CHEMISTRY 368

Course Outline

Administration; Introduction; History
Wave Mechanics; Schrodinger equation; Particle-in-a-box;
Postulates in Quantum Mechanics
Wave Mechanics; Schrodinger equation; Harmonic Oscillator; Rigid Rotor
Hydrogen atom ground state; Hydrogen atom excited states; Angular momentum
Approximate Methods; Variational principle; Perturbation theory
Many-electron atoms; Pauli exclusion principle
Term symbols; Self- Concistent Field Approximation

SPRING BREAK

Chemical Bond
Valence Bond model; Molecular Orbital model.
Homonuclear diatomics, Heteronuclear diatomics.
Molecular Spectroscopy
NMR
Computational chemistry
Group Theory
Polyatomic molecules; Hybridization; Multiple bonds;
Huckel Molecular Orbital Theory

General References

1. *Quantum Chemistry*, D. A. McQuarrie, University, Mill Valley, CA, 1983.

2. P.W. Atkins, *Physical Chemistry* 3rd Ed., W.H. Freeman, New York, 1990.

3. I. N. Levine, *Physical Chemistry* 3nd , Mc Graw-Hill, New York, 1988.

4. G. P. Matthews, *Experimental Physical Chemistry*, Clarendon Press, Oxford, 1985.

5. J. H. Noggle, *Physical Chemistry* 2nd , Scott, Foresman, Boston, 1989.

6. J. Rose, *Advanced Physico-Chemical Experiments*, John Wiley, New York, 1964.

7. D.T. Sawyer, W.R. Heineman, J.M. Beebe, *Chemistry Experiments for Instrumental Methods*, John Wiley , New York, 1984.

8. D.P. Shoemaker, C.W. Garland, J.I. Steinfeld, and J.W. Nibler, *Experiments in Physical Chemistry,* 4th Ed., McGraw-Hill , 1981.

9. R. C. Weast, Editor *Handbook of Chemistry and Physics*, Chemical Rubber Publishing Company, Cleveland, Ohio.

Quantum Chemistry

1.- M. W. Hanna, *Quantum Mechanics in Chemistry,* ,Benjamin, New York, 1965.

2.- Kauzmann, *Quantum Chemistry*, Academic Press, New York, 1959.

3.- Levine, *Quantum Chemistry*, 4 th Prentice Hall, New York, 1991.

4.- Atkins, *Molecular Quantum Mechanics*, 2 nd Oxford, New York, 1983.

Group Theory

1.- F. A. Cotton, *Chemical Application of Group Theory*, Wiley, New York, 1971.

2.- H. H. Jaffe and M. Orchin, *Symmetry in Chemistry,* Wiley, New York, 1965.

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