Laboratory Reports

Students are free to discuss with each other the laboratory reports, but **the written material must be your own**. The data given in your laboratory report must be the data that you (and your partner) collected in the laboratory. References to all literature explicitly used in the laboratory reports must be properly noted.

The written reports should be organized approximately as follows

I. **Introduction**: This section should contain a clear description, in your ***own words***, of the purpose of the experiment with background material sufficient to place the purpose in context. Based on your results you may want to raise certain questions to be answered by your experiment.

II. **Theory**: This section should be brief and may, in some cases, be combined with the Introduction. It is a summary, including equations, of what you expect to find as a result of your measurements. (maximum of 4 pages)

III. **Data**: This section should include all the relevant data in a clear and ordered format. Do not paste printed data from a software package. Instead, cut, organized, paste and photocopy the data.

IV. **Error Analysis**: This section should include the error analysis used to calculate any deviation from your experimental results.

V. **Discussion**: This section should explain any agreement and/or disagreement between theory, your experimental results and the literature results.

VI.

SPRING 2004

February 18: MATHEMATICA Review

February 25: Computational (prob. set): Normal modes of a circular drum; Mathematica animation
Experiment 9 (prob. set): Zero Potential Models

March 10: Experiment 3 (lab. report): Vibrational - Rotational Spectrum

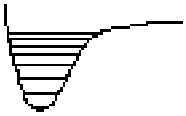
March 17: Experiment 10(prob. set): SCFLCAO Method for He

April 14: Experiment 7 (prob. set): Analysis of NMR Spectrum

April 21: Experiment 6 (lab. report): Interpretation of ESR Spectra of Aromatic

Anion Radicals

Mayo 5: Experiment 11: Gaussian 98.



Approximate Course Outline

	Date	Readings	Topics
Feb	9	Ch:1&2	Administration; Introduction; History, Motivation
	11	Ch:3	Schrödinger equation; Particle-in-a-box.
	16 – *18	Ch:4	Axiomatic Quantum Mechanics
	23 – *25	Ch:5	Schrödinger equation: Harmonic Oscillator, Rigid Rotor.
Mar	1 -3	Ch:6	Hydrogen atom ground state; Hydrogen atom excited states; Angular momentum.
	8 - *10	Ch:7	Variational principle; Perturbation theory.
	15 – *17	Ch:8	Many-electron atoms; Pauli exclusion principle; Term symbols; Self Consistent Field approximation
			SPRING BREAK
Apr	5 - 7	Ch:9	Chemical bond. Valence Bond model; Molecular Orbital model. Homonuclear diatomics, Heteronuclear diatomics.
	12 - *14	Ch:13	Molecular Spectroscopy
	19 - *21	Ch:14	NMR
	26 - 28	Ch:11	Computational Quantum Chemistry, Gaussian and extended basis sets
May	3 - *5	Ch:12	Symmetry operations; Symmetry elements; Group theory. Point Groups; Character tables; Applications of group theory.
	10 – 12	Ch:10	Polyatomic molecules; Hybridization; Multiple bonds; Huckel Molecular Orbital Theory.
	?		Final Exam (to be scheduled by the Registrar)

"Ch" refers to chapters in the text by McQuarrie and Simon
* indicates lab week