Week 1

???

1.1 Experimental Physical Chemistry: An Introduction

1/3:

- Questions:
  - Is "Introduction to Nanotechnology by Linsay" the same as "Introduction to Nanoscience by Stuart M. Lindsay?"
    - They'll check on this.
  - Access to Panopto recordings?
    - I have access now.
  - Recordings of class content?
    - Yes, if they can get the AV working.
- Intro by Hannah Lant (instructional professor to manage lab meetings). Tokmakoff handles lectures/non-in-lab stuff.
- Goals of the course.
  - Demonstrate and interrogate principles from your theory courses, e.g., from QMech/Thermo.
  - Learn practical techniques to characterize chemical and physical properties of molecules and nanomaterials, and the related spectroscopic techniques.
  - Analysis of data (in-class and in-lab).
  - What have you learned, and how can you communicate your findings to a scientific audience.
- Everything helps everything else; it's cyclical from experimental theory, to collecting data, to data analysis, to communication, and back to more theory.
- Lectures will be more like workshops/recitations. There are recordings for content.
- Rest of today: Logistics and individual experiments.
- Canvas page.
  - Syllabus.
  - Most info on the Modules page.
  - Fitting exercises will be in in-class meetings in the day to come.
  - Experiments.
  - Video lectures on Panopto.
- Watch the 15-min Lecture 1 before class on Thursday!

- 6/9 weeks in lab. Complete a total of 6 experiments.
  - Core experiments for weeks 2, 4-6 (UV/Vis, FT-IR, NMR, GC-MS).
    - Full lab report on one of these; short lab report on the other ones.
  - Choose your experiments for weeks 7-8.
    - Highlight content in nanomaterials and kinetics.
    - Week 7 requires a full lab report on that experiment.
    - Week 8 requires a group presentation on your experiment.
    - Survey to determine what you do before Friday of Week 2!
- Grading breakdown.
  - Prelab quizzes: 15% (2.5% per quiz).
    - About 5 questions.
    - Must get 80% or above to attend lab.
    - 2 attempts.
    - Focus on safety, but also thinking critically about the theory for the lab.
  - Short reports: 40% (10% per report).
    - How to do info — in the lab manual.
    - ACS citation style.
    - There will be rubrics posted on Canvas (grading is not subject to the whims of our TAs).
  - Full reports: 30% (15% per report).
  - Group oral presentation: 15%.
    - Attend a few other presentations and give ours during finals week.
- A full schedule of assignments and labs is available in the syllabus.
- See announcement for which lab cohort I'm supposed to be in!
- What the experiments are and what their purposes are (nontechnical because we haven't done the theory yet).
- Weeks 2, 4-6.
  - UV/Vis to get a vibronic spectrum of iodine (to get electronic/vibrational data on I_2).
  - FT-IR: Rovibrational information on HCl.
  - NMR: $C_5H_{11}OH$.
  - GC-MS: Separation science and MS. Analyze gasoline, which is a complex mixture of organic molecules.
- Week 7 (+ info on who should choose these; think about it next week after first lab).
  - Fluor: Fluorescence spectra of analytes, including pyrene.
    - Both spectroscopy and kinetics. If you're really interested in physical chemistry and kinetics, do this. Uses custom built stuff in the labs.
  - QDots: Cadmium and Selenium nanocrystals.
    - Applications of particle-in-a-box ideas, nanotechnology, synthesis, the prettiest one.
  - EChem: Developed by Anna Wuttig.
    - More training in CV. Look at a number of different electrodes, and assay their activity in the hydrogen-evolution reaction. Applications in renewable energy.
    - Will run both weeks 7-8.

    - Includes some interaction with Wuttig.
  - AFM: Atomic force microscopy.
    - Imaging a number of different materials, e.g., the grooves on a DVD. Great for anyone interested in nanoscience.

- Week 8:
  - Photo: Alternate addition this week.
    - Photodissociation of CO from that hemoglobin structure and then some kinetics.
- The PChem lab suite: Enter Jones laboratory and turn left. We'll go elsewhere for special instrumentation. Lant's office is next door.
- NMR and GC-MS in Searle 340 instrumentation center. Usually meet our TA in the PChem lab suite and then travel.
- Attendance.
  - You are required to attend all six lab sessions and record your own data (often in groups).
  - Excused absences include university travel, family emergencies, and illness; please be in touch with Prof. Lant as soon as possible to reschedule your lab.
  - Unexcused absences may be able to reschedule at a 20% penalty if availability allows (this is an overenrolled class).
- Safety.
  - General lab safety policies from Gen Chem and OChem still apply.
  - Bring your own goggles.
  - Acknowledge you've reviewed the polices on Canvas in the first lab quiz.
  - Safety tour of the lab space on your first lab day by your TA.
  - Lab aprons will be provided.
  - Specific safety concerns will be communicated in lab manuals and pre-lab quizzes.
- We're all coming in with diverse scientific experiences. Fill out a survey on Canvas > Assignments > surveys or at tinyurl.com/pchemlabsurvey!
- No formal lecture on Thursday in this room! There will be a series of about 7 video lectures over the first two weeks that cover what we need to know for our first core experiments (watch these!). Workshops during this period, too. E.g., if they find from the surveys that we don't have experience with fitting data very well, we'll work through that. There is an exercise for this on Canvas?? (Data Fitting Exercises.pdf explains it.)
- Tokmakoff puts a big emphasis on communication :)
  - "Any professional science is communicated; otherwise, it's just a hobby."
  - Should be nicely formatted with good figures, etc.
- My lab group: Thursday A.
- Schedule.
  - UV/Vis: 1/12.
  - FT-IR: 1/26.
  - NMR: 2/2.
  - GC-MS: 2/9.

1.2 Lecture 1: Principles of Spectroscopy

- **Spectroscopy**: Studying the properties of matter (e.g., molecules and materials) through its interaction with different frequency components of the electromagnetic spectrum. *Etymology* **spectron** from Latin "ghost" or "spirit."
  - More on the etymology: An apt description because you never see the molecule itself; you see a representation/image/apparition of it.
- Each type of spectroscopy gives a different picture (the *spectrum*).

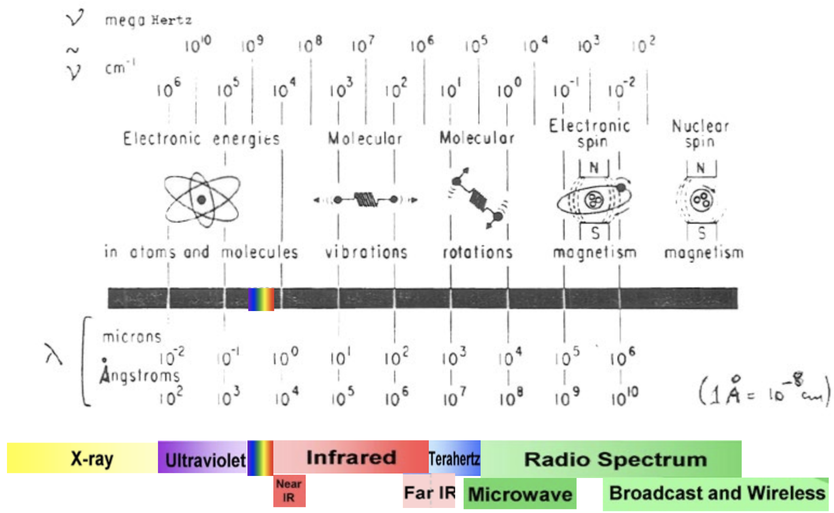

Figure 1.1: Types of light used by different forms of spectroscopy.

  - UV/Vis: Electronic absorption (esp. valence electrons).
  - Infrared: Vibrations.
  - Microwave: Rotations and crystal lattice vibration.
  - Radio: NMR.
- Goals.
  - Understand how light interacts with matter and how you can use this to quantitatively understand your sample (e.g., molecular structure, dynamics, reactivity).
  - Understand spectroscopy the way you understand other common tools of measurement (like a ruler).
  - See that spectroscopy is a set of tools that you can put together in different ways to solve the chemical problems that are of interest to you.
- A spectrum measures...
  - The interaction of light with a sample influences the sample and the light.
  - Two universal steps: Excitation and detection.
  - Light passes through the sample and then gets characterized on its way out (e.g., absorption, emission, scattering, reflection, dispersion, rotation). We can also characterize a change in the sample (e.g., photothermal, photoelectron and ionization, photochemistry).
  - In most cases, we characterize how a sample modifies the incident light.

- Two common measurements.
- **Absorption**: The attenuation of a light field passing through a sample.
  - Photodetectors measure intensity, which is related to the square of the electric field.
- **Emission**: Excitation induces light emission from the sample, typically of a different frequency.
- **Fluorescence**: Emission from singlet states.
- **Phosphoresence**: Emission from triplet states.
- **Raman scattering**: Light taken up shifts the frequency.
- The basics of an absorption spectrum.

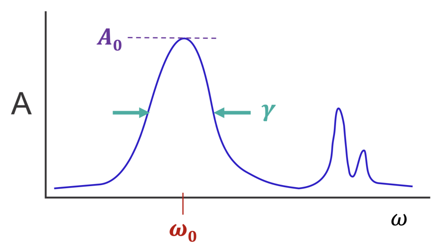

Figure 1.2: Features of an absorption spectrum.

  - x-axis: Characterizes the input light in terms of frequency (frequency, angular frequency, or wavenumber), wavelength, or energy.
  - y-axis: How the intensity of the light was attenuated at a particular frequency. Look at transmission ($T = I/I_0$) or absorbance ($A = -\log T = \epsilon(\nu)CL$, where ϵ is the extinction coefficient [unit $\mathrm{L\,mol^{-1}\,cm^{-1}}$], C is the concentration [unit M], and L is the sample pathlength [unit cm]).
  - Features: Resonance frequency ω_0, peak height A_0 or peak area, linewidth γ (different frequencies absorbed; gives information on dynamical processes), lineshape (actual functional form of the peak).
- How do you measure absorption spectra?
  - Measure the change of intensity of light at different frequencies as it passes through a sample.
  - Two types of spectrometers: Dispersive (common for visible spectrometers) and Fourier transform (more on this later).
- **Dispersive spectrometer**: A spectrometer that has a dispersive element, that is, one that takes white light and spacially spreads the colors of the rainbow.
  - Could be a reflection grating, prism, etc.
  - Measure the white light without the sample, and then with the sample and see what changes. Calculate the transmission, and then absorbance.
- That was basic definitions and variables.
- This time: We have defined some basic variables for an absorption spectrum.
- Next time: Molecular interactions of light. Analyze this mode: Driven electron on a spring.