Department of Chemistry

Brandon University

18:270 Physical Chemistry II: Quantum theory, Spectroscopy and Statistical Mechanics
Winter Term, 2013

Instructor: Dr. Adrian Weber (Office: 4-12 Brodie, webera@brandonu.ca, (204)571-7899)

Textbook:

P. W. Atkins and J. De Paula, 'Physical Chemistry' (9th edition), W. H. Freeman, New York (2010)

Course Outline:

1. Principles of Quantum Mechanics (Chapter 7)
   Energy quantization, Wave-particle duality, electron microscopy, the Schrodinger equation, the Born interpretation of the wave function, the uncertainty principle, postulates of quantum mechanics.
2. Techniques and Application (Chapter 8)
   Particle in a box, motion in two and more dimensions, tunneling, Scanning probe microscopy, vibrational motion, rotational motion, spin.
3. Atomic Structure and Spectra (Chapter 9)
   The structure and spectra of hydrogenic, many-electron and complex atoms.
4. Molecular Structure (Chapter 10)
   The Born-Oppenheimer approximation, valence-bond theory, molecular orbital theory for atoms, diatomics and polyatomics, computational chemistry.
5. Rotational and Vibrational Spectroscopy (Chapter 12)
   Experimental techniques, selection rules and transition moments, moments of inertia, rotational energy levels, rotational transitions, raman spectra, molecular vibrations of diatomics, anharmonicity, vibration-rotation spectra, vibration of polyatomics.
6. Molecular Electronic Spectroscopy (Chapter 13)
   Measuring intensity, electronic spectra of diatomics and polyatomics, vision, fluorescence and phosphorescence and applications.
7. Nuclear Magnetic Resonance (NMR) Spectroscopy (Chapter 14)
   The energies of electron and nuclei in magnetic fields, the NMR spectrometer, chemical shift, fine structure, conformational and exchange processes, pulse techniques, the magnetization vector, spin relaxation, magnetic resonance imaging (MRI), spin decoupling, the nuclear overhauser effect, 2D NMR, solid state NMR.
8. Statistical Mechanics (Chapter 15 and 16)
   Configurations and weights, the partition function, internal energy, statistical entropy, canonical ensemble, independent molecules, mean energies, heat capacities, equations of state, residual entropy.
9. Molecular interaction (Chapter 17)

Dipole moments and interactions, Polarizabilities, Polarization, repulsive interactions, intelligent drug design.

Evaluation:

Term tests (2)	25%
Problems	10%
Labs	20%
Final Exam	45%

Grading: A+ 90-100

A 85-89

A- 80-84

B+ 76-79

B 72-75

B- 68-71

C+ 62-67

C 59-61

C- 55-58

D 50-54

F 0-49