

## **Astrochemistry (ASTR/CHEM 450)** **Tuesday & Thursday, 2:00-3:20, Noyes 163**

Professor Ben McCall  
166 Roger Adams Lab  
bjmccall@illinois.edu  
4-0230  
Office Hours: TuTh right after class  
[or by email appointment]

TA: Brad Gibson  
164 Roger Adams Lab  
bmgibso2@illinois.edu  
4-3993  
Office Hours: M 1-2, W 10-11

### **Course Description:**

Covers the foundations of astrochemistry, a young field at the intersection between chemistry and astronomy. Topics to be discussed include the interstellar medium, atomic and molecular physics, interstellar chemistry, molecular astronomy, and unresolved enigmas in the field. The class will involve lectures, discussion, readings from the primary and review literature, and student presentations. Suitable for graduate students or advanced undergraduate students in chemistry, physics, or astronomy.

A tentative schedule of the topics to be covered follows:

Aug 27: Introduction to the Course

### **Topic 1: The Interstellar Medium**

Aug 29: Introduction to the Interstellar Medium

Conditions, time and length scales, constituents (elemental abundances, isotopic ratios, grains, radiation field, cosmic rays, shocks, magnetic fields).

Sep 3: Structure and Evolution of the Interstellar Medium

Three-phase interstellar medium. Heating and cooling. Life cycle of interstellar matter (astration). Types of interstellar environments (diffuse clouds, dense clouds, star forming cores, photodissociation regions).

### **Topic 2: Atomic & Molecular Physics**

Sep 5, 10, 12: Interaction of Radiation with Matter; Atomic Spectroscopy

Semi-classical approach, oscillator strengths and Einstein coefficients, introduction to spectroscopy. Atomic structure (principal, angular momentum, magnetic, and spin quantum numbers; fine structure; hyperfine structure) and atomic spectra.

Sep 17: Structure and Spectra of Diatomic Molecules

Energy level structure (electronic, vibrational, and rotational). Electronic spectra, vibrational spectra (dipole- and quadrupole-allowed), rotational spectra. Application to H<sub>2</sub>, C<sub>2</sub>, CH, CO.

Sep 19, 24: Structure and Spectra of Polyatomic Molecules

Energy level structure of spherical, linear, symmetric, and asymmetric tops. Rotation-vibration interaction. Application to H<sub>3</sub><sup>+</sup>, C<sub>3</sub>, H<sub>2</sub>O, HCO<sup>+</sup>.

Sep 26, Oct 1: Radiative and Collisional Excitation Processes

Radiative excitation and selection rules. Collisional excitation and de-excitation. Example: rotational excitation of C<sub>2</sub> and CO. Radiative transfer.

[Oct 3 – possible spillover lecture in case we're running behind]

[Oct 8 – no lecture; please spend this time working on the midterm project!]

### Topic 3: Interstellar Chemistry

#### Oct 10: H<sub>2</sub> Formation and Destruction

Formation of molecular hydrogen on interstellar grains.

#### Oct 15, 17: Chemical Kinetics and Rate Equations; Ion-Neutral Reaction Dynamics

Types of chemical reactions, endo/exothermicities, activation energies, rate expressions. Langevin cross-sections and temperature independence. Importance of ion-neutral reactions for interstellar chemistry.

#### Oct 22, 24: Chemical Modeling

Calculation of molecular abundances using chemical reaction networks, both steady state and time-dependent. Identification of primary formation/destruction pathways for individual molecules. Dependence on laboratory data.

#### Oct 29: Isotopic Fractionation

Quantum mechanical effects leading to fractionation of rare isotopes in molecules, and observational evidence.

### Topic 4: Molecular Astronomy

#### Oct 31: Detecting Interstellar Molecules in the Optical

Principles of optical spectrographs, and echelles.

#### Nov 5: Basics of Radioastronomy

Fourier transforms, single dish studies, mapping, backends for spectroscopy

#### Nov 7: Radio Interferometry

Principles of interferometry (aperture synthesis).

### Topic 5: Student Presentations on Individual Molecules

[week of Nov 12 & Nov 14 to be used for group collaboration and rehearsals for presentations]

Presentations: Nov 19, Nov 21, Dec 3, Dec 5, Dec 10

CH <sup>+</sup> , HCO <sup>+</sup> , H <sub>2</sub> CO	[Group 1]
NH, N <sub>2</sub> H <sup>+</sup> , NH <sub>3</sub>	[Group 2]
OH, H <sub>2</sub> O, H <sub>3</sub> O <sup>+</sup>	[Group 3]
C <sub>2</sub> H, C <sub>2</sub> H <sub>2</sub> , C <sub>3</sub> H, C <sub>3</sub> H <sub>2</sub>	[Group 4]
CN, HCN, HNC, HCNH <sup>+</sup>	[Group 5]

Participation: You are expected to actively participate in this course! Contribute to discussions during the lecture sessions! Seek out useful websites, books, review articles, and research articles! Do **not** be passive...take the initiative to learn about this exciting field!

Readings: There will be no formal textbook for this course. As a class, you will develop a list of useful reference books, websites, and articles on a wiki. The course will be based primarily on lecture notes, as well as readings from the primary and review literature. You are expected to actively seek out additional readings.

Midterm Project: In lieu of a midterm exam, a midterm project will be due October 22. It will require you to solve the excitation of a molecule such as CO, and use observational data to infer the density and temperature of the cloud. If you don't already know how to use some software to solve a simultaneous set of linear equations (i.e., matrix manipulation), start learning now!

Your Molecule(s): You will split up into groups of 3 or 4 [each with at least one undergrad and one grad student; each with at least one chemist and one non-chemist], and pick a set of 3 or 4 known interstellar molecules. Each of you will pick a molecule of your primary responsibility, but you will also be held responsible for the work of your entire group. Over the course of the semester, your group will develop wiki pages detailing all aspects of these interstellar molecules (including their energy level structures, their spectra, their chemistry, where they have been detected, and what they tell us as astronomical probes).

Final Project: In lieu of a final exam, each of you will present a ~20 minute talk about your primary molecule. These should be coordinated with your group members (and rehearsed in front of them) so that together you present a coherent picture of the astrochemistry of your set of molecules. A written final report on your molecule will be due during finals week (by 5pm on December 17), along with the final version of your wiki page.

Collaboration Policy: Please **do** collaborate, but don't copy! Feel free to discuss your approach to the homework problems (and the midterm project) with other students, but work out all of the solutions independently. The work on your individual molecules (wiki pages) naturally will be more collaborative in nature, but each person should do their fair share.

Grades: The course will not be graded on a curve. If everyone does great, I'll be very happy to give all A's! [And conversely...] The contribution of the various components of the course follows:

10%	Class participation
20%	Homeworks
20%	Midterm project
20%	Final presentation
15%	Final report
10%	Final version of your wiki page
5%	Final version of your group members' wiki pages

Astr/Chem 451: Offered in the spring semester, this laboratory course will provide you with an opportunity to align an optical spectrograph, use the historic (1896) 12" refractor at the Observatory to obtain a spectrum of interstellar CH, use a flame/discharge source to obtain a laboratory spectrum of CH, and utilize *ab initio* calculations, spectroscopic analysis, and chemical models to interpret these spectra. An exciting, hands-on introduction to astrochemistry!