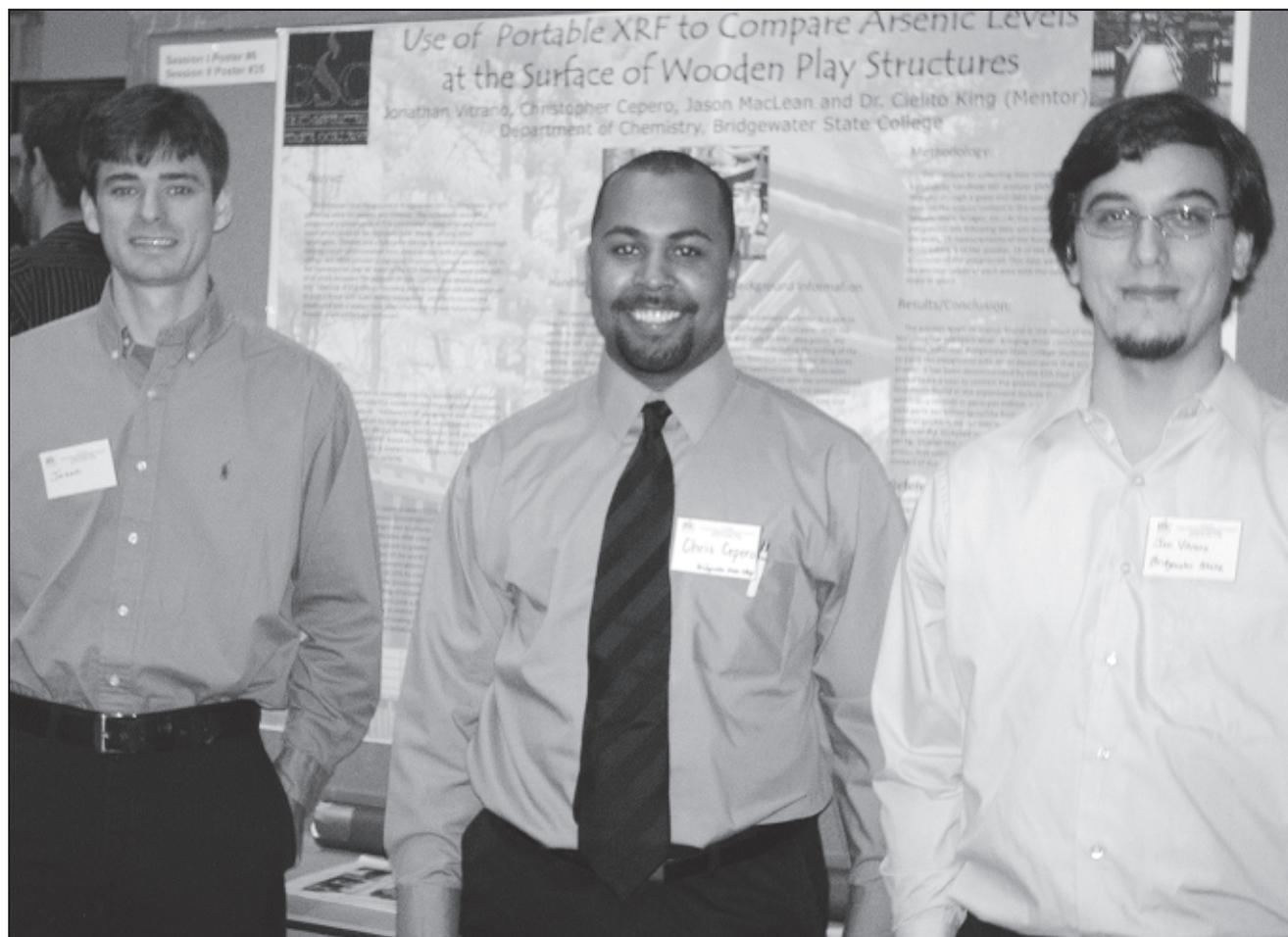


THE NUCLEUS

February 2010

Vol. LXXXVIII, No. 6



Monthly Meeting

NESACS Town Hall Meeting at Novartis

Summer Scholar Report

By Danielle Raad and Dr. Theodore Betley

Joanne Stubbe

An Interview by Mindy Levine

8th Annual Environmental Research Symposium

Joanne Stubbe

An Interview by Mindy Levine

When Joanne Stubbe, Novartis Professor of Chemistry and Biology at MIT, received a phone call late one night in September, she did not expect to hear John Holdren, President Barack Obama's science and technology advisor, on the line. Nor did she anticipate that he was calling to inform her that she had won the National Medal of Science, the highest domestic scientific honor. "It came as a complete surprise," Professor Stubbe said. "I had no idea."

Professor Stubbe, together with the 8 other National Medal winners, received her award from President Obama in a ceremony on October 7, 2009. One of the best parts of receiving the award, explained Professor Stubbe, was that "my family finally figured out that what I do is important." Nine of her family members were in Washington to witness the ceremony, characterized by Professor

Stubbe as "pretty inspiring" and "very emotional."

Impact on Career

Despite the importance of the award, Professor Stubbe does not anticipate that it will significantly impact her career. "Awards can sometimes give you visibility so you can attract better people," said Professor Stubbe. However, at a high-profile institution like MIT, such added visibility may be less important.

"In the long run, is the award the key thing?" Professor Stubbe asked rhetorically. "Not really. The key thing is solving the problems."

Research Activities

Professor Stubbe's research focuses on mechanistic investigations of biochemical pathways involved in nucleotide metabolism. This research has led to a number of successful applications, including the mechanism-based anti-cancer drug Gemcitabine, which is patented and distributed by Eli Lilly and Company. "The evidence is really strong that Gemcitabine works like other mechanism-based inhibitors we have studied in detail with an unusual

twist due to the second fluorine," said Professor Stubbe. "Why it works on cancer cells specifically is related to complex metabolism, and is something no one could have predicted *a priori*."

Professor Stubbe said that there are relatively few scientists interested in detailed enzymatic mechanisms today. "People today think they can look at a protein crystal structure and know how things work - and they don't have a clue. This is what we are up against."

Nonetheless, people can still be successful in this research area as long as they are willing to continually learn new things, which is good advice for all chemists in today's rapidly changing world, Professor Stubbe said. Mechanistic biochemical research remains an active and exciting research area, she said, because "there are a lot of problems left to solve."

Importance of Teaching

Despite such impressive research achievements, Professor Stubbe stated categorically, "I think my most important contributions have not been to research but to teaching." She said

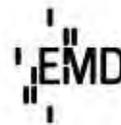
continued on page 12

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Complexes with transition metal-to-oxo multiple bonds stabilized by pyrrole-based ligands to target C-H bond functionalization. By Danielle Raad, Brown University and Dr. Theodore Betley, Harvard University.

Cover: *Pictured (R-L) are Jason MacLean, Christopher Cepero and Jonathan Vitrano of Bridgewater State College in front of their poster, "Use of Portable XRF to Compare Arsenic Levels at the Surface of Wooden Play Structures." They were mentored by Dr. Cielito King. Their poster was presented at the 8th Annual Undergraduate Environmental Research Symposium at Bridgewater State. (Photo courtesy of David Wilson, BSC Office of Institutional Communications).*

Deadlines: *April 2010 Issue: February 10, 2010*

May 2010 Issue: March 11, 2010

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Buchwald to Receive 2010 Esselen Award



Stephen L. Buchwald, Camille Dreyfus Professor of Chemistry at the Massachusetts Institute of Technology (MIT), has been selected to receive the 2010 Gustavus J. Esselen Award for Chemistry in the Public Interest from the Northeastern Section of the American Chemical Society (NESACS).

The Esselen Award is presented annually to recognize and reward a U.S. or Canadian chemist whose scientific and technical work has contributed to the public well-being and has thereby communicated positive values of the chemical profession. Professor Buchwald's selection recognizes his major impact on medicinal chemistry, due to his development of palladium and copper catalyzed processes to form carbon-nitrogen and carbon-oxygen bonds. These catalysts are used daily by the discovery groups of nearly every major pharmaceutical company worldwide. His catalysts have enabled the synthesis of novel, promising, small molecule drugs targeting a very wide range of diseases. His catalysts have also been instrumental in developing novel organic semi-conductors and in a wide range of other non-medicinal chemical syntheses.

Professor Buchwald joined the MIT Department of Chemistry in 1984 as an assistant professor after post-doc-

National Recognition for NESACS Student Chapters

The ACS Committee on Education has selected the following student chapters in the Northeastern Section to receive special recognition for the programs and activities described in their 2008-2009 reports:

Outstanding Recognition

Northeastern University, Boston, MA; Andrea Lebed, chapter president; Prof. Jordan Swift, faculty advisor.

Commendable Recognition

Stonehill College, North Easton, MA; Natalie Dogal, chapter president; Prof. Cheryl Schnitzer and Prof. Marilena Hall, faculty advisors

Suffolk University, Boston, MA; Urjana Porcei, chapter president; Prof. Doris Lewis, faculty advisor.

Honorable Mention

Keene State College, Keene, NH; Joseph Meany, chapter president; Prof. Colin Abernethy and Prof. Denise Junge, faculty advisors

They will be honored at the 239th ACS National Chemistry Meeting in San Francisco, CA, on Sunday, March 21, 2010. ◇

total work at the California Institute of Technology. He earned a B.S. in chemistry at Brown University in 1977, and an A.M. (1980) and a Ph.D. (1982) in chemistry from Harvard University. He has previously received the ACS Award in Organometallic Chemistry in 2000 and the ACS Award for Creative Work in Synthetic Organic Chemistry in 2006.

Professor Buchwald will receive the Esselen Award medal and a \$5000 prize at the Esselen award dinner and lecture at Harvard University on Thursday, April 8, 2010. ◇

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Summer Scholar

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Monthly Meeting

The 903rd Meeting of the Northeastern Section of the American Chemical Society

Thursday – February 18, 2010

Novartis Institutes for Biomedical Research
250 Massachusetts Ave, Cambridge, MA 02139

2:30 pm Board Meeting

4:00-6:00 pm Panel Discussion

Northeastern Section ACS (NESACS) Town Hall Meeting— “The Prospects for Chemistry in the Future US Economy”

- Julian Adams, panelist, President and CSO of Infinity Pharmaceuticals
- Chris Austin, panelist, Director of the NIH Chemical Genomics Center
- Scott Biller, moderator, VP of Global Discovery Chemistry, Novartis Institutes for Biomedical Research
- Joe Francisco, panelist, ACS President for 2010, Purdue University
- Robert Langer, panelist, Institute Professor and entrepreneur, Massachusetts Institute of Technology
- Jordan Swift, panelist, Co-Op Education Coordinator, Northeastern University Chemistry Department

6:00-7:00 pm Reception

ADVANCED REGISTRATION IS REQUIRED.

Registration details will be on the front page at www.nesacs.org. If you have any questions, please contact Leland Johnson at public.relations@nesac.org or ljohnson@creagenbio.com

Directions: From the Massachusetts Turnpike: Take exit 18 toward Brighton/Cambridge. Keep right at the fork to continue toward Cambridge St and merge onto Cambridge St. Continue onto River St/River St Bridge. Continue to follow River St. for 0.8 mi to Central Square. Turn right at Massachusetts Ave. Destination will be on the right in 0.5 mi.

Parking: Shaw's (Star) Supermarket parking garage, using the entrance on Franklin or Green Streets.

By Public Transportation: Take the MBTA Red line to the Central Square stop and proceed to 250 Massachusetts Ave.

February Meeting

Genesis of a Town Hall Forum: Reasons to Attend a NESACS Monthly Meeting

By Leland Johnson

About a year ago, January 15th, to be exact, I walked in early and picked an empty chair amongst a sea of empty place settings near the back of Whitney Hall B, Holiday Inn in Brookline. It was the night of the Monthly Meeting for NESACS, and as the YCC Chair at that time, I attended the NESACS board meetings, social hour, and an occasional dinner in order to meet with colleagues, make new connections, and listen to as much of the program as I could before heading home to help put my little guy to sleep for the night.

I put my coat on the back of the chair and a cloth napkin on my seat, and I headed back out into the function lobby for the social hour. After catching up with several colleagues from industry, volunteers for NESACS and those who were working on the NESACS-GDCh German Exchange Program, I returned with the masses to find nearly all of the seats occupied with section members, ACS scholars, NESACS board members, and other guests.

I was happy to find that my efforts to reserve a seat had succeeded, and there happened to be one last available seat directly to my left. A few minutes later, I introduced myself to Professor Joe Francisco as he sat down in the seat next to me. This was a pleasant surprise and, as it turned out, a stroke of luck. As the dinner progressed, table members engaged Joe and one another, and the conversation flowed around the table.

I talked with Joe for several minutes about the economy, prospects for chemistry, and my family. As the local YCC chair, I mentioned that several of my colleagues from various pharmaceutical and biotechnology companies in the area had missed the opportunity to talk with him during his stay.

Continued on page 12

New Members

Invitation to attend a meeting

You are cordially invited to attend one of our upcoming Section meetings as a guest of the Section at the social hour and dinner preceding the meeting.

Please call Marilou Cashman at 800-872-2054, 508-653-6329 or: [Mcash\(at\)aol.com](mailto:Mcash(at)aol.com) by noon of the first

Thursday of the month, letting her know that you are a new member. ◇

What exactly goes on at NESACS' monthly Board meetings?
www.nesacs.org/reports

The 8th Annual Undergraduate Environmental Research Symposium at Bridgewater State College

On Saturday, November 14, 2009, the 8th Annual Undergraduate Environmental Research Symposium was held in the John Joseph Moakley Center at Bridgewater State College. The Symposium was sponsored by Bridgewater State College, their Office of Undergraduate Research and Center for Sustainability, and by NESACS.

The Symposium ran from 9:00 AM to 2:30 PM and featured a record 58 poster presentations from undergraduate researchers, and was attended by over 140 students, faculty and guests representing eleven public and private colleges and universities in New England. Attendees were treated to a continental breakfast and lunch.

The Symposium was officially opened by Dr. Howard London, Provost and Vice-President for Academic affairs at Bridgewater State College. Dr. London praised the students for their work confronting urgent environmental issues, and fashioning acceptable and effective solutions. He congratulated the students on their work and also expressed his thanks to the faculty mentors who provided guidance and support.

The theme of the 2009 Symposium was "Environmental Analysis." The formal program began at 9:30 AM with a presentation by Dr. Carl Lamborg from the Department of Marine Chemistry and Geochemistry at Woods Hole Oceanographic Institution. Dr. Lamborg's talk was entitled, "Research into the Biogeochemistry of Mercury in the Ocean and its Impact on Public Policy."

The poster sessions began immediately following the presentation, running from 10:45AM – 2:15PM.



Guest speaker Dr. Carl Lamborg, Department of Marine Chemistry and Geochemistry, Woods Hole Oceanographic Institution, "Research into the Biogeochemistry of Mercury in the Ocean and its Impact on Public Policy"



Student researchers from Plymouth State University present their work, L-R: Kris Wojtusik, Rebecca Mailhot, and Ben Crawford, "Habitat preference of crayfish (*Orconectes virilis*) among three different macrophytes" (Photos by David Wilson)

The complete program with all presenters, titles and abstracts can be accessed from the symposium web page: <http://www.bridgew.edu/Environmental/>

The 9th Annual Environmental Research Symposium is tentatively scheduled for Saturday, November 13, 2010. ◇

Announcement

The Sixteenth Annual Northeastern Section Undergraduate Day

Saturday, February 27th, 2010

Hosted by the Department of Chemistry, UMass Boston

Sponsored by the Northeastern Section of the American Chemical Society

- 9:00** Registration (Directions at http://www.umb.edu/parking_transport/directions.html; park in the North Lot, Campus Center; come into the Campus Center and follow the signs to the registration desk)
- 9:30** Welcoming Remarks
- 9:45** Keynote Address – Berkeley W. Cue, Vice President, Pharmaceutical Sciences, Pfizer Global R&D (retired)
- 10:30** Coffee Break
- 10:45** Research Talks (choose one)
- 12:00** Lunch
- 12:30** Resume Review and Graduate School/Industry Fair
- 1:30** Panel Discussions (choose one):
1. Choosing and Applying to a Graduate School
 2. Careers in Chemistry without a Graduate Degree
- 2:15** Adjournment

There will be a \$10 registration fee to partially cover the cost of coffee and lunch, which will be provided. If you would like more information, or if your school or company would like to send a representative to the Graduate School and Industry Fair, please contact Marietta Schwartz – marietta.schwartz@umb.edu; phone 617-287-6146; fax 617-287-6030. ◇

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our editor by calling and saying you appreciate the quality and content of our newsletter. Our editor works hard to maintain a publication of interest to our membership. Oh, and by the way you could also give credit to our advertisers who financially support us.

February Historical Events in Chemistry

by Leopold May, The Catholic University of America, Washington, DC

February 3, 1893

Lenora Neuffer Bilger, a researcher in asymmetric nitrogen compounds, was born on this date. She also received the Garvan Medal from ACS in 1953.

February 5, 1840

John Boyd Dunlop, who developed pneumatic rubber tires, was born on this date.

February 6, 1860

One hundred and fifty years ago, Nikolai D. Zelinsky, was born on this date. He researched on the catalysis of disproportionation reactions of hydrocarbons and the bromination of fatty acids (Hell-Volhard-Zelinsky reaction).

February 7, 1850

John B. F. Herreshoff, who developed a method for manufacturing sulfuric acid, was born on this date.

February 8, 1777

Bernard Courtois, who was born on this day, discovered iodine in the liquor from the lixiviation of kelp in 1811.

February 8, 1866

Moses Gomberg, who synthesized the first stable free radical (triphenyl-methyl), was born on this date. He also did research on tautomerism.

February 11, 1847

Thomas A. Edison was an inventor who invented the incandescent lamp and the mimeograph. He was born on this date.

February 12, 1785

Two hundred and twenty-five years ago, Pierre L. DuLong was born on this date. He discovered nitrogen trichloride in 1813; and was a researcher on refractive indices and specific heats of gases. In 1819, he and Aléxis Thérèse Petit discovered the law of constancy of atomic heat and suggested that acids were compounds of hydrogen in 1815. He

devised a formula for measuring the heat value of fuels (DuLong Formula).

February 14, 1917

Twenty-five years ago in 1985, Herbert A. Hauptman and Jerome Karle shared the Nobel Prize in Chemistry for their outstanding achievements in the development of direct methods for the determination of crystal structures. Herbert A. Hauptman was born on this date.

February 18, 1745

Alessandro G. A. A. Volta, who was born on this date, invented the voltaic pile, *volta pila*, and observed the bubbling of methane in swamps. He developed a gas lantern that was electrically ignited. The unit of electric potential, the volt, is named in his honor.

February 20, 1937

Robert Huber, who did research on the three-dimensional structure of proteins involved in photosynthesis,

was born on this date. In 1998, he shared the Nobel Prize in Chemistry with Johann Diesenhofer and Hartmut Michel for the determination of the three-dimensional structure of a photosynthetic reaction centre.

February 24, 1913

William S. Johnson devised new and efficient methods to synthesize complex molecules including corticoid steroids. He was born on this date.

February 25, 1869

Phoebus A. T. Levene, who was born on this date, was a researcher on the biochemistry of proteins.

February 26, 1905

William J. Sparks, an innovator and developer in synthetic rubber, was born on this date.

Additional historical events can be found at Dr. May's website:

<http://faculty.cua.edu/may/ChemistryCalendar.htm>. ◇



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Northeast Region of the American Chemical Society, Inc.

CALL FOR NOMINATIONS FOR THE 2010 NORTHEAST REGION AND ACS AWARDS

Northeast Region Awards for 2010

- **THE ACS DIVISION OF CHEMICAL EDUCATION NORTHEAST REGION AWARD FOR EXCELLENCE IN HIGH SCHOOL TEACHING**
- **THE E. ANN NALLEY REGIONAL AWARD FOR VOLUNTEER SERVICE TO THE AMERICAN CHEMICAL SOCIETY**
- **THE ACS REGIONAL INDUSTRIAL INNOVATION AWARDS**
- **THE NORTHEAST REGION, ACS AWARD FOR ACHIEVEMENTS IN THE CHEMICAL SCIENCES**

The deadline for these awards is April 15, 2010

Award offered by the National ACS

**THE STANLEY C. ISRAEL REGIONAL AWARD FOR ADVANCING
DIVERSITY IN THE CHEMICAL SCIENCES**

The deadline for this award is March 1, 2010

Presentation of awards:

**The awards will be presented at the
2010 Northeast Regional Meeting (NERM)
Potsdam, New York
June 2 – 5, 2010**

***Specifics about each award and nomination forms may be found on the
webpage for the 2010 Northeast Regional Meeting (NERM)***

www.nerm2010.org

Call for Nominations

Awards of the Northeast Region of the American Chemical Society

All awards will be presented at the 2010 Northeast Regional Meeting (NERM) June 2nd – 5th, 2010, Potsdam, New York

THE ACS DIVISION OF CHEMICAL EDUCATION NORTHEAST REGION AWARD FOR EXCELLENCE IN HIGH SCHOOL TEACHING

Purpose: To recognize, encourage, and stimulate outstanding teachers of high school chemistry in the Northeast Region.

Eligibility: The nominee must be actively engaged in the teaching of chemistry or a chemical science in a high school (grades 9-12) on at least a half-time basis.

THE E. ANN NALLEY REGIONAL AWARD FOR VOLUNTEER SERVICE TO THE AMERICAN CHEMICAL SOCIETY

Purpose: To recognize the volunteer efforts of individuals who have served the American Chemical Society by contributing significantly to the goals and objectives of the Society through their Regional Activities.

Eligibility: The nominee must be a member of the ACS, residing in a Local Section within the Northeast Region, who has made significant contributions to the Section and Region of the ACS.

THE ACS REGIONAL INDUSTRIAL INNOVATION AWARDS

Purpose: To celebrate the successful innovations of industrial chemists and chemical engineers which contribute to the health of their local and regional economy and the corporate leadership for its advancement of a healthy economy. This award is given to an individual or team of individuals whose

creative innovations have contributed to the commercial success of their company and, consequently, to the good of the community and society.

Eligibility: Nominee must be a chemical professional and an ACS member. For team nominations, only one member needs to be an ACS member. Those who are not ACS members, but are employed by an ACS Corporation Associates Member Company, qualify for nomination.

THE NORTHEAST REGION, ACS AWARD FOR ACHIEVEMENTS IN THE CHEMICAL SCIENCES

Purpose: To recognize notably outstanding achievements by a chemist in the Northeast Region. The award is conferred annually on a scientist who has made meritorious research contributions leading to the advancement of pure or applied chemistry.

Eligibility: The nominee must be a member of the ACS, residing in the Northeast Region and whose work, on which the nomination is based, has been carried out during a period of residence in the area encompassing the Local Sections that comprise the Northeast Region.

The deadline for all of the above listed awards is April 15, 2010.

For most awards, a nomination form must be used. Please refer to the 2010 NERM Website for all forms and other guidelines. www.nerm2010.org

THE STANLEY C. ISRAEL REGIONAL AWARD FOR ADVANCING DIVERSITY IN THE CHEMICAL SCIENCES

Sponsor: ACS Committee on Minority Affairs

Purpose: The Stanley C. Israel Regional Award recognizes individuals and/or institutions that have advanced diversity in the chemical sciences and significantly stimulated or fostered activities that promote inclusiveness within the region. The award consists of a medal and a \$1,000 grant to support and further the activities for which the award was made. The award also will include funding to cover the recipient's travel expenses to the ACS

regional meeting at which the award will be presented.

Eligibility: Nominees may come from academia, industry, government, or independent entities, and may also be organizations, including ACS local sections and divisions. The nominee must have created and fostered ongoing programs or activities that result in increased numbers of persons from diverse and underrepresented minority groups, persons with disabilities, or women that participate in the chemical enterprise.

The Nomination Package must include:

- A letter of nomination
- A CV or resume containing relevant diversity-promotion activities and factual data on outcomes.
- At least one, but no more than three supportive letters, one of which must come from the nominee's ACS Local Section. Mailing address, phone number(s), and e-mail address of nominee/supporter must be provided.

Contact Information:

American Chemical Society
Department of Diversity Programs
1155 Sixteenth Street, NW
Washington, DC 20036
Fax: 202-776-8003
Email: Diversity@acs.org

Deadline for receipt of nominations: March 1, 2010. ◇

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Find yours at
www.nesacs.org/jobs

Summer Scholar Report

Complexes with transition metal-to-oxo multiple bonds stabilized by pyrrole-based ligands to target C-H bond functionalization

Danielle Raad, Chemistry Department, Brown University, Providence, RI

Dr. Theodore Betley, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA

Abstract

Complexes with high-valent metal-oxo multiple bonds are potential catalysts for the activation of typically inert C-H alkane bonds. We propose a group of transition metal complexes characterized by such metal to ligand multiple bonds, and stabilized by tridentate pyrrole-based ligand platforms. These tris(pyrrole)ethane, or TPE, ligands were prepared synthetically with substituted pyrrole moieties, in particular 2-mesityl pyrrole. These were subsequently deprotonated and metallated, with the insertion of a transition metal coordinated to the three pyrrole nitrogens. Further steps include oxidizing the metal center and producing metal-to-oxo multiple bonds stabilized by the TPE ligand. These reactive oxo, and analogous imide, complexes may have the potential to activate inert C-H bonds and subsequently catalyze their functionalization.

Background

Saturated hydrocarbons are typically unreactive, and have been historically inert in all but the most extreme of reaction environments. At elevated temperatures, combustion occurs indiscriminately, yielding the industrially useless products of carbon dioxide and water. Established methods to induce alkane reactivity include cracking, thermal dehydrogenation, and exposure to highly reactive species, which involve acute reaction conditions, are relatively expensive, and offer little control over product selectivity.¹ Facile methods for activation of these stable C-H bonds and conversion of ubiquitous alkanes into synthetically useful compounds could revolutionize the chemical industry, allowing the exploitation of naturally found hydrocarbons as a previously-untapped low-cost chemical feedstock.²

Practical insertion into the hydrocarbons of new bonds, such as C-C, C-O, or C-N, necessitates the use of effective transition metal catalysts, which are able to provide predictable selectivity.^{3,4} Functionalization can occur without the need for intermediates or waste products, decreasing unpleasant environmental consequences while optimizing atom and energy efficiency.⁵ Several catalysts have been thus far discovered with such functionalization abilities. A small-molecule iron catalyst has been shown to oxidize C-H bonds with hydrogen peroxide,³ while much research is focused on catalytic C-H amination, for example using copper⁵ or iron organometallic complexes.⁶

Often, the chemical species capable of such direct introduction of a new functional group into a stable hydrocarbon bond is characterized by a metal-ligand multiple bond. Oxygen, nitrogen, or carbon centers doubly or triply bound to late transition metals have been found to promote such transformations.⁷ This feature is successfully utilized by

nature; cytochrome P450 enzymes employ the use of an Fe=O intermediate to aid in the catalysis of C-H to C-O bonds of compounds in the human body.^{2,8}

Synthetic Methods

The initial step in building the catalyst complex is to assemble the ligand backbone. All manipulations were performed under inert atmosphere in a glove box, and heated reactions were carried out in air-tight bomb flasks in fume hoods. First, distilled pyrrole was carefully deprotonated with sodium hydride. The resulting sodium pyrrolide was reacted with 2-bromomesitylene in the presence of a palladium catalyst and zinc chloride to form 2-mesityl pyrrole (Scheme 1), according to a previously reported procedure.⁹ The mixture was heated at 100°C for two days. This 2-

Scheme 1

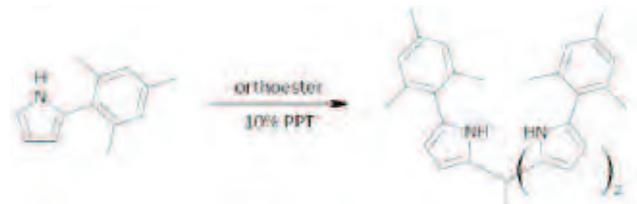
Synthesis of 2-Mesityl pyrrole



mesityl pyrrole was next reacted with trimethyl orthoacetate with the acid catalyst pyridinium p-toluene sulfonate (PPTS) at 70°C for one week (Scheme 2). The product is the stable tris(2-mesityl-pyrrole)ethane (TPE) tridentate ligand structure. To prepare for metallation, it is deprotonated and lithiated. A reaction with phenyllithium at low temperatures results in a lithium atom ligated to each of the three pyrrole

Scheme 2

Synthesis of tris-pyrrole ethane(TPE) ligand



nitrogens, with a THF molecule in the other coordination site (Scheme 3). Finally, with this ligand backbone, abbreviated (TPE)Li₃, a series of metallation reactions were run with different ruthenium, nickel, and cobalt compounds (Table 1), by mixing the two thawing reagents.

Results and Discussion

The synthesis of the TPE ligand resulted in pure material, although in sparse yields (10-20%). ¹H NMR shifts occurred at δ 7.33, 6.82, 6.16, 6.04, 2.19, 2.15, 1.81ppm (Figure 1). Though the TPE ligand was isolated in relatively pure yields, when reacted with the different metal precursors

in the following reactions, it produced metallic complexes in extremely low yields, or failed completely. An outline of the different metallation reactions can be seen in table 1. Two ruthenium precursors were used, $\text{RuCl}_2(\text{PPh}_3)_3$ and $\text{RuCl}_2(\text{COD})$. Both of the preliminary reactions, run by warming frozen reactants up to room temperature and stirring for 2 hours yielded no reaction (1, 2). The conditions for the reaction with $\text{RuCl}_2(\text{PPh}_3)_3$ were next altered to try to induce the reaction. Increasing the reaction time to 15 hours was unsuccessful (3). However, heating the reaction at 60°C for one day (4) produced small, unmeasurable amounts of a metallated ruthenium complex. Reaction of $(\text{TPE})\text{Li}_3$ with analogous nickel and cobalt compounds (5, 6) produced compounds that go through a series of color changes as the solvent is changed. This indicates ligand exchange with the solvent molecules. The reaction with cobalt chloride afforded no measurable product (7).

Future Directions

These preliminary tests show that it is possible to create organometallic complexes by inserting transition metals into the tridentate TPE ligand, with the appropriate reaction conditions. Future work on this project involves tuning these conditions to induce clean and efficient metallation reactions. Once the metallated complexes are stabilized, crystal structures will be determined in order to elucidate the identity of the additional ligands on the metal, and the structure of the complex.

The specific ligand used in the aforementioned experi-

Scheme 3

Lithiation of TPE ligand

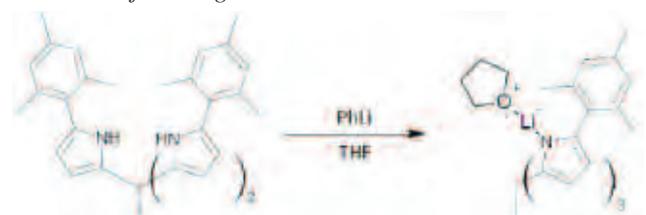


Figure 1

$^1\text{HNMR}$ of TPE Ligand

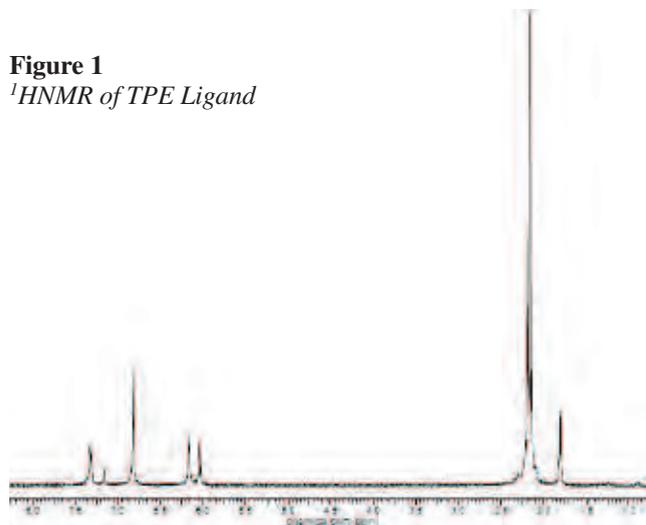


Table 1

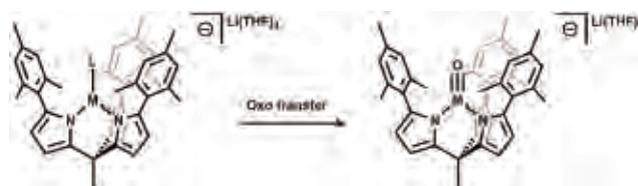
Summary of transmetalation experiments with lithiated TPE ligand

Entry	Metal Precursor	Temperature	t (hr)	Reaction ^a
1	$\text{RuCl}_2(\text{PPh}_3)_3$	RT	2	no
2	$\text{RuCl}_2(\text{COD})$	RT	2	no
3	$\text{RuCl}_2(\text{PPh}_3)_3$	RT	15	no
4	$\text{RuCl}_2(\text{PPh}_3)_3$	60°C	24	yes
5	$\text{NiCl}_2(\text{PPh}_3)_2$	RT	2	yes
6	$\text{CoCl}_2(\text{PPh}_3)_2$	RT	1	yes
7	CoCl_2	RT	1.5	no

ments has mesityl groups located off the δ position of the pyrrole groups. Substituents with larger mesityl analogues, such as 2,4,6-(R) $_3\text{C}_6\text{H}_2$, where R is CF_3 , ^iPr , or ^tBu may also be used, in addition to smaller molecules, such as the simpler isopropyl pyrrole and tert-butyl pyrrole.¹⁰ These will serve to sterically hinder the metal center around the C_3 -symmetric pocket of the ligand backbone, enough to prevent the formation of dimers. Tuning the substituents could produce slightly different results in the next step of the catalyst synthesis.

The next step after metallation will be oxo transfer to establish a metal to oxygen bond. A variety of oxygen transfer agents would be used, such as ONMe_3 , PhIO , O_2 , O_2CMe_2 , oxone, and H_2O_2 (Scheme 4). A similar group transfer reaction using amides will be performed to produce the electrically analogous nitrene functionality.

Scheme 4



The oxidation state of the resulting complexes would be +4, equivalent to the reactive iron metal center of the cytochrome P450 enzyme. Once these complexes with transition metals-to-oxo multiple bonds are stabilized, they will be characterized and compared. An attempt will also be made to oxidize them further; an oxidation state of +5 would increase their reactivity even more. Reactivity profiles with various alkanes will be determined, so that the ability to activate or even functionalize C-H bonds may be probed. Hopefully, this research will continue and culminate in the production of a new class of complexes with unique reaction chemistry suitable for functionalizing alkanes, with the potential to drastically impact the field of organic synthesis.

Acknowledgements

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continued on page 4

Joanne Stubbe

Continued from page 2

teaching can have a tremendous impact. For example, if there are 25 students in a class, and 5 of those students are inspired, each one can go on to make a major contribution to his or her field.

Recently Professor Stubbe gave a seminar at the University of South Carolina. While at the university, one of the faculty members approached her and said that her class was the best class he had ever taken. "I may not even remember a particular student," Professor Stubbe said, "but I think I am impacting the people who go into science."

Gender Issues

"I don't want to discuss this issue," Professor Stubbe said when the question of gender issues in chemistry was first raised, "even though I think it is a very important one." Nonetheless, as the first woman to be tenured in the MIT chemistry department, she is perhaps in a unique position to comment on the question. Professor Stubbe has spent a lot of time helping young faculty members, both men and women, adjust to life at MIT.

Professor Stubbe explained that there used to be discrimination against female academics of all disciplines, in areas such as compensation and the tenure process. There has been tremendous progress in reducing such discrimination over the years, said Professor Stubbe, so that "women coming in the present generation may not even realize how much energy went into changing the culture."

Advice about Academia

Professor Stubbe explained some advantages to choosing a career in academia. "A big plus for academics is that you can work on something that you are really passionate about," said Professor Stubbe. "For example, I have been fortunate my whole life to be paid to do my hobby."

Professor Stubbe cautioned new faculty members against spending excessive energy worrying about tenure decisions and departmental poli-

February Meeting

Continued from page 5

Around the time dessert was served, I had to confess to Joe that I would be unable to stay for his talk. As we wrapped up our own discussion, I asked Joe to come back to Boston for an open forum, inviting younger chemists to attend for a discussion and a Q and A session.

A few weeks later, I began the conversations with Alicia Harris (National ACS) regarding my invitation to Joe. He accepted, and in August we secured the date, February 18th. As the fall approached, it was time to secure a location and a sponsor. I emailed Scott Biller, VP of Global Discovery Chemistry at Novartis Institutes for Biomedical Research (NIBR). Within a few days, availability of space at NIBR was confirmed, and Scott informed me that Novartis would sponsor the event. Shortly thereafter, Scott, John McKew and I invited leaders from industry, government, and academia (many bridging at least two of these areas) to join the panel. By

tics. "Spend more time doing good science," she said, and hopefully the good science will be recognized appropriately. Moreover, in Professor Stubbe's opinion, the six-year period before tenure is really too short to make a substantial contribution, especially in the biological sciences.

Reflections on MIT

When asked to reflect on her career at MIT, Professor Stubbe said, "My career wouldn't be what it is at all without being at MIT. Being here has allowed me to set up outstanding collaborations, which has enabled me to do science that I otherwise couldn't have done. At MIT, there are so many people interested in science that if you use your energy wisely you can do just about anything. Being at MIT has allowed me the privilege of working with the best graduate students in the country."

Professor Stubbe concluded, "It is a tough place, but a very special place." ◇

December, we had merged the event with the February Monthly Meeting, and the schedule of events had been set.

The members of the panel, including Scott Biller as moderator, are:

- Julian Adams, President and CSO of Infinity Pharmaceuticals
- Chris Austin, Director of the NIH Chemical Genomics Center
- Joseph Francisco, ACS President
- Robert Langer, Institute Professor at MIT and entrepreneur
- Jordan Swift, Co-Op Education Coordinator, Chemistry Department, Northeastern University

We are looking forward to a discussion of, "The Prospects for Chemistry in the Future US Economy." Following introductory remarks and presentations beginning at 4 PM, there will be a Q and A session with members of the audience. There will be a reception from 6 to 7 PM following the discussion. This NESACS February Monthly Meeting is sponsored and hosted by Novartis, and I wish to personally thank Scott Biller and his team for facilitating this anticipated event. The NESACS monthly meetings provide great opportunities to network with colleagues, classmates, speakers leaders in the chemical sciences. In retrospect, I encourage more NESACS members to attend our monthly meetings. You can never tell who might sit next to you during dinner, and where that might lead. Networking is clearly a huge part of monthly meetings, and we encourage you to participate.

Advanced reservations are required and space is limited. To inquire about availability, please contact Leland L. Johnson, Jr., ljohnson@creagenbio.com.

The meeting will be held at NIBR in Cambridge at the 250 Massachusetts Avenue site. Parking will be at Shaw's (Star) Supermarket parking garage, using the entrance on Franklin or Green Streets. ◇

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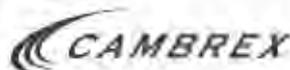
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Timothy F. Jamison (MIT)
Brandeis University, Gerstenzang 122
3:45 pm

Feb 02

Prof. Phil Dawson (Scripps Research Institute)
"Synthetic Protein Engineering"
Boston College, Merkert 130
4:00 pm

Feb 03

Thomas Rauchfuss (Univ. Illinois at Urbana
Champaign)
MIT, 6-120
4:15 pm

Feb 04

Karl Scheidt (Northwestern University)
MIT, 6-120
4:00 pm

Max Diem (Northeastern University)
"Micro-spectroscopy for Medical Diagnostics:
Infrared and Raman Microscopy of Human
Cells"
Univ. New Hampshire, Iddles L103
11:10 am

Feb 08

The Pfizer Symposium
David MacMillan (Princeton University)
Harvard, Pfizer Lecture Hall
4:00 pm

Feb 09

Prof. Daniel Raleigh (SUNY-Stony Brook)
Boston College, Merkert 130
4:00 pm

Feb 10

Malcolm Chisholm (Ohio State University)
MIT, Room 6-120
4:00 pm

Feb 16

Prof. Karl A. Scheidt (Northwestern University)
"New Discoveries with Carbene Catalysis"
Boston College, Merkert 130
4:00 pm

Feb 18

Helmut Schwarz (Technical University of
Berlin)
Harvard, Pfizer Lecture Hall
4:00 pm

Feb 22

Anna Croft (Bangor University, UK)
MIT, 56-114
4:00 pm

Feb 23

Prof. Brad Smith (Notre Dame University)
"Supramolecular probes for optical bioimaging"
Boston College, Merkert 130
4:00 pm

Feb 24

Elena Rybak-Akimova (Tufts University)
Harvard, Pfizer Lecture Hall
4:00 pm

Feb 25

Judith Herzfeld (Brandeis University)
Harvard, Pfizer Lecture Hall
4:00 pm

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