

**DEPARTMENT OF CHEMISTRY**  
**College of Arts & Sciences**

**SUMMER RESEARCH OPPORTUNITIES**  
**FOR UNDERGRADUATE WOMEN**

**APPLICATION DEADLINE: MARCH 1, 2002**

*The Department of Chemistry is pleased to offer the following research projects for the summer of 2002. Interested students are urged to contact the faculty member (s) directing the project (s) that most interest them. By contacting the faculty member, you can discover more about the project, learn what your responsibilities will be, and if possible, develop a timetable for the twelve-week research period.*

**Professor Bruce S. Ault**  
**Department of Chemistry**  
**401 Crosley x6-9238      Fax: (513) 556-9239      Email: Bruce.Ault@uc.edu**

**Matrix Isolation Studies of Reactive Intermediates.**

Our research interests lie with the exploration of the mechanisms of important chemical reactions by isolating, identifying and characterizing reactive intermediates that are created and destroyed during the course the reaction. The matrix isolation technique, which involves trapping the intermediates of interest in an argon crystal at nearly absolute zero, is employed to permit the study of very reactive intermediate species. High resolution infrared spectroscopy is the primary technique for characterization of the trapped species. The reactions of particular interest are those involving high valent transition metal oxo compounds, which are commonly used as oxidizing agents in organic synthesis, and as models for active sites of enzymes. The goal of this project will be the identification and characterization of reaction intermediates, from which we can obtain a better understanding of the mechanistic details of these oxidation reactions.

**Professor Thomas Beck**  
**Department of Chemistry**  
**402 Crosley x6-4886 Fax: (513) 556-9239      Email: Thomas.Beck@uc.edu**

My research centers on computational methods to study complicated systems in chemistry. We are developing new ways to study large chemical systems: chemical reactions, molecular electronics, etc. We use a cluster of PCs connected together (Beowulf) to perform the calculations. The student would learn how to use computers to do interesting calculations on chemical systems and relate the results to experimental data. She would also learn how to visualize the results using the computer graphics programs. Overall, it would be a challenging and rewarding experience in scientific computing.

**Professor Anna D. Gudmundsdottir**

**Department of Chemistry**

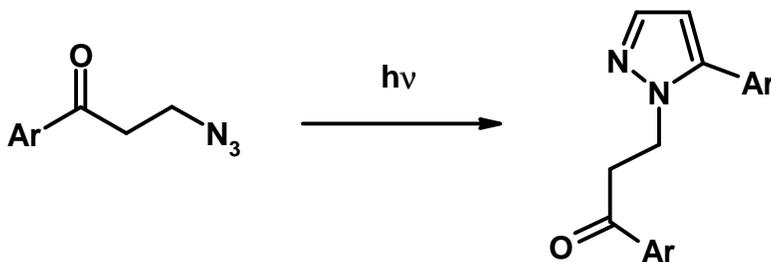
**805 Crosley x6-3380 Fax: (513) 556-9239 Email: Anna.Gudmundsdottir@uc.edu**

**Solid State Photoreactions: Green Chemistry.**

One of the advances of studying chemical reactions in the solid state is that it reduces the use and disposal of potentially hazardous solvents, an important consideration in this era of increased environmental awareness. Furthermore, due to the restricted motions of molecules in crystals, solid state reactions are generally more selective than their counterparts in solutions.<sup>1</sup> Crystal lattices can therefore pose as an effective technique for controlling chemical reactivity. We are interested in study the reactivity of azidoarylketones in the solid state, since they can be used to make interesting heterocyclic compounds.

A summer project would focus on synthesizing and characterizing various derivatives of the azidoarylketones. The photoproducts from solution and solid state photolysis of these compounds can then be isolated and characterized. Obtaining X-ray structure analysis of the starting material will allow us to connect the solid state reactivity with the structure of the starting material. By studying a series of closely related compounds we can attempt to correlate the molecular structure and the molecular packing arrangements in the crystals, a concept known as “crystal engineering”. The ultimate goal of this research is to control the regioselectivity of photochemical reactions by slight changes in the molecular structure of the substrates to obtain specific crystal lattices.

After spending a summer in my research laboratory the student will have gained experience in carrying out synthesis in solutions and in the solid state. The student will have contributed to the development of using crystals as a reaction media for synthesis.



1. Scheffer, J.R.; Garcia-Garibay, M.A.; Nalamasu, O.; *Org. Photochem.*, **1987**, 8, 249.

**Professor Apryll Stalcup**

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Chiral compounds are substances that contain a center of asymmetry and can exist as non-superimposable mirror image isomers or enantiomers. Many compounds of pharmaceutical interest have this property but are administered as the racemic or 50:50 mixture. Often, only one enantiomer has the desired properties while the other

enantiomers may be responsible for dose-limiting side effects. The analytical separation of these kinds of compounds has been considered among the most difficult of all analytical separations. The research will focus on developing new methods for performing these types of separations as well as investigating the separation mechanism. Students engaged in research on this project become familiar with high performance liquid chromatography, capillary electrophoresis and and/or various spectroscopic methods.

**Professor Pearl Tsang**

**804 Crosley x6-2301 Fax: (513) 556-9239 Email: Pearl.Tsang@uc.edu**

**Understanding the basis for the binding and interaction of protein with their ligands.**

The biochemical research in the Tsang laboratory is focused upon study of proteins that have important functions in immunology and metabolism. We are specifically interested in understanding how these proteins recognize and bind with high specificity and affinity to other molecules (otherwise known as ligands). The specificity of binding between these proteins and their ligands is important to understand because it can be useful for the development of molecules that block the interactions between these proteins and their respective ligands and this can lead to the development of drugs and diagnostic agents against certain diseases. Some of the proteins we actually study have important roles in diseases such as AIDS and cancer. Students involved in this research will learn about the synthesis and purification of some proteins and peptides and they will also gain experience with some UV-Vis absorption and NMR spectroscopy techniques.

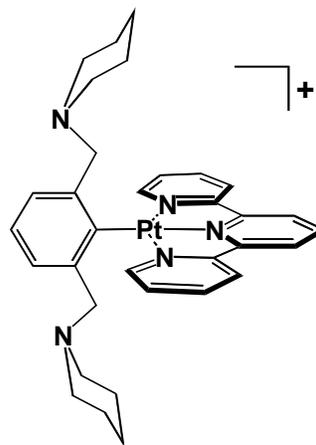
**Professor Bill Connick**

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**Designing Molecules for Photo-induced Two-Electron Transfer.**

Increasing worldwide energy demand is driving our efforts to improve solar energy technologies. In this field, the most difficult challenge we face is the conversion of sunlight energy to useful chemical energy. The traditional approach to this problem relies on molecules that, when excited by light, undergo one-electron transfer reactions. The resulting reduction and oxidation reactions can produce useful chemical fuels. Unfortunately, these systems tend to be inefficient.

Our goal is to explore a new approach to this problem that involves designing molecules that will transfer more than one-electron when excited by light. An example is illustrated in the adjacent figure. These molecules offer significant advantages over traditional solar catalysts. One of the side benefits is that they are expected to exhibit very slow rates of charge recombination. Therefore, these molecules



may be useful in designing molecular-scale optical and electronic devices. More importantly, investigations of these systems will provide insight into the mechanisms of catalytic reactions that are important to industrial and biological chemistry. This project will provide students with experience in the design, synthesis and characterization organic ligands and inorganic transition metal complexes. No prior chemistry research experience is necessary.

**Professor R. Marshall Wilson**

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**Email: Marshall.Wilson@uc.edu**

### Synthesis of Dihydrodioxin-Thymine Conjugates for Incorporation into Targeting DNA Cleaving Agents.

The methyl group of thymine provides an ideal site for the attachment of a wide variety of reagents that can interact with DNA, since attachment of groups to this site does not interfere the interstrand binding modes of DNA. For this reason, we have developed strategies for attaching **dihydrodioxins** (DHDs) to the methyl group of thymine. Upon photochemical activation, DHDs cut DNA. When simple DHDs are used to cut DNA, they will cleave the DNA backbone at random sites. However, when they are attached to DNA sequence-recognizing oligos they can be used to cut DNA at very specific sites. The goal of this project is to synthesis thymines with attached DHDs, incorporate these modified nucleotides into sequence-recognizing oligo, and see if these modified oligos can be used to knock-out specific genes in large DNA molecules. As the WISE component of this project, a summer student would prepare modified thymine molecules and learn the basic aspects of manipulating DNA.

