THE VORTEX

AMERICAN CHEMICAL SOCIETY
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CALIFORNIA SECTION
FEBRUARY 2012

A tour of the brewery and a talk on the science and benefits of beer

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THE VORTEX

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Volume LXXIII February 2012 Number 2

Chair's Message

Jim Postma

I am still a bit intimidated to be called "Chair" of a section with the history and complexity of the California Section. One way to make sense of it is to visit the Section website, www.calacs.org. I assume that most of you know this because it has become the major mechanism for disseminating the *Vortex* and most other information about Section events.

I also find it useful for exploring the Section and want to recommend that you do a little of that with me. I think you will find it informative but you may also find a program or event that entices you to get a bit more involved or encourage a colleague to do so. We are grateful to Doug Henry for his work to develop the site and to keep it operational.

Some of the interesting features that I would like to point out to you include a History of the Section (under "About Us"). I find it interesting to picture what chemistry was like 111 years ago, not to mention what the State of California was like. It is also fascinating to see some of the famous names of chemistry and note that they took time from busy careers to invest in the California Section. It is personally inspiring.

You can also discover the wide range of activities, committees, and projects that might interest you. There are Younger Chemists (the Section could benefit from someone volunteering to Chair the Senior Chemist Committee). There are projects for teachers and for students at all levels as well as contests (the Chemistry Olympiad) and awards for those who demonstrate excellence. Environmental events, science fairs, and industry tours are all features of our section.

The California Section includes a huge array of educational institutions; I have not had a chance to tally them up, but my sense is that only the Boston section may rival us in this regard. A potential area of growth for our Section is the large number of universities and colleges with their energetic chemistry clubs and science clubs.

"Surfing" the calacs website could occupy a lot of time, but I will warn you about linking from there to the American Chemical Society's website, www.acs.org. The range of activities of our parent organization and the resources that it offers to members, including students, academics, members from industry, and the general public is staggering. You could be "spelunking" for weeks. I encourage your exploration and hope that it leads to a satisfying involvement with the Section.

If you find errors or have suggestions about the Section's website, please pass them on to Lou Rigali, qpfans@qpfans.com

The Chico Subsection of the California Section
February Meeting

Speaker: Charlie Bamforth,Department Chair, Food Science & Technology
University of California, Davis
Date: Saturday, February 25, 2012
Time: 9:00 am Tour followed the talk at 1:00 PM at the Oxford Suites Hotel (across the freeway from the Brewery).
Place: Sierra Nevada Brewery, 1075 E 20th St. Chico, CA 95928
(530) 893-3520
Cost: Please call for information
Reservations: To prepay, please send check to Cal. Section, ACS at 2950 Merced Street, #225, San Leandro CA 94577
Directions: Take exit # 384 on Rte. 99 for E. 20th St., trun left onto 20th St., then turn left onto Sierra Nevada Ct.

Biography:

Education

B.Sc. Biochemistry, University of Hull, UK, 1973
Ph. D. Solubilization and properties of N-Methylglutamate dehydrogenase from Pseudomonas aminovorans and its role during growth on methylamine University of Hull, 1977
D. Sc. University of Hull, 1993

Career Positions

Department Chair, Food Science & Technology UC, Davis, 2005 – 2009
Anheuser-Busch Endowed Professor of Brewing Science UC, Jan 1999-Present
Director of Membership Services Brewing Research International, 1997-1998
Director (previously Head) of ResearchBrewing Research International, 1991-1997
Quality Assurance Manager Bass Brewers, Preston Brook Brewery, 1988-1991
Research Manager Bass Plc, 1984-1988
Senior Projects Manager Bass Plc, 1983-1984
Various including Head of Malt and Wort Production Brewing Res. Fdn.1978-1983
Independent Research Worker Department of Microbiology Univ. of Sheffield,1976-1978

Other:

Hundreds of publications related to the brewing industry

Professional Relations

Special Professor in the School of Biosciences, University of Nottingham

ELK-N-ACS

Evaldo Kothny

Phosphorus

"Phosphorous", is a grammatical mistake if one refers to the element and not to a valence state. Thus phosphorus refers to the element of valence 1, 3 and 5, whereas phosphorous are combinations of phosphorus of valence 3. Phosphorus was also the name given to Venus, the morning star. In the Sun's spectrum, investigated by Fraunhofer in 1815, only lines belonging to Na, Ca and Fe were found, but no lines for phosphorus.

In the last November article about nitrogen, the cosmogenesis of the lighter elements was explained. It all started with the burning of hydrogen at extremely high temperatures and formation of helium, which in turn is burning for the formation of heavier elements in stars such as nitrogen, sulfur, phosphorus, carbon and oxygen. The fact that in stars both hydrogen and helium comprise 99% of the matter and that only 1% are heavier elements, gives us an idea about the dilution of the world we are living in. By sure, we will not face another large event such as a precambrian episode comprising the first and second parting, (see below) or any other sequence of a cambrian style transformation that had only 1% of free oxygen available (comprising the third parting, see below). Before that moment, the geological science we know of, had just kicked in. Imagine condensation of a steaming hot atmosphere hitting disintegrating basalt, etc. and leaching out soluble substances including all halogens, alkalies, phosphoric substances and leaving behind some insoluble silicates (our new kitchen countertop? granite?)

In the first parting, the heavier molten rocks of Earth settled by gravity into the core. The core collected most iron, nickel, sulfur and carbon. Phosphorus was largely locked up in the iron-sulfur phase.

In the second parting, remaining iron minerals separated collecting most of the phosphorus as accessory minerals or as impurities in the sulfide phase.

In the third parting, the solid minerals weathered, disintegrated and transformed into sediments.The most resistant P mineral is apatite (a Ca halophosphate or hydroxyphosphate with a small impurity of As). During weathering, basalt, the primary carrier of P with about 1400 ppm P, loses most of its Ca as silicate, whereas Al, Fe and half of the P is retained in the freshly formed clay. Other substances containing P are granite, shale, and limestone. Since P is sensitive to pH changes, it might be solubilized in presence of nutrients by microorganisms. Thus organic acids generated by microorganisms (e.g., ketogluconic, lactic, glycolic, citric, formic and acetic acids) plus enzymes contained in humus and those segregated by plant roots solubilize P.

The stable isotope of P is that of atomic weight 31. Most unstable P isotopes of atomic weight 29, 30, 32, 33 and 34 are produced artificially except the isotopes of atomic weight 32 and 33 which also exist naturally in very small quantities. They all are beta emitters. All compounds of P are unstable in presence of moisture and are easily absorbed by Ca, Fe and Al compounds. In California, over 40 minerals containing P have been found; Apatite was found as small crystals in rocks of 11 counties, including Contra Costa Co. Apatite is found in bones, teeth and fluorescent lamps (optimized for efficient light output).

For optimal plant growth, Justus von Liebig predicted among others, the needs of P in agriculture. As example, nuts, soya, cocoa and cheeses have the highest content of P (3 to 7%), oats, rye, beef, poultry and fish, contain about 3% P, peas, beans and wheat have between 1 and 3%, potatoes, fruits and vegetables carry between 0.2 to 0.5%. Continuous harvesting of crops removes nutrients from the soil which have to be replenished for maintaining productivity. Traditionally, fertilization with P consisted of ground phosphate rock, bones, ammonium phosphate, Thomas

(Continued on page 10)

Recycling Water (Part 3)

Bill Motzer

In the December 2011 and January 2012 Vortex, I described some of California's recycled water (RW) characteristics, history, and monitoring requirements. Many chemical compounds occurring in waste water could also occur in RW, although in very low concentrations (in the ng/L or part per trillion range). Therefore, the California Department of Public Health (CDPH) and State Water Resources Control Board (SWRCB) maintain considerable oversight in regulating potential Groundwater Recharge Reuse Projects (GRRPs) involving RW usage and potential risks.

In California, about 50% of RW is used in agriculture and 20% is used for landscape irrigation such as golf courses, parks, and neighborhood residential common areas. The remaining 30% is used for industrial applications and groundwater recharge. So what human risks are associated with such applications? To answer this question, I have described four Pharmaceutical and Personal Care Products (PPCPs) followed by calculated human risks from varying exposure to different human receptors at different concentrations.

Ibuprofen (CAS: 15687-27-1) also known as (RS)-2-[4-(2-methylpropyl) phenyl] propanoic acid is an over-the-counter (OTC) medication primarily used for controlling fever, pain, and inflammatory diseases such as rheumatoid arthritis. Ibuprofen is in a class of PPCPs known as non-steroidal anti-inflammatory drugs (NSAIDs) with common trade names such as Advil and Motrin. Ibuprofen has a dose-dependent duration of action of approximately four to eight hours. The recommended dose varies with body weight, but 1,200 mg is considered the maximum daily dose for OTC use. However, under a doctor's care, the maximum amount of ibuprofen for an adult may be increased to 800 mg per dose or 3,200 mg per day. As a result, excess ibuprofen is excreted by the body over a short time period.

17-beta estradiol (CAS: 50-28-2) or (17β)-estra-1,3,5(10)-triene-3,17-diol, also known as oestradiol is an estrogen (sex hormone) both naturally produced and excreted by humans. It is the predominant reproductive hormone in women during their reproductive years, although smaller amounts occur in men resulting as a metabolic byproduct of testosterone production. Estradiol has a critical impact on reproductive and sexual functioning, but also affects other organs, including the bones. Synthetic estradiols have been prescribed for post menopausal women; however, recent reports suggest that it may result in breast cancer. Because of its widespread usage, estradiols have been found in treated wastewater effluent

DEET (CAS: 134-62-3) or N,N-Diethyl-meta-toluamide is the most common active ingredient in OTC insect repellents. It is commonly applied to the skin or to clothing providing protection against tick, chigger, and mosquito bites, and bites from other disease-transmitting insects. DEET generally enters the environment when washed off from skin by bathing. Although it probably does not bioaccumulate in organisms, it has slight toxic effects for some coldwater fish such as rainbow trout and tilapia and for some freshwater zooplankton species. As a result of production and use, DEET has been detected at low concentrations in water bodies, such as in the Mississippi River and its tributaries, where a 1991 study detected concentrations ranging from 5 to 201 ng/L.

Triclosan (CAS: 3380-34-5; 5-chloro-2-(2,4-dichlorophenoxy) phenol) is an antibacterial and antifungal compound in general use since 1972. It is added to many soaps (at concentrations ranging from 0.10 to 1.00%), deodorants, shaving creams, cleaning supplies, and toothpastes and mouth washes (to prevent gingivitis). It has also been incorporated into some plastics used in kitchen utensils, toys, and trash bags, and in bedding and socks. Triclosan is most effective in reducing and controlling bacteria on hands and showering or bathing with 2% triclosan solution is recommended for patients whose skin carries methicillin-resistant Staphylococcus aureus (MRSA).

During wastewater treatment, most triclosan generally degrades; however, some traces

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ACS Presidents

Marinda Li Wu 2012 ACS President-Elect

As we start the New Year, I want to thank you for your support over the years and also with the recent national ACS election. I feel very fortunate and honored to learn that I will become the 8th ACS President from the California Section and also the 8th woman elected as President in ACS' 135 year history. What is remarkable is that the number 8 is a very lucky number in the Chinese culture because the word for "eight" sounds similar to the word that means "prosper" or "wealth." In some regional dialects, the words for "eight" and "fortune" are also similar, according to Wikipedia.

When I learned the names of the previous ACS Presidents that I will follow, I am deeply humbled. The eight ACS Presidents of the Society from California Section are well known by most of us: E.C. Franklin (1923), Joel Hildebrand (1955), Melvin Calvin (1971), Alan Nixon (1973), Glenn Seaborg (1976), George Pimentel (1986), Attila Pavlath (2001), Marinda Li Wu (2013).

It was also interesting to learn from ACS that I will be the 125th ACS President after 136 years. Apparently a few Presidents served multiple terms although none have been within the recent history. The women elected as ACS Presidents include Anna J. Harrison (1978), Mary L. Good (1987), Helen M. Free (1993), Elsa Reichmanis (2003), E. Ann Nalley (2006), Catherine T. (Katie) Hunt (2007), Nancy B. Jackson (2011), Marinda Li Wu (2013).

Thus, I feel great responsibility and humility as I enter the ACS Presidential succession in this New Year. The countless supporting letters I received from ACS members around the world have strengthened the determination that I have long had to do my best to better our Society for all our members. Indeed, I hope to be a "catalyst for positive change."

I look forward to the challenges ahead and am starting to formulate plans for what I would like to accomplish as ACS President in 2013. While I certainly have ideas, I also value any thoughts or suggestions you might have on what more ACS can do to help its members.

Two of the areas I would like to focus on are:

1) Jobs and professional development, including advocacy to improve the business climate in the U.S.

2) Global outreach and international exchange/collaborations to benefit ACS members and the global chemistry enterprise

If you have any suggestions or ideas, I welcome your input at m.wu@acs.org. Of course, not all suggestions will be feasible, but your input will be heard and brought to the attention of the ACS for consideration. Thanks again for your support over the years! Happy 2012 to all!

Dr. Marinda Li Wu with students at the Western Regional ACS Meeting in Pasadena, CA on 11-11-11"

International Year of Chemistry

Attila Pavlath

Hopefully every chemist knows that 2011 was declared as The International Year of Chemistry (IYC11) by the United Nations. This was not a unique action. Previously, some years ago were declared as International Year of other sciences, e.g. Physics. However, the corresponding scientific societies of the world did not spend enough energy to provide enough publicity. In contrast, the chemical societies, made in 2011 a yearlong continuous effort to show the world how much essential benefits chemistry has provided in our everyday life. This is the real purpose of IYC11 which was badly needed, since the general public is continuously bombarded with possible occasional problems attributed to chemistry while ignoring hundreds of its benefits.

IUPAC had a well-publicized opening of IYC11 in Paris in January, followed by the North American celebration in Puerto Rico in July and was finished in December in Brussels by the closing ceremony. These alone would not have made it much more different from the other International Years. The chemical societies of the world used various ways to meet the goals: to publicize the benefits of chemistry. As in many other areas, our Section was a chief contributor by providing publicity materials for these celebrations. Their value did not diminish by the end of 2011. They will maintain publicity for the numerous beneficial chemical developments for years to come.

The ACS for years tried to increase the public awareness of chemistry as example in 2001, for the 125th anniversary of the Society, an electronic exhibit was created to display 80 chemical developments which play crucial beneficial roles in our everyday life by using layman terms. Due to its bulkiness its wide scale use was limited. A few years ago, when I chaired the California Section, I contacted the Hungarian Chemical Society to convert the exhibit into an easily transportable poster display. This was done not only successfully, but the colorful 32-poster display was also translated to Hungarian and became a traveling exhibit in Hungry.

The Hungarian Chemical Society obtained industrial support to create a virtual book available for viewing in eight languages (www.chemgeneration.com)

They also created a pamphlet summarizing the benefits of chemistry described in the display. Consequently, we used its English version and distributed both domestically and abroad.

A few years ago, in the UN Ethiopia started a campaign for an International Year of Chemistry. It was evident that some powerful tool was needed to make the IYC to be different from previous International Years. Based on the success of the display in Hungary, we started a successful worldwide effort to translate it to other languages. At the start of IYC11, it was already available in 30 languages (Africa, Asia and Europe). We uploaded them on a webpage (www.chemistryinyourlife.org) from where they could be downloaded freely.

For the Paris opening and the Brussels closing we provided the posters and helped to display them in both English and French as a gift from the California Section. We did the same in Puerto Rico using the English and Spanish versions for directing the attention to the benefits of chemistry. The appropriate versions were used for many countries throughout the world. Interestingly, even before the Paris opening, the Hebrew version was used to open IYC11 in Jerusalem in the Knesset. It was such a success that the Israel Ministry of Education distributed a CD to every high school in Israel. The Brazilian Chemical Society similarly promoted the use of the Portuguese version in Brazil.

This lead to further developments. We helped the Korean Chemical Society to convert it to a book, of which 3000 copies were distributed to schools and libraries in Korea.

We created a Committee of International Year of Chemistry to promote all of these activities. It will continue its activities in 2012 too. Both the display and the pamphlet version was distributed to a number of other Sections. It has also been shown at some meetings of our section. The abbreviated

(Continued on page 10)

Send us your designs and ideas

The California Section will be offering a number of products for sale on its website. The profits from these sales will be used to continue and expand various outreach efforts such as our Educational Grants program to schools.

The products offered will consist of items such as mugs, magnets, and a number of various garments such as t-shirts, golf shirts, hooded sweatshirts and other apparel all with chemistry or science related images or text. Names and other forms of personalization can also be added. Personalization will be by silk-screening, direct-to-garment-printing, or embroidery.

In addition to the science related products, one can also obtain custom apparel for any group activity in a school or company.

Send your designs and ideas to office@calacs.org All submittals will be acknowledged and those that are selected will be offered a percentage of sales. The program is scheduled to start around March 1, 2012. Write for details. Here are a couple of early suggestions.

Chromates.....(an image of two crows in same nest)
Adiabatic Demagnetization is Cool

Younger Chemist Committee

The Case of the Missing PEEPS - March 25th
Date: March 25th
Time: 2:00 - 4:00 PM
Location: Golden Gate Park in San Francisco RSVP for details

The Case of the missing PEEPS is a forensic mystery that only science can solve. This is a hands-on mystery party that gets you testing the evidence and grilling the suspects to find out what happened to those missing marshmallows. RSVP required and please indicate if you would like to play a suspect to squidbait@ymail.com. A voluntary donation to cover cost of supplies is greatly appreciated.

To check out other YCC events and postings visit: https://www.facebook.com/pages/Younger-Chemists-Committee-YCC-ACS-California-Section/164045583624244?v=wall

Recycling *(continued from page 6)*

may not occur in treated wastewater effluent. It may also adsorb onto sewage sludge. Undegraded triclosan may adsorb onto particles settling out of the water column, thereby contaminating sediments that may take more than 30 years to degrade. In the environment, triclosan may be degraded by microorganisms or it may photochemically degrade, forming other intermediate compounds, including between 3 to 12% of chlorophenols and dioxin, particularly, 2,8-dichlorodibenzo-p-dioxin (2,8-DCDD) and 2,4-dichlorophenol (2,4-DCP).

Risks of RW Exposure

In a study by the WateReuse Foundation, 10 PPCPs were subject to risk assessment calculations to determine the relative human risks from exposure to these compounds. Risk calculations are determined from dermal exposure, ingestion, and inhalation. Four of the above described PPCPs are listed as ricks. Actual concentrations are those at the 90th percentile from a review of RW studies where PPCPs were measured in RW. Acceptable concentrations are those calculated concentrations at which adverse health effects are not expected from RW exposure or are at levels at which RW contact is considered to be safe.

Due to space limitations a table showing exposure of PPCPs is included at the end of this issue

Phosphorus *(continued from page 5)*

meal (obtained from the removal of excess phosphor in steel) and diverse organic wastes (animal wastes, compost, manure, garbage, sewage). A healthy diet should provide a daily intake of nearly 1 to 2 grams of P.

The function of P as fertilizer is more important than that of N or K because of the complicated relationship between total and available P. The soluble P reacts quickly with hydrated Fe and Al minerals in the soil structure, thus remains hidden and unavailable as fertilizer. From a pH of 6 to 8 , the affinity of P for Fe in soil decreases markedly whereas the affinity of P for Al decreases between a pH of 7 to 9. Large ties of P with Fe and Al can be partially offset by presence of chelating organic acids. and active microorganisms. These mechanisms remove Fe and Al ions by complexation, whereas fertilization with N foster proliferation of microorganisms and releases some of the trapped P. More details can be found in "Chemistry of the soil" by Firman Bear (editor) (ACS Monograph #160 (out of print but available in libraries).

Therefore, walk to the library and read

IYCII *(continued from page 8)*

version of the exhibit is permanently displayed at SFSU. We are also seeking other places where either temporary of permanent displays are possible. The exhibit is also available in four Power Point presentations on Energy & Transportation, Communication & Information, Health & Medicine and Agriculture & Food. While officially IYC11 is ended, we want to continue its goal to increase the public image of chemistry.

If you are interested in giving a talk at your organization's luncheon or dinner, please email me (Attila@pavlath.org). We can also provide speakers for your organization or schools at any level interesting to students. We welcome any other suggestions how to reach these goals.

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(951 words)

Recycling Water
(Part 3)

by

Bill Motzer

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During wastewater treatment, triclosan generally degrades; however, some may not and therefore it can occur in trace amounts in treated wastewater effluent. It may also adsorb to sewage sludge. Undegraded triclosan may adsorb to particles settling out of the water column thereby contaminating sediments that may take more than 30 years to degrade. In the environment, triclosan may be degraded by microorganisms or it may photochemically degrade, forming other intermediate compounds, including between 3 to 12% of chlorophenols and dioxin, particularly, 2,8-dichlorodibenzo-p-dioxin (2,8-DCDD) and 2,4-dichlorophenol (2,4-DCP).

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In a study by the WateReuse Foundation, 10 PPCPs were subject to risk assessment calculations to determine the relative human risks from exposure to these compounds. Risk calculations are determined from dermal exposure, ingestion, and inhalation. Four of the above described PPCPs are listed in the table below. *Actual concentrations* are those at the 90^{th} percentile from a review of RW studies where PPCPs were measured in RW. *Acceptable concentrations* are those calculated concentrations at which adverse health effects are not expected from RW exposure or are levels at which RW contact is considered to be safe. *Relative exposure* is the time required for a person to be exposed to receive one dose or application.

PPCP	Person Exposed to RW	Concentration in µg/L		Relative Exposure at Actual Concentration (years)
		Actual Level	Acceptable (safe) Level	
Ibuprofin	Ag Worker Landscaper Golfer Child at play	0.5	1,700 530 1,600 890	28,000 8,600 26,000 67,000
17-beta estradiol	Ag Worker Landscaper Golfer Child at play	0.0084	0.18 0.05 0.15 0.39	16,000 5,000 13,000 160,000
DEET	Ag Worker Landscaper Golfer Child at play	1.5	17,000 5,200 38,000 18,000	85,000,000 26,000,000 190,000,000 110,000,000
Triclosan	Ag Worker Landscaper Golfer Child at play	0.49	3,100 7,600 2,700 1,400	7,600 2,400 6,600 17,000

Relative risks of known exposure to these PPCPs are extremely low. For example, risk of exposure to a child at play from 1.5 µg/L of DEET in RW used to irrigate plants would require 110 million years for that child to receive a single dose. Other risks such as ecological and metabolite risks (those from PPCP degradation products) are just now being researched and investigated. These will be discussed in a future series.