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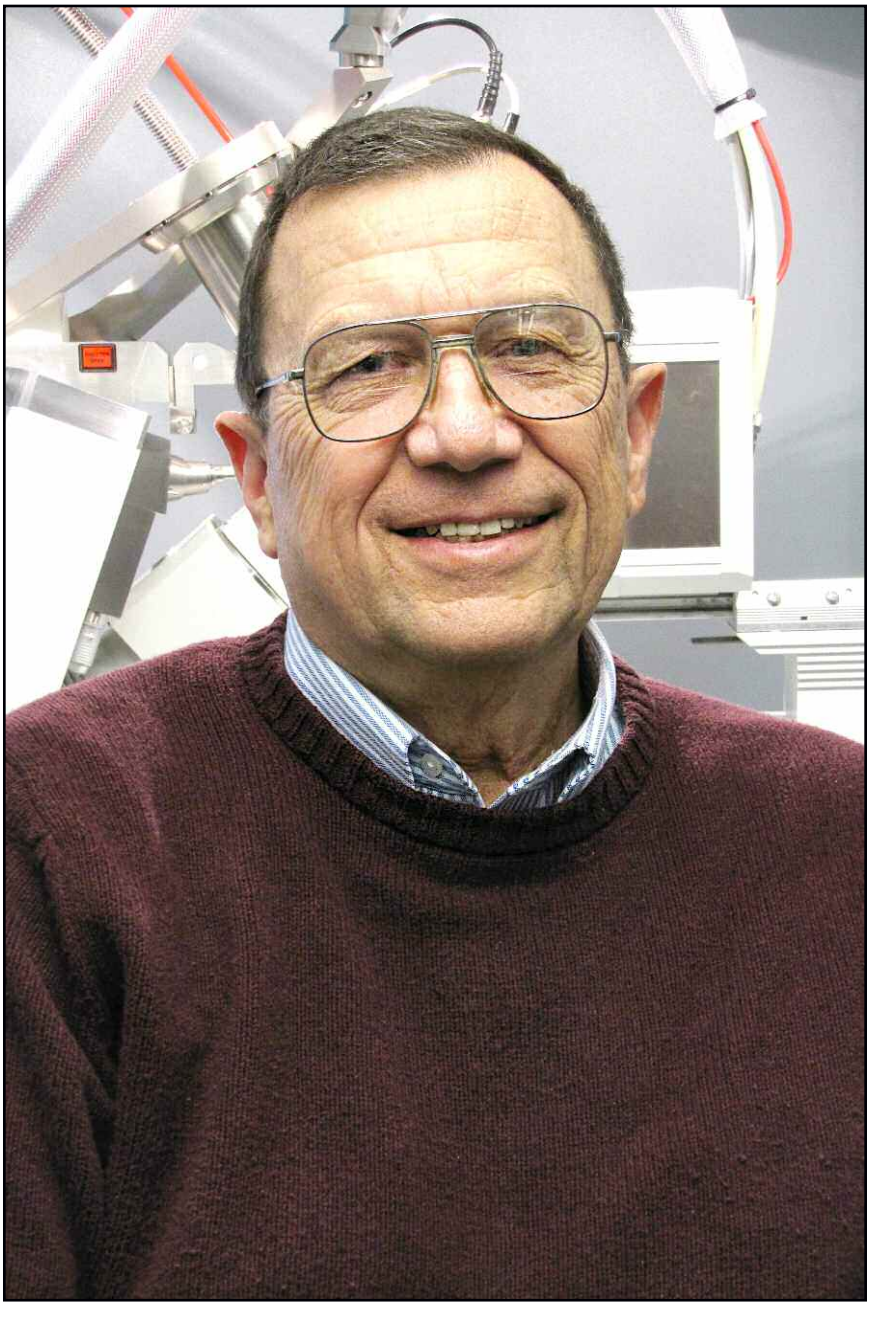

Monthly Meeting

NESACS Annual Meeting at Pfizer
Bethany Kormos to speak

Summer Scholar Report

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2016 Chair's Statement

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By Michael P. Filosa

Summer Scholar Report

Incorporating 4-Aminopyridyl Groups in Metal Organic Frameworks for Gas Separation

Jona Koka and David R. Manke , Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth, North Dartmouth, MA

Introduction:

The need for materials that can selectively separate carbon dioxide from other gases is great. The impacts of global climate change are becoming more evident, and isolation of carbon dioxide at the point of generation is one of the proposed methods of mediating this global challenge. According to the United Nations Intergovernmental Panel on Climate Change in its Fifth Assessment Report, human activity is "extremely likely (95-100%) to have been the dominant cause of the observed warming since the mid-20th century." It further states that the results of this climate change will have impacts that "include alteration of ecosystems, disruption of food production and water supply, damage to infrastructure and settlements, human morbidity and mortality and consequences for mental health and human well-being."[1] One method to offset human production of greenhouse gas is carbon dioxide capture and sequestration (CCS). The current industrial standard is wet scrubbing, where alkanolamines capture carbon dioxide through carbamate formation. While this method is effective, release of the carbon dioxide and regeneration of the capture media could increase overall energy consumption by as much as 40%.[2]

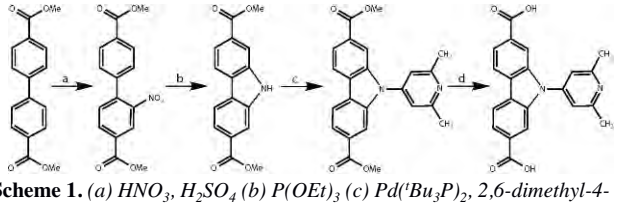
New materials are being investigated as potential carbon capture media, which must selectively adsorb carbon dioxide over other gases present in the atmosphere and in waste streams. It must be easy to regenerate, requiring a small energy input to release the pure carbon dioxide for sequestration or as a chemical feedstock. Metal-organic frameworks (MOFs) are emerging as promising materials for carbon capture. MOFs are crystalline, porous solids composed of metal ions and polyfunctional organic linkers. One major advantage of MOFs is that pore shape and size can be varied, and the functionality of the pores can also be controlled through ligand design and the coordination environment of metal centers.

Our strategy for the selective capture of carbon dioxide is to incorporate open Lewis base sites within the pores of MOFs. While carbon dioxide is a non-polar molecule, it does possess two polar C=O bonds, resulting in a partial positive charge on its carbon atom which can interact with an electron donor. The major components of the atmosphere (N_2, O_2) are homonuclear diatomics and non-polar, precluding such an interaction. An additional benefit of our strategy is that the interaction we are seeking to employ is strictly physical in nature (physisorption), which should be reversible at a lower energy cost than that observed in wet-scrubbing where a chemical change occurs (chemisorption) upon carbamate formation. Generating open Lewis base sites within MOFs is not trivial given the propensity of these functional groups to act as ligands, resulting in a relative scarcity of such solids in the literature.[3,4]

Linker Design, Synthesis and Structure:

Our lab has been exploring 9*H*-carbazole-2,7-dicarboxylate as a linker, generating frameworks from a variety of metals and with an assortment of structures.[5] Cadmium, zinc and zirconium networks have been reported in the literature.[6,7,8] In analyzing the gas sorption properties of networks with this linker, we have observed a relatively low selectivity for the adsorption of carbon dioxide versus dinitrogen. To increase this selectivity, we have been working to produce frameworks incorporating stronger Lewis base groups. The nitrogen atom of the carbazole presents a point of functionalization, and we have begun to couple pyridyl groups to this atom to yield a significantly more basic 4-aminopyridyl functionality. The strong basicity presents the problem that the pyridyl group can compete with the carboxylate for binding to the metal center. To help avoid this competitive binding, we have incorporated 2,6-substitution of the pyridyl ring, such that the steric hindrance could reduce the competence of the pyridine as a ligand, while maintaining the basicity for adsorption of carbon dioxide.

Synthesis of the desired pyridyl-carbazole starts with the commercially available dimethyl-4,4'-biphenyldicarboxylate and 2,6-dimethyl-4-hydroxypyridine via a multistep process (Scheme 1). The biphenyl dicarboxylate is mono-nitrated via literature procedure,[9,10] and the carbazole is generated via a ring-closing Cadogan reaction to yield dimethyl 9*H*-carbazole-2,7-dicarboxylate.[11,12] 2,6-dimethyl-4-hydroxypyridine[13] is converted to the 4-iodopyridine through the triflate complex via literature procedure,[1415-16] which is then coupled to the carbazole diester via a Buchwald-Hartwig cross coupling reaction.[17] Refluxing one equivalent of the carbazole diester with two equivalents of the iodopyridine, three equivalents of cesium carbonate and five mole percent of bis(tri-*tert*-butylphosphine)palladium in toluene under an inert nitrogen atmosphere yields a white/gray solid in 85% yield after washing with ethyl acetate. For use in solvothermal syntheses of coordination polymers, the carbazole ester is converted to the dicarboxylic acid via standard base hydrolysis methods in 92% yield.



Scheme 1. *(a) HNO_3, H_2SO_4 (b) $P(OEt)_3$ (c) $Pd(^tBu_3P)_2$, 2,6-dimethyl-4-iodopyridine, THF (d) KOH, H_2O/THF*

Single crystals of the pyridyl-carbazole ester suitable for an X-ray diffraction study were grown from the slow evaporation of dichloromethane. In the solid state, the compound crystal-

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Cover: *Professor Jerry P. Jasinski, 2016 NESACS Chair (Photo courtesy of Dr. Jasinski)*

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THE NUCLEUS

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2016 Chair's Statement

Jerry P. Jasinski, Keene State University, jjasinski@keene.edu

I consider it an honor and privilege to serve as Chair of the Northeastern Section (NESACS) of the American Chemical Society (ACS) for 2016 and to have served as Chair-Elect and Program Chair for 2015. NESACS is the largest and most influential section of the American Chemical Society with over 7,000 members. Its geographical range extends from the Southeastern, MA region through the Greater Boston area and includes New Hampshire. It embraces a unique connection and collaboration with the national organization and globally by bringing programs, activities and networking to our local area and promotes a variety and diversity of interactions including industrial and academic research, scientific entrepreneurship, student and young chemist activities, career services, government relations, and professional ethics amongst its charge. The Section is very active and sponsors national and local awards to honor outstanding chemists and chemical educators as well as grants and scholarships for students and faculty in support of research, travel and related activities.

As an ACS member residing within the boundaries of the NESACS you are automatically a member of this local section. Therefore, it is one of my goals to increase engagement and participation of our members not only in the Greater Boston area but also extending to the northern and southern sections of the organization as well. As a chemist, chemical engineer or chemical educator with a locally and/or globally oriented focus, the NESACS continues to work hard to deliver diverse scientific programs through its monthly meetings and to continue to host career workshops, support science outreach, recognize excellence in chemistry as demonstrated by teaching, research or student achievement. We, therefore, need you to step up and get involved for the advancement of its goals and to accomplish its mission. Visit http://www.nesacs.org to learn more about current and future NESACS activities.

Among my other goals for 2016 are to continue to support the activities of our award winning Younger Chemist Committee (NSYCC) and continue the active recruitment and engagement of our secondary school teachers particularly though the "Connections to Chemistry" program that our section supports annually as well as other committees programs including the annual exchange with their German counterparts. I wish to support and maintain the outstanding collaboration we enjoy with the activities of the medicinal chemistry group and am proactive in supporting international symposia and exchange programs which allow for a sharing of ideas and networking in a global environment.

We are here to serve you in any way possible to enhance your involvement in the activities of the local section. I am here to listen to your thoughts and ideas on how to step up and volunteer to experience all that the NEASAC has to offer at all levels of diversity, collaboration and professional enhancement.

All the best in 2016! ◇

ResMed: Residential School on Medicinal Chemistry and Biology in Drug Discovery
June 5-10, 2016
Wyndham, Florham Park, NJ

This graduate level course concentrates on the fundamentals that are useful in drug discovery spanning initial target assay evaluation through clinical development. Several case histories of recent successful drug development programs will also be presented. The five-day program covers:

Principles of Med Chem	DMPK
Chemoinformatics	Toxicophores
Lead ID & Optimization	GPCRs
Epigenetics	Kinase Inhibitors
Fragment-based Drug Design	Ion Channels
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For more information and application forms:
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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 Anna Singer at 781-272-1966 between 9am-6pm, or email: secretary(at)nesacs.org by noon of the first Thursday of the month, letting her know that you are a new member. ◇

Join NESACS on facebook
www.facebook.com/nesacs

Monthly Meeting

The 957th Meeting of the Northeastern Section of the American Chemical Society

Thursday, January 14, 2016

Pfizer, 610 Main Street, Cambridge, MA

4:00 pm NESACS Annual Meeting (1st floor seminar room)

4:30 pm NESACS Board Meeting (1st floor seminar room)

5:30 pm Social Hour (Cafeteria)

6:15 pm Dinner (Cafeteria)

7:15 pm Dr. Jerry Jasinski, NESACS Chair Presiding
Dr. Bethany Kormos, Senior Principal Scientist, Worldwide Medicinal Chemistry, Pfizer, Inc. "Using Computational Chemistry to Drive Drug Discovery: A LRRK2 Case Study."

For those who would like to join us for dinner, register by noon, Thursday, January 7, 2016 using PayPal: http://acssymposium.com/paypal.html. Select the pay with credit or debit card option and follow the additional instructions on the page. Cost: Members, $30; Non-members, $35; Retirees, $20; Students, $10. Dinner reservations not cancelled at least 24 hours in advance must be paid.

If you wish to join us for this meeting and not eat dinner, please register by noon, Thursday, January 7, using PayPal: http://acssymposium.com/paypal.html. Select "Seminar only". The fee is $1. New members or those seeking additional information, contact the NESACS administrative coordinator, Anna Singer, at secretary@nesacs.org or at (781) 272-1966 during regular business hours only.

THE PUBLIC IS INVITED TO THE EVENT. ATTENDEES NEED TO BE AWARE THAT THE HOST FACILITY IS A PRIVATE FACILITY WITH ITS OWN SECURITY AND GUIDELINES FOR ADMISSION. IT IS REQUIRED BY THE HOST SITE THAT ALL ATTENDEES BE REGISTERED IN ADVANCE. THOSE WHO FAIL TO REGISTER IN ADVANCE MAY NOT BE ADMITTED TO THE PROGRAM.

NESACS gratefully acknowledges support from Pfizer for this event.

Directions: The Pfizer 610 Main Street building is located in the MIT Osborn Triangle, the block spanned by Main, Portland, Albany, and Osborn Streets in Cambridge, MA.

The entrance to the Pfizer 610 Main Street lobby is at the corner of Albany and Portland Streets.

By Subway: 610 Main Street is a 10 minute walk from the Kendall Square or Central Square T stops on the Red Line.

By Bus: The #1 bus serving Harvard/Boston stops at the corner of Massachusetts Avenue and Albany Street. The CT2 bus serving Ruggles/Sullivan stops at the corner of Massachusetts Avenue and Vassar Street.

Parking: Metered street parking (2 hour limit) is available on Main Street, Albany Street, and Vassar Street.

Garage Parking: Two locations for unsubsidized garage parking are at the Technology Square Garage and the Franklin Street Garage near Star Market/Le Meridien, entrance on Green or Franklin Street. ◇

Biography

Bethany Kormos graduated summa cum laude from Mercyhurst College in Erie, PA with a B.A. in Chemistry and a B.S. in Biochemistry. As an undergraduate, she spent a summer at the University of Southern California as a visiting scholar in the group of Prof. Arieh Warshel, which solidified her early interests in computational chemistry.

She went on to earn a Ph.D. in Chemistry at the University of Minnesota with Prof. Christopher Cramer for the study of organic reactions and organometallic systems using *ab initio* computational chemistry methods.

After earning her doctorate, she was awarded a Ruth L. Kirschstein National Research Service Award from the National Institutes of Health for the study of induced fit in U1A-RNA complexes using molecular dynamics simulations, which funded her postdoctoral work with Profs. David Beveridge and Anne Baranger at Wesleyan University.

Bethany is currently a Senior Principal Scientist at Pfizer in Cambridge, MA where for the past eight years she has driven computational chemistry and modeling strategies to advance projects in the Neuroscience Chemistry Group.

Her research interests include homology modeling, potency prediction and molecular dynamics simulations, as well as understanding substrate recognition by aldehyde oxidase and mitigation of hERG liabilities.

In addition to her work, Bethany is involved in the Women's Leadership Network at Pfizer, and enjoys yoga and playing volleyball. She has been a member of the American Chemical Society

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October Meeting Photos

By Morton Z. Hoffman

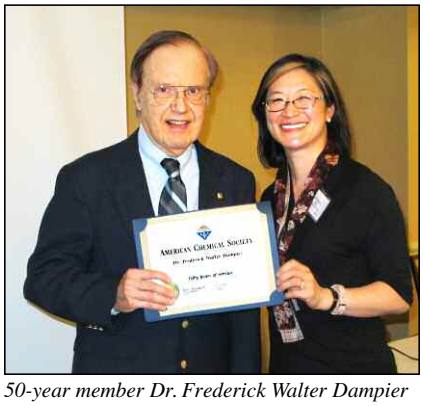
Each October we honor the recipient of the Henry A. Hill Award for Meritorius Service to the Northeastern Section. This years recipient of the Hill Award was Christine Jaworek-Lopes, Professor of Chemistry at Emmanuel College. We also honor NE-SACS members who have been members of the American Chemical Society for 50 years and 60 years. ◇

Christine Jaworek-Lopes (2015 Hill Award recipient) with son Zach and husband Josh.

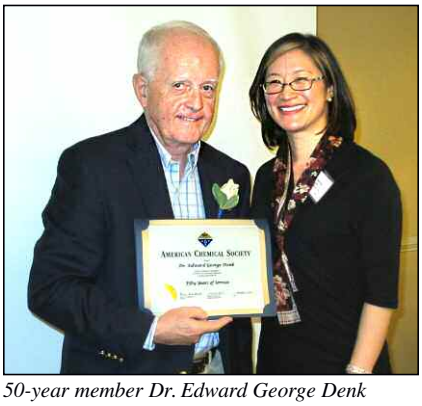
(L-R) Doris Lewis (NESACS Awards Committee, 2003 Hill Award recipient), Dorothy Phillips (Chair, NESACS Awards Committee, 2006 Hill Award recipient), Christine Jaworek-Lopes (2015 Hill Award recipient), Katherine Lee (NESACS 2015 Chair), Anthony Hill (Son of Henry Hill).

50-year member Dr. Russell R. Bessette with Katherine Lee

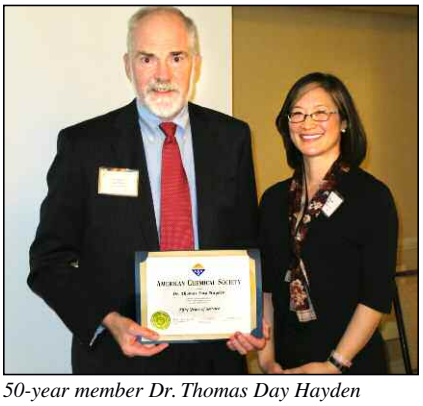
50-year member Mr. Thomas Patrick Brady, Jr.



50-year member Dr. Frederick Walter Dampier



50-year member Dr. Edward George Denk



50-year member Dr. Thomas Day Hayden

50-year member Dr. James A. Kaufman

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Changes in the Nucleus

By Michael P. Filosa

If you have been paying attention, you already realize that the December issue of the Nucleus was the last issue of the Nucleus to be printed *en masse* and mailed to our membership.

Effective January 1, 2016 only those who opted-in for a printed copy will continue to receive *the Nucleus* via third class mail. At this point the number who opted-in is 117. The remainder of our membership will receive notification of the availability of *the Nucleus* electronically via email. This has been the standard policy for new members to NESACS for several years. This policy and eliminating complimentary copies mailed to members of the Central Mass Section of ACS reduced circulation from approximately 7000 to 4500. However, the cost of producing and mailing 4500 copies proved prohibitive as advertising revenue plummeted in recent years.

To maintain our third class mailing permit we need to maintain at least 200 mailed copies. My plan is to merge the mailing list of those receiving copies via first class mail with the list receiving copies via third class mail. We were mailing approximately 225 copies via first class mail at a substantial cost per copy. Most of these copies were sent to ACS-affiliated student groups at a number of local colleges and universities. Sending these copies to the student groups is still good policy but could fall to the budget ax as we assess our budget situation in 2016.

Our printer has also scaled back printing and offered a reasonable price for printing 500 copies. Approximately half will be mailed and the rest will be distributed at various NESACS events.

More changes are likely in the future. The budget will be the major determinant of the future of *the Nucleus*. At some point *the Nucleus* may be solely distributed electronically. Many ACS sections have already done this.

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Call for Applications

YCC+EYCN Young Chemists Crossing Borders (YCCB) Exchange Program to attend the 6th EuCheMS Conference in Seville, Spain (September 2016)

The European Young Chemists' Network (EYCN, www.eycn.eu) and the American Chemical Society Younger Chemists Committee (YCC, http://ycc.sites.acs.org/yccbcrossingborders.htm) invite you to apply for the YCCB exchange program to attend the *6th European Association for Chemical and Molecular Sciences (EuCheMS) Chemistry Congress* as a delegate from NESACS. **The one week cultural and scientific exchange program will occur in Seville, Spain from September 9th to September 17th, 2016.**

As part of an international collaboration, the YCCB program provides an opportunity for local young professionals, new professors, post-docs and graduate students in the chemical sciences to experience the younger chemists' network operating across Europe. Delegates of the 2016 Exchange program will present their research at the EuCheMS congress (http://euchems-seville2016.eu/) and will have many international networking opportunities. During the week, delegates will engage in discussions on research activities and international relations between and amongst like-minded scientists. They will attend professional development workshops, as well as tour industrial and academic facilities.

The Northeastern Section of the American Chemical Society (NESACS, www.nesacs.org) is coordinating the applications process for 2016 YCCB Exchange. Applications are available on the Northeastern Section Younger Chemists Committee (NSYCC) (http://www.nsycc.org) and NESACS (http://www.nesacs.org) websites. Up to 6 younger chemists (applicants **must** be <35 years of age) will be asked to represent the NESACS Local Section in this international exchange.

Applicants **must** demonstrate a strong commitment to the field of chemistry, active engagement in the ACS community, and exhibit high standards of scientific qualifications. Qualified candidates will interview in February 2016 through a process overseen by the NESACS German Exchange Steering Committee, with representatives from National YCC and EYCN. While travel and accommodations will be covered, applicants with travel grants or stipends through work or academia are strongly encouraged to apply.

For more information, contact Felicia Lucci, Chair - NSYCC at felicia.lucci@nsycc.org

Deadline for applications: Friday, January 29, 2016 at 11:59 pm ◇

75 Years of Polaroid Chemistry

Spoken In Honor of Dr. Edwin Land at the August 13, 2015 dedication of the first National Historic Chemical Landmark in Massachusetts

By Michael P. Filosa

I am highly honored to be speaking at this dedication of the first National Historic Chemical Landmark in Massachusetts. I want to thank the ACS for creating this program 20 years ago and the National Historic Chemical Landmarks Subcommittee for recognizing the important contributions of Edwin Land.

I think it pretty amazing that this program had yet to dedicate an NHCL in Massachusetts despite all the iconic chemists who have spent their careers here. Although Land was by training a physicist, he inspired and employed a legion of chemists. His ideas, whether the sheet polarizer or instant photography, required chemists to reach fruition. Much as Pharma and Biotech are magnets for talented scientists in today's Cambridge, Polaroid was a similar magnet and employer of first choice for several generations of chemists and chemical engineers.

By the time I joined Polaroid in the fall of 1979, Polaroid chemistry was 40 years old and Polaroid was at its peak as a company. The "Chemistry Set" was immense with hundreds of chemists working in the research labs at 730-750 Main Street, Osborn St.; the 10X, pilot, and process groups at 600 Main Street, and chemical manufacturing facilities in Freetown and Waltham.

The bulk of Polaroid's research, development and manufacturing were in eastern Massachusetts. Land's visionary ideas and their development into successful commercial products had an enormous impact on the local community.

I mentioned to Keith Lindblom that Land was responsible for the creation of a Disneyland for chemists. I thought it a bit of a trite comment, but it was very true. We had great infrastructure, great colleagues, a great history, quite a bit of freedom, and an environment tuned to creativity and problem-solving.

The chemistry set started slowly. Black and white instant film was done fairly quickly and did not require a complex set of chemicals. However, the effort to create color instant photography required a great increase in the synthetic chemistry capability of the company. This took many years and the first instant color film was not introduced until 1963.

Among the first generation of Polaroid-affiliated chemists were R. B. Woodward of Harvard and his student, friend and protégé, Elkan R. Blout. Woodward won the Nobel Prize in 1965 and was a consultant extraordinaire to Polaroid right up to his death in 1979. Blout was a prolific scientist in multiple fields.

The fundamental invention of the dye-developer, which led to color instant photography, is rightly credited to Howie Rogers, but on many of those dye-developer patents you will also find the names of Woodward and Blout.

That Polaroid chemistry was both complex and sophisticated in no small part stems from the contributions of these men, and one of Woodward's first Ph.D. students, Myron S. Simon.

Also among these early chemical contributors was Vivian Walworth. She joined Polaroid in 1944 two years after receiving her B.S. in Chemistry from University of Michigan.

Vivian worked in research at Polaroid starting with Vectograph images during WW2. She has maintained a passion for Vectrograph images which you can see at tomorrow night's event here at the M.I.T. Museum. She also presented a Vectrograph image of the SX-70 sheet as evidence in the landmark Polaroid/Kodak lawsuit.

Just as Victor McIlheny is Land's pre-eminent biographer, Vivian has been, and still is Polaroid's scientific biographer. She co-authored with Land and Rogers the chapter "One-Step Photography" in "Neblette's Handbook of Photography and Reprography". She was also an author of sections on instant photography in several editions of the Kirk-Othmer Encyclopedia of Chemical Technology, and she served for several years as editor of the IS&T journal Imaging Science and Technology.

Polaroid was very supportive of the involvement of its scientists and engineers in professional societies whether it was the ACS or the IS&T. Many Polaroid chemists have been important leaders and contributors to the Northeastern Section as chairs and as heads of committees.

You can't mention these early Polaroid chemists without mentioning Saul Cohen. In 1945 Land hired Saul Cohen, a recent Ph.D. from Paul Bartlett's physical organic chemistry group at Harvard. A recent tribute by Professor Irving Epstein describes Saul's pathway, which

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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

75 Years of Polaroid

Continued from page 8

far transcended his time at Polaroid: "*In 1950, Saul left Polaroid to join the faculty of Brandeis. By 1966 Saul had already served as Brandeis' first chair of the School of Science, first dean of faculty, and first University Professor. He had played a key role in transforming a tiny college with uncertain prospects into a thriving research university.*"

After this first generation of Polaroid chemistry we had a second generation come and grow Polaroid and the chemistry at Polaroid. One such was a Smith College professor and Woodward Ph.D. student, Stanley M. Bloom. Stan was, along with Myke Simon's group, the prime inventor of the opacification system, which was the most critical new chemical invention necessary for Land's ultimate creation, Instant Integral film and the SX-70 camera.

Other significant second generation chemists were Marty Idelson, Frank Meneghini, Alan Borror, James W. Foley, David Waller, and Lloyd Taylor.

Lloyd Taylor was an eminent polymer chemist from BC and MIT who was a mentor and inspiration to his colleagues both young and old. Lloyd was honored by Polaroid in 2000 at an event held at the Museum of Science for having over one hundred patents. Lloyd was not the only one with a raft of patents. Polaroid was not only a patent machine for Dr. Land, but for many of his coworkers, not the least of which were the chemists.

However, soon after I started at Polaroid and Land departed for the Rowland Institute, Sony demonstrated the Mavica digital camera with a Dye Diffusion Thermal Transfer printer (D2T2) and many felt the death of instant photography was certain.

We had some notable successes in the following years and we had many talented people. However, the death of the instant imaging cash cow was inevitable. I often like to say that to survive the death of chemical-based imaging, Polaroid or Kodak would have had to become a smart phone manufacturer like Apple or Samsung and a social network like Facebook. That is how photos are taken and shared these days.

Land's instant photography legacy does live on in the efforts of ZINK Imaging and the Impossible Project. You can see examples of ZINK's latest technology at tomorrow night's event at the MIT Museum. ZINK's future has brightened significantly under new ownership.

Impossible Project CTO Steve Herchen will also be at tomorrow night's event to discuss the latest with Impossible. They truly did tackle the impossible just as Dr. Land would have. They have had to rebuild Land's chemistry set from scratch. This has presented huge challenges.

Land's legacy also lives on in third generation chemists who, like the first generation chemists, started their careers at Polaroid, but then moved on to bigger and better things. A few examples are: Steve Telfer, Steve Sofen, Judy Giordan, Ken Waterman, and John Warner.

ACS meeting attendees will have the opportunity to hear from some of these individuals at Sunday's symposium on Edwin Land and Instant Photography, presented by the ACS Division of the History of Chemistry and co-presented by ACS President Diane Grob Schmidt.

Edwin Land certainly had a profound effect not only on chemistry, but on science. This NHCL is a tremendous recognition of his impact and significance.

And as a final comment: Vivian added in an email yesterday what I was missing in the previous sentence: "Land's interest in art, his friendship with Ansel Adams, Ansel as a consultant, Land's support of outstanding photographers and the Polaroid Collection.

What a guy!" ◇

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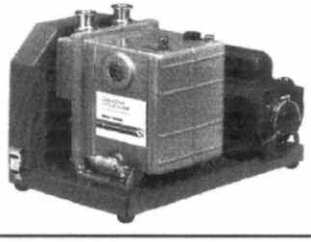

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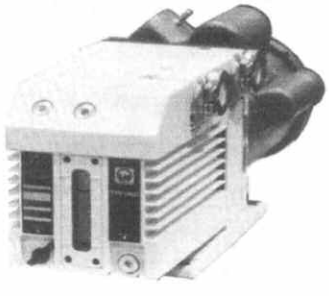

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Selected Written Reports from the December Monthly Meeting

Compiled by Michael Singer, NESACS Secretary

Public Relations: Jack Driscoll

National Historic Chemical Landmark (NHCL)

Edwin Land and Instant Photography was designated an ACS NHCL in Dec. 2014. The American Chemical Society (ACS grants) Landmark (NHCL) status to seminal achievements in the history of the chemical sciences and provides a record of their contributions to chemistry and society in the U.S. The dedication of the plaque was held at 4:30 PM at the MIT Museum (265 Massachusetts Ave., Cambridge, MA) on August 13, 2015. Opening remarks were made be by Diane Schmidt, President of the ACS, world's largest scientific organization with 161,000 members worldwide. The ACS Board of Directors was also present. We had > 150 people in attendance. A seminar on Edwin Land and Instant Photography was held on Sunday Aug. 2015 at the ACS Fall National Meeting in Boston. This will be sent to the Nucleus and the long version will be posted on our website. It can be found on my Scribed site using the following link: https://www.scribd.com/doc/292498412/First-National-Historic-Chemical-Landmark-in-MA-815

NCW

On Oct. 25, 2015 (1-5 PM), a NESACS Cape Cod Science Café was held at Camp Greenough, Yarnouth, MA in conjunction with the Wicked Cool Autumn Festival of the Cape and Islands Council of the Boy Scouts of America (C&ICBSA). There were more than 300 in attendance

The event consists of hay rides, carving pumpkins, building your own bat house fishing on Lake Greenough, archery, visit with a blacksmith, creating cider with an antique cider press and experiencing STEM and Scouting. This will be sent to the Nucleus and the long version will be posted on our website. It can be found on my Scribd site using the following link: https://www.scribd.com/doc/292508702/ACS-NCW-2015-Boy-Scouts-*Autumn-Festival-2015*

A writeup on our NESACS activities was in chemical & Engineering News Dec. 7, 2015 http://cen.acs.org/articles/93/i48/COLORFUL-CELEBRATION.html

STEM Journey III April 2, 2016

Next year (April 2, 2016), our theme will be Transportation and the title is "STEM Journey III: Transportation: Air, Ground and Sea". One of our Keynote speakers will be discussing Autonomous Vehicles. We do expect to have 50 organizations, 150 volunteers and 1,500 visitors on April 2, 2016 at Cape Cod Community College. A full description can be found on my Scribd site using the following link: https://www.scribd.com/doc/292511228/STEM-Journey-III-Announcement-1115

Social Media Training Workshop

On Saturday November 14, 2015, Jennifer Maclachlan facilitated an onsite social media training workshop together with two members of the ACS Office of Public Affairs, at Nazareth College, Rochester, NY. Jennifer presented for an hour on how local sections can leverage social media (specifically Facebook and Linked-In) to increase volunteer participation and attendance at local section events followed by working with small groups on a social media plan for specific events for the Rochester Local Section. Jennifer is currently the Chair of the Communication Technology subcommittee of the ACS National Committee on Public Relations and Communications.

Government Relations: D. Lewis

This is a critical time for the federal budget. Appropriators are now in the process of determining how funds will be divided between federal programs and agencies. We need to send a message to Congress that strong investment in science is vital to the innovation enterprise driving the American economy. ACS is asking us to use the Act4Chemistry program to send a message to our representatives in Congress. Once you have entered your address information in Act4Chemistry the letters to your representatives are automatically generated and you can modify them if you wish. Please consider taking just a few minutes to take this important action.

Additionally, the long holiday recess between December 18 and mid-January gives us a good opportunity to visit our congressional representatives in their home offices. Please let me know if you would like me to schedule a visit for you and accompany you on a visit.

NERM: M. Hoffman

The next Northeast Regional Meeting (NERM) will be hosted by the Binghamton Local Section of the ACS, and will take place Wednesday-Saturday, October 5-8, 2016, at the Binghamton University Downtown Center in Binghamton, NY, with Wayne Jones (SUNY Binghamton) as the General Chair. The meeting website is <http://nerm2016.sites.acs.org/>.

The following dates have been announced:

- Tentative Opening of Abstract Submission and Registration - June 1, 2016
- Abstract Deadline - August 19, 2016
- Early Registration Deadline - August 26, 2016

NERM 2016 will also be the occasion for the annual meeting of the Board of Directors of the Northeast Region of the ACS, Inc. (NERACS), which consists of representatives of the following local sections: Binghamton, Central Massachusetts, Central New York, Connecticut Valley, Cornell, Corning, Eastern New York, Green Mountain, Maine, Mid-Hudson, New Haven, Northeastern, Northern New York, Penn-York, Rhode Island, Rochester, Western Connecticut, Western New York. The officers of NERACS are Anthony Noce (Eastern New York), Chair; Willem

Continued on page 11

December Meeting

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Leenstra (Green Mountain), Vice Chair; Alyssa Thomas-Kuelling (Central New York), Secretary; Wayne Jones (Binghamton), Treasurer.

Summerthing 2016: D. Lewis
Save the date of May 12 for our NESACS event at Fenway Park, Red Sox vs. Houston Astros- our 2016 tickets are the best seats ever!

YCC: F. Lucci
Northeast Student Chemistry Research Conference and Career Symposium DATE CHANGED to Saturday April 16, 2016 and Sunday April 17, 2016

Industry Tour Series
On December 2, 2015, 19 members of NSYCC toured Vertex and learned about drug discovery. The event was organized by Jeremy Green (Vertex, Senior Director, Chemistry), Mark Ledeboer (Vertex, Research Fellow) and Kyle Cole (NSYCC).

Reverse Science Fair
On November 13, 2015, Catherine Rawlins and Ray Borg spent the afternoon presenting chemistry demos at East Boston High with Jerry Gilligan. They worked with Dr. Kristen Cacciatore's AP Chemistry class. The experiments will be used by the students for their annual Science Day where they will conduct and explain the experiments in front of their parents.

Young Chemists Crossing Borders Applications are now available at http://www.nsycc.org/young-chemists-crossing-borders/
Applications are due by January 29, 2016

YCC / GDCh exchange: L. Johnson / J. O'Neil
On behalf of the committee, we wish to thank the board of directors of NESACS and those who participated in the interview process, including alumni of our program as well as Sandy Gregorakos from Strem Chemicals.

For the Kiel trip from March 12 through March 20, 2016, we have selected ten graduate students and two undergraduates. These delegates are citizens of the United States, China, and Nepal. With our 2016 delegate from Nepal, the German Exchange Committee has selected representatives from eighteen (18!!) countries. The schools represented include Boston College, Boston University, Brandeis, Northeastern, Tufts, and the University of New Hampshire.

Thanks to everyone who participated in the interviews and selection process, including Mike Strem, Ruth Tanner, Mort Hoffman, Andrew Scholte, Felicia Lucci, Pat Cappillino, Gulbenk Anarat Cappillino, Elise Miner, Emel Adaligil, and Leland Johnson.

We would not be able to perform our functions without the strong support of our board and corporate and society sponsors.

We plan to have at least one social event where the delegates can meet each

Continued on page 14

October Meeting Photos

Continued from page 6

50-year member Mr. Neil Kaufman

50-year member Mr. Lewis John Klunk, Jr.

50-year member Dr. Doris Ingram Lewis

50-year member Mr. Paul D. Lubin

60-year member Mr. L. Louis Hantman

R: 60-year member Dr. Morton Z. Hoffman

Summer Scholar

Continued from page 2

lizes with half a molecule in the asymmetric unit; the carbazole and ester groups lie in a plane that varies from the plane of the pyridine ring by 43.3 degrees. The molecules are aligned in the solid-state by intermolecular π-π interactions between the six-membered rings of the carbazoles and those of the pyridines. Figure 1 shows the molecular structure of the compound, and the packing of the molecule.

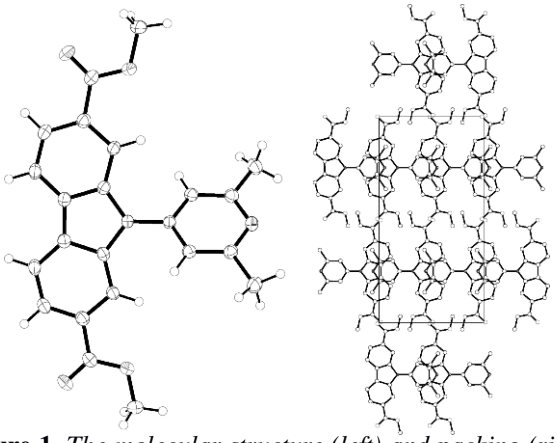

Figure 1. *The molecular structure (left) and packing (right) of the pyridyl-carbazole ester.*

Coordination Polymer Synthesis and Structure

A cadmium coordination polymer was synthesized in a thick-walled glass tube, when 0.0239 mmol of the pyridyl-carbazole diacid and 2 equivalents of cadmium (II) nitrate tetrahydrate were combined in 3 mL of dimethylformamide. The tube was degassed via three freeze-pump-thaw cycles. The evacuated tube was sealed with a methane-oxygen torch and placed in a 110 °C oven for two days, after which pale gold needle crystals had formed. The crystals were isolated and analyzed by X-ray diffraction.

The crystalline network has a linear trimetallic cadmium secondary building unit with six bridging carboxylates and two dimethylformamide molecules (Figure 2). The cluster is capped by two pyridine groups from the carbazole. We have observed similar SBUs in cobalt and manganese coordination polymers using the parent carbazole linker, and similar SBUs have been reported in the literature.[18,19,20,21] The packing of the framework is shown in Figure 3. The trimeric SBUs are connected by the carboxylate linkages to generate two dimensional sheets. The coordination of the pyridine groups at the two terminal cadmium atoms joins these sheets together to generate a three dimensional network. While two of the pyridine groups are coordinated to cadmium centers, one out of every three is still left open the structure. Unfortunately, the binding observed in this structure leads to a structure that is not porous, with a void volume of only 11.6%.

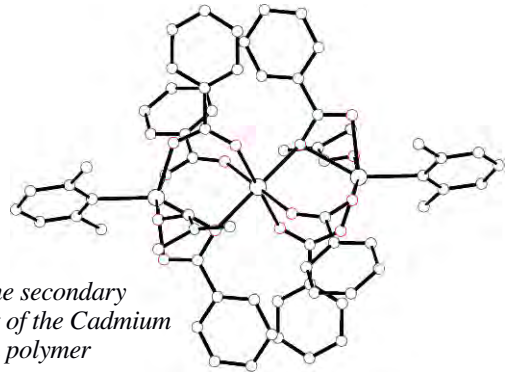

Figure 2. *The secondary building unit of the Cadmium coordination polymer*

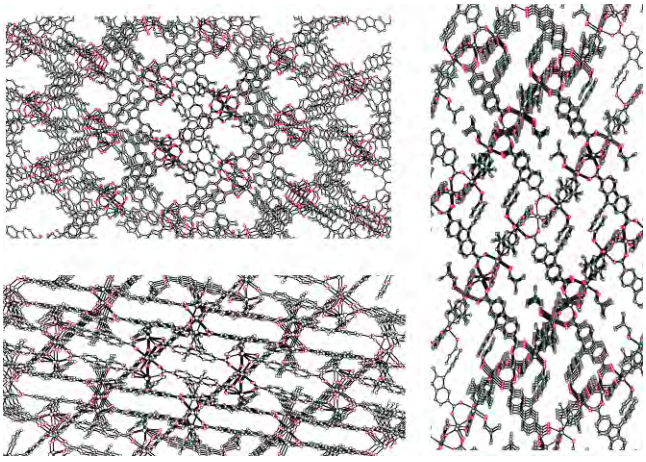

Figure 3. *The packing of the Cadmium coordination polymer shown along the A face (top left), the B face (right) and the C face (bottom left).*

Future Directions:

While we have managed to synthesize our targeted ligand and structurally characterize a cadmium coordination polymer with this linker, the resulting solid does not possess the porous structure that we desire. To address this, we are exploring solvo-thermal syntheses with a variety of metal ions, including transition metals and lanthanides, to produce secondary building units that yield a porous material. As our other target is to have open Lewis base sites within the network, the reported structure having two out of three pyridines coordinated to metal centers is not desirable. To address this issue, we are altering the 2,6-substitution of the pyridine (Ph, ^{t}Bu), such that the steric hindrance reduces the competence of the pyridyl group as a ligand, while still being accessible for carbon dioxide. When we gain our targeted network – porous with open pyridine groups – the gas adsorption properties, selectivities and heats of adsorption will be analyzed using a Micromeretics ASAP2020 Physisorption analyzer. We have also begun *ab initio* calculations to examine the interactions of carbon dioxide with our linkers.

Acknowledgements:

Research conducted by Jona Koka was funded by the Norris-Richards Undergraduate Summer Research Scholarship awarded by NESACS. She would like to thank Dr. David Manke for his insight, guidance and encouragement, former student Amanda Stubbs for previous work on the project, and Dr. James Golen for his contribution in the determination of

Continued on page 13

Biography

Continued from page 5

since 2000, and belongs to the Computers in Chemistry and Medicinal Chemistry technical divisions. ◇

Summer Scholar

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crystal structures. The work was also supported by two NSF instrumentation grants (CHE-1229339 and CHE-1429086).

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NESACS Web-Streaming of Meetings

Dear NESACS members: My name is Ajay Purohit and on behalf of the Board of Publications, I would like to introduce to you a new WebEx feature, through MM Start Visuals, that we would like to roll out starting with our January 2016 monthly meeting.

This web-based service will allow our members to dial in and listen/view remotely, presentations organized by the NESACS during monthly meetings. We hope that this service will allow members who are unable to attend these meetings to still engage and participate.

Please see the Monthly Meeting section for more details regarding how to access this service and system requirements. We would also like to solicit feedback on this feature/service. Please email me at purohian@verizon.net or call me at 508 735 9693 with any questions or comments. Thank you. ◇

Directions for Logging into NESACS Web-Streaming

Go to www.mmstartvisuals.com.

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System Requirements:

- Network connection to the StartVisuals server through HTTP and HTTPS
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- Mac OS X with Firefox or Apple Safari 1.1
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- Macromedia Flash 8.0 or higher - (*when using the recording feature) See considerations below*
- Cookies and Scripting enabled in browser ◇

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December Meeting

Continued from page 11

other before they visit Strem Chemicals and before the trip in March 2016

BAGIM: K. Mattes
A new executive board has been elected for BAGIM (Boston Area Group for Informatics and Modeling)
They have received sponsor donations to keep the group going. A new LinkedIn site has been generated.
https://www.linkedin.com/groups/Boston-Area-Group-Informatics-Modeling-8129238

Phyllis A. Brauner Memorial Lecture Committee: D. Lewis

The Committee met on November 1 and Bassam Shakhashiri reminded us that 2016 will be an important anniversary for National Chemistry Week, formerly National Chemistry Day, and that Phyllis A. Brauner organized the first of many successful lectures on that occasion. All are invited to submit any information they have about this event or past NCW or National Chemistry Day events and to offer their ideas and participation to help us organize a successful commemoration of this event in the fall of 2016. ◇

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Calendar

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Note also the Chemistry Department web pages for travel directions and updates.
These include:
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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

January 11
Prof. Mircea Dinca (MIT)
Brandeis, Gerstenzang 121
4:00 pm

January 25
Prof. Bart Kahr (NYU)
"Optical Activity of Achiral Compounds"
Brandeis, Gerstenzang 121
4:00 pm

January 27
Prof. Christopher Scarborough (Emory University)
University of New Hampshire, Parsons N104
11:10 am

January 28
Prof. Rick Danheiser
"Reproducibility in Synthetic Organic Chemistry"
MIT, Room 6-120
4:00 pm

Notices for The Nucleus Calendar of Seminars should be sent to:
Xavier Herault, email: xherault(at)outlook.com
◇

Changes in the NUCLEUS

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We may also ultimately implement a newer web-based format similar to that used by the Washington, D.C. Section, or MIT's Chemformation Newsletter: http://www.capitalchemist.org/ http://chemistry.mit.edu/news-events/chemformation/current.

However, I greatly prefer the current format. I am not the one who will immediately drive that type of change. *The Nucleus* is in its 94th year. I imagined, when I first started as editor of *the Nucleus*, serving as editor during its centennial year (2021). At that point I will have served 16 years as editor, matching Arno Heyn's tenure, but still far short of that of Avery Ashdown.

I haven't given up on that idea yet. ◇

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