



*The Bulletin*  
of the  
Virginia Section  
AMERICAN CHEMICAL SOCIETY

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**SEPTEMBER MEETING NOTICE**

● **AWARDS MEETING** ●

*Virginia Commonwealth University  
Richmond, Virginia*

*Friday, September 23, 2005*

**RECEPTION:**                   **5:00 - 6:45 p.m.**  
Lobby/Atrium  
Temple Building  
901 West Main Street

**AWARDS PROGRAM:**   **7:00 p.m.**  
Room 1160  
Temple Building

**MENU:**                       Light Appetizers (5:00-5:30); Shrimp, Meatballs, Roast Beef,  
Rolls, Cheese, Fruit, Brownies, Lemon Bars (5:30 - 6:45);  
Soft Drinks, Beer, and Wine

**PRICE:**                       Members/Guests - \$12.00; Students, High School Teachers/  
Spouses, Retired ACS Members/Spouses, Retired Teachers/  
Spouses - \$6.00

**RESERVATIONS:**       Please make reservations by NOON on **Wednesday,**  
**September 21** by calling Mrs. Diane Ruff at (804) 828-1298

**HOST:**                       Dr. Sally Hunnicutt, (804) 827-0531, sshunnic @ vcu.edu

**PROGRAM:**               **DISTINGUISHED SERVICE AWARD: Dr. Ann Sullivan**

**SEPTEMBER 2005**

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			reservations due		meeting	
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## ***DISTINGUISHED SERVICE AWARD***

### ***Dr. Ann Sullivan***

Ann Sullivan received her doctoral degree in physical chemistry from Virginia Commonwealth University in December 1992. In January 1993 she joined the faculty of J. Sargeant Reynolds Community College in Richmond as an instructor of Chemistry; she has since risen to the rank of full professor, while teaching mostly introductory science and general chemistry courses. Ann received her Bachelor of Science degree in chemistry from Virginia Tech and spent most of the time between the two degrees working on her doctoral degree and having her first child, Bryan. When she started her work at VCU, she was already married to a local Richmonder, David, whom she had met at Virginia Tech. She has remained in Virginia since first moving to Northern Virginia in 1972. Before relocating to Virginia, she lived in six other states while attending school in eight different systems. After working for several years at the community college, she had a second child, Patrick. Ann has been very active in the local section since she attended a Section meeting at Randolph- Macon College and was talked into becoming the Entertainment Chair by Bill Myers. She has served the section as secretary, vice chair, chair elect, and chair, and now holds three positions: Alternate Councilor, Webmaster and the Chemical Olympiad Chair.



In recent years, much of Ann's teaching has involved a service component. In 1996, she participated in the VCEPT grant project sponsored by Virginia Commonwealth University to develop courses designed for students interested in becoming mathematics or science teachers in middle school. She continued this interest by developing several workshops and summer programs that involved elementary school teachers in designing science curriculum and activities centered around the Standards of Learning. She also helped develop activities for the BioTechnology Bonanza, which was a two week summer program for over 60 middle school students. These activities were sponsored by SCHEV and the Dwight D. Eisenhower professional development program. In the process of developing these activities and in an attempt to get her introductory students more interested in the course materials, she became very interested in how to use toys and other common materials to help teach her courses. She came across several books that galvanized her to become more active in this endeavor. Since then she presented this concept to students who are interested in becoming teachers and thinks she has influenced a few to consider science as a major

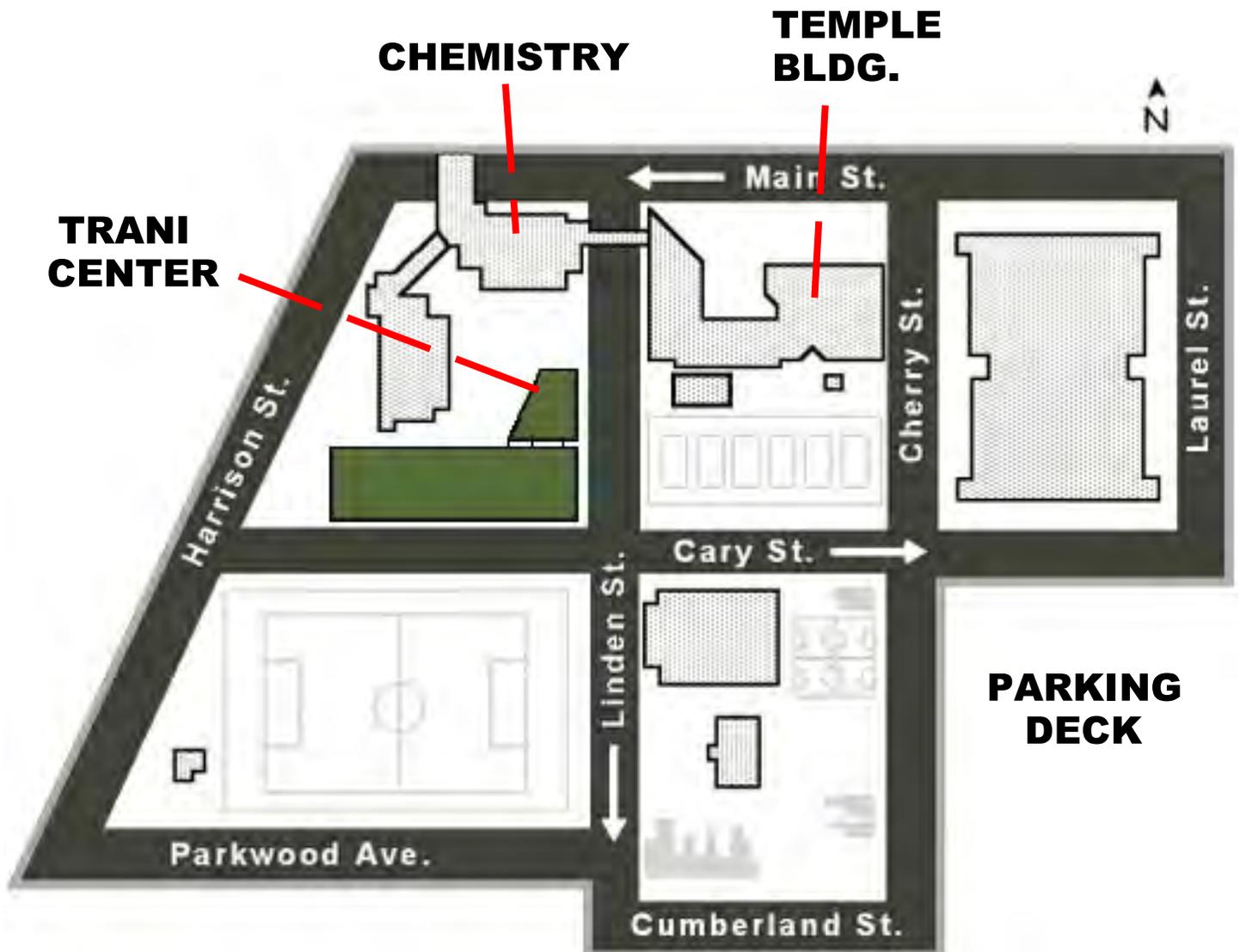
### ***“Teaching Science Using Toys ”***

Concepts in science and mathematics are often difficult to understand for some students. By using toys and common materials, students can manipulate abstract ideas with an object that relates the science concept to a real life example. Several objects that are easily purchased will be discussed and it will be shown how they can be used to teach physics and chemistry concepts to students who are often afraid of science.

## DIRECTIONS

The Reception will be held in the lobby of the Temple Building (formerly the General Purpose Academic Building) at Virginia Commonwealth University. The Temple Building is at 901 West Main Street in Richmond, one block west of Richmond's Landmark Theater (formerly the Mosque). This is just south of the Chemistry Department which is housed in Oliver Hall, 1001 W. Main Street. Note that Main Street is one-way west and Cary Street is one-way east, and that you cannot turn left from Main Street on to Linden. There is parking on the streets around the Temple Building and in the Main Street Parking Deck, 801 W. Main Street (enter from Cherry or Laurel Streets). The Awards Program and Dr. Sullivan's talk will be held in Room 1160 on the first floor of the Temple Building.

## MAP



\*\* VIRGINIA SECTION NEWS \*\*

### **FUTURE MEETINGS OF THE SECTION**

DATE: October 21, 2005	DATE: November 18, 2005
LOCATION: Mary Baldwin College Staunton, Va.	LOCATION: Mary Washington College Fredericksburg, Va.
HOST: Dr. Elizabeth Hairfield	HOST: Dr. Roy Gratz
PHONE: (540) 887-7117	PHONE: (540) 654-1412
SPEAKER: Dr. Matthew Neurock	SPEAKER: Dr. John J. Meister
TOPIC: "From Computational Chemistry to Catalyst and Materials Design"	TOPIC: "Your Garbage = My Reactants: Trash Recycling"

DATE: December 2, 2005	
LOCATION: Afton Research Center Richmond, Va.	
HOST: Rob Davidson, (804) 788-6327	
SPEAKER: Dr. Kevin M. Dunn	
TOPIC: "Caveman Chemistry: Hands-On Projects in Chemical Technology" <b>Presentation of Teaching Awards</b>	

### **QUESTIONS FROM THE PAST**

This question was asked in the Summer Bulletin: April was a special month for the Virginia Section. Two meetings were held. The speaker for the Richmond meeting was a woman chemist, Florence E. Wall, who spoke on "Cosmetics as a Field of Chemical Research." Later that month in Williamsburg there was a joint meeting with the Hampton Roads Section. Speakers were R.C. Herman of the Johns Hopkins University who spoke on "The Origin of the Elements," and Rev. A.E. Acey of Portsmouth who treated the subject "Noblesse Oblige" with deftness and humor. The same month saw the Section sponsor a Seminar on Research and Development that was planned and directed by the Virginia-Carolina Chemical Corporation. The panel of speakers included Dr. S.S. Negus, Dr. Allan Gwathmey, Dr. Lauren

B. Hitchcock, Dr. Milton Harris, and Dr. John Weiss. The concluding address was by the Hon. Colgate W. Darden, President of the University of Virginia and former Governor of the Commonwealth. He spoke on "Scientific Research and Our American Way of Life." **In what year was this month of memorable Section activities?** The year was 1952. The speaker at the April 18 meeting, held in the Baruch Auditorium at the Medical College of Virginia, was Florence E. Wall, Consulting Chemist in New York City. Ms. Wall identified several problems in the field of cosmetics that awaited further research. These included allergenic substances in cosmetics, new types of hair coloring, the relationship between systemic conditions and cosmetic treatments, and the use of surface-active agents in cosmetics. Dinner at the Richmond Hotel cost \$2.00 that evening.

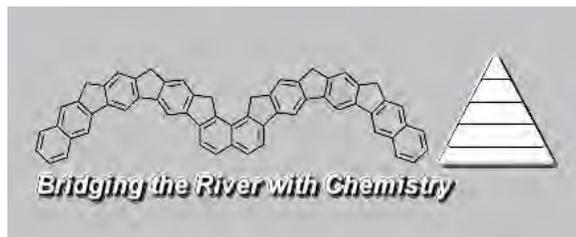


Florence E. Wall

A new question from the past: When it was first chartered in 1915, the Virginia Section encompassed the entire Commonwealth of Virginia. The state is now divided into three local sections—Virginia, Virginia Blue Ridge, and Hampton Roads. In addition, a few counties in northern Virginia are part of the Washington Section, four counties in Southwest Virginia belong to the Northeast Tennessee Section, and there are some rural counties that are not part of any local section. The Virginia Blue Ridge Section was carved out of the Virginia Section in 1931. The Hampton Roads Section was formed some years later. The new Tidewater local section had 54 charter members (the Virginia Section had 301 at the time). **In what year was the Hampton Roads Section chartered?**

## SOUTHEAST/SOUTHWEST JOINT MEETING

The joint Southeast/Southwest regional meeting will be held at the Peabody Hotel in Memphis, Tennessee, November 1-4, 2005. The meeting program will include many special events, symposia and workshops. Abstracts for symposia, general sessions, and poster sessions can be submitted through the online abstract system .



Examples of symposium topics include:

- a. Innovations in the Teaching of Chemistry (CHED)
- b. Guided Inquiry in the Chemistry Curriculum (CHED)
- c. Computational Chemistry
- d. Environmental Health and Safety
- e. Advances in Chiroptical Methods: A New Resource for Chiral Chemistry
- f. AFM and STM
- g. Chemistry and the Law
- h. Nanomaterials and Composites: Synthesis, Properties and Applications
- i. Developments in NMR Spectroscopy
- j. NMR and Structural Biology
- k. Biomedical Applications of Polymers
- l. Spectroscopy of Matrix-isolated Species
- m. Frontiers in Nucleic Acid Chemistry
- n. Cope Award Symposium
- o. Biosensors
- p. Bioactive Lipids

There will be workshops on ACS Insurance, Hygiene and Safety, and How to Start a Co-op program. The ACS Office of Career Services will present workshops and hold a Regional Employment Clearinghouse onsite.

Other special events will include a "Meeting in Miniature" for undergraduate student presentations and posters. (Papers must be submitted through the online abstract system .)

A Graduate School Fair will be held in conjunction with the undergraduate meeting.

The program will also include the Southern Chemist Award Address, and the SE and SW Industrial Innovations Award presentations.

An exhibition will take place during the middle two days of the meeting, Wednesday and Thursday, November 2nd and 3rd, and the Graduate School Fair will be held on Friday, November 4.

Richard Peterson is the General Chair of the regional meeting, Roger Lloyd is Associate Chair, Henry Kurtz is the Program Chair, and Bill McLaughlin is Exhibits Chair. Full information on the meeting can be found at [www.chem.memphis.edu/acs/seswrm.html](http://www.chem.memphis.edu/acs/seswrm.html).

## **JAMES WEBB COLE, JR.** **1910 - 2005**



Dr. James Webb Cole, Jr., Professor Emeritus of Chemistry at the University of Virginia, died on August 7, 2005. He was 95 years old. Dr. Cole served as Chairman of the Virginia Section in 1943-44. A native of Norfolk, Virginia, he completed his undergraduate and graduate studies at the University of Virginia, receiving a Ph.D. degree in Inorganic Chemistry in 1936. After two years of work as a research chemist with the DuPont Company, he joined the faculty of the University of Virginia. He remained there until his retirement in 1975. In 1958, he became dean of the Division of General Studies and Services (now known as the School of Continuing and Professional Studies). He was President of the Virginia Academy of Science in 1967-68. Dr. Cole is survived



by two sons and two grandchildren.

## **2005 CHEMISTRY OLYMPIAD RESULTS**

The 2005 Chemistry Olympiad was a huge success! Nearly 800 students from 29 schools participated in the competition. The First Year Exam was taken by 592 students and 184 students took the Second Year Exam. Team awards were given to schools in several categories. A Team Award is given to a school that has the highest combined total for three students. The winners of the 2005 Team Awards were:

### **First Year Examination:**

Category	School
Small School	The Stewart School
Governor's School	Maggie Walker Governor's School
Large School	Harrisonburg High School

### **Second Year Examination:**

Category	School
Small School	St. Stephen's & St Agnes' School
Governor's School	Maggie Walker Governor's School
Large School	Charlottesville High School

The twelve highest-scoring students were invited to compete at the second level by taking the national exam (no more than two students from a school are allowed to participate in the national exam). Five of those who were selected took the exam. Sydney Creutz, a junior at Albemarle High School, did very well on the national exam and was selected as one of 20 students to attend the International Chemical Olympiad study camp at the Air Force Academy in Colorado (more information on Ms. Creutz and additional Olympiad results appear below). Students selected to participate in the national examination:

School	Student
Albemarle High School	Sydney Creutz*, Sofia Fleyshmann*
Charlottesville High School	Brian Bills, Sarah Harrison
Harrisonburg High School	Riddhi Kothari, Elliot Kulakow*
Maggie L. Walker Governor's School	Yuan Rao, Yang Han
Maggie L. Walker Governor's School	Connor Broaddus*, Xun Zhou* (alternates)
Matoaca High School	Charlie Sutliff, Camille Kump
Potomac Falls High School	Oleg Krogus
New Horizons Governor's School	Ken Kania

\*participated in national examination



**Students who took the National exam:  
Xun Zhou, Elliot Kulakow, Connor Broaddus,  
Sofia Fleyshmann, and Sydney Creutz  
(left-to-right)**

At each school, the student with the highest score received a National Olympiad pin. Here are the highest-scoring students:

SCHOOL	FIRST-YEAR EXAM	SECOND-YEAR EXAM
Albemarle High School		Sydney Creutz
Charlottesville High School		Brian Bills
Chesapeake Bay Governor's School - Warsaw	Joshua Flickinger* Brienne Oltermann *	
Chesapeake Bay Governor's School - Glens	Leah Hendrix	Jennifer McConnell

SCHOOL	FIRST-YEAR EXAM	SECOND-YEAR EXAM
Christian Fellowship School	Caitlin Dronfield	
Commonwealth Governor's School	Bennett Childs	
Deep Run High School	Daniel Kaczka	
Douglas Freeman High School		Daniel Schwartz
Fredericksburg Academy	Michael Weaver	
Harrisonburg High School	Nathan Seifert	Riddhi Kothari
Highland School	Charlotte Selbo	
Highland Springs High School	James Vaughan	Peter Kauffmann
James River High School	Ryan Dougherty	Yuwei Jiang
Louisa County High School		Janelle Conley
Maggie Walker Governor's School	Gregory Leffert	Yang (Helen) Han
Matoaca High School	Sean Yaworsky	Charlie Sutliff
Miller School of Albemarle	Joo Hyun Song	
New Horizons Governor's School		Ken Kania
Potomac Falls High School	Robert Bowen	Oleg Krogus
Prince George High School	Jolisa Parham	Bethany Magee
Spotswood High School	Samuel DuVal	
St. Stephen's & St. Agnes School	Hayley Deavel	Will Killmer* Jeffrey K. Cubeta*
Stafford High School		Patrick Bales
The Blue Ridge School	Kenton Kilmer	
The Steward School	Michael Delaney	Andrew Frank* Douglas Smith *
The Southside Governor's School - Alberta	Rebekah Sykes	
The Southside Governor's School - Keysville	Amanda Thomas	

\* tied for top score

The students with the three highest scores from all participating schools, separated by category and by test, received a \$25 gift certificate from Barnes and Noble for first place, a \$15 gift certificate for second place and a \$10 gift certificate for third place. Those students who were also nominated for the National Exam received a \$25 gift certificate, instead of their place amount. The top scorers:

**FIRST-YEAR OLYMPIAD LOCAL EXAMINATION:**

PLACE	SMALL SCHOOL	GOVERNOR'S SCHOOL	LARGE SCHOOL
First	Michael Delaney – The Steward School	Gregory Leffert – Maggie L. Walker Governor's School	Christopher Stevens – Harrisonburg High School
Second	Michael Weaver – Fredericksburg Academy	Geoffrey Ramsdell & Wenying Wu – Maggie L. Walker Governor's School	Nathan Seifert – Harrisonburg High School
Third	Charlotte Selbo – Highland School	Katherine Seidel – Maggie L. Walker Governor's School	Sean Yaworsky – Matoaca High School

**SECOND-YEAR OLYMPIAD LOCAL EXAMINATION:**

PLACE	SMALL SCHOOL	GOVERNOR'S SCHOOL	LARGE SCHOOL
First	Jeffrey Cubeta – St. Stephen's & St. Agnes' School	Yang (Helen) Han * – Maggie L. Walker Governor's School	Sydney Creutz * – Albemarle High School
Second	Will Killmer – St. Stephen's & St. Agnes' School	Yuan Rao * – Maggie L. Walker Governor's School	Brian Bills * – Charlottesville High School
Third	William Schafer – St. Stephen's & St. Agnes' School	Connor Broaddus * – Maggie L. Walker Governor's School	Sarah Harrison * – Charlottesville High School

\*these students were invited to take the National Olympiad Examination (Olympiad rules allow only two students from a school to take the National Examination, and each participant must be an American citizen)

**ALBEMARLE HIGH SCHOOL STUDENT HONORED**

Sydney Creutz, a junior at Albemarle High School in Charlottesville, was selected to participate in the 2005 U.S. Chemistry Olympiad Study Camp. The Camp was held at the United States Air Force Academy in Colorado Springs, Colorado from June 5 through June 19. Ms. Creutz was one of only 20 students invited to attend the Camp. The Camp participants engaged in intensive activities in preparation for the 37<sup>th</sup> annual International Chemistry Olympiad competition. Four students from the Camp were selected to represent the United States in the International contest that was held in Taipei, Taiwan, July 16-25. Although Ms. Creutz was not among the final four, her selection for the Study Camp was a great honor. The selection was based on her performance on the national Chemistry Olympiad Examination. Her chemistry teacher at Albemarle High School is Mr. Marvin Curry, who received the Virginia Section's Distinguished Service Award for High School Chemistry Teaching in 1987. Congratulations to Ms. Creutz, Mr. Curry, and Albemarle High School for this outstanding achievement.



## **INTERNATIONAL OLYMPIAD RESULTS**

As usual, students from Asian countries dominated the 37<sup>th</sup> International Chemistry Olympiad, which took place in Taipei, Taiwan from July 16 to 25. South Korea received top honors, followed by Vietnam, Iran, Russia, and Taiwan. Alexey Zeifman of Russia had the top individual score. The U.S. team finished in the middle of the pack of 59 countries that competed. Perennial powerhouse China declined to participate in this year's event. The U.S. team consisted of Allen Cheng of Arcadia, California, who earned a Silver Medal; Nicholas Sofroniew of Los Angeles, also a Silver Medal winner; Scott Rabin of Miami, Florida, a Bronze Medal winner; and Jacon Sanders of River Edge, New Jersey, recipient of a Silver Medal. A total of 26 gold, 48 silver, and 79 bronze medals were awarded to the 225 student competitors. The 2006 International Chemistry Olympiad will take place next July in Gyeongsan, South Korea.

## **CHEMISTRY SEMINARS AT THE UNIVERSITY OF VIRGINIA**

September 1 - **Professor Karl Hale**, University College London

September 3 - **Professor Paul Murphy**, University College Dublin

September 23 - **Professor William Klemperer**, Harvard University

Chemistry colloquia are held at 4:00 p.m. in Room 304 of the Chemistry Building. The complete colloquium schedule is on-line at <http://www.virginia.edu/chem/newsandevents/seminars/>.

### **NATIONAL CHEMISTRY WEEK**

**October 16-22, 2005**

**Theme: "The Joy of Toys"**

Information: <http://www.chemistry.org>

## **ABSTRACTS OF POSTER PRESENTATIONS APRIL 15, 2004 - UNIVERSITY OF VIRGINIA**

**Conversion of Carboxylic Acids to Dimethylaminomethyl Esters, Adepeju Ligali, Matthew Roberts, Heather Petruzzi, Tsegahiwot Belachew, Seann Mulcahy, Ivanka Kamenova, Stuart Clough, John Gupton, and Robert Miller, Department of Chemistry, University of Richmond, VA 23173**

Heating carboxylic acids in DMF in the presence of silver carbonate provides a new route to dimethylaminomethyl esters. The reaction appears to have a wide range of applicability working equally well with aliphatic, aromatic, and  $\alpha,\beta$ -unsaturated carboxylic acids. The silver ion appears to be playing the role of a catalyst and an intermediate adduct of DMF and the carboxylic acid appears to be undergoing a self oxidation reduction to form the product. Evidence for this mechanism will be presented. The synthetic utility of this unique system is being explored and ongoing results will be reported.

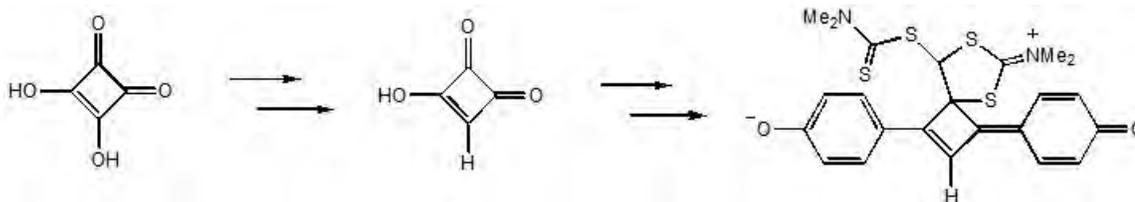
**Photochemistry of Humic Substances: Quantum Yields of Singlet Oxygen, Paul Walsh and Charles Sharpless, Department of Chemistry, University of Mary Washington, Fredericksburg VA**

This poster will present the results of preliminary experiments conducted to examine singlet oxygen generation from humic substances. Humic substances come from plant matter and can be found everywhere in the environment. Singlet oxygen reacts with many different chemicals found in the environment, including many pollutants. To date, experiments have been conducted to set up and test a chemical probe method for measuring  $^1\text{O}_2$  in solution via its reaction with furfuryl alcohol (FFA). Two experimental arrangements have been tested using a sensitizer dye (Rose Bengal). In an open container, oxygen concentration was kept constant and the decrease in furfuryl alcohol was measured. In a closed system, the furfuryl alcohol concentration was increased to keep a constant concentration. The oxygen concentration was measured. Results were used to calculate reaction kinetics. The two systems will be compared. Initial experiments have now begun with humic substances. These results will be presented and future work outlined.

**Design of Chromophore for Chiroptical Molecular Switches Based on Dithiocarbamate – Iminodithiolane Interconversion, Daryl A. Guthrie and John D. Thoburn, Department of Chemistry, Randolph Macon College, Ashland, VA 23005**

We have recently shown the potential for using interconversion of chiral dithiocarbamate and iminodithiolanes as molecular switches. This molecule changes handedness and dipole moment upon interconversion and is thus suitable information storage. The next key step is incorporation of a suitable chromophore that will absorb light in the visible region. The chromophore will act as an “antenna” to harvest energy for photochemically cleavage of the weak C-S bond thereby initiating the switching process.

The key synthetic step in the formation of these switches is the coupling of lithiated methylene(bis)dithiocarbamates with a ketone. Thus incorporation of the chromophore requires that it have an appropriate carbonyl. Condensation products of squaric acid are promising candidates for this purpose because of their ease of synthesis, their robustness, and intense color. Electron donating effects however necessitate a chromophore based on semi-squaric acid. Efforts toward synthesis of these new molecular switches will be described.



**The Effect of Detergent Micelle Environments on the Conformation of BtuB Outer-membrane Protein, Kwo Wei Ho and David Cafiso, Department of Chemistry, University of Virginia, Charlottesville VA 22904**

The versatility of detergents in solubilizing protein and their usefulness in purifying protein have virtually made the science in detergent a unique section in chemistry. However, the effects of detergent on the protein itself have often been overlooked, especially when it comes to X-ray crystallography and the NMR study of membrane protein. In this project, the membrane protein BtuB, found on the outer membrane of gram negative bacteria, was solubilized into various detergent micelles. The dynamics of various parts of the protein were recorded with Site-directed spin labeling (SDSL) technique. A comparison between the spectra of the normally reconstituted protein and the detergent-solubilized protein was made, and the detergents tested were categorized into three classes: 1. Detergents that both destabilized the barrel region, the region facing immediate phospholipids, and the Ton-Box region, a region which becomes unbound in the presence of substrate. These detergents include the alkyl glucoside series, SDS, C8E4, TTAB and D7PC; 2. Detergents that destabilized

barrel region but maintained the natural mobility of Ton-Box. The detergent LDAO fell into this category; 3. Detergents that maintained the natural mobility of both the barrel region and Ton-Box. These detergents include bile salt derivatives, Cholic acid, CHAPS and CHAPSO.

The titration of OG to the reconstituted protein with various spin-labeled residues on the barrel and Ton-Box were conducted to analyze the interaction between the two regions. The primary interpretation of the results showed that there were no direct correlations between the mobility changes in both regions. This result indicated that the increased dynamics of both barrel and Ton-Box were not correlated, as one would speculate from a published paper concerning the effect of OG on BtuB<sup>1</sup>. The insight gained from this project could be used on the further study of BtuB with NMR, which requires solubilization of protein in micelle conditions. The results also demonstrate how different the effects of the solubilizing detergent can be on the dynamics of a protein.

#### Abbreviations:

Lauryl-dimethylamine-oxide (LDAO); CHAPS Cholic acid, CHAPSO; 1,2-Diheptanoyl-sn-Glycero-3-phosphocholine(D7PC) ; sodium-n-dodecylsulfate (SDS); n-Octyl- $\beta$ -D-glucoside (OG); n-Nonyl- $\beta$ -D-glucoside nonylglucoside(NG); n-Heptyl- $\beta$ -D-glucoside nonylglucoside(HG). Tetra-oxyethylene octyl ether (C8E4); tetradecyltrimethylammonium bromide (TTAB).

1. Gail E. Fanucci; Jae Y. Lee; David S. Cafiso. J.AM. CHEM.SOC.2003, 125,13932-13933

#### **Microwave Accelerated Reactions for the Formation of Pyrroles from Vinamidinium Salts, Nick Lauerman, John Solano, John Gupton, Rob Miller, and Stuart Clough., Department of Chemistry, University of Richmond, Richmond, VA 23173.**

We have previously described the preparation of highly functionalized pyrroles from the condensation of vinamidinium salts with  $\alpha$ -aminocarbonyl compounds under basic conditions with heating. We have begun to examine the use of microwave radiation to accelerate such reactions and the initial results of our studies will be presented.

#### **Synthesis and Characterization of Water-Soluble Diphosphine Ligands and their Platinum Complexes, Samantha L. Hopkins and Serge Schreiner, Department of Chemistry; Randolph-Macon College; Ashland, VA**

The synthesis of the water-soluble, chelating phosphines 1,2-bis(bis(hydroxymethyl)phosphino)ethane (1,  $n = 0$ ; DHMPE), 1,2-bis(bis(hydroxybutyl)phosphino)ethane (2,  $n = 3$ ; DHBuPE), 1,2-bis(bis(hydroxypentyl)phosphino)ethane (3,  $n = 4$ ; DHPePE), and 1,2-bis(bis(hydroxyhexyl)phosphino)ethane (4,  $n = 5$ ; DHHePE). These ligands were used to facilitate degrees of water solubility of platinum complexes, depending upon the length of the hydrocarbon chain. For example the water-soluble, bis-chelated complexes Pt[DHMPE]<sub>2</sub>Cl<sub>2</sub> (5), Pt[DHBuPE]<sub>2</sub>Cl<sub>2</sub> (6), Pt[DHPePE]<sub>2</sub>Cl<sub>2</sub> (7), and Pt[DHHePE]<sub>2</sub>Cl<sub>2</sub> (8) were synthesized. Furthermore, the water-soluble, mono-chelated platinum complexes, PtCl<sub>2</sub>[DHMPE] (9), PtCl<sub>2</sub>[DHBuPE] (10), PtCl<sub>2</sub>[DHPePE] (11), and PtCl<sub>2</sub>[DHHePE] (12) were also formed after heating for 14 days at approximately 60 °C. All of the ligands were characterized by <sup>1</sup>H, <sup>13</sup>C{<sup>1</sup>H}, <sup>31</sup>P{<sup>1</sup>H}, and <sup>195</sup>Pt{<sup>1</sup>H} NMR.

#### **Synthesis and Reactivity of 2,5-dimethylfuran Complexes, Matthew Olsen and W. Dean Harman, Department of Chemistry, University of Virginia, Charlottesville VA 22904**

A pi basic metal complex has been developed for the purposes of dearomatizing organic molecules. Several heterocycles that have been coordinated in a dihapto fashion, including 2,5-dimethylfuran. Spectroscopic data suggests that at low temperatures and acidic conditions access to the open ring isomer is granted. Research is being performed to see if this isomer can be manipulated to provide synthetic routes to dihydrofurans and pyrans. Preliminary results strongly indicate that when the open ring isomer is exposed to a hydride source, tandem addition has resulted.

**Synthesis and Purification of Various Acyl-ACP Derivatives, Kathy Goodson<sup>1</sup>, R.M. Cicchillo<sup>2</sup>, N.M. Nesbitt<sup>2</sup>, D. Iwig<sup>2</sup>, M. Baker<sup>2</sup>, S.J. Booker<sup>2</sup>; <sup>1</sup>Department of Chemistry and Physics, Virginia State University, Petersburg, VA 23806; <sup>2</sup>Department of Chemistry, The Pennsylvania State University, University Park, PA**

Lipoyl synthase is the primary enzyme that is responsible for the synthesis of lipoic acid, a unique biological cofactor that is involved in cellular respiration. The substrate for lipoyl synthase is the acyl carrier protein that contains an octanoyl chain tethered to its phosphopantetheine prosthetic group. In order to study the lipoyl synthase reaction, efficient methods for preparing the substrate must be established. Octanoyl-ACP can be synthesized by the enzyme acyl-ACP synthetase from *Vibrio harveyi*, the *Escherichia coli* acyl-ACP synthetase, or by a chemical method. The objective of this research was to establish an efficient means of preparing octanoyl-ACP using *Escherichia coli* acyl-ACP synthetase.

**Characterization of Potential Drug Interactions Between Dextromethorphan, Fluoxetine, and PMMA, Richard B. Keithley, Sarah E. G. Porter, Sarah C. Rutan, Department of Chemistry, Virginia Commonwealth University, Richmond, VA**

The metabolism of dextromethorphan catalyzed by the liver enzyme cytochrome P450 isoenzyme 2D6 (CYP2D6) in the presence of fluoxetine and p-methoxy methamphetamine (PMMA) is being studied. Dextromethorphan is an over the counter cough suppressant, fluoxetine is a popular antidepressant sold under the trade name Prozac®, and PMMA is an illicit amphetamine. A liquid chromatography (LC) method was developed to separate all of the substrates, metabolites, and an internal standard, levallorphan. *In vitro* incubations of the substrates with the CYP2D6 in the presence of NADPH cofactor are being conducted. Separations of these incubations will be run on a Waters 2795 LC coupled to a Thermo Finnigan Deca XP ion trap mass spectrometer with an electrospray ionization source. In order to obtain kinetic profiles, several data analysis methods will be employed including multivariate curve resolution with alternating least squares (MCR-ALS) and wavelet transforms. The mechanisms and kinetics of this reaction can be used to characterize how PMMA and fluoxetine affect the metabolism of dextromethorphan, which can reveal information about the chance of these drugs causing dangerous side effects when taken simultaneously.

**Platinum Recovery: An Inherently Dangerous Procedure For Only the Most Dispensable of Lab Students, K.M. Knott, S.L. Pitts, Y. Qu, N.P. Farrell. Department of Chemistry, Virginia Commonwealth University, Richmond, VA 23284**

Platinum, or “Pt” as we have affectionately named it in our lab, has many uses. These include adorning the necks of our nation’s finest hip-hop stars, high-limit credit cards, catalytic converters, staples, and most importantly, cancer chemotherapeutic compounds. Since the days of antiquity, man has searched for ways to transmute metal into gold. Here at VCU, we have resurrected this ancient technique, alchemy, and made (recovered) large quantities of “Pt”. The Farrell group’s primary focus is the development of next-generation anticancer platinum compounds. All liquid and solid waste from the synthesis and testing of these compounds was collected over a time of 3.5 years. Over a period of three months, this waste was converted into our starting compound, K<sub>2</sub>PtCl<sub>4</sub>, using a refined published method. With the price of platinum at about \$900/oz, near an all time high, recovery of the laboratory’s platinum waste saved the lab at least \$15,000.

**Dihapto-Coordinated Carbonyl Complexes and Their Role in Chemistry, Yunqing Lin and Dean Harman, Department of Chemistry, University of Virginia, Charlottesville VA 22904**

The  $\delta$ -basic metal fragment {TpW(NO)(PMe<sub>3</sub>)} forms thermally stable  $\zeta^2$  complexes with acetone, acetaldehyde. Dihapto coordination of the CO group drastically reduces the electrophilic nature of the carbonyl and activates it towards electrophilic attack. Methylation of the TpW(NO)(PMe<sub>3</sub>)( $\zeta^2$ -Acetone) by methyl-triflate demonstrate the exceptional strength of the nucleophilicity of metal-bounded acetone complexes.

**Synthesis and Characterization of  $\text{TpW}(\text{NO})(\text{PMe}_3)(\eta^2\text{-4H-Pyran-4-one})$ , My-Linh Nguyen, Kevin Welch, and W. Dean Harman, Department of Chemistry, University of Virginia, Charlottesville VA 22904**

The metal fragment  $\{\text{TpW}(\text{NO})(\text{PMe}_3)\}$  (Tp=hydridotris(pyrazolyl)borate) has been identified as a versatile  $\pi$ -base capable of  $\eta^2$ -coordination with arenes and heterocycles, effectively activating aromatic compounds towards electrophilic addition and cycloaddition reactions. Coordination of this W(0) system to 4H-pyran-4-one was investigated and found to occur  $\eta^2$  across the carbonyl.  $^1\text{H}$  NMR and COSY data indicated the presence of only one coordination isomer, whose structure has been unambiguously determined. The  $\text{TpW}(\text{NO})(\text{PMe}_3)(\eta^2\text{-4H-Pyran-4-one})$  complex was found to be stable over several weeks in acetone solution. The complex will hopefully give rise to the development of the first  $\eta^2$ -pyrylium system.

**The Reactivity of Naphthalene Facilitated by an Unusually  $\pi$ -Basic Molybdenum(0) Metal Fragment, Tim Reichart, Chris Mocella, and W. Dean Harman, Department of Chemistry, University of Virginia, Charlottesville VA 22904**

An unusually  $\delta$ -basic molybdenum(0) metal fragment was synthesized and the chemistry of the bound naphthalene was explored. Current studies are exploring the effects of changing one ligand to modulate the electronic and steric effects on the reactivity of the bound naphthalene.

**Determining the Effects of Tethered Urea Groups on Imidazole-Catalyzed Baylis-Hillman Reactions, H.S. Sanders, D.K. Williams, Jr., J. Rock, and P.H. Mueller, Hampden-Sydney College, Hampden-Sydney, Va 23943**

The Baylis-Hillman reaction, a condensation between an electron deficient alkene (generally an acrylate ester or unsaturated ketone) and an aldehyde, is catalyzed by a tertiary amine. The intermediate of the reaction, formed via Michael addition of the amine to the electron deficient alkene, is a zwitterion that functions as a enolate nucleophile in an addition reaction to the carbonyl of the aldehyde. Two separate urea-tethered imidazole catalysts have been synthesized and used to catalyze Baylis-Hillman condensations: N-Phenyl-N'-[(1H-imidazol-1-yl)propyl]urea and N-Phenyl-N'-[(1H-imidazol-1-yl)propyl]thiourea. The products and yields of these reactions are reported.

**Copolymerization of Heteronorbornenes with Styrene and Acrylates via Copper-Mediated ATRP, Ted V. Shaner<sup>1</sup>, Gregory S. Long<sup>2</sup>, and April D. Hennis Marchetti<sup>1</sup>. (1) Department of Chemistry, Randolph-Macon College, Ashland, VA 23005, (2) NMT-11, Los Alamos National Laboratory, Los Alamos, NM 87544**

This project describes efforts to synthesize novel materials through the copolymerization of traditionally radically polymerized monomers with 7-oxa heterosubstituted norbornene derivatives (heteronorbornenes) via radical and ATRP mechanisms. To this end, oxanorbornene derivatives functionalized at the 2 (R') and 3 (R'') positions have been synthesized, where R'=H, R''=C(O)OCH<sub>3</sub> (Species 1), R'=H, R''=CN (2), and R'=R''=COOH (3). In addition, exo-7-oxabicyclo[2.2]hept-5-ene-2,3-dicarboxylic anhydride (4) has been synthesized and characterized by published methods. Species 1, 2, and 3 have been characterized by  $^1\text{H}$ ,  $^{13}\text{C}$ ( $^1\text{H}$ ), DEPT, COSY, and HMQC NMR spectroscopy, and have been shown to include both exo and endo isomeric forms of the substances. Separation of the isomers has been affected in order to determine relative prevalence and reactivity of each isomeric form. In addition, radical and ATRP homopolymerization data trials have been performed, as well as copolymerization trials with the traditionally radically polymerizable monomers styrene and methyl methacrylate.

**WORDS OF WISDOM FOR SEPTEMBER :** "You Can't Turn Back The Clock, But You Can Wind It Up Again"

### Preparation of a Synthetic Receptor for the Age Determination of Cognac, Elizabeth M. Spero and Serge Schreiner, Department of Chemistry, Randolph-Macon College, Ashland, VA

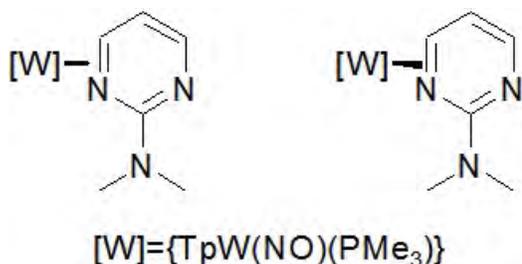
As wine or cognac ages in oak casks, gallic acid and its derivatives are extracted from the oak. The goal of this project was to determine the age of certain cognacs by determining the quantity of gallic acid and gallic acid like derivatives in commercial cognac samples. In order to accomplish this goal, a synthetic receptor, 1-aminomethyl-2,4,6-triethyl-3,5-N-(imidazoline-2-yl-aminomethyl)benzene, needed to be synthesized capable of binding the extracted acids. The synthesis of the receptor is a multi-step synthesis of which the first four steps have been accomplished thus far. The reaction of 1,3,5-triethylbenzene, paraformaldehyde and a 31% HBr/acetic acid solution yields 1,3-bis(bromomethyl)-2,4,6-triethylbenzene(1). Reaction of (1) with KBr, H<sub>2</sub>SO<sub>4</sub> and glacial acetic acid yields 1,3,5-tris(bromomethyl)-2,4,6-triethylbenzene (2). The third step is the reaction of (2) with sodium azide in DMF yielding 1,3,5-tris(azidomethyl)-2,4,6-triethylbenzene(3). The fourth step is conversion of (3) in the presence of triphenylphosphine in THF to 1,3,5-tris(aminomethyl)-2,4,6-triethylbenzene(4). All compounds were characterized by <sup>1</sup>H NMR and <sup>13</sup>C{<sup>1</sup>H} NMR spectroscopy.

### Investigation of Palladium-Initiated Insertion Polymerization from Inorganic Surfaces, Caleb Strepka<sup>1</sup>, Gregory S. Long<sup>2</sup>, and April D. Hennis Marchetti<sup>1</sup>. (1) Department of Chemistry, Randolph-Macon College, Box 5005, Ashland, VA 23005, (2) NMT-11, Los Alamos National Laboratory, Los Alamos, NM 87544

This project describes the synthesis and characterization of a supported palladium catalyst that has shown activity toward addition polymerization of olefinic monomers. This novel method of surface polymerization improves upon current (radical) mechanisms, which involve lengthy post-polymerization catalyst removal procedures and produce polydisperse polymer products. To this end, alumina and silica particles were modified by affecting a condensation reaction in which various (trihalo)silane compounds containing an alkyl halide group were tethered to the surface. The surfaces produced were analyzed by thermogravimetric analysis to confirm silanation. Results indicate approximately 5-7% silanation, varying by surface and silane employed. Additional evidence for successful silanation was obtained by initiating styrene polymerization off the modified surface via an ATRP mechanism. Zerovalent palladium complexes were then oxidatively added to the pendant alkyl halide groups. Metal attachment was confirmed via TGA; the percentage of active sites varied depending upon silane and surface. The metal catalysts showed activity toward norbornene polymerization in the presence of NaBAr<sub>4</sub><sup>-</sup>; this reaction is consistent with an addition-type polymerization mechanism.

### Synthesis and Reactivity of $\eta^2$ -Diazine Tungsten (0) Complexes, Yogesh Surendranath, Hill Harman, W. D. Harman, Department of Chemistry, University of Virginia, Charlottesville, VA

Several complexes of aromatic diazines coordinated to the  $\pi$ -basic transition metal fragment, {TpW(NO)(PMe<sub>3</sub>)} (Tp = hydridotrispyrazolylborate), have been synthesized. Unsubstituted diazines show a strong preference for binding to the metal through the nitrogen lone pair in an  $\eta^1$  manner. However, the addition of pendant groups to the aromatic heterocycle can lead to the formation of isolable  $\eta^2$  linkage isomers. The location and nature of the substituents on the ring can be used to control which  $\eta^2$  linkage isomer is obtained. Examples of  $\eta^2$ -species bound on the carbon-carbon double bond, as well as the carbon-nitrogen double bond, have been observed. The steric environment surrounding the nitrogen lone pairs and the electronic properties of the ligand dictate binding specificity. The reactivity of these novel  $\eta^2$ -diazines is currently under investigation.



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## CAN YOU IDENTIFY THESE PERSONS?



The photograph is from 1991 when these three persons were involved in an important activity sponsored by the Virginia Section. Two of them were the General Chairpersons of that event, while the third was the Meeting Chairman for a similar event that the Virginia Section sponsored in 1969. Two served as Chairs for the Virginia Section—one in 1972 and the other in 1981. Each of the three was a recipient of the Section's Distinguished Service Award—one in 1979, one in 1982, and the other in 1985.

Summer Bulletin was Vada C. Miller who received the Section's Distinguished Service Award for High School Chemistry Teaching in 1952.

