Frontiers in Spectroscopy

Chemical Physics 894A and 894

Winter 2003

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Course Description: This course will provide students with an overview of topics on the frontier of spectroscopic research. It will exploit internationally renowned lecturers, as well as outstanding OSU faculty, to cover topics ranging from very fundamental to quite applied. General areas to be covered will include fundamental characteristics of molecular quantum structure, electromagnetics, new experimental techniques, remote sensing, ultra-high sensitivity analytical techniques, astrophysical applications, etc. It is planned that the course will be offered multiple times, with topics and speakers varying with each offering. The lecturers for the upcoming Winter quarter are listed below.

Each topic will be covered by lectures on Wednesday and Friday mornings, 9:00-10:18AM, MP2015, with a discussion period 9:00-10:18AM on Thursdays in MP2015.

Prerequisites: Chemistry 866 or Physics 780.04 or permission of the instructor

Required Text: None; suggested articles for reading will be supplied prior to the lecture on a given topic.

Syllabus:

List of speakers and dates scheduled:

January 15-17 Peter Bernath, University of Waterloo

Click here: 1, 2, 3, 4, 5 to access readings for these lectures.

- Molecular Astronomy
  Our recent laboratory and astronomical work on a variety of molecules including VCl, CrH, SO, hot CH4, and hot H2O as well as on hydrogenated amorphous carbon thin films will be presented. The main theme of the talk is the interaction of laboratory spectroscopy and observational infrared and near infrared astronomy. Laboratory infrared emission spectra were recorded with a Fourier transform spectrometer. Astronomical spectra of sun spots, cool dwarf stars, brown dwarfs, protoplanetary nebulae and the Jovian moon Io were recorded with a variety of telescopes and spectrographs. For example, high resolution infrared spectra of brown dwarfs were just recorded with the Phoenix instrument at the 8 meter Gemini South telescope in Chile.
- Infrared Emission Spectroscopy
  Infrared emission spectroscopy is an unjustly neglected technique. We will review the advantages and disadvantages of working in emission with a wide variety of results from our laboratory. Recently, we have developed a new source that combines a high temperature furnace with an

electrical discharge. This source has led to the discovery of gas-phase BeH2, the simplest neutral polyatomic molecule.

- The Atmospheric Chemistry Experiment (ACE): Spectroscopy from Orbit
  The main goal of the ACE mission is to measure and to understand the chemical and dynamical processes that control the distribution of ozone in the upper troposphere and stratosphere, with a particular emphasis on the Arctic region. A comprehensive set of simultaneous measurements of trace gases, thin clouds, aerosols, and temperature will be made by solar occultation from a satellite in low earth orbit.
  A high inclination (74 degrees) low earth orbit (650 km) will give ACE coverage of tropical, mid-latitudes and polar regions. The vertical resolution will be better than 4 km from the cloud tops up to about 100 km. The solar occultation advantages are high sensitivity and self-calibration.
  A high-resolution (0.02 cm-1) infrared Fourier Transform Spectrometer (FTS) operating from 2 to 13 microns (750-4100 cm-1) will measure the vertical distribution of trace gases, and the meteorological variables of temperature and pressure.
  Aerosols and clouds (e.g., Polar Statospheric Clouds, PSCs) will be monitored using the extinction of solar radiation at 0.525 and 1.02 microns as measured by two filtered imagers as well as by their infrared spectra. A spectrograph called MAESTRO has been added to the mission to extend the wavelength coverage to the 280-1000 nm spectral region. The PI for MAESTRO is T. McElroy from the Meteorological Service of Canada (MSC). As secondary science both the FTS and MAESTRO can record spectra in the nadir direction. The FTS and Imagers have been built by ABB-Bomem in Quebec City, while the satellite bus has been made by Bristol Aerospace in Winnipeg.
  ACE has been selected in the Canadian Space Agency's SCISAT-1 program for a planned launch by NASA in the May 2003.

January 22-23
NOTE: Third lecture to be given 2pm in 2136 Newman-Wolfrom
William Happer, Princeton University

Click here to download references 1, 2, and 3 .

These lectures will review the fundamentals processes of optical pumping[1] to produce spin polarized atoms. We will also discuss some of the more important applications of optically-pumped systems, for example, medical imaging[2] with hyperpolarized 3He and 129Xe, and atomic clocks based on optically pumped Rb and Cs atoms.

- Lecture 1. We will review what types of atoms are most suitable for direct polarization by optical pumping, in particular, the alkali-metal atoms, Na, K, Rb and Cs, metastable He atoms, and the group-II atoms, Zn, Cd and Hg. The nuclei of noble-gas atoms can be polarized by spin-exchange with optically pumped alkali-metal atoms [2]. The atomic polarization is conveniently described with density matrices. The two direct pumping mechanisms are depopulation and repopulation pumping. Optical and other ways to detect atomic polarization will be reviewed.
- Lectures 2. We will review spin-relaxation mechanisms for spin polarized atoms. Some of the most important mechanisms include radiation trapping, collisions in the gas phase, diffusion to the container walls and diffusion through magnetic field gradients. We will review the most important spin-dependent interactions that lead to ground-state spin-relaxation, including the spin-rotation interaction for electron or nuclear spins, the quadrupole interaction, the collisional shift of the Fermi-contact interaction of alkali-metal atoms, spin-exchange and spin-axis interaction for colliding pairs of alkali-metal atoms. Modifications of the optical pumping process by collisions of the optically excited atoms will also be discussed.
- Lecture 3. We will review some applications of optical pumped systems, including medical

imaging [3], atomic clocks, magnetometers, polarized targets for nuclear and high-energy physics, and tests of fundamental symmetry laws.

1. S. Appelt et al. "Theory of spin-exchange optical pumping of 3He and 129Xe," Phys. Rev. A 58, 1412, (1998).
2. T. G. Walker and W. Happer, "Spin-exchange optical pumping of noble-gas nuclei." Reviews of Modern Physics, 69, 629 (1997).
3. M. Salerno et al. "Dynamic Spiral MRI of Pulmonary Gas Flow Using Hyperpolarized 3He: Preliminary Studies in Healthy and Diseased Lungs," Magn. Reson. Med., 46, 667 (2001).

January 29-31 Peter Weber, Brown University Click here to download references 1, 2, 3, 3 continued and 4 .

Pump-Probe Electron Diffraction - Pump-probe electron diffraction is a new technique to probe structures of molecules in excited and transient states. The talks will discuss the information content, technical aspects of the experiment, and issues relating to the analysis, of pump-probe diffraction experiments.

- **Lecture 1**: The foundations of electron diffraction The first lecture provides an overview of the promise and challenges of time-resolved diffraction on molecules in excited states. We will review the foundations of electron diffraction by discussing the relevant approximations and equations. Experimental techniques of electron diffraction in general will be reviewed.
  Outline:
  Diffraction methods
  Diffraction methods in molecular spectroscopy: prospects and challenges
  Review of Scattering theory
  Experimental considerations in electron diffraction
- **Lecture 2**: Pump-probe electron diffraction for probing excited states and chemical dynamics The second lecture focuses on the implementation of pummp-probe electron diffraction for the measurement of excited state structure and dynamics. We will review the experimental requirements for the experiments, and discuss results and the data analysis of the ring-opening reaction of 1,3-cyclohexadiene to form 1,3,5-hexatriene. Theoretical studies of excited state diffraction will be presented and discussed.
  Outline:
  Pump-probe diffraction experiments
  Topics related to data analysis
  Theoretical studies: diffraction signals from excited molecules

February 12-14 Jaan Laane, University of Texas A&M Click here to download references 1, 2, 3

Vapor-phase far-infrared spectra, Raman spectra, ultraviolet absorption spectra and jet-cooled fluorescence spectra along with quantum mechanical computations are utilized to determine the one-, two-, and three-dimensional vibrational potential energy surfaces for selected molecules of conformational interest in their ground and excited electronic states. From these potential surfaces the energy differences between various structures and the magnitudes of the forces determining the structures can be ascertained. The investigations of cyclic and bicyclic molecules and those with internal rotation are emphasized.

March 4-6 Takeshi Oka, University of Chicago (talks Tues, Wed and Thurs). Click below to download references Reading 1 - an encyclopedia article which covers all the material, especially Lecture 1

Reading 2 - A review article for Lecture 2 and 3

Reading 3 - an article for Lecture 2 Also useful is "compass" on page 59 of the same issue.

Reading 4 - Review for Lecture 3 Look up p. 2363-2559 of the same issue for more information.

Microwave and Infrared Spectra of Molecular Ions in the Laboratory and Astrophysical Plasmas

Lecture 1. Introduction — The big Picture, Ions and Chemistry, Historical Sketch

Experimental — Plasmas, High Sensitivity Laser Spectroscopy

Individual Ions — Protonated ions H_3^+, HCO^+, HN_2^+, $HCNH^+$, H_3O^+, NH_4^+

Primary ions CO^+, H_2O^+, NH_3^+, $HCCH^+$

Anions OH^-, NH_2^-, HC_2^-

Lecture 2. Intra-molecular Dynamics Proton Tunneling CH_3^+, $C_2H_3^+$, CH_5^+, H_3^+

Ions in Space — Comets CO^+, H_2O^+ Molecular Clouds HCO^+, HN_2^+, HCS^+, $HCNH^+$, H_3O^+, $HOCO^+$, Ubiquitous H_3^+

Lecture 3. The H_3^+ Spectrum

H_3^+ in Planets — Jupiter, Saturn, Uranus, Protoplanet (?), Exo-planet (?)

H_3^+ in Interstellar Space — Dense (Molecular) Clouds, Diffuse Clouds, The Galactic Center, Extra-galactic (?), Supernove (?)

Grading: Satisfactory/Unsatisfactory options: Class attendance and participation

Letter grade option: Class attendance and participation plus term paper

(Grades will be assigned solely by OSU faculty.)

19525-2 (3 hours) Call number for ChemPhys 894 (S/U option)

19524-7 (3 hours) Call number for ChemPhys 894A (letter grade option - prerequisite=a previous spectroscopy course at OSU in Chemistry or Physics or prior permission of the instructor)

Chemical Physics 894 - 1998 Chemical Physics 894 - 1999 Chemical Physics 894 - 2000 Physics 880G20 - 2001 Physics 880G20 - 2002