Syllabus: Astrochemistry Laboratory (ASTR/CHEM 451)

This course is intended to be a hands-on introduction to the practice of astrochemistry, including laboratory spectroscopy, astronomical spectroscopy, quantum chemical calculations, simulations of molecular spectra, and theoretical analysis and modeling of interstellar chemistry. Labs will be conducted by small groups (2-3) of students, and are designed to be significant intellectual challenges, not pre-prepared activities. Because of the diversity of the laboratory activities and the need for good weather for observations, along with the constraint that we only have one telescope and spectrograph, Labs 1-6 will be conducted by students on their own schedule and in a different sequence by each group, subject to some ordering restrictions. The labs will be preceded by an involved orientation process ("Lab 0") and followed by a one-week period in which the students will synthesize all of their data ("Lab 7"). Detailed write-ups will be required for all students for Labs 0-7. For students electing to earn 4 credit hours, a final report (written in LaTeX in the style of the *Astrophysical Journal*) synthesizing all of the work performed will be required at the end of the course. Note that students are expected to need to spend about as much time outside of the laboratory (doing background reading of the literature, designing the experiments, and writing lab reports) as they spend in the laboratory environment itself.

Lab 0: Orientation [1 week]

Note: This lab will be completed during the first week of the semester.

Students will be introduced to all of the relevant equipment, including the laboratory equipment, the computer systems, and the telescope. Following this introduction and the completion of safety training, students will be granted 24/7 access to the laboratory via a card-swipe system.

Lab 1: Spectrograph Configuration [3 weeks]

Note: This lab must be completed before attempting lab 2 or lab 6.

Students will teach themselves the principles behind an optical spectrograph, and proceed to configure the bench spectrograph essentially "from scratch." They will learn how to interface a computer to the CCD, and how to use common astronomical data reduction packages to reduce spectra. They will then obtain calibration spectra of various standard arc lamps, as well as a solar spectrum.

Lab 2: Laboratory Spectroscopy of an Interstellar Molecule [2 weeks]

Students will utilize a flame source to produce a molecule of interstellar interest that has an optical spectrum (CH). They will then use the bench spectrograph to obtain a laboratory spectrum of that molecule and measure the transition wavelengths and intensities. These will be compared with the results of their simulations in lab 4.

Lab 3: Quantum Chemical Calculations [1 week]

Note: Lab 3 must be completed before lab 4.

Using a quantum chemistry package, students will calculate the electronic spectrum and equilibrium structure of the target molecule (CH). The results from these calculations will be compared with their observed spectra, and used in the simulation of the spectrum.

Lab 4: Simulation of Molecular Spectrum [2 weeks]

Students will utilize the molecular parameters they have calculated to simulate the spectrum of the target molecule under interstellar conditions as well as under the conditions in their laboratory experiment. These simulations will be used to interpret the laboratory and astronomical spectra.

Lab 5: Chemical Modeling of a Diffuse Interstellar Cloud [2 weeks]

Students will conduct a literature review and analyze the key formation and destruction mechanisms for the target molecule. They will then perform a steady-state analysis of the abundance of the target molecule in diffuse clouds. Subsequently, students will learn the conceptual basis for kinetic modeling of interstellar clouds, and will use the state-of-the-art modeling code NAHOON (developed by the OSU modeling group) to create their own model of a diffuse cloud. They will use these models to predict the abundance of the target molecule, for comparison with their results from lab 6.

Lab 6: Astronomical Spectroscopy of an Interstellar Molecule [3 weeks]

Students will couple the historic 12" refracting telescope in the dome of the Observatory to the bench spectrograph using fiber optics. Using information from the astronomical literature, and with guidance from the instructor, they will select a bright star to serve as a background source, and will observe the spectrum of the target molecule in that sightline.

Lab 7: Synthesis [1 week]

Note: This "lab" will be completed in the last week of the semester.

Once they have completed Labs 1-6, students will synthesize all of their results (in their groups). This synthesis will include comparing the observed astronomical spectrum with their laboratory spectrum (lab 2), with their simulations (lab 4), and with the results of their chemical model (lab 5). For students electing to take the course for 4 credit hours, a final report must be written in the format of a paper in the *Astrophysical Journal*, and should include a comprehensive literature review.

<u>Readings</u>: There will be no textbook for this course. Students, together with the professor and the TA, will develop a TWiki site that contains the basic operating procedures of the equipment involved and some suggested internet resources, journal articles, and monographs to consult to figure out how to make the experiments work. But on the whole, students will be left to their own devices (of course, with guidance from the professor and TA as needed) so they will have an authentic research experience.

<u>Contact Hours:</u> The course will have one lecture hour per week, which will also include an opportunity for discussion of students' results. Students will work on the experiments on their own schedules, which is necessary due to limited experimental resources and good weather. The professor and TA will be available (by appointment) at the Observatory to offer advice and guidance to the students. Students are expected to spend an average of 8 hours per week in the laboratory [equivalent to two four-hour lab sessions in other chemistry lab courses], and an average of 8 hours per week outside of the laboratory performing preparatory work, analyzing their results, and writing their reports. Some of the computer-based labs may be performed outside of the Observatory laboratory, if that is more convenient.

<u>Evaluation</u>: Students taking the course for 3 credit hours will be evaluated by a combination of their reports on each lab (~80%), and effectiveness in the laboratory as judged by the professor and the TA (~20%). Students taking the course for 4 credit hours will be evaluated by a combination of their reports on each lab (~50%), their final report (~30%), and their effectiveness in the laboratory as judged by the professor and the TA (~20%).

Tentative Schedule for Spring 2009

<u>Note:</u> This schedule is subject to change. Please consult the TWiki site for the most up-to-date information.

Week:	Activities:
1/26	Orientation (Lab 0); Begin astrochemical analysis/modeling (Lab 5)
2/2	Continue analysis/modeling (Lab 5); report due on 2/9
2/9	Quantum chemistry (Lab 3); report due on 2/16
2/16	Learn and practice data reduction (part of Lab 1)
2/23	Group 1: Build spectrograph (Lab 1); report due 3/9
3/2	Group 2: Spectral simulations (Lab 4); report due 3/9
3/9	Group 1: Spectral simulations (Lab 4); report due 3/30
3/16	Group 2: Build spectrograph (Lab 1); report due 3/30
3/23	[Spring Break]
3/30	Both groups perform laboratory and astronomical spectroscopy over this period (Labs 2, 6); reports due 5/4
4/6	
4/13	
4/20	
4/27	
5/4	Synthesis (Lab 7); report due 5/11
5/15	Final Report Due [last day of finals week]

Contact Information

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TWiki site: http://dib.uiuc.edu/451 — check this frequently, and participate in building it up!

<u>SCS account:</u> Ben will give you a username/password for the VizLab computers in SCS. Please change your password ASAP by going to http://passwords.scs.uiuc.edu. Your account will expire on June 15, so if you want to keep your work you'll need to move it off by then.

<u>Astro account:</u> If you don't already have an account on the Astro cluster, please fill out the Account Request form on http://w3.astro.uiuc.edu. You will need this account to run IRAF.

Lab computers: Computers will be set up in the lab shortly; authentication will use your NetID.