Ch6 INDEPENDENT PROJECT

If you have taken one term of Ch6 already, then with instructor's permission, you can choose to do an optional independent project, which will SUBSTITUTE for TWO labs. It should take approximately four weeks worth of time to complete. Since we cannot possibly design projects to cover every physical chemistry technique, the independent project will allow you to work on any (feasible) physical chemistry project of interest without having a pre-designed lab. This will give you wide flexibility in the systems studied and the methods used.

Students will do two regularly scheduled experiments in the first five weeks. The project will be done in the last two periods, but you will be required to propose and design the experiment in the first half of the class. Only students who have had one term of Ch6 will be permitted to do this project.

EXAMPLES

1. Measure electron transfer rates between a donor and acceptor by varying the acceptor concentration and comparing to predictions based on calculation using Marcus theory
2. Characterize isotope shifts, effect of substitution, etc. by spectroscopic characterization (using at least two methods, e.g. IR and Microwave) of two species and compare with quantum chemistry calculation
3. Unimolecular decomposition of an ion in a trap; compare to statistical rate theory
4. Measure rates of a gas phase reaction using the diode laser apparatus to follow the loss of reactant or formation of a product.
5. Size-dependent spectroscopic properties of quantum dots
6. ESR and UV/Vis or IR to study properties of environment of a metal in a metal-containing protein.

SCHEDULE

Week 2. Project proposal (1-2 pages) due Friday (latest).

Weeks 3-5. Develop details of project design. Update of plan should be turned in weekly. Detailed design of experimental plan due at middle of week 5. Preparation (reagents, glassware, machining etc) should also be anticipated and done/ordered.

Weeks 6-9. Execute experiment. Perform analysis.

Week 10. Complete analysis. Turn in laboratory notebook.

GUIDELINES:

Content. This is a physical chemistry laboratory experiment. You are to design an experiment to test a physical chemistry hypothesis using physical experimental methods. We strongly discourage (a) instrument building/new techniques (due to time problems), (b) try-it-and-see experiments with no hypothesis/prediction, (c) projects which involve substantial time spent on nonphysical or nonexperimental aspects, e.g. synthesis, computation.

Experimental emphasis. Since this is a physical chemistry lab, the project should have a significant experimental component. We expect that you will spend a minimum of 12 hours in the lab, preferably more. There is a limited budget for new glassware, machining, chemicals, etc. You are encouraged to apply more than one method that you have learned/is available.

Due to the severe time constraints (and Murphy's Law), you must limit your experiment to existing, functioning apparatus, except for minor changes, e.g. straightforward modifications, adaption of apparatus. Past attempts at similar projects which involve new have too often ended in students spending the entire time trouble-shooting with no results and no time spent doing science per se.

You may use methods available in other labs, e.g. the dye laser system in the BI Laser Resource Center, pending permission of the relevant authority figures.

Analysis. The analysis should involve concepts and methods developed during Ch6 or Ch21/24. You are expected to apply error analysis as needed. It can involve computational work, e.g. quantum chemistry, but these should not be the major emphasis of the project.

Writeup. To be consistent with the rest of the course, we ask that you turn in a detailed notebook following the guidelines set forth in the course for other labs.

HOW DO WE DECIDE WHAT PROJECT TO DO?

Ideally, we would like you to come up the idea for the project on your own. However, since this may be very difficult, some ideas for projects are listed above. If you have any other ideas, even if they are very general, feel free to talk to the TA and work together to come up with a more specific idea. Otherwise, you can use one of the general ideas below and develop a more specific plan (or modify one of the plans). If you think a project listed below sounds interesting but you don't know how to proceed, then feel free to talk with the TA.

Week 1-2. Proposal

Once you have decided on a project and worked with the TA to come up with an initial plan, you will need to write up and submit a proposal. This should be submitted as soon as possible into the term, but no later than the end of Week 2. This will let you start working on preparing for your project.

Your proposal should include

- OBJECTIVE. a concise statement of the goals (what you want to measure/do) including a ***statement of your hypothesis.***
- INTRODUCTION. A brief summary of the background (why is this interesting)
- PLAN OUTLINE. What needs to be done.
- TIMELINE (a schedule).

The proposal should be about 1-2 pages long. This proposal will factor into your grade for the project and will be graded on clarity, completeness, and understanding of the project.

Week 3-4. Develop Detailed Experimental Plan

When your proposal is approved you should start writing down a more detailed plan for your experiment. This should be

Itemize what needs to be done in detail (what reagents, how much, where will they be ordered; what instruments, what modifications need to be done, if any;
Signal-to-noise considerations (will it work; what sensitivity is required, how much stuff do you need)
Analysis and Error analysis plan
Anticipate possible problems.

You have a small budget to purchase supplies. You will need to purchase them 1-4 weeks in advance, to allow for typical order processing and delivery times, so do not delay!

If you use departmental instrumentation, you may need to line up permission and scheduling in advance. For some instruments, e.g. NMR, you or the TA may need training.

Week 5-9. Experiment Time

You should primarily work independently on your project; however the TA will be available to show you how to work the instruments, help troubleshoot, and answer other questions.

Week 9-10. Analysis and Writeup

Grading

Grading will be based in equal parts on

1) Proposal
2) Planning and Preparation
3) Experimental approach; problem solving

Analysis (including quantitative use of statistics