CHEMISTRY DEPARTMENT SUMMER RESEARCH ON THE HILL 2004

Douglas Beussman – Mass Spectrometry/Course Development Research Opportunities

There will be several opportunities for students to engage in my research during the summer of 2004. One project might include collaborating with researches in the Biology Department on the Identification of isolated proteins, using mass spectrometry techniques with the new LC-MS instrument. This may also involve developing methods to reduce the amount of sample required for protein identification. A second research area might include development in LC-MS techniques for the analysis of dietary supplements or performance enhancing drugs. There may also be opportunities to help develop laboratory experiments for two new courses to be offered at St. Olaf in 2005.

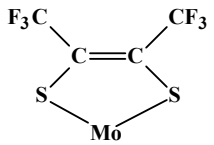
Bob Hanson -- Web-Based Chemical Informatics

Current plans for research in the Hanson group this summer are in the area of chemical informatics, particularly as it relates to chemical education. "Chemical Informatics" is the "computer-assisted storage, retrieval and analysis of chemical information, from data to chemical knowledge." This is a reviving of a project we started some years ago that culminated in a student co-authored paper, "Data-Driven Chemistry: Making Molecular Models (Literally) from Electron Diffraction Data," a book, "Molecular Origami," and an extensive website (http://www.stolaf.edu/people/hansonr/mo).

Our interest now is in using the latest web-based technology to allow immediate student on-line access to extensive and detailed structural information relating to molecular geometry and bonding. The project is based on the idea that learning from real data more closely resembles actual science than typical book learning, but learning from real data is only possible when real data are readily available. In collaboration with Scot Wherland at Washington State University, we will be developing a chemical structure database (see http://www.stolaf.edu/people/hansonr/mo/struc for its preliminary form) and associated educational lessons. Plans are to submit this work for publication by the end of the summer and also present this work at the Biennial Conference on Chemical Education in July. Additional projects will be developed that are consistent with the particular interests of group members. Student coworkers should have an interest in molecular structure and bonding and be able to work and learn independently (with guidance, of course). Students with an interest in web programming (HTML, JavaScript) but not necessarily any background in such are encouraged to apply. Course background should include Chemistry 125 and 126.

Gary Miessler: Dithiolene Complexes of Molybdenum and Tungsten

My main research interests are in organometallic chemistry of molybdenum and tungsten. Primarily I hope to develop syntheses of new compounds of these metals that contain dithiolene ligands in addition to organic ligands such as CO and h5-C5H5. Some important molybdenum- and tungsten-containing enzymes have dithiolene ligands, (the structure of one dithiolene is shown below) and I hope to synthesize compounds that might serve as models for the metal sites in such enzymes.



A dithiolene ligand bonded to Mo

In the laboratory, students participating in this work will gain experience in vacuum line synthesis and purification techniques beyond the scope of our regular synthesis laboratory courses. Students will also use a variety of instruments, especially the NMR, IR, and UV-vis, and will perform web-based searches of the chemical literature. The department's new mass spectrometer should also be a valuable tool in this project.

Biochemistry research opportunities with Greg Muth

Gene regulation in bacteria often occurs by protein factors binding to DNA near the site of the start of transcription. It is also clear that regulation can occur by direct interactions of small molecule co-factors (vitamins) with the mRNA after it has been transcribed. What has not been well established is a detailed biochemical model of the RNA structures that form in the presence of co-factors and a mechanism of discrimination used by these RNA structures to differentiate between potentially very similar co-factors. The goal of this project is to study the mRNA regulatory region and effector molecules in the biosynthesis of the vitamin co-factor thiamin from bacteria *Rhizobium etli*.

The project is a hybrid between molecular biology, biochemistry and synthetic organic chemistry utilizing skills and techniques from each of these disciplines.

Ligand Synthesis and the Preparation of Transition Metal Complexes: Pat Riley

My research interests are developing new ligands to support inorganic and organometallic chemistry. Ligand synthesis has been a cornerstone of research in chemistry for many years. In this context, we have decided to examine the synthesis and reactivity of complexes containing hydroxyindole ligation. Once these ligands have been prepared and purified, we will conduct reactivity studies with early transition metal halides and metallocene halides. The resulting complexes may be useful as olefin polymerization catalysts or as homogeneous models for hydrodenitrogenation catalysis.

Students working on this project will learn techniques and use instrumentation commonly employed in organic synthesis, organometallic, and inorganic chemistry.

Jeff Schwinefus, Chemistry, Summer 2004 Research

Why are proteins thermally stabilized in most cosolvent-water mixtures while the DNA double helix is destabilized? As an example, glycerol thermally stabilizes protein structure while decreasing the melting temperature of double-stranded (ds) DNA. Since dsDNA and proteins are both polyelectrolytes with hydrophobic cores, why is there such a difference in cosolvent influence on dsDNA and protein structures? Interestingly, cosolvents that stabilize protein structure are generally excluded from the protein surface. Are cosolvents then accumulated near the DNA surface, disrupting hydration of the DNA helix? As of yet, the answer is unknown. This is rather surprising considering the understanding of dsDNA physical chemistry in cosolvent-water mixtures has potential meaning for cosolvent mediated protein-DNA interactions and the polymer coil-globule transition.

Students involved in my research during the summer of 2004 will measure cosolvent accumulation or exclusion near the surface of calf-thymus (ct) DNA using high precision density measurements. Our ultimate goal is the determination of dsDNA water-cosolvent transfer free energies to piece together the thermodynamic cycle of dsDNA thermal destabilization. Students involved in this research will gain exposure to biophysical chemistry concepts, thermodynamics, and analytical techniques for the study of biopolymers.

Paul T. Jackson: "Investigating Environmental Contamination in the Cannon River Watershed: Caffeine and the Other Actors"

During the summer of 2004, there are opportunities for interested students to work with me on projects related to separation science and environmental analysis. Pharmaceuticals and personal-care products contain numerous chemicals designed to illicit specific biological responses. What happens to these unmetabolized or unreacted materials after we "flush" them down the drain? The focus of this project is to extend the chemical assessment of surface waters to include largely rural, agriculturally dominated river watersheds. Specifically, my research group is interested in identifying and quantifying therapeutics

and personal care products in wastewater output from rural communities with populations between 10,000 and 25,000. Therapeutic agents, metabolites, and a suite of chemicals related to personal care products have been traced to effluents emanating from wastewater treatment works, and the exact impact of such chemicals on the river ecosystem is not well understood. Our initial hypothesis is that rivers flowing through rural communities are at a similar risk of contamination as compared to their larger urban cousins, such as Minneapolis-St. Paul.

I hope to have students apply gas and liquid chromatography, mass spectrometry, and sampling/extraction techniques to answer two questions. In the past, we have found levels of caffeine in the Cannon River. Since caffeine is an excellent indicator of anthropogenic (human) influence on the water system, what can it tell us? More specifically, what is the temporal and spatial concentration of caffeine in the Cannon River around Northfield? Secondly, the USGS found a significant number of surface water systems contaminated with steroidal chemicals (including hormones) and non-prescription medications. Which of these chemicals exist in the surface waters of the Cannon River and at what concentration level?