

CINTACS



Newsletter of the Cincinnati Section of the American Chemical Society February, 2004
Vol. 41, No. 5

Meeting Calendar

| | |
|---------------------------|--|
| Wed., Feb. 25 | Chemist of the Year at Givaudan Flavors <i>Discussion Groups:</i> * Organic Chemistry * Biochemistry * Chemical Information |
| Wed., March 24 | Don Tomalia at Miami University |
| Thurs. Apr. 22 | Arthur Ford, USGS at NKU |
| Fri. May 21 | Party Night! Melting Pot Restaurant |

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Awards Note: The award for Research Associate of the Year will not be given this year, since no nominations were received (despite extensive efforts by members of the awards committee). We look forward to receiving qualified nominations from all sectors next year.

2004 Cincinnati Chemist of the Year

Professor Thomas L. Beck
Department of Chemistry
University of Cincinnati

*How a Pre-med Biology Major
Ended up in Chemical Physics and
then Came Back to Biology*



Abstract

Sometimes career paths take a jagged course. This talk will describe such a course, starting with pre-med biology studies, moving to a summer research job in physical organic chemistry, and then on to a major change of plans (graduate school in chemical physics) resulting from a growing interest in mathematics and physics. During those graduate studies, I was drawn to statistical mechanics and the computer simulation of condensed phase systems as an 'experimental tool' to study complex behavior. This tool was applied to studies of melting transitions in small atomic clusters: how small can a particle be and still exhibit a phase transition like melting? A brief stint at Los Alamos led to an interest in methods for doing similar simulations but with quantum mechanics instead of classical me-

(Continued on page 4)

About the Awardee

Thomas Beck studied biology and physiology at the University of Minnesota, and graduated in 1982 magna cum laude with University Honors. He earned the Ph.D. in Chemical Physics from the University of Chicago in 1987. A postdoctoral appointment at Los Alamos preceded his appointment in 1989 as an Assistant Professor of Chemistry at the University of Cincinnati. Since 1997 he has held Professor rank. Dr. Beck's research interests are in areas of theoretic-

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THE CINTACS NEWSLETTER**Vol. 41, No. 5 Feb., 2004**

Editor.....Bruce S. Ault
 Advertising.....Ed Hunter

CINTACS is published eight times a year (October through May) by the Cincinnati Section of the American Chemical Society. The submission deadline will be approximately March 4 for the April, 2004 issue. Electronic submission is strongly preferred, except for original photos. All materials should be sent to:

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From the Chair

Congratulations to the 2004 Cincinnati Chemist of the Year, Professor Thomas Beck of the University of Cincinnati. We will be celebrating Tom's award at the February 25th meeting, to be held at Givaudan Flavors. We thank Givaudan for sponsoring and hosting the meeting, and Phil Christenson for making the meeting arrangements.

Dr. Tom Beck is a physical chemist who emphasizes computer modeling and theoretical calculations in his work. The impact of Tom's modeling has been felt in many areas. For example, his work on the theory of liquids has contributed substantially to the understanding of substrate properties in liquid chromatography. Tom collaborates with a variety of researchers—at the UC Medical Center, for example, where his work has implications for active transport across biological membranes. His talk will be an interesting saga of how a pre-med biology major ended up as a theoretical physical chemist.

The February 25th meeting will also host three Discussion Groups before dinner. The Biochemistry Discussion Group will hear Eileen Jaffe of the Fox Chase Cancer Center; organic chemists will host Zhongwu Gou of Case Western Reserve University; and Kathleen Schmidt of *Chemical Abstracts* will meet with the Chemical Information Discussion Group.

Three days after our February meeting, on Saturday, February 28, the Younger Chemists Committee will sponsor a Chemistry Career/Job Search Conference at Xavier University. This workshop is open to all chemists who want to maximize their resume-writing, interviewing, and job-search skills. Dr. Richard Bretz, Special Assistant to the Provost at Youngstown State University, will conduct the workshop under the auspices of the Office of Career Services at the ACS. The morning will be devoted to talks and discussion of the above skills, while the afternoon will provide time for practice interviews for interested attendees. The workshop is appropriate for undergraduates, graduate students, and any chemists in or about to be in the job market. Breakfast and lunch will be available and everything is **FREE!** See the announcement on page 7 and contact Joy Henderson if you are interested in attending this event.

Finally, I want to remind high school chemistry teachers that the Cincinnati Section will again be sponsoring several Project SEED students this summer. This program, with the goal of encouraging economically disadvantaged students to pursue careers in the chemical sciences, was very successful last year. If you know of any students who might qualify for SEED or have questions about the program, contact Bill Connick at the University of Cincinnati (556-0148; bill.connick@uc.edu).

See you on February 25th.

Joel Shulman

February Monthly Meeting Wednesday, February 25, 2004

Givaudan Flavors
1199 Edison Dr.
Cincinnati, Ohio

Sponsored by Givaudan Flavors

Featuring Thomas Beck, 2004 Cincinnati Chemist of the Year

Program

| | |
|----------------|--|
| 5:30 – 7:00 pm | Registration |
| 5:30 – 6:30 pm | Biochemistry Discussion Group CDR # 2 (see page 4 for details) Chemical Information Discussion Group R&D conf. room (see page 5) Organic Chemistry Discussion Group CDR # 1 (see page 5) |
| 6:00 – 7:00 pm | Social Hour : Cheese with crackers and grapes, veggies with dip, punch, lemonade, iced tea, soft drinks (note: alcoholic beverages cannot be served at this meeting) |
| 7:00 - 8:00 pm | Buffet Dinner, House Salad, Sliced Glazed Ham, Chicken Portabella Marsala, Baked Salmon with a Lemon Parmesan Crust, Glazed Baby Carrots, Wild Rice, New York Style Cheesecake \$25.00 (\$12.00 students, emeritus, unemployed and new members) |
| 8:00 pm | Meeting and Featured Speaker Cincinnati Chemist of the Year Professor Thomas L. Beck <i>“How a Pre-med Biology Major Ended up in Chemical Physics and then Came Back to Biology »</i> |

Dinner Reservations: The meeting reservation form is online at <http://www.che.uc.edu/acs/cinacs.html>. This is the best and easiest way to register. As a lesser alternative, you may send your reservations by email to kim.carey@uc.edu. If it is absolutely impossible for you to make reservation via the internet, call 513-556-0293 (please leave name, affiliation, a contact phone number and state if you are in one of the ½ price categories). Deadline for reservations is 12:00 noon on Fri. Feb. 20.

Directions:

From I-75 North, take the Towne St. exit. Go right at the end of the exit. Turn left at the light onto Paddock Rd. At the first light, turn left onto Edison Dr. and enter the TechSolve Research Park. Givaudan Flavors is on the left, however, continue on Edison past the visitors entrance and park in the employee parking lot which is behind the building. Use the entrance near the south end of the parking lot. The entrance will be marked.

From I-75 South, take the Paddock Rd exit and turn left at the end of the exit onto Paddock Rd. Turn right at the third stoplight onto Edison Dr. and continue as above.

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chanics as the underlying theory. After arriving in Cincinnati, collaborations motivated applications of these methods to some real-world problems, and to development of other simulation methods. One application concerns the basic driving forces for retention in reversed phase liquid chromatography. A new method we are working on is an alternative way to do quantum chemical calculations without basis sets. Finally, in the last year we have collected all these computational approaches and started a project studying biological ion channel proteins: how do they select certain ions and how do they gate?

(Continued from page 1)

cal chemistry, especially density functional theory and its application via computational methods. He utilizes multigrid analysis for computer modeling of large molecular arrays and has developed a 64-processor cluster for this purpose. Dr. Beck is interested in a wide range of highly practical and important problems. He collaborates with scientists from within and outside the Chemistry Department at the University of Cincinnati, and is particularly active within the Department of Physics, the Medical Center, and the College of Engineering. His work on the theory of liquids has contributed substantially to the understanding of substrate properties in liquid chromatography. Additional areas of research focus include the properties of porous membranes, active transport across biological membranes, and electron transport in nano-scale molecular devices. Dr. Beck has published approximately 60 papers and book chapters. He is in high demand as an invited lecturer. His past honors include the Cincinnati Technical Societies Young Scientist of the Year (1991) and the Hans Jaffe Chemistry Faculty Award for Excellence (1997). *When Dr. Beck is not doing chemistry he enjoys performing with his local jug band, The Cincinnati Dancing Pigs. Other interests include backpacking and mountaineering.*

**Visit the
Section's Home Page**

<http://www.che.uc.edu/acs>

Biochemistry Discussion Group

*A Novel Structural Paradigm for
Allosteric Regulation of Protein Function*

Dr. Eileen K. Jaffe

About the discussion group leader

Eileen K. Jaffe received a B.S. in chemistry from SUNY Cortland in 1975 where she worked with Arden Zipp on spectroscopic studies of sulfoxide adducts of vanadyl acetylacetonate. This led to an interest in the relatively new field of bioinorganic chemistry. Dr. Jaffe obtained her Ph.D. in 1979 from University of Pennsylvania, with Mildred Cohn. The work in Dr. Cohn's lab was on the stereochemistry of enzyme-bound metal-ATP complexes using the diastereomers of adenosine phosphorothioates and ³¹P NMR. Dr. Jaffe then moved toward the field of enzymology with a post-doctoral experience with Jeremy Knowles in the chemistry department at Harvard University. Since 1981 Dr. Jaffe has held a number of academic positions in Philadelphia, PA, including Haverford College and University of Pennsylvania. Dr. Jaffe is currently a Senior Member at the Fox Chase Cancer Center. Although she has pursued a number of research projects since becoming an independent investigator, Dr. Jaffe has retained 22 years of NIH funding to study the fascinating metalloenzyme, porphobilinogen synthase, which was initially undertaken because it is a target in lead poisoning. Work on porphobilinogen synthase has included such diverse methodologies as enzyme kinetics, ¹³C NMR, classic chemical modification techniques, Raman spectroscopy, artificial gene synthesis, mutagenesis, X-ray crystallography, and phylogenetic analysis.

Abstract

Allosteric regulation of protein function is generally described on a phenomenological level as involving an equilibrium between two different "states" of the protein, where one state has high activity and the other state does not. Allosteric regulators bind to one or both of these states and perturb the equi-

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librium so as to favor one state. In general allosteric proteins are multimeric, lie at the first committed step of a metabolic pathway, and the detailed structural difference between the two states is not understood. Recent work on porphobilinogen synthase (a.k.a. delta-aminolevulinic acid dehydratase), which catalyzes the first common step in the biosynthesis of the tetrapyrrole pigments (heme, chlorophyll, vitamin B12), identifies a novel structural paradigm for allosteric regulation of protein function and implicates the enzyme in the regulation of chlorophyll biosynthesis. In this case the fundamental difference between the high activity state and the low activity state is the quaternary structure of the protein, and divalent magnesium is the allosteric regulator molecule. X-ray crystal structures provide insight into the molecular basis for the difference in activity between a high activity octamer and a low activity hexamer.

Chemical Information Discussion Group

*SciFinder –
What is really happening with my search?!*

Kathy Schmidt
Applications Specialist
with Chemical Abstracts Service

About the Discussion Group Leader

Kathy Schmidt is an Application Specialist for CAS. Her primary responsibilities include: assuming technical lead for CAS 2004 Eseminar series and customer training in online searching on STN - specializing in polymers, agriculture, and food science. She was conferred an MS in Organic Chemistry with studies in Materials Science from The Ohio State University. She spent four years as a bench chemist for Owens Corning studying the fundamentals of glass/polymer interphases and has additional experience in the analytical chemistry of livestock feeds, meat, and arsenic remediation from drinking water.

Abstract

This will be an opportunity for users of SciFinder to talk with a live specialist about puzzling results they may have received from their search attempts and to learn more about what happens during the actual query process. Potential session attendees are encouraged to submit actual search questions to the discussion group chair, Michael Clager (clager.mr@pg.com), up through Friday, February 20th so that the speaker can formulate appropriate responses.

Organic Chemistry Discussion Group

*Chemical synthesis of complex glycoconjugates and
their applications as cancer vaccines*

Professor Zhongwu Guo
Case Western Reserve University

About the Discussion Group Leader

Zhongwu Guo was born in China (1964) and received his bachelor and master degrees in medicine from Second Military Medical University in 1984 and 1987. He then joined Professor Xikui Jiang's (Academician, Chinese Academy of Sciences CAS) group at Shanghai Institute of Organic Chemistry (SIOC) to pursue his Ph.D. study in physical organic chemistry. In 1989, he was chosen by SIOC to partici-

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Cincinnati Section Meeting Sponsors 2003-2004 Program Year

October 10: University of Cincinnati, Department of Chemistry
November 12: Advanced Testing Laboratory
December 10: Procter and Gamble Pharmaceuticals
January 14: The Procter and Gamble Company
February 25: Givaudan Flavors
March 24: Marshall Wilson
April 22: Robert Laughlin
May 21: Rick Fayter

(Continued from page 5)

pate in a joint training program between CAS and Polish Academy of Sciences (PAS) and was sent to Institute of Organic Chemistry, Warsaw, where he obtained his Ph.D. in 1991 under the supervision of Professor Alesander Zamojski, focusing on organometallic chemistry. He finished his postdoctoral training at SIOC in 1994, and was thereby appointed assistant professor and half a year later promoted to associate professor. His research interests focused on isolation and structural studies of bioactive polysaccharides, chemical and chemoenzymatic synthesis of complex oligosaccharides, new synthetic methodology for carbohydrates, and development of new inhibitors of carbohydrate-related enzymes. He joined Professor Tomoya Ogawa's group at RIKEN, Japan on a prestigious RIKEN fellowship in 1996, where he worked on solid-phase glycopeptide synthesis. He was appointed assistant research officer of National Research Council of Canada and thus moved to Ottawa in 1997. He started his career at the Department of Chemistry, Case Western Reserve University as an Assistant Professor in 1999. His present research interests mainly focus on chemical synthesis of complex carbohydrates and glycoconjugates, new methods for carbohydrate and glycopeptide synthesis, design and development of novel cancer vaccines, and study of new carbohydrate-based materials for selective drug delivery. He received an Alexander von Humboldt Fellowship (Germany) in 1996 and a Research Innovation Award (USA) in 2001. His research projects are funded by NIH, ACS, American Cancer Society, Research Corporation, and Ohio Cancer Research Associates.

Abstract

Immunotherapy is considered an ideal treatment for cancer, whereas an important problem with this therapy is immunologic tolerance to tumor-associated antigens (TAAs). A new strategy is developed to overcome the problem, which is based upon glycoengineered modification of cancer cells. First, an artificial analog or derivative (neoantigen) of a tumor-associated carbohydrate antigen (TACA) is applied to inoculate cancer patients. Once a specific immune response against the neoantigen is established, the patients are treated with the correspondingly modified monosaccharide precursor of the TACA to initiate the exclusive expression of the

neoantigen on tumor cells. Then, the pre-stimulated immune system will react to eradicate the specifically marked tumors. A series of N-modified mannosamines and GM3 antigens were synthesized. The former were studied as precursors for the bioengineering of cancer cells, and the immunologic properties of the latter are carefully compared. Moreover, *in vitro* and *in vivo* studies of the glycoengineered immunotargeting of RMA with alpha(2,8)polysialic acid as the target TACA and N-propionyl mannosamine as the bioengineering precursor proved the principle of the new strategy.

Surplus Computers and Lab Equipment

Hamilton County, to include the Hamilton County Coroner's Crime Laboratory and all other agencies, now disposes of its excess equipment and supplies on an on-line auction site. This is an "e-bay style" site run by litegov.com and can be found by visiting www.hamilton-co.org. Teachers may especially be interested in periodically checking the site for items to augment their programs or provide the core of student's science projects. Bargain hunters of all types should check in often because the items are constantly changing. Recent offering included computer equipment, office furniture, and photographic supplies.

Nominations for Officers Sought

The time for the election of officers for the Cincinnati Section is rapidly approaching. The Nominating Committee will meet in only a few weeks. Thus, if you would like to run for any of the Section's offices (Chair-elect, Second Vice-Chair, Secretary, Treasurer, Auditor, Councilor, and Alternate Councilor), please contact Allan Pinhas, who is Chair of the Nominating Committee, by E-mail (allan.pinhas@uc.edu) or by telephone (513-556-9255). The Cincinnati Section is one of the best because it has great members who are willing to become officers, so please consider running.

Chemical Educators' Discussion Group

An Environmental Evening for Teachers

Just in time for those Spring term lesson plans! On Thursday, March 4, the teachers will gather in Shirley Frey's classroom at McAuley High School to experience environmental chemistry demonstrations by Al Conklin. Al is a professor of Agriculture and Chemistry at Wilmington College. Some of the concepts he plans to cover are cation exchange, flocculation, diffusion, buffering capacity, organic sorption, and electric flow in soils. Each demo is designed to work safely in the high school laboratory and to occupy only short amounts of classroom time. Handouts will be provided; one "make-and-take" is promised! Please feel free to invite your environmental science teachers to this event. The meeting will begin at 6:30 PM for social time and announcements. The program will start at 7 PM and conclude by 8:30 PM. Light refreshments will be served.

McAuley is located at 6000 Oakwood Avenue in College Hill. Exit the Ronald Reagan Highway at Hamilton Avenue. Proceed south on Hamilton Avenue to North Bend Road. Turn right on to North Bend and travel about 1/2 mile west to Oakwood. Turn left onto Oakwood; the school will be on the left side of the street. You can park on the circular drive in front of the school. Enter the lower level near the cafeteria. The stairway is on your left or the elevator is to the right. Go up 2 floors and head into the new wing. Shirley will post signs leading to her classroom, room 201. I am sure that Shirley will be happy to take teachers on a tour of the beautiful new lab rooms at McAuley.

This will be the last meeting of the discussion group for this academic year. I am looking for program ideas and meeting places for the 2004-05 school year. Please send your ideas or offers to host to Linda Ford at Linda.ford@7hills.org.

The area teachers have a hydrogen fuel cell demonstration kit to share. If you would like to get

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Chemistry Career/Job Search Conference

The Younger Chemists Committee is sponsoring a chemistry career/job search conference to assist those in the local area who are seeking to maximize the interviewing, resume writing, and other related employment search skills needed to succeed in the job market. The event will feature a speaker from ACS National Career Services presenting a workshop entitled "Managing An Effective Job Search" (to address resume preparation, interviewing techniques, and targeting the job market), a panel discussion about job searching in the Cincinnati area, and optional one-on-one practice interviews conducted by local employers. Even if you are stable in your current position, the information offered may be useful down the road, should your situation change. Or, you may know of someone who would benefit from this event. **It is open to anyone in the local area-- not just YCC-types!** This includes students nearing the end of an undergraduate or graduate studies program, recent graduates, and those who are or will be in transition from a current position. All are welcome and the conference is FREE!!!

This event will be held at Logan Hall at Xavier University on Saturday, February 28. Breakfast refreshments will be available at 8:30 AM. The workshops listed above will begin at 9 AM, with lunch following at noon. The panel discussion will begin at 1 PM with optional practice interviews running in 30-minute increments from 1 PM to 2:30 PM.

To register for this FREE conference, please contact YCC Chair Joy Henderson, Barr Laboratories, 513-731-9900 x 87227, henderj@barrlabs.com. For more information contact Joy and/or view the YCC web page at <http://www.che.uc.edu/ycc/index.html>

There is no cost for this conference, but you must **REGISTER BY MONDAY FEBRUARY 23** in order to obtain parking passes and event details and to allow YCC to plan for refreshments and site accommodations.

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- Be exposed to the status of contemporary pharmacologic thought and drug therapy - where progress is being made and where advances will likely be made

About the Instructor

Joseph G. Cannon, Emeritus Professor of Medicinal Chemistry, University of Iowa, is the author or co-author of more than 200 articles in organic chemistry, medicinal chemistry, and pharmacology. He is one of the highest rated instructors in the ACS Continuing Education program and is the recipient of the Smissman-Bristol-Myers-Squibb Award sponsored by the ACS Division of Medicinal Chemistry.

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Definitions

Survey of appropriate literature of pharmacology

Membrane models, ion channels, structure of liquid water, implications to pharmacology

Absorption and distribution of drugs: active and passive transport

Blood-brain barrier

Drug metabolism, storage, and excretion

Enzyme induction

Drug-receptor interactions

Theories of drug activity

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Nervous System

Anatomy and physiology of the nervous system

Nerve impulse transmission

Autonomic nervous system

Autonomic physiology and pharmacology

Noradrenergic system: receptors, agonists, antagonists, mixed acting drugs

Dopaminergic system: physiology, Parkinsonian syndrome

Cholinergic system: receptors, agonists, antagonists, acetylcholinesterase inhibitors, Alzheimer's syndrome, other forms of cognitive dysfunction

Central nervous system drugs

Definitions

Aspects of CNS anatomy and physiology

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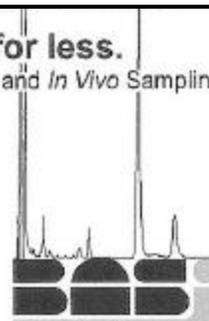


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Analgesics and related agents

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 Placebo effect
 Antiinflammatory analgesics: the inflammatory response, role of prostaglandins, survey of drugs in this category
 "Coal tar" analgesics, possible mechanisms of action, metabolic aspects, toxicity
 Opioid analgesics-survey of chemical types, "MPTP," receptors, mechanisms of actions, endogenous peptide analgesics

Cardiovascular Agents

Aspects of cardiovascular anatomy and physiology
 Hypertension
 Physiology of blood pressure regulation
 Renin/angiotensin system
 Antihypertensive drugs: physiology and pharmacology

Arrhythmias

Aspects of physiology
 Agents used: pharmacological mechanisms
 Physiology of muscle fiber contraction
 Ion channels
 Myocardial ischemia (angina pectoris)
 Physiological aspects
 Drugs employed

The course fee will be \$800 (ACS members) and \$900 (non-ACS members) and includes all course materials, continental breakfast, lunch, refreshment breaks for all 3 days (**compare to \$1,345 and \$1,445 at ACS National meeting or Pittcon**). Please call Rick White at 513-622-1624 to confirm your registration and arrange to have check or money order (Sorry, we cannot accept credit cards) sent to: (**Please make check payable to "Cincinnati Section ACS"**)

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on the list to have the kit in your classroom, please e-mail Linda. The kit is rotated among the schools on a weekly basis. It is easy to use.

If you are looking for a great summer pro-

fessional development opportunity, the 18th Biennial Conference on Chemical Education (BCCE) will be held on July 18-22 at Iowa State University in Ames, Iowa. To learn more about this conference visit the website at www.chem.iastate.edu/bcce or e-mail questions to bcce@iastate.edu.

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