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THE NUCLEUS

April 2014 *Vol. XCII, No. 8*

Monthly Meeting

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Summer Scholar Report

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By Amanda W. Stubbs and David R. Manke

ACS Northeastern Section at Fenway Park!

Red Sox Game Tuesday, May 6

Developing a Passion for Science

By Rajeev Chorghade, rajchorghade@gmail.com

In March 2010, as a graduating high-school student, I was fortunate to publish an article in the Nucleus[1] describing my career aspirations, and how my progressive research internships helped guide my interests and passion for science. I am extremely grateful for an opportunity to write a follow-up article detailing my experiences since that time, and how I have continually sought out opportunities to conduct research and work towards bringing my goal of being admitted to an M.D./Ph.D. degree program to fruition. I was thrilled to work with several extraordinarily distinguished scientists, and I was struck by how remarkably well they mentored, guided and inspired their students.

I am currently a senior majoring in chemistry with a minor in biomedical engineering at Carnegie Mellon University. I strive to ultimately pursue a career in academic medicine. This aspiration was instilled in me at a very young age, fueled by a love and passion for sports, science and medicine, and a desire to help people. To complement my determination and excitement at the prospect of advancing science, an entrepreneurial mindset was essential in seeking out opportunities for conducting research.

For my first laboratory experience, I was fortunate to secure a research appointment at the California Institute of Technology under Professor Robert Grubbs. Working under a Nobel Laureate was truly an inspiring experience. I studied olefin metathesis by the Grubbs catalyst and performed chiral reductions with menthol as an auxiliary[2]. This opportunity developed my technical skills and introduced me to the problem-solving mindset necessary to carry out scientific research. From my first experience in a chemical laboratory, I was hooked. I loved research, and I knew that solving problems using precise scientific methodology would be instrumental in reaching my ultimate goal of becoming a physician.

Next I secured a research appointment at the Beth Israel Deaconess Medical Center, under the mentorship of Dr. Vikas Sukhatme, Chief Academic Officer. In my first exposure to cell culture work, I treated cancerous A549 cells with combinations of anticancer drugs to determine their synergistic efficiency in blocking mitochondrial function and causing selective apoptosis. This incredible experience, allowed me to work with a living organism, and directly see the benefits of advancing science at the cellular level.

I then worked in the field of organic chemistry at Harvard University under the supervision of Professor Eric Jacobsen. The Massachusetts Life Sciences Center awarded me a highly competitive internship in the "Internship Challenge". I designed and implemented thiourea catalysts for enantioselective synthesis. This project allowed me to delve into mechanistic studies of reactions, promising to give me a greater insight into the molecular basis of medicine.

During a study abroad semester at the University of Cambridge, I worked in flow chemistry under the mentorship of Professor Steven Ley. This was truly an amazing experience to learn both the science and culture of England and life in the hallowed halls of Trinity College. I worked to optimize the Oppenauer oxidation and Meerwein-Ponndorf-Verley reduction using hydrous zirconia catalysts.

Oxidation is an extremely important step used in the synthesis of numerous commercial pharmaceutical drugs. However, there is currently no perfect method to perform oxidation without the use of expensive heavy metals, toxic reagents, or harsh conditions. My goal was to develop a faster, cheaper, safer system to perform Oppenauer oxidations in a more sustainable manner, using green solvents, less toxic reagents, and mild conditions[3].

Hydrous zirconia was chosen as a catalyst because it is cheap, recyclable, stable to high temperatures, and was shown to work well in MPV reductions. The hydrous zirconia catalyst was calcinated at different temperatures to increase its active surface area. Below, Figure 1 shows the ketone products of benzylic alcohols obtained through the use of acetone as an oxidant at 80 °C.

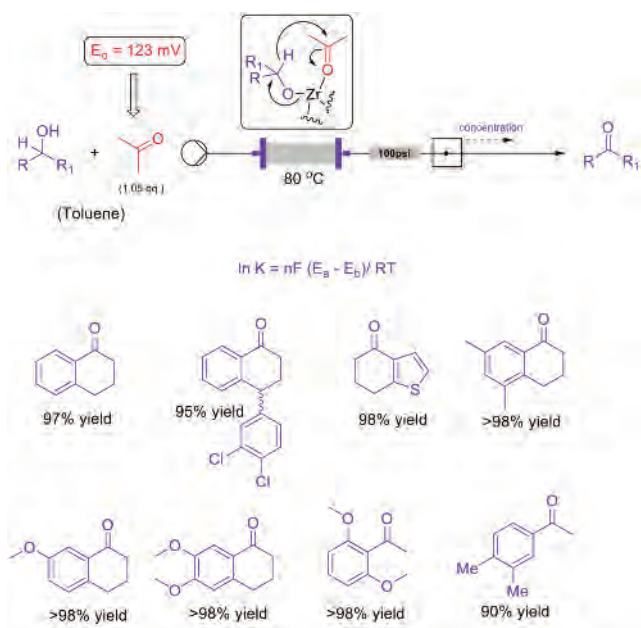

Figure 1: *Oxidation products using acetone as oxidant*[3]

With acetone used as the oxidant, the above products were obtained in high yield, with very few aldol condensation side products. These products had relatively low oxidation potentials, and, due to their relatively flat, fixed geometries, they were readily able to bind to the catalyst in the proper conformation to carry out the electron-transfer mechanism. However, to oxidize alcohols with higher oxidation potentials, a large excess of acetone would be needed, which would result in greater aldol side product

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September 2014 Issue: July 15, 2014

THE NUCLEUS

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Call for Nominations

The 2014 James Flack Norris Award for Outstanding Achievement in the Teaching of Chemistry

Deadline: April 15, 2014

Nominations are invited for the 2014 James Flack Norris Award, which consists of a certificate and an honorarium of $3,000 and is given annually by the Northeastern Section (NESACS). The presentation will take place at a ceremony and dinner in November, 2014, and will include a formal address by the awardee. The Award was established in 1950 by NESACS to honor the memory of James Flack Norris (1871-1940), a professor of chemistry at Simmons College and M.I.T., chair of NESACS in 1904, and ACS President in 1925-26.

Nominees should have served with special distinction as teachers of chemistry at any level: secondary school, college, and/or graduate school. With the presentation of the first Award in 1951, awardees have included many eminent teachers at all levels whose efforts have had a wide-ranging effect on chemical education. The recipient will be selected from an international list of nominees who have served with special distinction as teachers of chemistry with significant achievements.

A nomination in the form of a letter should focus on the candidate's contributions to and effectiveness in teaching chemistry. The nominee's curriculum vitae should be included and, where appropriate, a list of honors, awards, and publications related to chemical education. Seconding letters may also be included; these should show the impact of the nominee's teaching for inspiring colleagues and students toward an active life in the chemical sciences, and attest to the influence of the nominee's other activities in chemical education, such as textbooks, journal articles, or other professional activity at the local, national, and international level.

The nomination materials should consist of the primary nomination letter, supporting letters, and the candidate's curriculum vitae. Reprints or other publications should NOT be included. The material should not exceed thirty (30) pages, and should be submitted electronically in Adobe PDF format through April 15, 2014 to Ms. Anna Singer, NESACS Administrative Secretary <secretary@nesacs.org>. For more information about the Award, see <http://www.nesacs.org/awards_norris.html>.

Questions about the Award or the nomination process should be directed to the Chair of the Norris Award Committee, Professor Doris Lewis, <Dorisilewis@gmail.com>. ◇

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Monthly Meeting

The 940th Meeting of the Northeastern Section of the American Chemical Society – Esselen Award Meeting

Thursday, April 10, 2014

Harvard University, Cambridge, MA

Harvard Faculty Club, 20 Quincy Street

4:30 pm Board Meeting

5:30 pm Social Hour

6:30 pm Dinner

8:15 pm Award Meeting, Mallinckrodt Building, 12 Oxford St. Pfizer Lecture Hall (MB23), ground floor.

Dr. Catherine Costello, NESACS Chair, presiding

Welcome and Award History – Dr. Mukund Chorghade, Chair, Esselen Award Committee

Introduction of the Award Recipient – Professor George Whitesides, Harvard University

Presentation of the Award - Gustavus J. Esselen, IV

Dr. David R. Walt, Robinson Professor of Chemistry and Howard Hughes Medical Institute Professor, Tufts University

Esselen Award Address: *Microwell Arrays: From Genetic Analysis to Ultra-High Sensitivity Diagnostics*

Dinner reservations are required no later than NOON, Friday, April 4. Reservations are to be made using PayPal services: http://acssymposium.com/paypal.html. Select pay with credit or debit card option and follow the additional instructions on the page. Members, $30; Non-members, $35; Retirees, $20; Students, $10. Reservations for new members and for additional information, contact the secretary Anna Singer at (781) 272-1966 between 9am and 6pm or e-mail at secretary@nesacs.org. Reservations not cancelled at least 24 hours in advance must be paid.

THE PUBLIC IS INVITED - reservations for the public lecture portion of the evening are also required, an can be made using the paypal site.

Free Parking in the Broadway Street garage (3rd level or higher), enter from Cambridge St. via Felton St. ◇

Abstract

"Microwell Arrays: From Genetic Analysis to Ultra-High Sensitivity Diagnostics"

We have developed microwell arrays as a platform for performing bioanalytical measurements. In one scheme, microwells are filled with size-matched microspheres containing receptors for performing high-throughput genetic analysis. In another scheme, the microwells are used as miniature reactor chambers to confine single molecules.

Digital measurements, based on counting single molecules, enable extremely high sensitivity because low background signals can be readily distinguished, making for a much lower limit of detection. We have used the microwell arrays to develop a method to measure the concentration of proteins more than a thousand times lower than ELISAs. Both of these applications of microwell arrays have been commercialized. ◇

Biography

David R. Walt is Robinson Professor of Chemistry, Professor of Biomedical Engineering, Professor of Genetics, and Professor of Oral Medicine at Tufts University and is a Howard Hughes Medical Institute Professor. Dr. Walt is the Founding Scientist of Illumina, Inc. and has been a Director and Chairman of its Scientific Advisory Board since 1998.

Dr. Walt is also the Founding Scientist of Quanterix Corporation and is a Director and Chairman of its Scientific Advisory Board since 2007.

He has received numerous national and international awards and honors for his fundamental and applied work in the field of optical sensors and arrays.

Dr. Walt is a co-chair of the Board on Chemical Sciences and Technology of the U.S. National Academy of Sciences. He is a member of the U.S. National Academy of Engineering, American Academy of Arts and Sciences, a fellow of the American Institute for Medical and Biological

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CAREER DEVELOPMENT

Being an active participant in NESACS activities will enable you to network with major institutions and corporations in our area and can open up new career opportunities.

The NESACS Board of Publications, which is responsible for both the *Nucleus* newsletter and the NESACS website, is looking to increase its activities in this arena.

We would like to expand our capabilities for keeping our membership informed on what is happening in our field and how to adapt to changing times and new technologies.

You can help us do that. All we ask of you is a few hours a month and a smile.

Call or email to see what opportunities are available.

contact -- Vivian Walworth
NESACS Board of Publications
Phone - 978-369-3735

Email vwalworth@comcast.net

Passion for Science

Continued from page 2

condensation and a lower yield. Hence cyclohexanone and trimethylacetealdehyde were used as oxidants in the oxidation of alcohols with higher oxidation potentials. Below, Figures 2 and 3 show the products obtained using cyclohexanone and trimethylacetaldehyde, respectively, as oxidants over a temperature range of 40-80 °C.

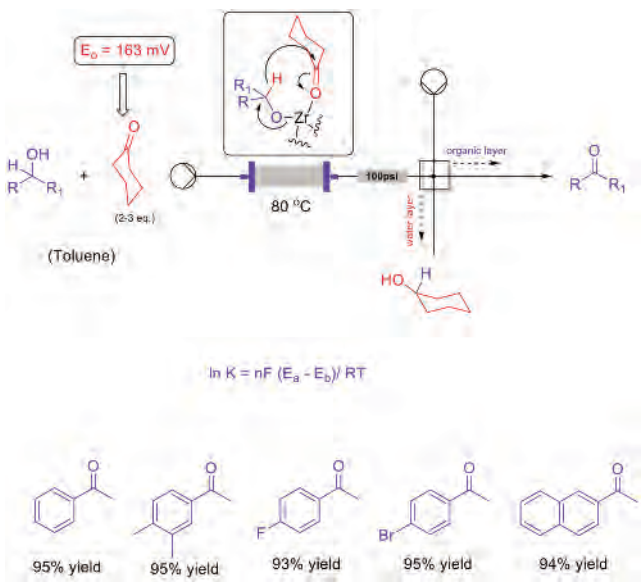

Figure 2: *Oxidation products obtained using cyclohexanone as oxidant*[3]

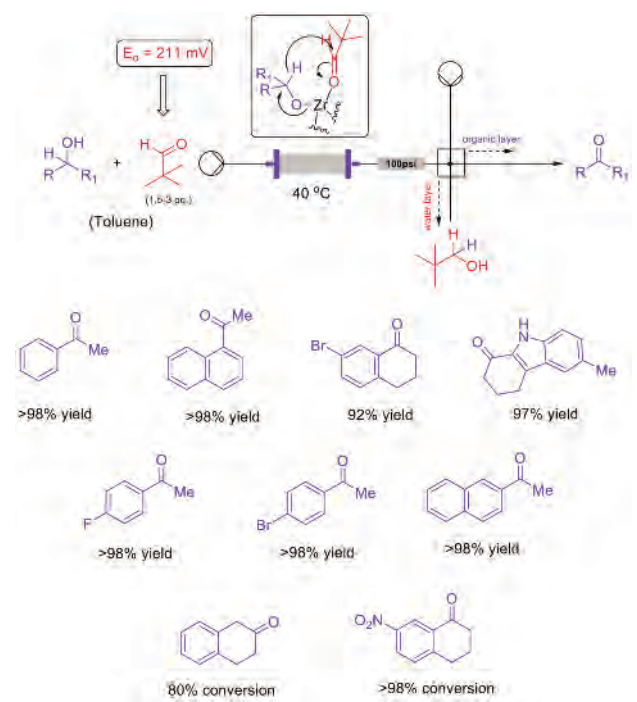

Figure 3: *Oxidation products obtained using trimethylacetaldehyde as oxidant*[3]

This Oppenauer oxidation method proved to be extremely effective and offered the advantages of being extremely cheap, using mild conditions and less toxic reagents, allowing for fast delivery of products, (within 8-25 minutes) and causing a reduced downstream work-up process.[3] In addition to this project, I conducted cerium oxide enhanced Sonogashira reactions by perovskite catalysts.[4] A flow procedure was chosen to contain the heterogeneous catalyst, reduce downstream processing, and deposit the catalyst onto the solid support surface. The perovskite catalysts were previously used by the Ley group for Sonogashira and Suzuki reactions in batch, and were very attractive due to extremely low level palladium loading and high ability for reuse without loss of turnover. A solid support was necessary to both contain the catalyst and help prevent the leaching of palladium from the catalyst. Cerium oxide is commonly used in the water gas shift reaction, and cerium oxide-supported nanoparticles have shown high stability and catalytic turnover. Although the perovskite catalysts contained extremely low levels of palladium and iron, it was shown that they were effective in catalyzing Sonogashira reactions using different substrates with varying electronic effects at high yield. In addition, it was shown that as the level of cerium oxide was increased the yield of the reaction increased, demonstrating a synergistic effect from the cerium oxide. This method showed the advantages of being extremely cheap, using an extremely low level of palladium, allowing for fast delivery of products, and a high potential for reuse without a loss of catalytic turnover. Below, Figure 4 shows the products of Sonogashira reactions obtained through this method.

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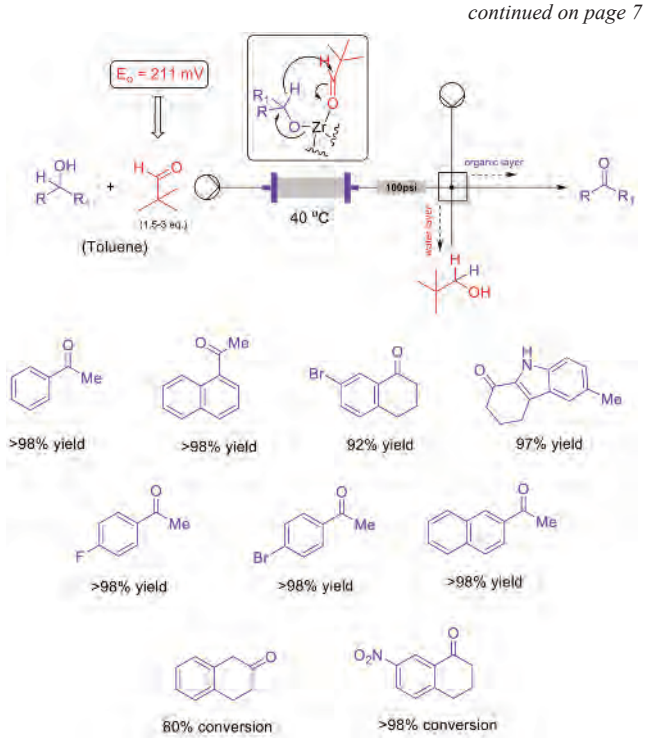

Figure 4: *Sonogashira products using perovskite catalysts*[4]

Passion for Science

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Currently, I am working under Professor Danith Ly at Carnegie Mellon University, synthesizing guanidinium-rich peptide nucleic acids (PNAs) for use in gene correction. I am continually working to further develop my technical and analytical skills, and to gain a greater understanding of the mechanism of medicine at the molecular level. This research has helped me grow tremendously as a researcher, and is allowing me to use chemistry knowledge and skills to attempt to ultimately provide a useful treatment to help save lives. This experience is extremely rewarding to me, and provides me further motivation to apply knowledge of chemistry towards a medical career.

These numerous laboratory-based research experiences were extremely inspiring and motivating and they helped bolster my desire to actively use research as a means for advancing clinical practice. To gain a greater understanding of how medicine is administered in a clinical setting, I conducted research at Massachusetts General Hospital under Dr. Ravi Thadhani. I recruited patients, collected blood samples, and performed statistical analysis for "Predictive Biological Markers for Hepatorenal Syndrome" and "Perceptions of CVVH" observational clinical trials. Working in a hospital setting was awe-inspiring and extremely humbling. I was given the opportunity to directly interact with patients every day in the intensive care unit, and I learned the importance of effective communication skills. Working with extremely sick patients was initially very jarring, but provided further motivation for me to work tirelessly to improve their lives.

Late last summer, I was honored to be offered an advisory position with Empiriko. The central theme of Empiriko is to connect drug discovery to patient outcomes, so the right therapies are developed for the right subpopulation, and physicians are able to treat patients more effectively. Led by my father, Dr. Mukund Chorghade, scientists are progressing in the design and development of proprietary oxidative catalysts to conduct and predict metabolic profiling of drugs, both *in vitro* and *ex vivo,* using chemosynthetic livers rather than human liver cells.[5]

These catalysts (commercialized under the name Biomimiks™) work to mimic the function of Cytochrome P450. With this technology, drug discovery scientists can quickly screen a series of compounds by reacting them with permutations of the patented oxidative catalysts, co-oxidants and non-aqueous solvents. This powerful combination serves as an "*in vitro* cocktail" that reduces the elapsed time for drug screening from several days to a matter of hours[5]. In addition, Biomimiks™ can be used by clinicians to dynamically measure a patient's response (drug-to-drug interactions, dosing levels and regimens) to a spectrum of drugs and incorporate the results into more effective diagnosis and patient treatment. The long-term strategy is to continuously enhance the Biomimiks™ platform by developing a "Chemosynthetic-liver-on-a-chip" and other future applications (e.g., defining CYP-specific reactions and delineating bioequivalence among species, liver dialysis). Currently, I am involved in performing soft-spot analysis of drug molecules, predicting metabolism pathways and profiles and correlating mass spectrometry data to potential metabolites.

The accountability, responsibility, and leadership and critical thinking skills I learned from these research experiences make me a perfect fit in the highly collaborative and motivated environment within a medical team. I aim to use my extensive research experience to secure an M.D./Ph.D. degree, and discover causative and curative factors in sports medicine. Receiving this joint training is essential to further understanding medicine at the molecular level. It will allow me to use this research-based problem-solving approach, coupled with knowledge of anatomy and physiology, to develop novel treatments to save and improve lives.

References:

1. Rajeev Chorghade, "My Internship Experiences", *The Nucleus,* LXXXVIII (7), March 2010.

2. Christopher S. Daeffler, Rajeev Chorghade, Mukund Chorghade and Robert H. Grubbs, "The Asymmetric Reduction of Acetophenone," *The Nucleus*, LXXXVIII (7), March 2010.

3. Rajeev Chorghade, Claudio Battilocchio, Joel M. Hawkins, and Steven V. Ley. "Sustainable Flow Oppenauer Oxidation of Secondary Benzylic Alcohols with a Heterogeneous Zirconia Catalyst." *Organic Letters*, **15** 22 (2013) 5698-5701.

4. Claudio Battilocchio, Benjamin N. Bhawal, Rajeev Chorghade, Benjamin J. Deadman, Joel M. Hawkins, and Steven V. Ley, "Flow Based Cerium Oxide Enhanced Low Level Palladium Sonogashira and Heck Coupling Reactions by Perovskite Catalysts," *Israel Journal of Chemistry*, Manuscript in Press. May 2013.

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http://www.youtube.com/watch?v=6C1pE0LS8i8 ◇

Summer Scholar Report

Carbazole-based metal-organic frameworks for gas separations

Amanda W. Stubbs and David R. Manke
Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth, North Dartmouth, MA

Introduction

The United Nations Intergovernmental Panel on Climate Change recently released its Fifth Assessment Report, in which they stated with 95% certainty that human activity was responsible for the climate change observed over the past half century. Since the beginning of the Industrial Revolution, the concentration of carbon dioxide in the atmosphere has increased by 40%, the greater part of which is attributed to the burning of fossil fuels.[1] One method to offset human production of green house gas is carbon dioxide capture and sequestration. The current industrial standard is wet scrubbing, where alkanolamines capture carbon dioxide through carbamate formation. While this method is effective in the capture of carbon dioxide, release of the CO_2 and regeneration of the capture media could increase overall energy input by as much as 40%.[2]

New technologies are being investigated as potential carbon capture media, with metal-organic frameworks (MOFs) emerging as one possible solution. MOFs provide many advantages over other materials, including large open pores and structural regularity. Perhaps most beneficial is that the materials can be readily modified through the judicious selection of metal ions and organic linkers. Pore shape and size can be varied, and the functionality of the pores can also be controlled.

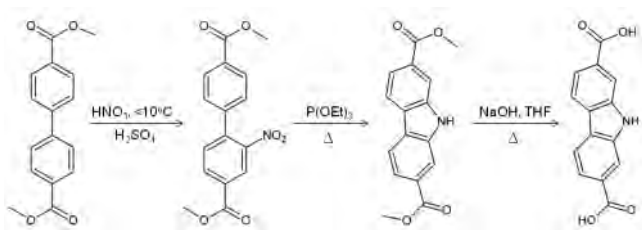
Our approach to carbon dioxide capture is the inclusion of open Lewis base sites within the pores of an MOF. Primary atmospheric gases (N_2, O_2) possess non-polar bonds, while carbon dioxide's polar bonds result in a partial positive charge on the carbon atom. Materials with open Lewis base sites included should selectively adsorb carbon dioxide due to a Lewis acid/base interaction. If this interaction is strictly physical in nature (physisorption), then the reversibility would have a lower energy cost than observed in wet-scrubbing where a chemical change occurs (chemisorption). Generating open Lewis base sites within MOFs is not trivial, given the propensity of these functional groups to act as ligands. This has resulted in a relative scarcity of such solids in the literature. Herein are described some efforts towards producing such materials.

Linker Synthesis

The structure and functionality of an MOF is greatly impacted by the selected organic linker. For this project, derivatives of carbazole dicarboxylates were chosen. The dicarboxylate motif has demonstrated great success in the production of highly porous MOFs.[3] The carbazole group provides a single Lewis base site sufficiently removed from the carboxylates to avoid chelation or competition for binding. Additionally, the nitrogen-containing carbazole provides a site for interaction with carbon dioxide and can also be substituted with other functionalities to enhance the Lewis base character in the pores.

Synthesis of the desired carbazole from commercially available dimethyl biphenyl-4,4'-dicarboxylate can be accomplished via two routes, both of which begin with mono-nitration of the biphenyl, as reported by Olkhovik, et al.[4] The literature method for carbazole formation involves three steps, the first of which is reduction of the nitro group to an aniline, a reaction that runs for ten days. The amino group is converted to an azide, which then undergoes a thermal ring closure to carbazole over 40 hours. To avoid the use of an azide and long reaction times, alternative reaction conditions were explored.

One method for the generation of carbazoles is a Cadogan reaction; the reaction of 2-nitrobiphenyls with organophosphorous reagents.[5] One previous attempt to synthesize the targeted carbazole via a Cadogan reaction was reported using triphenyl phosphine, but demonstrated low yield and low purity.[4] We were able to optimize a Cadogan reaction to produce pure dimethyl 9*H*-carbazole-2,7-dicarboxylate in 45% yield (**Scheme 1**). Refluxing 4,4'-dimethyl-2-nitrophenyl dicarboxylate in neat triethyl phosphite for 12 hours, followed by cooling of the reaction mixture, resulted in precipitate formation. After filtration and washing with benzene, an off-white solid was isolated that proved to be the pure carbazole. While the yield for this reaction is lower than that of the azide route (45% vs. 79%), we feel that the quickness, ease of purification, and removal of the azide step make it a favorable alternative. For use in solvothermal MOF syntheses, the carbazole ester was hydrolyzed to its acid form. This was accomplished via standard base hydrolysis methods in 94% yield.



Scheme 1. *Synthesis of 9H-carbazole-2,7-dicarboxylate accomplished via nitration, a Cadogan reaction, and base hydrolysis.*

Metal-Organic Framework Synthesis and Structure

Utilizing this carbazole acid, a manganese MOF was synthesized in a thick-walled glass tube, when 0.125 mmol of 9*H*-carbazole-2,7-dicarboxylic acid and 1 equivalent of manganese(II) nitrate tetrahydrate were combined in 3mL of dimethylacetamide. The tube was degassed via three freeze-pump-thaw cycles. The evacuated tube was sealed with a

Summer Scholar

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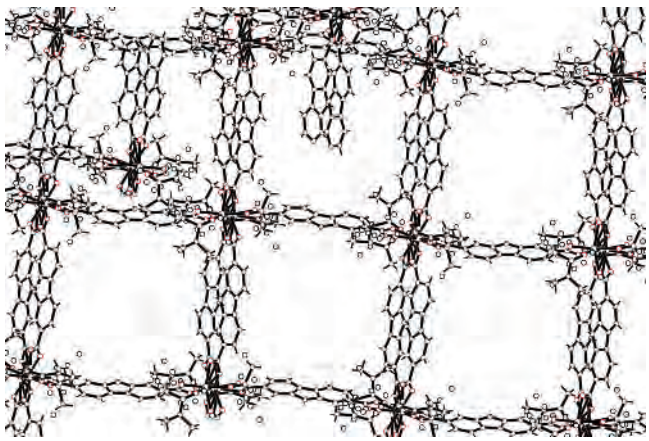


Figure 1. *The solid state structure of the carbazole-based Mn MOF.*

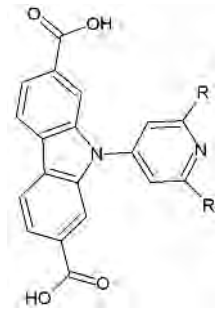
methane-oxygen torch and placed in a 110ºC oven for seven days, at which point tan to pale orange rectangular crystals had formed. The crystals were isolated and analyzed by X-ray diffraction (**Figure 1**).[6] In the asymmetric unit, there are three distinct metal centers arranged in a linear trinuclear cluster. The two terminal manganese centers are bound by four oxygen atoms from three carboxylates and two solvent oxygen atoms each. The central manganese atom is bound by six oxygen atoms from six carboxylates. All three metal centers are in pseudo-octahedral configuration. Similar Mn_3 secondary building units (SBUs) have been previously observed.[7-10] The trimanganese hexacarboxylate units combine to form two-dimensional sheets that are connected through N–HO hydrogen bonds. The Platon program SQUEEZE[11] was used to address unrefined solvent, which was treated as 12 dimethylacetamide molecules that when removed generate a void volume of 2064 Å.^{3} Gas adsorption studies are currently being performed on this material and will be reported at a later date.

Future Directions

Beyond producing MOFs with 9*H*-carbazole ligands, we are seeking to couple pyridyl groups at these positions to generate linkers with the motif proposed in **Figure 2**. The 4-aminopyridyl functionality of this linker would enhance the basicity of the open Lewis base site. The addition of 2,6-dialkyl substitution on the pyridyl ring should temper the ability of the pyridine to compete with the carboxylate as a metal binder. The steric hindrance should not greatly impact interaction with small molecules like carbon dioxide.

To this end, I began to explore the coupling of 2,6-lutidines to the carbazole. This began with the production of 2,6-dimethyl-4-triflatopyridine from 4-hydroxy-2,6-dimethylpyridine.[12] The utilization of this yellow oil proved to be difficult, as it decomposed to form the dipyridinium ether 4,4'-oxybis(2,6-dimethylpyridinium)bis(trifluoromethanesulfonate) (**Figure 3**). Colorless crystals of this decomposition product were isolated and analyzed by X-ray

Figure 2. *Proposed organic linker with a 2,6-disubstituted-4-aminopyridine motif. (R=alkyl)*



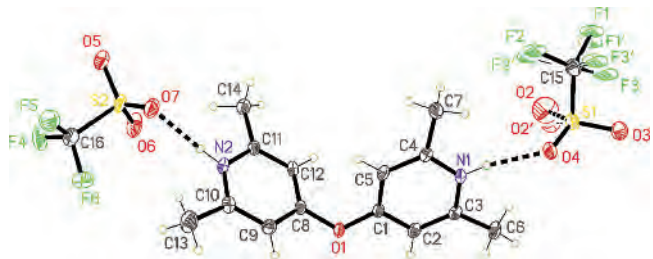


Figure 3. *The molecular structure of the 4,4'-oxybis(2,6-dimethylpyridinium)bis(trifluoromethanesulfonate), with displacement ellipsoids drawn at the 50% probability level.*

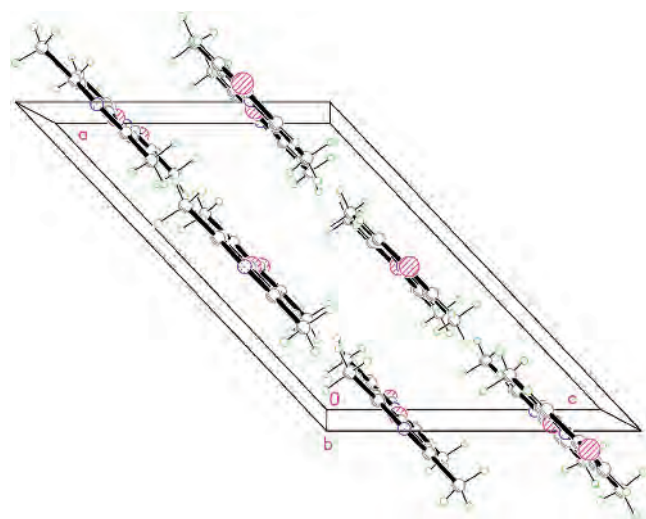


Figure 4. *The unit cell of 4-iodo-2,6-dimethylpyridine along the b-face.*

diffraction.[13] The structure is typical of a dipyridyl ether, with a C–O–C bond angle of 119.3º and C–O bond lengths of 1.364 Å and 1.389 Å.[14] The dissimilar C–O–C–C torsion angle of 61.5º and 15.1º result in what is defined as a skew conformation for bridged diaryls.[15]

To avoid the stability issues associated with the pyridyl triflate, it was converted to the 4-iodo-2,6-dimethylpyridine (**Scheme 2**).[16] The crystal structure of the resulting solid was also determined. The structure of the pyridyl ring is as expected, but the molecules arrange in sheets (**Figure 4**) held together by short N–I contacts of 3.161Å. The coupling reaction conditions are still being optimized, and work is being done to modify the 2,6-alkyl groups to bulkier substituents.

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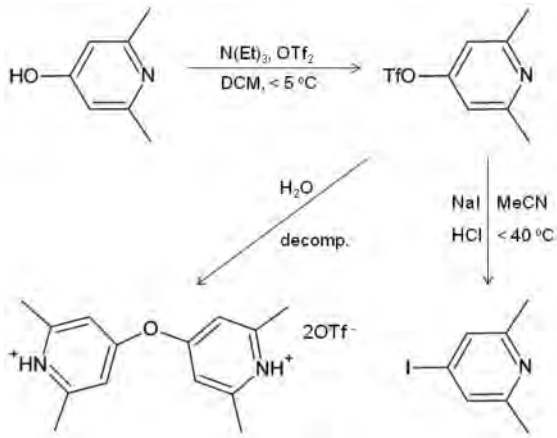

Scheme 2. *Synthesis of 2,6-dimethyl-4-triflatopyridine, its decomposition in the presence of moist air, and its conversion to 4-iodo-2,6-dimethylpyridine.*

Acknowledgements

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Calendar

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April 22 continued

Prof. Steven L. Tait (Indiana Univ.)
"Supramolecular Self-Assembly at Surfaces"
Tufts University, Pearson, P-106
4:30 pm

Apr 23

Prof. Curtis Berlinguette (U. of British Columbia/U. of Calgary)
Harvard Univ., Pfizer Lecture Hall
4:15 pm

Apr 24

Prof. Melanie Sanford (U. of Michigan)
MIT, 6-120
4:00 pm

Dr. Yu-Sheng Chen (Harvard Univ.)
"Advanced Crystallography with Synchrotron"
Harvard Univ., Pfizer Lecture Hall
2:00 pm

Prof. David DeMille (Yale University)
Harvard Univ., Pfizer Lecture Hall
4:15 pm

Apr 26

Prof. David Schuster (NYU)
"Electron Transfer Processes in Supramolecular Artificial Photosynthetic Systems Incorporating Fullerenes"
U. Mass, Lowell, Cumnock Hall Auditorium
3:30 pm

Apr 28

Prof. Andrew G. Myers (Harvard Univ.)
Boston University, Metcalf, Rm 113
4:00 pm

Prof. Nathaniel Rosi (Pittsburgh)
Brandeis University, Gerstenzang 121
4:00 pm

Notices for The Nucleus Calendar of Seminars should be sent to:

Xavier Herault,
email: xherault(at)netzero.net ◇

Biography

Continued from page 5

Engineering, a fellow of the National Academy of Inventors, and a fellow of the American Association for the Advancement of Science.

He received a B.S. in Chemistry from the University of Michigan and a Ph.D. in Chemical Biology from Stony Brook University. ◇

Malta-VI Workshops

Continued from page 12

connection with the problems created by the dual use of chemicals for both peaceful and terrorist purposes.

Science Education at All Levels

In addition to the presentations on innovative pedagogy, systemic assessment, and the use of technology, there were several that attracted particular interest. The talk on the ethics of scientific research emphasized the importance of stressing the basic values of honesty, reliability, and objectivity in all of science education. A representative from Saudi Arabia described the enormous progress made by women scientists in the Arab world with a particular focus on her own country where there has been a significant increase in the number of highly qualified women scientists although career opportunities remain limited. A speaker from Egypt reminded the audience that the use of gas weapons in North Africa and the Middle East against civilians engaged in peaceful political protests puts an ugly face on the public perception of chemistry.

For more details about Malta-VI, see <www.MaltaConferencesFoundation.org>. ◇

ACS Northeastern Section at Fenway Park!

Red Sox Game Tuesday, May 6

Northeastern Section members are encouraged to bring their families, friends, and colleagues to this NESACS traditional outing. We are hoping again this year for pleasant weather, good company, and a winning team.

On Tuesday, May 6th, we have right-field box seats for the Red Sox - Cincinnati Reds game. Our tickets reflect the lowest possible cost under the new Red Sox ticket pricing policy; $45 includes handling charges and a small donation to the Northeastern Section. Reserve your seats by mailing your check (payable to NESACS) to Anna Singer, 12 Corcoran Road, Burlington, MA 01803. Questions may be sent to secretary@nesacs.org. ◇

Fenway park photo from Boston.redsox.mlb.com

Summary of the Workshops at Malta-VI

By Morton Z. Hoffman

At the conference, Frontiers of Science: Research and Education in the Middle East, held in November 2013 (Malta-VI), workshops examined scientific, educational, and regional issues.

Chemistry and Bio-Medicinal Chemistry

A wide range of topics were explored in this workshop, including cancer therapy, tumor markers, HIV activity, and myocardial infarction, as well as chemical synthesis and computational studies. Of great interest was a presentation on clinical trials on the analysis of breath samples for the early detection of lung cancer in which chemical nanoarrays and GC-MS are used for the comparison of the signatures and compositions of the exhaled volatile organic compounds that are created as a result of the biological pathways that occur in the human body. The results show a clear distinction among 1) head and neck cancer patients and healthy controls, 2) lung cancer patients and healthy controls, and 3) head and neck cancer patients and those with lung cancer. Other clinical trials aimed to explore the difference in the breath print of the four most widespread cancers in the developed world (lung, prostate, colorectal, breast), which account for half of the cancer deaths; the results showed that each cancer has a unique pattern of volatile organic compounds when compared with healthy patients.

Analytical, Nanotechnology, and Material Science

The current trends in these areas that were described included the atmospheric measurement of pesticides, the extraction, separation, and analysis of lignans, and electron transfer in biological systems. The realm of complex functional bio-composites has attracted a good deal of interest, in particular plant cystoliths, which are mineralized objects formed by specialized cells in the leaves of certain plants, that scatter incident light. Cystoliths are regularly distributed in the epidermis of leaves and protrude into the photosynthetic tissue such that the photosynthetic pigments generate a steep light gradient in the leaf. Under most illumination regimes, the outer leaf layer is light saturated, rendering the photosynthetic apparatus kinetically unable to use the excess light for photochemistry.

Energy, Environment, Air and Water Quality

This workshop had many interlocking components. Inasmuch as collaborations that involve renewable energy among several Middle East countries are currently ongoing, this aspect of the workshop concentrated on current research activities; the hope was expressed that new collaborations could be established to lead to the further development of sustainable resources that do not impact adversely on the environment, particularly air quality. With regard to water, the shared resources are under heavy natural and human pressures in terms of quantity and quality, which affect every aspect of life from ecosystems and the environment to food security and health. Because of population growth and urbanization, and despite a general improved standard of living in the region, many communities still lack access to safe drinking water and basic sanitation. The problem of water scarcity provides important opportunities for cooperation and conflict prevention, and could be at the core of programs to promote peaceful coexistence and collaboration among people in Israel, the Palestinian Authority, and Jordan, to the mutual benefit of all the stakeholders.

Chemistry Safety and Security

The awarding of the 2013 Nobel Peace Prize to the Organization for the Prohibition of Chemical Weapons (OPCW) placed in clear focus the work of that group in the development of the international Chemical Weapons Convention (CWC) and the removal of chemical weapons from current areas of conflict in the Middle East. Especially relevant is the fact that some of the participants at Malta-VI were from the several countries that have not ratified or signed the CWC. It was pointed out that OPCW is working toward the creation of an international code of conduct for chemists, especially in

continued on page 11

2014 German Exchange

Pre-travel meeting on March 1 for the 2014 German Exchange; (l-r) front row: Emily Lewis (Tufts, NSYCC Chair), Brian Sneed (B.C.), Mike Strem (Strem Chemicals, German Exchange Steering Committee Chair), Jackie O'Neil (Alkermes, Inc., NSYCC Vice-Chair), John Podobinski (Moderna Therapeutics, German Exchange Steering Committee), Stephanie Maiocco (B.U.); second row: Emel Adaligil (Tufts), Peter Frank (UNH), Ekaterina Vinogradova (MIT), Peter Thill (MIT), Felicia Lucci (Tufts), Ruth Tanner (UMass Lowell, German Exchange Steering Committee); last row: Lee Johnson (Conditas Biotechnology Group, German Exchange Steering Committee), Thomas Sisto (B.U.), Elise Miner (Northeastern), Matthew Marcinkowski (Tufts), June Lum (Natick Soldier Systems Center, NSYCC Career Chair). Not present: Gloria Hong (Harvard), John Nicoludis (Harvard).

Photo by Morton Z. Hoffman

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Abstracts: abstracts@nsycc.org

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Northeastern Section Younger Chemist Committee (NSYCC)
Boston University Younger Chemist Committee (BUYCC

Calendar

Check the NESACS home page for late Calendar additions: http://www.NESACS.org

Note also the Chemistry Department web pages for travel directions and updates.
These include:
http://www.bc.edu/schools/cas/chemistry/seminars.html
http://www.bu.edu/chemistry/seminars/
http://www.brandeis.edu/departments/chemistry/events/index.html
http://www.chem.harvard.edu/courses/seminars.php
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http://www.umassd.edu/cas/chemistry/
http://www.uml.edu/Sciences/chemistry/Seminars-and-Colloquia.aspx
http://www.unh.edu/chemistry/events

Apr 1
Prof. Cynthia Friend (Harvard Univ.)
U. New Hampshire, Room N104
11:10 am

Prof. Liz Nolan (MIT)
Tufts University, Pearson Chemistry Building, P-106
4:30 pm

Apr 2
Prof. Ben L. Feringa (Univ. Groningen)
"Exploring Chiral Space in Asymmetric Synthesis"
Boston College, Merkert 127
4:00 pm

Apr 3
Prof. Ben L. Feringa (U. Groningen)
"Catalytic Asymmetric C-C bond Formation"
Boston College, Merkert 127
4:00 pm
Prof. Jeremy Hutson (Durham Univ.)
Harvard Univ., Pfizer Lecture Hall
5:00 pm

Apr 4
Prof. Ben L. Feringa (U. Groningen)
"Dynamic Molecular Systems; from switches to motors"
Boston College, Merkert 127
4:00 pm

Apr 7
Prof. Brian Shoichet (U. of Toronto)
Brandeis University, Gerstenzang 121
4:00 pm

Prof. Ryan Shenvi (Scripps Research Institute-Florida)
Boston University, Metcalf Science Center, Rm 113
4:00 pm
Prof. Michael Krische (Univ. of Texas)
Harvard Univ., Pfizer Lecture Hall
4:15 pm

Apr 8
Prof. Bruce M Foxman (Brandeis University)
"Single-Crystal Reactions and Phase Transitions: Methods, Solutions and Puzzles"
Harvard Univ., Pfizer Lecture Hall
2:00 pm

Apr 9
Prof. Peidon Yang (Harvard Univ.)
Harvard Univ., Pfizer Lecture Hall
4:15 pm

Apr 10
Prof. David Nicewicz (U of North Carolina)
MIT, 6-120
4:00 pm

Apr 14
Prof. Barry Trost (Stanford University)
Boston University, Metcalf Science Center, Rm 113
4:00 pm

Prof. Suzanne Bart (Purdue University)
Brandeis University, Gerstenzang 121
4:00 pm

Apr 15
Prof. Eric Strieter (U. Wisconsin)
Boston College, Merkert 130
4:00 pm

Dr. Dannon Stigers and Dr. Ryan Kopreski (Cytec Industries)
"Global Industrial Energy Reduction Through Scale Inhibition"
U. New Hampshire, Room N104
11:10 am

Dr. Bob He (Bruker-Axs Inc.)
"2D XRD Applications in Materials Science"
Harvard Univ., Pfizer Lecture Hall
2:00 pm

Dr. Deepak Shukla (Eastman Kodak)
Tufts University, Pearson, P-106
4:30 pm

Apr 16
Prof. Joel Rosenthal (U. Delaware)
Boston College, Merkert 130
4:00 pm

Apr 17
Prof. Abigail Doyle (Princeton) and Prof. Seth Herzon (Yale)
MIT, 6-120
4:00 pm

Apr 22
Prof. Rachelle Gaudet (Harvard Univ.)
"Data collection and phasing for macromolecular structure determination"
Harvard Univ., Pfizer Lecture Hall
2:00 pm

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