CHEM*4880 TOPICS IN ADVANCED PHYSICAL CHEMISTRY: STATISTICAL THERMODYNAMICS AND QUANTUM CHEMISTRY
WINTER 2006
COURSE OUTLINE

Instructor: Professor John D. Goddard **e-mail:** jgoddard@uoguelph.ca
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Recommended Texts:

Physical Chemistry: A Molecular Approach.
D. A. McQuarrie and J. D. Simon. University Science Books (1997).
Physical Chemistry.
T. Engel and P. Reid. Pearson Benjamin Cummings (2006).
Quantum Chemistry and Spectroscopy.
T. Engel. Pearson Benjamin Cummings (2006).
Quantum Chemistry. 5th ed.
I. N. Levine. Prentice Hall (2000).

Calendar Description:

CHEM*4880 Topics in Advanced Physical Chemistry W(3-0) [0.50]:
Selected topics in advanced physical chemistry.(Offered in even-numbered years.)
Prerequisites: (CHEM*2820 or PHYS*3240), (CHEM*3860 or PHYS*3230)

Topics

Topic A: STATISTICAL THERMODYNAMICS.

1. Statistical Viewpoint. Review Classical Thermodynamics. Microstates. Distributions. Probability. Permutations. Combinations. Combinatory Rule. Most Probable Distribution. Stirling's Theorem.
2. Derivation Maxwell-Boltzmann Distribution Law. Basic Postulate Statistical Mechanics. Lagrange's Method Undetermined Multipliers. Energy Levels. Quantum States. Molecular Partition Function. Average Values. Physical Significance of β. Distribution Law and the Equilibrium State.
3. Statistical Basis of Entropy. Boltzmann-Planck Equation. S = k ln W. Additive Entropies, Multiplicative Microstates. Plausibility of S = k lnW. Ideal Gas Expansion. Volumes and Probabilities. Connection to Classical Thermodynamics.
4. Partition Functions and Thermodynamic Properties. Properties of the Partition Function. Calculation of Temperature, Energy, Entropy, Helmholtz Energy, Pressure, Heat Capacity, Enthalpy, Gibbs Energy.Factorization Partition Function.
5. Translational Partition Function. Gases. Indistinguishability. Counting Complexions for Gases. Dilute Gas Limit. Maxwell-Boltzmann Distribution for Gases. Thermodynamic Functions for Gases. Ideal Gas Equation of State. Translational Partition Function. Energies and Degeneracies Translational Motion.

6. Internal Partition Functions: Nuclear. Electronic, Vibrational, Rotational. Nuclear Degeneracy. Ortho and Para. Electronic Degeneracy. Vibration. Harmonic Oscillator. Diatomic and Polyatomic Molecules. Characteristic Temperature of Vibration. Rotation. Rigid Rotor. Symmetry Numbers. General Exclusion Principle. H_2 and D_2.
7. Molar Heat Capacities of Gases. Diatomic and Polyatomic Molecules. Hydrogen at Low Temperatures.
8. Quantum Effects. Bose-Einstein Statistics and Distribution Law. Fermi-Dirac Statistics and Distribution Law. Classical Limit of Quantum Statistics. Electrons in Metals. Liquid Helium.

Topic B: QUANTUM CHEMISTRY.
1. Review of the Postulates of Quantum Mechanics and Their Consequences. Dirac Bra-ket Notation.
2. Proof of the Variation Theorem. Linear Variation Functions. Determinants. Simultaneous Linear Equations. Matrices, Eigenvalues and Eigenvectors.
3. Non-degenerate Time-independent Perturbation Theory. First and Second Order Corrections to Eigenvalues and Eigenfunctions. Degenerate Perturbation Theory. Helium Atom Ground and Excited Electronic States by Perturbation Theory.
4. Electron Spin. Pauli Principle. Slater Determinants. Many Electron Atoms and Molecules. Hartree product. Hartree-Fock Self-Consistent-Field method. Orbitals. Electron Correlation. Atomic and Molecular Hamiltonians. Slater-Condon Matrix Element Rules.
5. Thomas-Fermi model. Basic Density Functional Theory (DFT) for the electronic structure of atoms and molecules.
Hartree-Fock-Slater. Xα. Hohenberg-Kohn Theorem. Hohenberg-Kohn Variational Theorm. Kohn-Sham method. Local Density Approximation. Kohn-Sham DFT calculations.

Class Schedule:
Lectures: Monday, Wednesday, Friday 09:30 – 10:20 MACN 201

Evaluation:

Problem Assignments	**30**	
Mid Term Exam	**30**	**(Probably during lecture time on Wednesday, March 1,2006.)**
Final Exam	**40**	

TOTAL	**100**	