



WHAT'S v...

October/November 2001 Issue

in the Pitt Chemistry Department

What's v is officially back in business! A new year, a new concept. As in previous issues, you'll find important departmental news and see notice of upcoming events...but for your pleasure, we've added a few new sections for scientific posterity as well as a touch of lighthearted fun. Some new sections include '5 minutes with...' (interview), 'the chef's choice' (submit your recipes!), and more. We will aim to publish What's v every two months, pending your response of course! Please let us know if you have any new ideas or have something you would like to be published. Please don't hesitate to contact us and let us know what you think too! Thanks and best wishes for a great semester!

Olivier Guise and Tracy Thompson, editors.

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Welcome New Students!!!

This year the department welcomes 28 new incoming first years. In case you missed out on the department New Student Picnic, which was a great success, we have listed the new students and their respective undergraduate universities. Please take some time to welcome all these new faces!

Twenty-eight incoming full-time PhD students are beginning their studies this Fall. These students (and their former institutions) include: **Zhi Chen** (Xiamen), **Kenneth Cutler** (Valparaiso-IN), **Kadir Diri** (Bogazic Univ.), **Joe Dukes** (Winthrop-SC), **Apsara Gopalarathnam** (Indian Institute of Technology-Madras), **Nilukshi Jayasuriya** (Rutgers-New Brunswick), **Hee-Kyung Kim** (Korea Univ.), **Petro Kondratyuk** (Kiev Shevchenko Univ.), **William Kowallis** (Pitt), **Mustafa Kucukkal** (Bilkent Univ.), **Bradley Lambie** (Edinboro-PA), **Min Liu** (USTC), **Wang Liu** (Jilin), **Petro Maksymovych** (Kiev Shevchenko Univ.), **Michael Martucci** (Millersville-PA), **Jamie McCabe** (Hamilton-NY), **Paul Mills** (Fairmont State-WV), **Branko Mitasev** (Davi&Elkins-WV), **Gregg Morgan** (Thiel-PA), **Paul Morgan** (California Univ. of PA), **Jaehyeon Park** (Seoul National), **Jeremy Walker** (Colgate-NY), **David Waller** (Georgia), **Kan Wang** (USTC), **Andrew Wasmuth** (Rochester-NY), **Tracy Wazenegger** (Indiana Univ.-PA), **Ao Yang** (Beijing Normal), **Fanglong Yang** (Shanghai Institute), and **Zhihua Zhang** (starting this spring).

...And New Professors!!!

On top of the new student additions to the department, we also have some new faculty to welcome. They include...

Kay Brummond
Associate Professor
Synthesis of Biologically Relevant Targets,
Organometallic Chemistry Applied to
Synthesis, Solid-Phase Synthesis
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The Brummond group is involved in: 1) the development of new synthetic methods to facilitate the construction of complex molecules in a stereo- and regioselective manner; 2) the application of these new methods to the synthesis of biologically important compounds; and 3) the design of novel methods for the attachment of small molecules to the solid support for the application to library preparation.

Stéphane Petoud
Assistant Professor
Inorganic Chemistry



email: spetoud@pitt.edu

Stéphane Petoud studied chemistry at the University of Lausanne, Switzerland and received his M.S. degree in 1992. He obtained his Ph.D. degree in 1997 from the Institute of Inorganic and Analytical Chemistry, University of Lausanne, Switzerland in the area of lanthanide coordination chemistry under the supervision of the Professors Jean-Claude G. Bünzli and Claude Piguet. At the end of 1997, he joined the research group of Professor Kenneth N. Raymond at the University of California, Berkeley. He has worked on two topics related to lanthanide coordination chemistry: the synthesis of contrast agents for application in magnetic resonance imaging and the development of a new generation of luminescent lanthanide probes dedicated to applications in high throughput screening. The work on luminescent agents has resulted in the filing of several patents and the creation of a start-up company, co-founded by Dr. Petoud.

Dr. Petoud is looking forward to join the Department of Chemistry at the University of Pittsburgh as an assistant professor in January 2002. He will start a multidisciplinary research program dedicated to the development, study and control of molecules with specific electronic properties, tailored for specific applications. One of the particular interests of this work is the development of luminescent molecules and materials with enhanced properties for modern technologies. This includes luminescent probes and sensors for application in biology, biotechnology, medical diagnostics and imaging, and luminescent materials (solid state and liquid crystal) for the development of a new generation of self-luminescent alphanumeric color displays.

Dr. Petoud will be visiting the department in early October and will be available to speak with first year students. Since his research program will span many areas of chemistry, students with interests in synthetic, inorganic, physical and analytical chemistry will find opportunities in his group. Speak with Dr. Meyer if you would like to be on his schedule.

Sunil Saxena
Assistant Professor
Analytical Chemistry
Magnetic Resonance Studies of Macromolecular Dynamics and Function



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Research in our laboratory will focus on the use and development of multidimensional Fourier transform (FT) electron spin resonance to study the microscopic details of macromolecular dynamics, structure and interactions. New experiments will be designed to probe large spin distances (of up to 50-80 Å), fast domain dynamics, and spin relaxation properties and correlations at conventional and at ultra-low fields. Significant biological processes occur in the ns-ms timescale and involve large changes in separations between groups. These new FT-ESR methods will thus provide insights, hitherto unobtainable, into the role of dynamics towards functionality in biological systems. Our methods will be complemented by NMR techniques already well-established but useful for problems that require the characterization of smaller distances and slower dynamics.

•Pr. Rex E. Shepherd has been invited by the Brazilian National Academy of Sciences to be their plenary lecturer at their national conference of chemistry to be held in San Carlos, Brazil October 22 - 25, 2001. He will be giving a talk on "*Bio-compatible ruthenium nitrosyl complexes as NO carriers : [Ru(NO)(bleomycin)] and related small molecule Ru(NO)-complexes*".

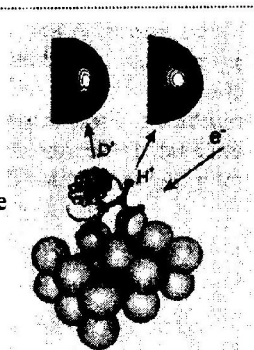
Also, Pr. Shepherd was appointed as of July 2001 to the Board of Editors of *Inorganica Chimica Acta*, the international journal of inorganic chemistry. The Board of Editors is made up of 25 inorganic chemists from around the world, plus three distinguished elder chemists (F.A. Cotton (Texas A&M), J. Lewis (Cambridge,UK), and A. Yamamoto(Tokyo, Japan)). Those from the USA among the 25 include J. K. Barton (Cal-Tech), H. B. Gray (Cal-Tech), F. Basolo (Northwestern), R. H. Holm (Harvard), S. J. Lippard (MIT), A. Wojcicki (Ohio State). Other international members of note include B. F. G. Johnson (Cambridge, UK), V. Balzani (Bologna, Italy), D. Sellman (Erlangen, Germany), H. Sigel (Basel, Switzerland), and K. Matsumoto (Tokyo, Japan).

• Pr. John Yates and Pr. Dennis Curran have recently been named "HighlyCited" researchers (Top 100) in Chemistry by the Institute for Scientific Information (ISI). See: <http://isihighlycited.com>

ISI, a Thomson Company, announced the launch of *ISIHighlyCited.com* at the 22nd American Chemical Society National Meeting held in Chicago. *ISIHighlyCited.com* is the free, online gateway to the world's most cited and influential scientific authors. *ISIHighlyCited.com* brings together the publication and achievement records of preeminent researchers. Researchers are selected for inclusion based on the total number of citations received by their articles within a given category—a quantifiable demonstration of their impact or influence—as recorded in the ISI Citation Database for the period 1981-1999. In addition, researchers will be able to access and update their profiles regularly. Since new material is published daily and citation counts are adjusted at the same time, ISI will regularly expand the list of highly cited researchers as new leaders emerge.

PITT SURFACE CHEMISTS INVENT NEW METHOD TO MEASURE MOLECULAR STRUCTURES OF ADSORBED MOLECULES

An adsorbed organic molecule presents outward-directed C-H bonds. It has been found that the direction of these C-H bonds may be accurately measured by observing the direction of H⁺ emission following local ionization by electron impact. Also, by selectively substituting C-D bonds in known positions and measuring the C-D bond directions, one may perform "molecular triangulation." This permits the conformation of the molecule to be accurately measured. In a *Chemical Physics Letter* (*Chem. Phys. Lett*, 2001 340, 21-25) recently authored by J. T. Yates, Jr. and coworkers, the 4-picoline molecule was conformationally analyzed and found to tilt and twist on the surface as it experiences various intermolecular forces. This new surface science measurement method holds much promise for understanding the structure of self-assembled monolayers. Such monolayers are important as electrode modifiers, for corrosion passivation, and for molecular electronics of the future. The conformation of 4-picoline is shown in the figure and illustrates the exciting possibilities which the new measurement method promises for understanding organic chemistry on surfaces.



Check out www.chem.pitt.edu for other important information regarding departmental news!

Self Assembled Monolayers (SAMs) show great potential as insulating films, ultrathin photoresist films in microelectronics, and building blocks of molecular electronics due to their structural controllability and electronic tunability at the molecular scale. Many SAM applications require patterning of SAMs, i.e., growing or modifying SAMs at desired locations. The mechanisms by which photons interact with SAMs during photopatterning have yet to be fully understood.

In a recent paper (*Langmuir* 2001, 17 4497-4500) authored by graduate student Tao Ye and Pitt undergraduate students Russell Dudek and Darren Wynn, from Dr. Borguet's group, contact angle, FTIR and Atomic Force Microscopy (AFM) measurements are combined to probe the reactive species and reactive sites of Octadecylsiloxane (ODS) SAM degradation under UV illumination in air. It was shown that a combination of oxygen and UV was necessary for the degradation. This suggests that oxygen radical species are the active agents in ODS SAM photodegradation. AFM measurements on submonolayer coverage SAMs provide direct evidence of the photodegradation of ODS SAMs and reveal the role of defects in the degradation process. In contrast to alkanethiol SAM photooxidation on Au, which has been reported to proceed via a heterogeneous defect mediated process, we have shown that photooxidation of alkylsiloxane SAMs on SiO₂ proceeds via a homogenous chain shortening mechanism. A microscopic mechanism of the ODS photoreactivity involving hydrogen abstraction is suggested based on the mechanism of gas-phase oxidation of alkanes.

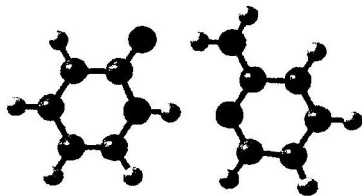
These results have implications for photoresist micropatterning and nanotechnology applications. Further understanding of the mechanisms may enable one to tune photopatterning conditions, such as wavelength, intensity and ambient atmosphere, to improve the resolution and contrast of the patterned films.

Probing The Double Helix

J. R. Roscioli, D. W. Pratt

The hydrogen bonding structure within the Adenine-Thymine and Guanine-Cytosine base pairs is responsible for the general structure and stability of the DNA double helix. Understanding the strength and geometry of these bonds, therefore, is crucial to further understanding role and functionality of the DNA molecule. In the Dr. Pratt's lab, the

2-Aminopyridine/2-Pyridone heterogeneous dimer, the simplest analog of the Adenine/Thymine heterogeneous dimer, has been created in the gas phase and probed with a high resolution UV spectrometer. In addition, rovibronic (Stark) spectra of the dimer within a static electric field were obtained. This was the first such investigation of the hydrogen bonds present in DNA at rotational resolution. From the experimental fits of these spectra, we are able to determine the transition moment, dipole moment, and structure of the dimer in both ground and excited electronic states. This information will provide us insight into forces that hold the Adenine-Thymine base pair together.



Be sure to submit your group's science news for next issue! Contact dr5@pitt.edu for information.

5 minutes with...FRAN NAGY!
(your very own grad secretary!)

What's v: *What's your birthday?*

F.N.: Oh man...

What's v: *You don't have to tell us the year*

F.N.: Ok, December 10th

What's v: *Tell us about your family*

F.N.: I'm married. I've been married for, well, it will be 27 years this month. I have two children, two daughters, a 21 and a 18 years old. They are both students at Pitt.

What's v: *Tell us about what you do exactly for the Department, an overview of your activities.*

F.N.: I keep track of all the graduate students and their progress. I keep updated files on them. I answer any questions that they may have, millions of questions. I do job interviews for students that are getting ready to leave; we have companies coming to interview and contact the students. I let them know the companies are coming. And hopefully they get a job from them. I make sure they are on the right track when they register, and when the time comes for them to conquer certain milestones. They have to pass their preliminary exam, their comp., their proposal, and then their thesis. And there are certain things that have to be done beforehand; so just to remind them I send them little nudges along the way. They're all like my own little kids.

What's v: *Where can we find you on Saturday at 4pm?*

F.N.: Probably at home watching TV. Relaxing. Or cleaning my kitchen...

What's v: *What is the last book you've read?*

F.N.: Actually right now I'm reading one: "Chicken soup for a mother's soul".

What's v: *The last movie you've seen?*

F.N.: I don't actually go out to movies. We rent. Every weekend.

We get about 4 or 5 movies a weekend. "Thirteen Days". It's a good movie as a matter of fact.

What's v: *Approximately how much money do you have in your wallet?*

F.N.: I think...21 dollars.

What's v: *What is the last thing you purchased? The last time you spent money?*

F.N.: My daughter bought me lunch today, so.. I probably bought a cappuccino yesterday.

What's v: *What is your favorite hobby? (Besides enjoying the company of the students)*

F.N.: Yeah, right! It used to be going to see my kids competing at swimming, but they don't swim anymore so there's a big hole in my life. It used to be photography but I don't have time for that anymore. I don't have a hobby (*pretending she cries*).

What's v: *The best way to contact you?*

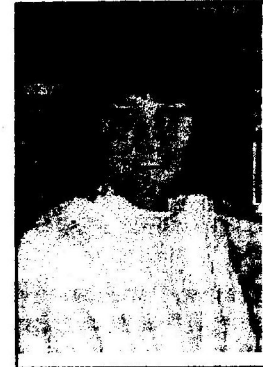
F.N.: At work, not at home! Stop down and see me, cause 95% of the time I'm there.

What's v: *Can you recommend us a good place to go out in Pittsburgh?*

F.N.: Baum Vivant (5102 Baum Blvd. 412-682-2620 see www.pittsburgh.com/auto_docs/dining/7535.html)

What's v: *Any additional comments?*

F.N.: Not really. I really enjoy working with all the students, and I do truly think of them as my little family. And they listen to me better than my own children do.



Chef's Choice!

You will need:

- 2 cups of graham cracker crumbs
- 1 stick of margerine (melted)
- 2 cups of powdered sugar
- 2 eggs
- 1 stick of softened margerine
- 3 large bananas
- 1 #2.5 can crushed pineapple
- Chopped nuts
- Maraschino cherries
- 1 regular container of Cool Whip

The famous Banana Split Cake from Margie Augenstein

1. Mix the graham cracker and the 1st stick of melted margerine in a 13x9 pan and pat it.
2. Whip the eggs, sugar and second stick of softened margerine until fluffy; spread on crumb mixture
3. Drain #2.5 can crushed pineapple; spread on icing
4. Slice 3 large bananas on top of pineapple
5. Spread Cool Whip on top of bananas
6. Sprinkle chopped nuts on top of Cool Whip
7. Place maraschino cherries on top (if preferred, cut cherries in half).
8. Refrigerate for a couple of hours before serving

<<Entertainment News>>

Benedum Center (412-456-6666)

11/20/2001 through 12/02/2001

This dramatic musical is based on Victor Hugo's famous novel of 19th century France. The action begins in 1815 as Jean Valjean, a man condemned to 19 years of hard labor for stealing a loaf of bread, finds only hatred and suspicion when he is released on parole. From his adoption and love of the orphan Cosette, to the darkly funny plots of the thieving Thénardières, from the soaring revolutionary fire of the student rebels who fight on the barricade in the streets of Paris to the final confrontation between Jean Valjean and the righteous police inspector Javert, the story of LES MISÉRABLES is one of love, courage and redemption.



Heinz Hall (412-392-4900)

Beethoven & Rachmaninoff

Friday, October 19, 2001 at 8.00p.m.
Saturday, October 20, 2001 at 8.00p.m.
Sunday, October 21, 2001 at 8.00p.m.

Ludwig Van Beethoven: Concerto No. 4 in G Major for Piano and Orchestra, Opus 58
Sergei Rachmaninoff: Symphony No. 2 in E minor, Opus 27

Bach, Brahms & Zukerman

Friday, November 02, 2001 at 8.00p.m.
Saturday, November 03, 2001 at 8.00p.m.
Sunday, November 04, 2001 at 8.00p.m.

Johann Sebastian Bach: Brandenburg Concerto No. 3 in G Major, BWV 1048
Igor Stravinsky: Suite from Pulcinella
Johannes Brahms: Serenade No. 2 in A Major, Opus 16
Johannes Brahms: Sextet No. 1 in B-flat Major, Opus 18

Stephen Foster Memorial Theatre (412-624-7529)

Canterbury Tales

October 24 – November 11

The Knight, the Prioress, Oswald the Reeve, and a host of others (including Chaucer himself) invite you to join their lively pilgrimage to the shrine of Saint Thomas à Becket in Canterbury. Pack lightly and prepare yourself for the ultimate in entertainment, as each of your traveling companions will amuse, educate, and serenade you with their lively, bawdy tales.

Byham Theatre (412-456-6666)

Oedipus Rex

November 9-10

Join us for a rare and exotic seventh destination: a cross-cultural production of *Oedipus Rex*, presented by Japan's Shizuoka Performing Arts Center and directed by the world-renowned Tadashi Suzuki.

Important Information

Survival Skills and Ethics Workshops

Saturday, October 6 Making Oral Presentations

Saturday, November 3 Teaching

Saturday, December 1 Advancing in your career

Workshops run from 9.00a.m. to 3.00p.m.

Check www.pitt.edu/~survival for a detailed schedule



Have important department news? Let us know! Send important dates, seminar notes, new scientific discoveries and any other relevant information to the What's v? staff...

Meetings!!!

GSAB: Please be sure to drop any comments or departmental/student concerns in the suggestions box outside of room 234.

OPEN FORUM PLU & GSAB

October 19th at 5pm.

Look for signs and details to follow. All are welcome to attend!

Meeting to discuss concerns of graduate students (chemistry only) for the upcoming year. Free food and drink provided. Please come with ideas and suggestions as well as problems that you have encountered. Come one come all, and bring a friend!

Seminars

Thursday, October 11 Pr. Marisa Kozlowski, Univ. of Pennsylvania (12B CSC – 2.30p.m.)

Identification of Novel Ligands for Asymmetric Synthesis.

Thursday, October 11 Pr. Mostafa El-Sayed, Georgia Tech (12B CSC – 4.00p.m.)

Small is Different: Some Interesting Properties of Material Confined to the Nanometer Size of Different Shapes

Wednesday, October 24 Dr. Chris Miller, Wyeth Research (132 CSC – 4.00p.m.)

Discovery and Preclinical Pharmacology of ERA-923: A New SERM for the Treatment of ER+ Breast Cancer

Thursday, October 25 Dr. John Scott, Bristol-Myers Squibb (12B CSC – 2.30p.m.)

The Continuing Evolution of Process Research and Development

Thursday, October 25 Pr. Christopher Chidsey, Stanford Univ. (12B CSC – 4.00pm.)

Long Distance Electron Tunneling: Towards a Tunneling-Based Nanoelectronics

Thursday, November 1 Pr. Pat Harran, Univ of Texas (12B CSC – 2.30p.m.)

Diazonamide

Thursday, November 1 Pr. Jianshu Cao, MIT (12B CSC – 4.00p.m.)

Statistical Analysis of Single Molecule Measurements

15th ANNUAL KAUFMAN LECTURES – Pr. Mark Ratner, Northwestern Univ.

Thursday, November 8 5.30p.m. 12B CSC

Electron Transfer and Transport-Some Mechanistic Issues

Friday, November 9 3.30p.m. 12B CSC

Molecular Deformations and Molecular Writings

Thursday, November 15 Pr. Stephan Stranick, NIST (12B CSC – 4.00p.m.)

Near-Field Microscopy and Spectroscopy for Chemical and Materials Nanoanalysis

Please be sure to submit your own news!!! Send information to tlt5@pitt.edu or oguisse@pitt.edu

NEWS-NEWS-NEWS

- Elevators in Chevron end construction phase...appear to work quite well!
- Congratulations to Ken Contaldo (machine shop) on his nearing retirement. Ken will be with us through the end of October. Thank you Ken for all of your hard work and dedication!!!
- Construction in Eberly Hall is nearing completion. Approximate date for movement of chemistry groups into the upstairs floors is approaching. More updated information to follow.
- Concerns regarding safety issues should see Paul Floreancig, who will be the head of regular safety inspections for the graduate department.
- Please see Dorcas Baumgart (234) regarding new ordering procedures. Be sure to give her your feedback regarding new ordering policies.

**Send us your news and
announcements!**

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