Ionic Polymerization (IP2013) was held in Awaji Island, Japan, 23-28 September 2013. The scientific program of IP2013 consisted of 49 invited, 9 contributed oral, 20 short oral (for young researchers), and 70 poster presentations, which addressed contemporary research, both fundamental and applied, in the areas of anionic, cationic, and ring-opening polymerizations, as well as other techniques of living/controlled polymerizations. The program also incorporated papers on the analysis of polymeric materials. The quality of the posters was evaluated by an international

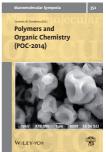
task group (6 foreign and 3 Japanese professors). The task group awarded three IUPAC Poster Awards as well as three RSC Polymer Chemistry Poster Awards.

The steering committee, attended by 19 members, approved the next IP meeting, to be held in Bordeaux, France (see http://ip15.sciencesconf.org).

Among the 49 invited speakers, 6 were from industry, while 3 of the 9 contributed orals were from industry. These numbers are relatively large in this series of symposia, and reflect the high standard of the Japanese polymer industry. The topics from industry are also wide-spread, covering anionic synthesis of acrylic block copolymers, practical applications of controlled/living radical polymerizations, and ring-opening polymerizations.

1. Polymer News, 1996, 21, 352-359; *Prog. Polym. Sci.*, 1997, 22, 1381-1395.

www.ms-journal.de



Polymers and Organic Chemistry

Macromolecular Symposia Vol. 352, June 2015 Symposium Editor: Corneliu-Mircea Davidescu

The IUPAC-sponsored conference

on Polymers and Organic Chemistry, POC-2014, took place in Timisoara, Romania, 10-13 June 2014. The conference was organized by Politehnica University Timisoara with the support of the Timisoara Branch of the Romanian Society of Chemistry (SChR) and the Institute of Chemistry Timisoara of the Romanian Academy.

The conference was the 15th scientific event sponsored by IUPAC in a series that has continued the tradition of biannual meetings travelling from one continent to another since the 1st edition held in 1982 in Lyon, France. These meetings aim to present, discuss, and share recent results in the fields of polymer and organic chemistry, and in the synthesis and applications of polymers, in order to promote their importance in science and technology. The last editions of POC were held in:

Tianjin, China (9th Ed. 2000) → San Diego, USA (10th Ed. 2002) → Prague, Czech Republic (11th Ed. 2004)

→ Okazaki, Japan (12th Ed. 2006) → Montreal, Canada (13th Ed. 2009) → Doha, Qatar (14th Ed. 2012)

POC-2014 was recognized as a very successful scientific event, and was attended by over 100 registered participants from 28 countries (Austria, Canada, Chile, China, Czech Republic, Egypt, France, Germany, Greece, Hungary, Iran, Israel, Italy, Japan, Mexico, Poland, Portugal, Qatar, Romania, Switzerland, Russia, Serbia, Spain, The Netherlands, Turkey, Ukraine and USA), located on 5 continents (Africa, Asia, Europe, North America, South America).

The conference presentations focused on 6 topics: advances in polymer synthesis; novel functional polymers; biocatalysis in polymer synthesis; polymers for catalysis and energy applications; polymers for separations and environmental protection; and polymers in medicine, biochemistry and agriculture. The main conference presentations were offered by 2 Keynote Speakers: Dr. Bogdan C. Simionescu, Department of Natural and Synthetic Polymers, Institute of Macromolecular Chemistry, Iasi, Romania, lectured on "Polymer engineering focusing on drug/gene delivery and tissue engineering: from simple towards complex architectures and hybrid materials"; and Dr. Ghislain David, Institut Charles Gerhardt, Ecole Nationale Superieure de Chimie de Montpellier, France, which lectured on "Phosphorus-containing polymers: New trends". Additionally, the conference featured 12 Plenary Invited Lectures delivered by prominent scientists from different countries, as well as 28 Oral Presentations. Two Poster Sessions, with 63 presentations, showcased the latest results obtained by younger scientists.

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Macromolecular Complexes

Macromolecular Symposia Vol. 351, May 2015 Symposium Editor: Anthony Guiseppi-Elie

These proceedings are intended for scientists, engineers, and other technical personnel who seek a current assessment of the state of the science and technological opportunities presented by the rapidly growing field of macromolecular complexes.

The book is the result of technical contributions to the 15th International Symposium on MacroMolecular Complexes (MMC-15) endorsed by IUPAC.

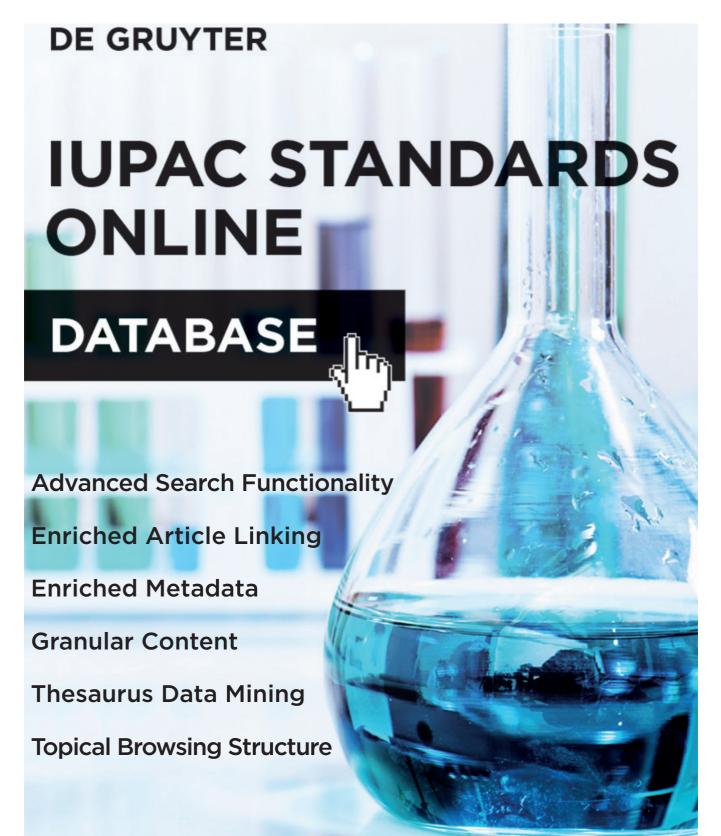
Under the chairmanship of Prof. Dr. Anthony Guiseppi-Elie and organized by faculty and students of the Center for Bioelectronics, Biosensors and Biochips at Clemson University's Advanced Materials Research Center, MMC-15 was held on 13-16 August 2013 in Greenville, South Carolina and on the campus of Clemson University in Clemson, South Carolina, USA.

The keynote address was delivered by Prof. Cato T. Laurencin (University of Connecticut, USA), while seven plenary addresses were delivered by Prof. Gero Decher (Strasbourg, France), Prof. Joseph M. DeSimone (University of North Carolina, USA), Prof. Sabine Flitsch (The University of Manchester, UK), Prof. Kazuhiko Ishihara (Tokyo University, Japan), Dr. Mkhulu Mathe (CSIR, South Africa), Prof. Hiroyuki Nishide (Waseda University, Japan), and Prof. Eduardo Pereira (University of Concepcion, Chile).

Thematically, the book is organized according to the topical conferences of the symposium. The themes for MMC-15 were Energy Harvesting and Energy Industry, Sustainability and Green Chemistry, Biotechnology and Biomedicine, and Global Health. These are pressingly important areas where macromolecules play a vital role in transforming technology for the betterment of human kind. Among the topics addressed were: in the area of energy-superior polyelectrolyte membranes for fuel cells and polymers for low-cost high emissive light emitting diodes (OLEDs); in the area of sustainability and green chemistry—polymers for biodegradable packaging and monomers and polymers from biomass sources; in the area of biotechnology and biomedicine—bioactive hydrogels and supramolecular polymer assemblies for targeted drug delivery; and in the area of global health-polymer fibers for controlled flow in low-cost lateral-flow diagnostic devices and polymer membranes for desalination. Conference sponsors were BIODOT, Milliken, ACS Poly, ACS PMSE, Wiley, ABTECH Scientific, Inc., Clemson Bioengineering, Milliken, Western Carolina Section of the ACS, Michelin USA, and Clemson Chemical and Biomolecular Engineering.

MMC-16 will be held at Wrocław University of Technology (WUT), Poland, 10-14 August 2015, under the chairmanship of Prof. Andrzej W. Trochimczuk.

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INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Conference Call

POLYCHAR 23 World Forum Advanced Materials

by Michael Hess

The 23rd World Forum on Advanced Materials (POLY-CHAR) (derived from Polymer Characterization) returned to the United States for the first time since 2003, when this Conference began changing venues annually. Previously, it had been hosted by the University of North Texas for the 11 years from its founding in 1992 by Witold Brostow, Michael Hess, and Kevin Menard. In the year 2015 POLYCHAR was hosted by the University of Nebraska, Lincoln (UNL), USA, and organized by a local organization committee (the Department of Mechanical & Materials Engineering and the College of Engineering) and an international organization committee with members from Belgium, France, South Korea, and Nepal, chaired by Prof. Mehrdad Neghaban (UNL). The conference was supported by IUPAC, the IUPAC Polymer Division (Samsung Fund), the American National Science Foundation, the University of Lincoln (UNL), the Office for Research and Educational Development (UNL), the College of Engineering (UNL), the Department of Mechanical & Materials Engineering (UNL), the City of Lincoln Convention and Visitors Bureau, and the John A. Woollam Company.

Previous conferences have been held in Denton, Texas; Guimaraes, Portugal (2004); Singapore (2005); Nara, Japan (2006); Buzios, Brazil (2007); Lucknow, India (2008); Rouen, France (2009); Siegen, Germany (2010); Kathmandu, Nepal (2011); Dubrovnik, Croatia (2012); Gwangju, South Korea (2013); and Stellenbosch, South Africa (2014).

In 2015, there were six Plenary Lectures (two Young Scientists Plenaries), the Flory Medal Talk, and 13 individual Sessions in two parallel events:

- Characterization Methods and Structure-Properties Relations (15 contributions) Keynote: Jean-Michel Guenet (France), Characterization and Properties of Hybrid Materials from Polymers and Self-Assembled Systems
- Predictive Methods, Modelling and Simulation (11) Keynote: Jean-Marc Saiter (France), Physical Aging and Cooperative Relaxation in Glassy Polymers
- Biomaterials, Drug Delivery and Tissue Engineering Materials - Green Polymers, Green Engineering and Recycling (11) Keynote: Valerio Causin (Italy), Nanocellulose-Reinforced Gels for Biomedical Applications; Victor Castano (México), Advanced

Natural Materials: From Rice Husk to Aerospace Systems

- Fibers, Interfaces and Composite (6)
- Nanomaterials and Smart Materials (10) Keynote: Yuri Dzenis (USA), Simultaneous Strong and Tough Continuous Polymer Nanofibres and Nanocomposites
- Dielectric-, Electrical-, Magnetic-, Optical- and Optoelectronic Properties (8)
- Polymers in Electronics and Optoelectronic Devices (5)
- Progress in Polymer Synthesis (5) Keynote: Daniel Grande (France), Design, Synthesis, and Characterization of Functional Doubly Porous Crosslinked Polymers; Betty López (Colombia), A New Method to Modify Poly(arylene ethers) with a Mild Sulfonating Agent
- Characterization with Scanning Probe Microscopy (4) Keynote: Dalia Yablon (USA), Advances in Atomic Force Microscopy Based Methods to Characterize Polymer Materials on the Nanoscale
- Rheology, Solutions and Processing Mechanical Properties and Performance (5)
- Processing and and Properties of Semicrystalline Polymers (6) Keynote: Jean-Marc Lefebvre (France), In-Situ SAXS/WAXS Investigation on Deformation Induced Structural Evolutions in Amorphous and Semi-Crystalline Polymers; Andrezej Galeski (Poland), Crystallization and Melting Phenomena in Nanofibers Reinforced Polymer Nanocomposites

These Sessions included 87 oral contributions (including 10 keynote speakers and 14 invited speakers), and 45 Posters in one session, with 103 registered participants (including 42 students) from 21 countries and 5 continents. In addition to the US, there were participants from France, Belgium, Nepal, Singapore, Poland, South Korea, Germany, Japan, China, Malaysia, Austria, Portugal, Canada, India, Georgia, Colombia, China (Taiwan). Mexico, and Ireland.

As indicated by the list of Sessions above, the topics were broadly distributed, with a focus on Characterization & Structure-Properties, Bio-related Materials/Applications, and Smart Materials.

The six Plenary Speakers were:

Gila Stein (Young Scientsts' Plenary), University of Houston, USA: Grazing Incidence Small-Angle X-Ray Scattering: Principles, Models, and Application for Nanostructured Thin Films

Abby Whittington (Young Scientsts' Plenary), Virginia

Tech: Polymer Characterization of Medical Devices for Use in Cancer Patients

Harald Ade, North Carolina State University, USA: Soft X-Ray Characterization Methods: Utility and Opportunity Stephen Cheng, University of Akron: Giant Polyhedra and Giant Surfactants Based on Nano-Atoms: Tuning from Crystals, to Quasicrystals, to Frank-Casper Phases: An Interconnection Between Soft and Hard Matter

Richard Laine, University of Michigan, USA: *Synthesis, Processing and Properties of Silesquioxane Macromonomers and Polymers*

Rachel Seligman, University of California, Santa Barbara: *Using Bioinspired Polymers to Explore the Role of Sequence on Controlling Polymer Properties*

There was an additional talk on Recent Developments in the IUPAC Polymer Division by Michael Hess, informing participants about the general work and the educational aspects of the work of the Division. The full program can be found at: http://polychar23.unl.edu/downloads/Sessions_Program.pdf

The Short Course consisted of nine contributions (each including a 50 min + discussion):

- Dynamic-Mechanical Analysis (Michael Hess, University of North Texas, USA)
- Rheology & Processing (Dirk Schubert, University Nuermberg-Erlangen, Germany)
- Characterization of Polymeric Nanostructures with Combined Scanning Probe and Fluorescent Microscopy (Holger Schoenherr, University Siegen, Germany)
- Glasstransition and Glasstransition Temperature (Jean-Marc Saiter, Universite de Rouen, France)
- Micromechanics of Polymers: Micro- and Nanoscopic Processes of Deformation and Fracture (Sven Henning, Fraunhofer Institute for Mechanics of Materials, Halle, Germany)
- Solid State NMR (Bernhard Bluemich, University Aachen RWTH, Germany)
- Basics of Scattering Techniques: X-Ray, Neutron, Light (Jean-Michel Guenet, Institute Charles Sadron and Universite Strasbourg, France)
- Photochemistry in Polymer Science (Brett Fors, Cornell University, USA)
- Friction, Wear and Scratch Resistance of Polymers (Natalie Hnatchuk, University of North Texas, USA)

Short Course lecturers were available for further

discussion throughout the Conference. There were about 47 Short Course participants—mostly, but not exclusively, students.

The Conference was opened by the Conference Chair, Mehrdad Neghaban (UNL), followed by welcome addresses by the Vice-Chancellor for Research & Economic Develoment at UNL, Prem Paul; the Chair of the Department of Mechanics & Materials Engineering, Jeff Shield; the Dean of the College of Engineering, Tim Wei; and Michael Hess, IUPAC Polymer Division (University of North Texas).



The prestigious Paul J. Flory Research Prize 2015 went to **Kohji Tashiro**, Toyota Technological Institute, Japan, for his Clarification of Microscopically-Viewed Structure-Property Relationship of Polymer Materials.

The International Materials Research Prize was given (ex aequo) to Valerio Causin, University of Padua, Italy, for his contribution to the structural and morphological characterization of materials by small-angle X-ray scattering, wide-angle X-ray dif fraction, thermal analysis, optical and electronic microscopy, and his contribution to polymer analysis in forensics; and to Victor Castano, Universidad Nacional Autónoma de México, México City México. Victor Castano founded the Center of Applied Physics





and Advanced Technology of the National University of Mexico and created a number of new materials for diverse applications, including medical as well as water treatment technologies.

The IUPAC Poster Prizes were given to:

Evan Schwahn, UNL Mechanical and Materials Engineering Department, USA: Controlled Curing of

Conference Call

Acrylate: System Modelling and Application in Stereolithography;

Franz Lanyi, University Erlangen-Nuremberg Institute of Polymer Materials, Germany: *Novel Chart For Representation of Material Performance and Reliability;*

Taylor Stockdale, UNL, Mechanical and Materials Engineering Department, USA: *Manufactoring of Polyimide Fibre-Reinforced Nanocomposites*



The Bruce Hartmann Prize for Young Scientists went to: **Brett Fors**, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, USA: *Deterministic Control of Polymer Molecular Weight Distribution*

The Jürgen Springer Prize for Young Scientists went to: Carolina Gonçalves, Faculty of Engineering, University of Porto, Portugal: Xanthan Gum and Chitosan as Natural Adhesives for Cork



Three Carl Klason Student Awards went to:

Yoga Salim, Department of Chemistry, Faculty of Applied Sciences, Universiti Malaya, Kuala Lumpur, Malaysia: Thermal Degradation in the Melt Reaction between Poly (3-hydroxybutyrate-co-3-hydroxyhexanoate) and Epoxidized Natural Rubber;

Kaspars Maleckis, UNL Mechanical and Materials Engineering Department, USA: *Ultrahigh-Performance Nanofibres from DNA and Proteins:*

Hao Liu, Department of Polymer Science, University of Akron, USA: *Two-Dimensional Nano-Crystals of Molecular Janus Particles*

Diplomas of Distinction went to:

Taria Jamil, Polymer Engineering Department, University of Akron, USA: *Mechanism of Molecular Interaction of Superplasticizer Oligomers with Hydrated Cement Phases;*

Xue Li, Chemistry University of Alberta, Canada: *Polymer-Based Materials for Building Artificial Muscles and Three Dimensional Structures by Self-Rolling*;

Yaping Ding, University Erlangen-Nuremberg Institute of Polymer Materials, Germany: *Electrospun PHB/PCL/Fumed Silica Fibrous Structure for Bone Tissue Engineering*;

Wenglong Li, UNL Mechanical and Materials Engineering Department, USA: *Characterization of the influence of depth in photo curing of acrylate: a method based on rapid-scan FTIR during laser curing on an ATR;* **Simon Schönherr**, Graphene-Based Nanotechnology, University Siegen, Germany: *Investigation of Electronic*

Properties of a Graphene Field Effect Transistor

Limited funds were granted by IUPAC for the support of graduate students and young scientists from underprivileged countries. However, due to high expectations by the applicants and visa problems, it was only possible to support one young scientist in the end:

Bishnu Prasad Neupane, School of Health and Allied Sciences, Pokhara University, Nepal: Conversion of Waste Paper into Bioplastics—Poly(lactic acid)

Mehrdad Neghaban, his colleagues, and collaborators at the University of Nebraska, Lincoln, deserve our thanks for their effective organization of the Course and the Conference. Good organization is a necessary condition for a creative and comfortable atmosphere, which was appreciated by the participants in Lincoln.

POLYCHAR 24 is scheduled for Poznan, Poland, end of April/early May 2016, POLYCHAR 25 is planned in Kuala Lumpur, Malaysia, 2017.

Science Assessments and Research Integrity: Reconcilable or Antagonistic?

At the recent **4th World Conference on Research Integrity** (31 May—3 June 2015, Rio de Janeiro, Brazil, www.wcri2015.org), attended by around 500 participants from more than 50 countries on five continents, the ICSU Committee on Freedom and Responsibility in the conduct of Science (CFRS) organised a symposium on "Research assessment and quality in science."

Speakers with different perspectives, from higher education to government and policy, with a national context and including young scientists, explored the implications of science assessments [1]. The goal of the symposium was to generate discussion on how to shape assessments to facilitate scientific work of high integrity for the benefit of society. This reflected a context that **Lex Bouter**, Professor of Methodology and Integrity at the Free University of Amsterdam in the Netherlands, characterised in his keynote as "hypercompetition" for positions, funding, and resources as a

Conference Call

result of an exponential rise in the number of scientists in recent times.

In the CFRS symposium, Ellen Hazelkorn, Director of Research and Enterprise at the Dublin Institute of Technology in Ireland, who has been involved in the review of higher education systems around the world, pointed out that rankings have become the de facto indicators of global scientific competitiveness since the early 2000s. Reinforced by the global financial crisis and a resulting call for increased public accountability, quantitative rankings have "emerged as a game changer" in higher education landscapes and in university reward structures by influencing government policies and resource allocation. Dr. Hazelkorn stressed the importance of combining indicator-based quantitative data with qualitative information, to recognise differences between research disciplines and to ensure that assessment processes were appropriate and fitfor-purpose.

Speaking from his perspective as lead coordinator for OECD's Global Science Forum, Carthage Smith emphasised that science evaluations and metrics were important tools for the organisation's mission to measure and promote economic development. By assessing the relation between government spending on higher education and scientific output in terms of numbers of publications, PhDs awarded, and patents filed, OECD provided governments with comparative information on the efficiency of science systems. Although agreeing that this benchmarking did determine scientific behaviour "to some extent," Dr. Smith noted that countries and science systems require these data to set their own priorities.

As someone working in a science system in an emerging economy, **Robert McLaughlin**, from the Office of Research Integrity at the University of Cape Town in South Africa, noted the challenges of aspiring to improve a university's or science system's rank worldwide while addressing local needs and supporting research integrity principles. Dr. McLaughlin noted that "the role of science in society is broadly discussed in South Africa," reflecting the challenge for the higher education system to balance an ambition to meet expectations and build capacity at the national level with an aspiration for international recognition.

Representing the Global Young Academy, **Tatiana Martins**, Professor at the Federal University of Goiás in Brazil, argued that increased pressure on young scientists to build a career posed threats to research integrity in academia. As a countermeasure, she suggested including research integrity as a criterion to be measured in assessments, helping to change the reward



From left to right: Ellen Hazelkorn, Carthage Smith, Robert McLaughlin, Merry Bullock, Tatiana Duque Martins, Roger Pfister, and Leiv K. Sydnes

system. Beyond this, Dr. Martins expressed concern that the present assessment and reward systems were further aggravating the brain drain by contributing to international competition for the best scientists.

The ICSU Committee on Freedom and Responsibility in Science [2], chaired by Leiv Sydnes, is developing a discussion paper that explores the issues highlighted in this invited Symposium [3].

Comments on the discussion paper are welcome, and can be shared by writing to the Committee's Secretariat, Roger Pfister at roger.pfister@icsu.org.

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www.icsu.org/news-centre/news/top-news/science-assessments-and -research-integrity-reconcilable-or-antagonistic

Notes

- www.icsu.org/freedom-responsibility/researchintegrity/science-assessments-and-research-integrity
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Trans Mediterranean Colloquium on **Heterocyclic Chemistry**

12-15 November 2015, Antalya, Turkey

The Organizing Committee, the Chemist Society in Turkey, the Scientific Committee of Trans Mediterranean Colloquium on Heterocyclic Chemistry (TRAMECH), and IUPAC are pleased to announce that TRAMECH VIII will be held at the Akka Antedon Hotel in Antalya, Turkey on 12-15 November 2015.

The first TRAMECH, in Marseille, France in 2000, was held in a friendly and informal atmosphere in order to provide the maximum interaction between the participants of Mediterranean countries. A great deal of chemists from the Mediterranean countries and all over the world participated and shared their ideas with great enthusiasm. They appreciated the high quality and interactive nature of this Colloquium. TRAMECH VIII follows on from:

TRAMECH VII, Rabat, Morocco (2013) TRAMECH VI, Tunis, Tunisia (2009) TRAMECH V, Tafila, Jordan (2007) TRAMECH IV, Aveiro, Portugal (2006) TRAMECH III, Marrakech, Morocco (2004) TRAMECH II, Bari, Italy (2002) TRAMECH I, Marseille, France (2000)

The main goals of TRAMECH VIII are:

- Presenting the latest research carried out in the field of Heterocyclic Chemistry by scientists and students from the universities of Mediterranean countries and all over the world.
- Providing opportunities to the delegates to exchange new ideas and application experiences
- Establishing research relations and finding global partners for future collaboration.

TRAMECH VIII is part of the new collaborative network involving Countries of the Mediterranean Sea Area, closely linked to IUPAC, in order to build and foster a sustainable program of high-quality heterocyclic chemistry research, education, and chemistry-based applications, especially in less developed countries of North Africa. See more at www.iupac.org/project/2011-006-2-300

For full details, visit www.tramech8.org

COSPAR 2016

30 July-7 August 2016, Istanbul, Turkey

The 41st Scientific Assembly of the Committee on Space Research (COSPAR) will be organized in Istanbul from 30 July - 7 August 2016. The Assembly will be held at the invitation of the Scientific and Technological Research Council of Turkey. Approximately 125 meetings covering the fields of COSPAR Scientific Commissions (SC) and Panels will be organized. Abstract Deadline: Mid-February 2016. The following is a short preview:

SC A: The Earth's Surface, Meteorology and Climate: SC B: The Earth-Moon System, Planets, and Small Bodies of the Solar System; SC C: The Upper Atmospheres of the Earth and Planets Including Reference Atmospheres; SC D: Space Plasmas in the Solar System, Including Planetary Magnetospheres; SC E: Research in Astrophysics from Space; SC F: Life Sciences as Related to Space; SC G: Materials Sciences in Space SC H: Fundamental Physics in Space; Panel on Satellite Dynamics (PSD); Panel on Scientific Ballooning (PSB); Panel on Potentially Environmentally Detrimental Activities in Space (PEDAS); Panel on Radiation



Belt Environment Modelling (PRBEM); Panel on Space Weather (PSW); Panel on Planetary Protection (PPP); Panel on Capacity Building (PCB); Panel on Education (PE); Panel on Exploration (PEX); Panel on Exoplanetary Exploration (PEPE); Special events: interdisciplinary lectures, round table, etc.

Selected papers will be published in Advances in Space Research and Life Sciences in Space Research, fully refereed journals with no deadlines open to all submissions in relevant fields.

Scientific Program Chair: Prof. Ersin Gogus, Sabanci University, COSPAR Secretariat, 2 place Maurice Quentin, Paris, France, Email: cospar@cosparhq.cnes.fr

http://www.cospar-assembly.org

Organic Chemistry of Sulfur

24-29 July 2016, Jena, Germany

The 27th International Symposium on Organic Chemistry of Sulfur, with the specific theme of from fundamental research to application, will take place in Jena, Germany, from 24-29 July 2016.

The Conference Chair, Professor Wolfgang Weigand, is organizing a rich program, including the following topics: Advanced materials, Agricultural chemistry, Bio-organic, bioorganometallic (coordination chemistry), Environmental issues, Catalysis, Medicinal chemistry, Sulfur-polymer composite materials, Nanotechnology, Organic Chemistry of Sulfur, Primordial chemistry, Stereoselective synthesis.

The conference will take place at the Friedrich-Schiller-University Jena, surrounded by the picturesque vineyards and shell limestone mountains

of the Saale-Valley. Only a few years after the political revolution in the Eastern part of Germany took place,

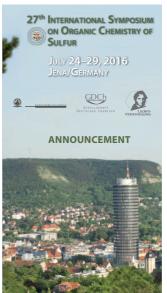
Jena emerged as a city of economic, scientific, cultural, and social prestige. It is the home of world-renowned institutions, including two Leibniz Institutes and three Max-Planck-Institutes, and looks back on an impres-

sive history in the field of optical works and research strongly associated with names such as Carl Zeiss and Ernst Abbe. Nearly 25,000 students contribute to Jena's image as Thuringia's intellectual center, which is mainly based on philosophers of international prominence like Schiller, Goethe and Hegel.

Contact:

Conventus Congress Management & Marketing GmbH
Felix Angermüller
Carl-Pulfrich-Straße 1
D-07745 Jena, Germany
Phone +49 3641 31 16-301
felix.angermueller@conventus.de

www.isocs-27.org



SOLID URBAN WASTE MANAGEMENT

XXI IUPAC CHEMRAWN CONFERENCE

Topics

- Energy from urban waste
- Materials recycling, transformation and recovery
- From organic waste to resource
- Education to sustainable waste management

April 6 7 8, 2016

CNR Piazzale Aldo Moro 7 - Rome (Italy)



ADVANCED TRAINING COURSE ON EMERGING BIOTECHNOLOGIES FOR SUSTAINABLE WASTE MANAGEMENT

April 4 5, 2016 University of Naples Federico II - Naples, Italy

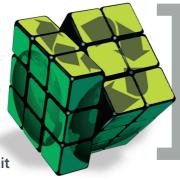


The Advanced Training course is sponsored by the EU funded project BIOASSORT (318931)

www.iupac-rome2016.it









20TH IUPAC CONFERENCE ON CHEMICAL RESEARCH APPLIED TO WORLD NEEDS

06-09 November 2015, Dhaka, Bangladesh

Theme Herbal Medicine for Health Care in the 21st Century











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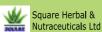


Companies





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Hamdard Laboratories (wafq) Bangladesh



Hamdard University Bangladesh



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27-30 January 2016 • POLYSOLVAT-11 • Kolkata, India

Polymer-solvent Complexes and Intercalates (POLYSOLVAT-11)

Dr. Sudip Malik (convenor), Polymer Science Unit, Indian Association for the Cultivation of Science, Kolkata, West Bengal, India, Tel: +913324734971 (Ext-1564),

E-mail: psusm2@iacs.res.in or polysolvat11@iacs.res.in, www.iacs.res.in/conferences/polysolvat11

16-18 March 2016 • Young Scientists • Blankenberge, Belgium

Chemistry Conference for Young Scientists 2016

Geert-Jan Graulus, Ghent University, Polymer Chemistry & Biomaterials Research Group, E-mail: geert-jan. graulus@chemcys.be or ChemCYS (Koninklijke Vlaamse Chemische Vereniging vzw),

E-mail: support@chemcys.be, www.chemcys.be

6-8 April 2016 • XXI IUPAC CHEMRAWN Conference • Rome, Italy

Solid Urban Waste Management

Dr. Mario Malinconico, Research Director, Institute for Polymers, Composites and Biomaterials (IPCB-CNR), Pozzuoli (Na) Italy,

E-mail: mario.malinconico@ictp.cnr.it or info@iupac-rome2016.it, www.iupac-rome2016.it

6-9 April 2016 • Agrochemicals Protecting Crops, Health and Natural Environment • New Delhi, India

3rd International Conference on Agrochemicals Protecting Crops, Health and Natural Environment -"New Chemistries for Phytomedicines and Crop Protection Chemicals"

Dr N. A. Shakil, Division of Agricultural Chemicals, ICAR-IARI, New Delhi, India;

E-mail: iamshakil@gmail.com

6-10 June 2016 • Mycotoxins • Winnipeg, Canada

9th World Mycotoxin Forum & XIVth International Symposium on Mycotoxins

Prof. Rudolf Krska (Program co-chair), University of Natural Resources & Life Sciences, Tullin, Austria, E-mail: rudolf.krska@boku.ac.at and Prof. Hans P. van Egmond, Institute of Food Safety, Wageningen, Netherlands,

E-mail: hans.vanegmond@wur.nl, Ms. Helena B. Bastiaanse (coordinator), Bastiannse Communication,

E-mail: wmf@bastiaanse-communication.com, www.WMFmeetsIUPAC.org

3-8 July 2016 • Physical Organic Chemistry • Sydney, Australia

23rd International Conference on Physical Organic Chemistry (ICPOC-23)

Prof. Jason Harper, School of Chemistry, University of New South Wales, Sydney, Australia,

E-mail: j.harper@unsw.edu.au, www.icpoc23.unsw.edu.au

17-21 July 2016 • Macro • Istanbul, Turkey

IUPAC World Polymer Congress (Macro 2016)

Prof. Yusuf Yagci, conference chair, Istanbul Technical University,

E-mail: yusuf@itu.edu.tr; Congress Secretariat: bilge.yuksel@brosgroup.net, www.macro2016.org

17-22 July 2016 • Carbohydrate • New Orleans, Louisiana, USA

28th International Carbohydrate Symposium

Dr. Albert French, Organizing Chair; E-mail: Chair.ICS2016@gmail.com;

Mrs. Mary An Godshall, Executive Secretary; E-mail: execsec.ics2016@gmail.com, www.ics-2016.org

24-29 July 2016 - Solubility Phenomena - Geneva, Switzerland

International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP17)

Dr. Montserrat Filella, Institute F.-A. Forel, University of Geneva, Versoix, Switzerland,

E-mail: montserrat.filella at unige.ch, http://issp17.unige.ch/

4-8 September 2016 - Green Chemistry - Venice, Italy

6th International IUPAC Conference On Green Chemistry

Prof. Pietro Tundo, Chairman, Organizing committee, Dipartimento di Scienze Molecolari e Nanosistemi, University Ca' Foscari Sede: Santa Marta, Venezia, Italy.

E-mail: secretary@greeniupac2016.eu,

www.greeniupac2016.eu

Index 2015

Book

Chemical Processes for a Sustainable Future 27(4)

Ionic Polymerization: Part I & II 39(5-6)

Macromolecular Symposia—Recent Volumes 28(3)

Polymers and Organic Chemistry 39(5-6)

Volumes Properties: Liquids, Solutions and Vapours 27(3)

Conference Call

100 volumes of IUPAC's Solubility Data Series by David Shaw 30(1)

Boron Chemistry by Michael A. Beckett 28(1)

Chemistry Education by Judith Poë 33(1)

Data Sharing for Sustainability 32(2)

FloHet-2014 By Eric Scriven 30(1)

Green Chemistry by Liliana Mammino 34(1)

Human Errors and Quality of Chemical Analytical Results 30(3)

Isoprenoids by Pavel Drašar 29(1)

Nanomaterials and Human Health by Vladimir Gubala 31(1)

Pesticide Chemistry by Kenneth Racke 27(2)

Photobiology by Silvia Braslavsky 28(2)

POLYCHAR 23 World Forum Advanced Materials 42(5-6)

Science Assessments and Research Integrity 44(5-6)

Solubility Phenomena and Related Equilibrium Processes by Marcus Altmaier 30(2)

Features

Books of Secrets: Writing & Reading Alchemy by Neil Gussman 4(2)

Chemical Speciation of Environmentally Significant Metals: An IUPAC contribution to reliable and rigorous computer modelling by Kipton J. Powell, et. al. 15(1)

Chemistry: Meeting the World's Needs? by Natalia Tarasova 4(1)

Concepts in Toxicology: Development of Online Instructional Modules by D.J. Huggins, M. Schwenk, D.M. Templeton, and J. H. Duffus 12(1)

Drug Design and Development: Part II—Reflections from an Academic-based Center by Paul Erhardt 12(3)

MATECSS: A global network enabling capacity-building for sustainable energy by Jennifer MacLeod 8(1)

Medicinal Chemistry in IUPAC by Robin Ganellin 17(5-6)

Meeting the Google Expectation for Chemical Safety

Information by Leah McEwen and Ralph Stuart 12(5-6)

Mind the Gap: Comparison of the Role Played by Women in the Departments of Chemistry of Two Universities and the Influence of Gender on Their Participation 10(4)

A Perspective on Chemistry Education 8(4)

Progress of Chemistry in South Korea by Choon H. Do 4(5-6)

Systematic Flexibility and the History of the IUPAC

Nomenclature of Organic Chemistry by Evan Hepler-Smith 10(2)

Taking IUPAC Literally: An International Union of Pure and Applied Chemistry by Jeffrey I. Seeman 4(3)

Towards a Uniform Description System for Materials on the Nanoscale 3(4)

Twitter in Chemical Education and IUPAC by D. Brynn Hibbert 10(3)

What's in a Name? Quite a Lot, as it Happens! by Mark I. Borkum and Jeremy G. Frey 7(2)

Youth Views on Sustainability: PMMA, from plexiglass window to a packaging for an implantable glucose sensor by Elke Van De Walle 16(3)

Youth Views on Sustainability: Chemical Waste Management at Clinical Laboratories by David Yafté Díaz-Sánchez 21(5-6)

From the Editor by Fabienne Meyers (1) Guest Editorial by James R. Bull (3)

IUPAC Wire

The 2014 AAAS Award for Science Diplomacy goes to Zafra M. Lerman 17(2)

OPCW-The Hague Award Presented at 19th Conference of States Parties 17(2)

2015 IUPAC-SOLVAY International Award for Young Chemists 21(1)

African Leaders Endorse a Science Funding Platform 20(3)

Awardees of the IUPAC 2015 Distinguished Women in Chemistry or Chemical Engineering Announced 15(4)

Berhanu Abegaz heads the UNESCO International Basic Sciences Programme (IBSP) scientific board 28(5-6)

Call for Nominations for IUPAC International Award in Crop Protection Chemistry 17(4)

Cefic Sustainability Report 2013-2014 23(1)

Chemical World Tour—4th Edition 18(4)

Chemistry International Survey 22(1)

CHEMRAWN VII Prize for Green Chemistry Call for Nominations 25(5-6)

Christo Balarew receives Presidential Honors 28(5-6)

De Gruyter to Launch Chemistry Standards Database 26(5-6)

Election of IUPAC Officers and Bureau Members—Call for Nominations 15(2), 21(3)

The EuCheMS Award for Service: Call for Nominations 20(3)

The Franzosini Award goes to Magdalena Bendová and Slobodan Gadzuric 16(4)

ICSU announces Dr. Heide Hackmann to be Executive Director and Dr. Lucilla Spini to be Head of Science Programmes 16(2)

In Memoriam: Anthony R. H. Goodwin 21(3), John William Lorimer 21(4), Nikola Kallay (1942-2015) 29(5-6), Peter A.S. Smith 21(3)

IUPAC Announces the Winners of the 2015 IUPAC-SOLVAY International Award for Young Chemists 15(4)

IUPAC 2015 Distinguished Women in Chemistry or Chemical Engineering—Call for Nominations 20(1)

IUPAC Elections for the 2016-2017 Term 20(1)

IUPAC Office move 18(2)

IUPAC Physical Chemistry Cartoon Competition 18(2) IUPAC-SOLVAY International Award for Young

Chemists 24(5-6)

IUPAC-ThalesNano Prize in Flow Chemistry Call for Nominations 25(5-6)

Laudation on Behalf of the 80th Birthday of Koichi Hatada 19(4)

Launch Event for SDGs Review Held at UN in New York 19(3)

L'Oréal-UNESCO Awards for Women in Science 2015 Announced 27(5-6)

Measurements and Light 16(2)

No Price Increase in 2015 for Pure and Applied Chemistry 23(1)

PhosAgro/UNESCO/IUPAC Research Grants 20(1)

Polymer International-IUPAC Award-Call for Nominations 17(4)

Thieme-IUPAC Prize 2016 Call for Nominations 24(5-6)

Tom Kariuki to Head the Alliance for Accelerating Excellence in Science in Africa 18(4)

Science an Important Theme at Post-2015 Negotiations in New York 19(4)

Solubility Data Series Books now Available on Web 27(5-6)

Standard Atomic Weight of Ytterbium Revised 26(5-6) Strengthening the Ties Between IUPAC and the Chinese Chemical Society 22(1)

Thieme Chemistry Website Relaunched 21(1)

UNESCO partners with Nature Education and Roche to Launch a Free Online Science Education Resource 23(1)

Making an imPACt

Brief guide to the nomenclature of inorganic chemistry 37(5-6)

Definitions of terms relating to individual macromolecules, macromolecular assemblies, polymer solutions, and amorphous bulk polymers 23(3)

Guidelines for checking performance and verifying accuracy of rotational rheometers: viscosity measurements in steady and oscillatory shear 24(3)

The NPU format for clinical laboratory science reports regarding properties, units, and symbols 24(3)

Immunochemical Recognition and its Diagnostic and Therapeutic Applications by Douglas Templeton and Michael Schwenk 20(2)

IUPAC Glossary of terms used in neurotoxicology 37(5-6) Latest Updates from PAC Conference Reports by Hugh Beckett 36(5-6)

Nomenclature and graphic representations for chemically modified polymers 23(3)

Reference correlations for the viscosity and thermal conductivity of fluids over an extended range of conditions: hexane in the vapor, liquid, and supercritical regions 23(3)

Spectroscopy of Water 25(3)

Time-resolved fluorescence methods 23(3)

Mark Your Calendar

Listing of IUPAC-sponsored Conferences and Symposia, 37(1), 35(2), 35(3), 33(4), 49(5-6)

NOTeS

On the Use of Quantity Calculus by Tomislav Cvitas 26(2)

Officers' Columns

The First IUPAC Congress in Korea by Myung Soo Kim 2(2)

Refocus on Contacts by Mark Cesa 2(1)

Ringing the Changes—For the Future by John Corish 2(5-6)

Secretariat on the Move by Colin Humphris 2(3)

Scientific Knowledge and Interdisciplinary Research by Natalia Tarasova 2(4)

Provisional Recommendations

Glossary of Terms Used in Extraction 38(5-6) Glossary of Terms Used in Neurotoxicology 19(2), 22(3) Source-Based Nomenclature for Single-Strand Homopolymers and Copolymers 38(5-6)

The Project Place

Accelerating the Participation and Leadership of Women in Chemistry 26(4)

Chemistry Beyond Chlorine 25(1)

The Emerging Problem of Novel Psychoactive Substances 24(1)

The Environmental and Health Challenges of E-Waste and its Management 22(4)

Increasing IUPAC's Social Media Presence 22(3)

IYC 2011 Description and Analysis of Activities 23(4)

Measurement of Photoluminescence Quantum Yields 31(5-6)

Nomenclature for polymeric carriers bearing chemical entities with specific activities and names 30(5-6) Nomenclature of Carbon Nanotubes and Related

Index

Substances 24(1)

Storing Energy: with special reference to renewable energy sources 30(5-6)

Terminology for Modeling and Simulation of Polymers 24(1)

Young Ambassadors for Chemistry (YAC) 32(5-6)

Stamps International by Daniel Rabinovich

The Chemistry of Vision 26(3)
The Discovery and Demise of Wodanium 28(4)
Let There Be light! 27(1)
Otto Wichterle: An Eye for Hydrogels 19(2)
Dreams Make Good Stories 3(5-6)

Where 2B & Y

Anatolian Conference on Synthetic Organic Chemistry, 16-19 March 2015, Antalya, Turkey 35(1)

Chemical Biography In the 21st Century, 9-12 September 2015, Aveiro, Portugal 36(1)

CHEMRAWN XX—Herbal Medicine for Health Care in the 21st Century, 6-9 November 2015, Dhaka, Bangladesh 3(3)

COSPAR 2016, 30 July—7 August 2016, Istanbul, Turkey 46(5-6)

Functional π -Electron Systems, 19-24 July 2015, Seattle,

WA. USA 33(2)

Green and Microscale Chemistry, 27-29 May 2015, Ciudad de México, Mexico 33(2)

IUPAC's role in achieving UN Sustainable Development Goals—2015 WCLM, 12 August 2015, IUPAC General Assembly, Busan, Korea 29(4)

Macromolecules & Materials, 7-10 September 2015, Port Elizabeth, South Africa 33(3)

Novel Aromatic Compounds, 5-10 July 2015, Madrid, Spain 34(2)

Research in Chemical Education, 22-27 November 2015, University of Venda, Thohoyandou, South Africa 34(3)

Research in Chemical Education, 22-27 November 2015, University of Venda, Thohoyandou, South Africa 31(4)

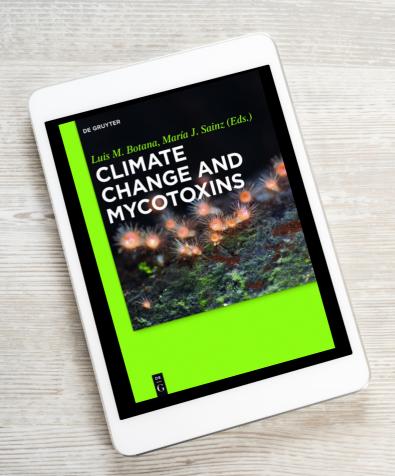
Selenium in the Environment and Human Health, 18-21 October 2015, Cuiaba, Brazil 36(1)

Trans Mediterranean Colloquium on Heterocyclic Chemistry, 12-15 November 2015, Antalya, Turkey 46(5-6)

Water and Life in the Universe, 9-13 November 2015, Foz do Iguacu, Brazil 35(1)

Pull-Out

Brief guide to the nomenclature of inorganic chemistry (5-6)



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IUPAC is a non-governmental organization of member countries that encompasses more than 85% of the world's chemical sciences and industries. IUPAC addresses international issues in the chemical sciences utilizing expert volunteers from its member countries. IUPAC provides leadership, facilitation, and encouragement of chemistry and promotes the norms, values, standards, and ethics of science and the free exchange of scientific information. Scientists have unimpeded access to IUPAC activities and reports. In fulfilling this mission, IUPAC effectively contributes to the worldwide understanding and application of the chemical sciences, to the betterment of the human condition.

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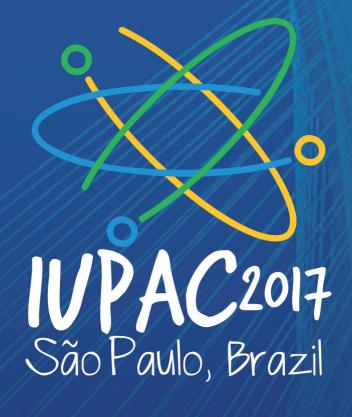
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