

# CINTACS



Newsletter of the Cincinnati Section of the American Chemical Society

January, 2003  
Vol. 40, No. 5

## Calendar

*New online registration!*

Thursday, Jan. 16, 2003	Dr. Steven D. Ittel at P&G HCRC
Wednesday, February 12	Dr. Paul Lahti at Vernon Manor
Wednesday, March 12	Cincinnati Chemist at Givaudan
Wednesday, April 9	Mr. Frederick Wallace at Northern Kentucky
Friday, May 16	Party Night! Robert Mondavi Montgomery Inn Boathouse

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## “Late Transition Metal Catalysts for Ethylene Copolymerization”

Steven D. Ittel and the Versipol® team.  
DuPont Central Research; Experimental Station

### abstract

Growing out of a discovery in the laboratory of Professor Maurice Brookhart at the University of North Carolina, DuPont has collaboratively developed a new technology for the homo- and co-polymerization of ethylene with a variety of polar comonomers. This discovery has sparked an intense competition around the world as scientists try to take advantage of the unique features of these catalysts. This lecture will focus on DuPont's advances.

The initial UNC discovery started with palladium and nickel catalysts bearing sterically encumbered, bidentate diimine ligands. These catalysts would homopolymerize ethylene to branched or hyperbranched polymers through a mechanism

*(Continued on page 4)*

## About the Speaker

Steve Ittel was born in Hamilton, Ohio (1946) and received his BS in chemistry from Miami University in 1968. After two years of studying photochemical smog in the greater New York City area for the USPHS, he attended Northwestern University where he received his PhD in inorganic chemistry in 1974 with Jim Ibers. Joining DuPont's Central Research, he was involved in the elucidation of fluxional processes in five and seven coordinate molecules. After work on C-H activation and diamagnetic and paramagnetic agostic M-H-C interactions, he moved to research management. Never straying far from the scientific

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**THE CINTACS NEWSLETTER****Vol. 40, No. 5     January, 2003**

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

CINTACS is published nine times a year (September through May) by the Cincinnati Section of the American Chemical Society. The submission deadline will be approximately January 22 for the March, 2003 issue. Electronic submission is strongly preferred, except for original photos. All materials should be sent to:

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**from the Chair**

The January meeting will be held at P&G's HCRC in Mason. The meeting will be sponsored by Advanced Testing Laboratory, whom I would like to thank for their help. The speaker will be Steve Ittel from duPont who will discuss "the crooked path taken from the laboratory to commercialization" of an ethylene polymerization process. In addition, there will be two discussion groups--Chemical Information and Colloid. I would like to thank Joel Shulman for all his help in making the arrangements at HCRC.

There is some misunderstanding about the need for meeting sponsors, which I hope to clear up. Meeting Sponsors such as Advanced Testing Laboratory for the January meeting or Bob Laughlin for the December meeting are very important. Believe it or not, the biggest expense for the Section every year is the monthly meetings. The reason for this is that the full price charged for dinner is approximately what it actually costs the Section for that meal. In other words, we are not making money on the meals. In addition, a number of folks, including those who are retired and students, get half price meals. Another cost for each meeting is the airfare, hotel, and other expenses associated with the after-dinner speaker and the discussion group speakers. What I have done this year is to have many of the out of town after-dinner speakers also give seminars at UC to help split the costs. The bottom line is that the monthly meetings cost more than we take in from the dinner receipts.

This is where the meeting sponsors come in. They help defray a significant percentage of the cost over run. It would be very difficult to continue to have monthly meetings without the help of these generous donations.

I have heard members ask about the anonymous donation and why that money cannot be used for the meetings. When the donation of \$50,000 was made to the Section, it was made as an *in perpetuity* grant specifically earmarked for NCW (50%), the Olympiad (25%), and Project Seed (25%). The match of \$50,000 from ACS National was only possible because the donation was restricted in this way and to these three areas. In fact, the Section does not have the \$100,000. The principal is being held and invested by ACS National. Each year we receive an interest check (this year the interest rate is approximately 3%). When asked, we need to show how the money was spent. Thus, the anonymous donation cannot be used for supplementing the meeting expenses.

Therefore, I again would like to thank those who have donated and those who will donate in the future. These donations make it possible for us to continue our tradition of first-rate monthly meetings.

(Continued on page 4)

**January Monthly Meeting**  
**Jan. 16, 2003**  
**Procter and Gamble Health Care Research Center**  
**Joint with Iota Sigma Pi**

*Sponsored by Advanced Testing Laboratory*

**Featured Speaker**  
**Dr. Stephen Ittel**

**Program**

- 5:30 – 7:00 pm Registrations and before dinner snacks: Cheese/Veggie/Fruit Display w/ French Bread Crackers, Salty Snack Mix, Beer – reg/light, Wine – red/white/blush, Soft Drinks / Bottle Water
- 6:00 – 7:00 pm Chemical Information Discussion Group, Harvard Room  
Group Discussion: “Getting Your Work Published in Scientific Journals”
- Colloid Discussion Group, Room DS2-206  
Professor Carl Seliskar, University of Cincinnati (see page 4 for details)
- 7:00 – 8:00 pm Buffet Dinner, \$24.00 (half-price for students, emeritus, unemployed and new members)  
Caesar Salad, Penne & Farfalla Pastas, Marinara & Alfredo Sauce, Italian Marinated Chicken Strips & Italian Meatballs, Italian Veggie Medley, Homemade Garlic Bread, Asst. Desserts, Asst. Beverages – soft drinks / bottled water, Coffee – reg / decaf, 1 glass of wine w/ dinner
- 8:00 pm meeting and featured speaker  
Dr. Stephen Ittel  
*“Late Transition Metal Catalysts for Ethylene Copolymerization”*

**Reservations: New!** A meeting reservation form is now 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](mailto:Kim.Carey@uc.edu). If absolutely impossible to make reservations via the internet, telephone 513-556-0293. Deadline for reservations is Monday, January 13, 2002. Include your name, affiliation, and state if you're in one of the 1/2 price categories. As a reminder, if you decide you must miss a meeting after you have made reservations, please call to cancel. If you do not cancel, the Section will have to charge you because it will have been charged by the University.

**Directions:** Follow 71 N to the Fields-Ertel exit. This is the first exit past 275. Make a left at the light onto Mason-Montgomery Rd. Stay on Mason-Montgomery Rd for approx. 2 miles. Natorps is on the left, there is a Biggs and a Lowes on the right. You will be able to see the HCRC (Health Care Research Center) after Mason-Montgomery Rd crosses Irwin-Simpson Rd. Stay on Mason-Montgomery and turn right at the first P&G sign. Follow the road straight to the main entrance where the flag poles are. Park outside the main entrance in the visitor's lot.

*(Continued from page 1)*

named "chain walking." Copolymerizations with functional comonomers would yield new structures of copolymers. A mechanistic investigation of all steps of the catalytic reactions has led to a better understanding of the factors which control catalyst activity and polymer structure. While the chain walking mechanism allows remarkable new structures, it also imposes limits on the rate of polymerization of ethylene and other monomers.

The technology base has been greatly expanded. Iron-based catalysts with tridentate pyridylbisimine ligands are highly active for the formation of high density polyethylene, giving remarkable few branches in the resulting polymer. When the steric constraints of the ligand are reduced, such as changing to isopropyl groups to methyl or even to one ortho substituent, the catalysts produce olefins at high catalyst activities. The olefins are of high quality, being very linear and have a low internal olefin content – features which make them attractive commercially.

It was quickly realized that the ligands for active catalysts were not limited to the diimine class. A broad screening program was undertaken to identify new catalyst structures and the particular activities of each of these ligands. Several new classes of anionic ligands have been developed for the nickel catalysts, improving selected copolymerizations with polar comonomers. Some of the original bidentate anionic ligands were based upon salicylaldimine ligands, but more recently, P-N and P-O structures have been developed.

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edge, he has been involved in small molecule catalysis including hydrocarbon oxidation, fluoro-organometallic chemistry, and olefin hydrocyanation. The molecules started getting a little bigger as his interests turned toward elastomeric polypropylene, catalytic chain transfer in free radical polymerizations, and most recently, ethylene polymerization with polar comonomers. He has over eighty publications, thirty patents or published patent applications and a book to his credit. Another interest having both technical and non-technical aspects is the styling and maintenance of his collection of about 80 bonsai.

*(Continued from page 2)*

Speaking of Project Seed, we need some one to be the coordinator. This person will have to help find the students and to make arrangements for the laboratories in which the students will work. As I just mentioned, we have some money from the anonymous donation for Project Seed, and once we get started with this, Project Seed will become a regular line item in our budget.

In my last statement, I mentioned that I had written it before the Oesper Banquet and before NCW. Thus, a few comments are in order at this time. The Oesper banquet was one of the best-attended meetings ever for the Section. I, for one, was very entertained and learned a great deal at Dick Zare's seminar on bubbles. The Oesper Symposium was a true success. I would like to thank Bill Heineman and especially Kim Carey for all they did to make the banquet and symposium a success. I saw Royce and Mirtha Murray the week after the banquet and symposium in Chapel Hill. They both told me how they were impressed with and grateful for the ACS meeting and the symposium.

National Chemistry Week was very popular this year. We had a large number of demonstrations at local libraries, including some new libraries. Based on the number of pictures I saw and the number of thank you notes I received, NCW was bit hit. I think we owe a great deal to Gloria Story for all the arrangements she made to make NCW the big success it was.

The February meeting will be at the Vernon Manor in Clifton and the speaker will be Paul Lahti who is on the faculty at the University of Massachusetts.

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## Nominations for 2003 - 2004 Officers Sought

Yes, it's just after the New Year, so it's time to begin thinking of who will be our new officers for 2003/2004. The list of officers whom we need to elect is:

1st Vice Chair	2nd Vice Chair	Secretary
Treasurer	Auditor	Councilor
Alternate Councilor		

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## Colloid Discussion Group

### *Preparation, Properties and Dynamics of Thin Films of Chemically-Selective Optical Materials*

C. J. Seliskar, Chemistry Department  
PO Box 210172, University of Cincinnati  
Cincinnati, OH 45221-0172

#### Abstract

The preparation of thin films of new selective optical composite materials by the sol-gel process and by blending is described. The optical properties of these films have been determined by a variety of techniques including spectroscopic ellipsometry, scanning electron microscopy and UV-Vis-NIR spectroscopy. The optical properties have been tailored to match the requirements for use as thin chemically-selective films on the surfaces of chemical sensors. The dynamics of film functioning on sensor surfaces have been measured *in situ* and the results describe the detailed physical changes that occur within the films during the selective incorporation of a small molecule (analyte) from aqueous solution. Future areas of related work are described.

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## Chemical Information Discussion Group

cosponsored by  
Women Chemists Committee and Iota Sigma Pi

### **Open Discussion -- Getting Your Work Published In Scientific Journals** *Guest speakers - YOU!*

Publication in scientific journals is one of the chief ways a scientist gains prestige and validation of his or her professional standing. Getting published isn't always easy or straightforward. You are invited to join us in a discussion of your problems and successes in getting your research published and to learn from other Section members how to smooth the path to publication.

## “The History of the Chemistry Set”

Chemical Educators' Discussion Group  
Monday, February 24<sup>th</sup>

Bill Jensen, chemistry historian at the University of Cincinnati, has invited us to his chemistry museum to enjoy a very visual lecture on the evolution of the chemistry set from 1770 to 1980 and to view the extensive collection. For some of us who were enjoying our own chemistry sets in the 50's and 60's, it will be a trip down memory lane. For younger teachers it might very well be a I-can't-believe-they-let-kids-have-that experience. We will meet in the conference room (Room 518) of Rieveschl Hall at 6:30 PM for light refreshments and announcements. At 7 PM we will walk the short distance down the hall to Room 520 for the program. Please bring a friend or colleague for this special occasion.

**Directions:** You are heading for the main campus of the University of Cincinnati. From I-75, take the Hopple Street exit, turn left, and proceed up the hill toward campus. Hopple St. will turn into Martin Luther King Drive. When you get to the top of the hill, turn right onto Clifton Avenue and then make a quick left onto College Court. (College Court is nestled between the DAAP building and Wilson Auditorium.) This short drive will take you straight into a parking garage under Rieveschl Hall. **Park and bring your parking ticket upstairs with you. It will be validated with a stamp to save you the cost of parking.** From I-71, take the Taft Road exit and travel west toward campus. As you cross Vine Street, Taft Road becomes Calhoun Street. Stay on Calhoun until it dead ends into Clifton Avenue. Turn right onto Clifton Avenue and travel a short distance past several university buildings until you get to College Court. Turn right and travel back to the parking garage.

The teachers will meet again on Monday, March 3<sup>rd</sup> at Raymond Walters College. Dick Barnes, analytical chemist, has invited us to his instrumental laboratory to explore analytical methods applicable to the high school curriculum

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Stanley N. Deming, Stephen L. Morgan, Instructors

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- Learn how to match appropriate experimental designs to real-world problems
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- Develop a firm foundation for understanding advanced design techniques
- Receive a brief introduction to Taguchi methods
- Learn about commercial software packages for data treatment
- Improve your skills in communicating research strategies to co-workers

**About the Instructors**

**Stanley N. Deming** is Professor Emeritus of Chemistry at the University of Houston, Texas. He is also the President of Statistical Designs, a firm that offers short courses and consulting in methods development, process optimization, statistical experimental design, and the statistical analysis of laboratory data. Dr. Deming is the author or co-author of more than 90 publications in the areas of analytical chemistry and related disciplines. He is co-author (with Dr. Morgan) of the Elsevier text, *Experimental Design: A Chemometric Approach*, 2nd edition (1992).

**Stephen L. Morgan** is Professor of Chemistry at the University of South Carolina. His current research inter-

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ests include optimization and experimental design in chemistry, pattern recognition on chemical information, and data preprocessing strategies. Additional research in his laboratory involves the application of computers in chemistry, experimental design, and multivariate statistics. Dr. Morgan is the author of more than 100 publications in the field of analytical chemistry and analytical biochemistry. He and Dr. Deming have co-authored (with F. H. Walters and L. R. Parker, Jr.) , Sequential Simplex Optimization (CRC Press, 1991).

Fees will depend on the number of participants, **but are guaranteed to be significantly less than what you would pay at a National meeting or Pittcon (\$1,345 ACS members, \$1,445 non-members)**. Course seating will be limited, so indicate your interest now and be among the first to receive the final announcement, fees and registration details. Send an e-mail with your name, company, and telephone to white.dr.2@pg.com.

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## Science History Tour 2003

Here is your opportunity to visit Holland and Belgium in the company of a group of most congenial people. Dates are not yet set, but it will probably be from June 25 to July 10. We shall end the tour in London, where we will attend a conference at the Royal Society on (Yvonne's hero!) Robert Hooke. Hooke died in 1703 and this conference will be held jointly by Gresham College and the Royal Society to honor Hooke, an under appreciated genius.

The broad plans are to begin the tour in Amsterdam, where there are a number of sites of interest in the history of science. The Boerhaave Museum, the Teyler Museum, porcelain manufacturers and brewing interests will all be included. Many aspects of Holland's history as a maritime and trading nation will be studied. Then we will move on to Belgium, with visits in Brussels and the lovely town of

*(Continued on page 8)*

## John J. Alexander 1940 - 2002



John J. Alexander, Ph.D. died at his residence in Clifton on Friday evening November 15, 2002 at the age of 62 years. Born in Indianapolis, IN., the first child and only son of John G. Alexander, a grocer, and Inez Snedaker, a schoolteacher, Dr. Alexander received his elementary and secondary education in the parochial schools in Indianapolis. In 1962, he received a A.B. in Chemistry from Columbia University in New York City, followed by a Ph.D. from Columbia in 1967 for work done under the supervision of Professor Harry B. Gray. After two years of postdoctoral study at Ohio State University in Columbus, Ohio, Dr. Alexander accepted a faculty position with the Department of Chemistry of the University of Cincinnati in 1969.

During his 33 years at the University of Cincinnati, he taught introductory Chemistry to thousands of undergraduates, supervised the thesis work of more than a dozen graduate students and served as chair of both the Freshman and Inorganic Chemistry Divisions. In addition to more than 40 technical papers and reviews in his chosen field of organometallic chemistry, Dr. Alexander also co-authored an internationally known textbook of inorganic chemistry which has passed through several editions and has been translated into both Spanish and Japanese. Dr. Alexander also served the Cincinnati Section of the ACS in many capacities, including Chair of the Section in 1980-81.

Dr. Alexander is survived by his mother Inez (of Indianapolis, IN.) sister Maryann Traut of Columbus, Indiana, and nephews Greg and Terry Brodnik. Contributions in John's memory may be made to the John J. Alexander Summer Research Experience for Undergraduates Scholarship Fund in the Department of Chemistry, University of Cincinnati, P.O. Box 210172, Cincinnati, OH 45221.

We'd like to have the nominations completed in a timely manner, so the election can be completed and the results announced at the May Meeting/Party.

Being an officer is a rewarding experience. Please look over the list of current officers at

<http://www.che.uc.edu/acs/officers0203.html>

and consider who amongst your colleagues would be most suited for these jobs. You may contact me at hgrieb@one.net, or call 513-385-8363.

Thanks!

Hank Grieb  
Trustee and immediate Past Chair

*(Continued from page 7)*

Bruges. We will make our way to the coast and travel to England by cross-channel ferry, then pay a visit or two in the south of England - Hooke was born in the Isle of Wight. Our last stay will be in London, in a very nice hotel near Hyde Park. In addition to the RS Conference we will visit other notable science venues in London.

Graduate credit is available. CPDUs are also available for teachers. See the following pages for a web presentation on our past trips.

<http://www.ncusd203.org/north/depts/science/chem/marek/>

Details of itinerary, dates and cost will be available later, but if you are interested in this trip, e-mail either Yvonne Twomey <ytwomey@mindspring.com> or Lee Marek <LMarek@aol.com> or call Yvonne at 630-961-9811, or even send mail to her at 841 Kinston Court, Naperville, IL 60540 People are signing up for this trip already, so an early inquiry is advised - numbers are limited.

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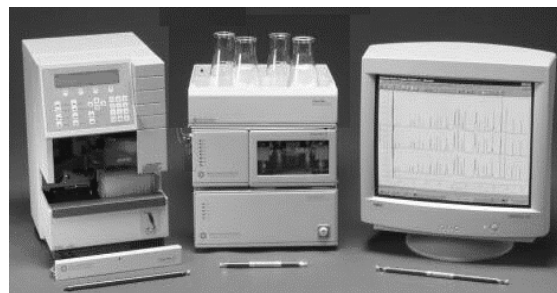


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## Chemical Information Update

### Lost and Found Data in the CRC Handbook

Edlyn Simmons  
Chair, Chemical Information Discussion Group

Everyone is familiar with the CRC Handbook of Chemistry and Physics, the compendium of physical data of chemical substances of all kinds. This invaluable collection of data is now in its 83<sup>rd</sup> edition, with much new and updated information. The 83<sup>rd</sup> edition was published in September, 2002, with a CD-ROM version due to be published in 2003.

The new edition of the CRC Handbook contains much new information, but the handbook

format limits the amount of information that can be included. As new information was added to recent editions of the Handbook, some of the older data were removed. Chemists were disappointed to discover that their new, up-to-date edition of the Handbook omitted tables of valuable data. They began asking the editor-in-chief, David Lide, where they could find the missing data, and Dr. Lide obliged by creating a list of the tables that were removed from recent editions or whose data had been reorganized.

"Tables Relocated or Removed from CRC Handbook of Chemistry and Physics, 71st through 79th Editions" can be found in the Internet at [http://www.indiana.edu/~cheminfo/crc\\_xtabs\\_71-79\\_alpha.html](http://www.indiana.edu/~cheminfo/crc_xtabs_71-79_alpha.html). This document directs you to data that has been moved to a different location in the 83rd edition or to the latest edition of the Handbook that contained the missing table. If you have access to a library with a collection of superceded editions of the Handbook (or if you or a colleague have kept an older edition), the lost data can be found.

## Helen M. Free Award for Public Outreach

Nominations for the Helen M. Free Award for Public Outreach are being solicited. This award is for "Public Outreach" activities, defined as those that reach the lay public. The award selection committee will consider such factors as the nominee's personal advocacy and involvement in public outreach initiatives; development or expansion of ideas, materials, and/or resources for volunteer programs; and overall impact on the public. Activities that qualify include lectures, presentations, demonstrations, seminars, symposia, and exhibits; newspaper or magazine articles and interviews; radio and television appearances; and hands-on science activities with children and/or adults.

The nominee must be an ACS member in good standing whose efforts have increased the public's awareness of the importance of chemistry or chemical engineering. The nominee must have made a major effort to reach the public with positive messages about the contributions of the chemical sci-


ences to a better quality of life. The nominee must have been involved in these activities for more than 5 years and performed them without financial compensation. Please submit names to Gwen Baumann, PR Chair, (gcbaumann@alum.mit.edu) by February 1st.

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