CHM 629: Principles of Physical Chemistry

Instructor: Dr. D. L. V. K. Prasad
Office: FB 425, Tel: 7295
Email: dprasad@iitk.ac.in
Lectures: M 1530 – 1700 @ FB434
Tu 1530 – 1700 @ FB434
Office Hours: F 1700 – 1730 @ FB425
Units: 3-0-0-0 (9)
Web: http://home.iitk.ac.in/~dprasad/

Prerequisites: Only for Ph.D students

Course Contents: Atomic and Molecular structure, Molecular Spectroscopy, Concepts of Statistical Thermodynamics, Electrochemistry, Chemical Kinetics, Photochemistry.

Atomic and Molecular Structure: Review of quantum mechanics, approximate methods in quantum chemistry and many electron atoms. Molecular orbital description, application of the variation theorem to calculate MOs, Valence bond description, sigma orbitals and pi orbitals, ionic bonds, dipole moment, resonance, delocalization, aromatic molecules and solids. (10)

Molecular spectroscopy: Rotational and vibrational spectra, P, Q and R branches, Raman spectra. Electronic spectra, fluorescence and phosphorescence, principle of laser action. (6)

Concepts of Statistical Thermodynamics: Molecular energy levels and Boltzmann distribution, partition function and calculation of thermodynamic quantities. Einstein and Debye models for solids, chemical equilibrium constant. (10)

Electrochemistry: Ionic equilibrium, activity and activity coefficients, Debye-Huckel theory, EMF of chemical cells, Nernst equation, concentration cells, applications, potentiometric titrations, solubility product, pH and pK. (4)

Chemical Kinetics: Rates of chemical reactions, steady state approximation, temperature dependence, activation energy, molecular reaction dynamics, collision and activated complex theory, theories of unimolecular reactions. Techniques of fast reactions and their applications. (8)

Photochemistry: Laws of photochemistry, quantum yield, radiative and non-radiative processes, photosensitized reactions, some applications of photochemical reactions. (4)

Reference textbooks:
- P. W. Atkins and Julio de Paula, *Physical Chemistry*
- D. A. McQuarrie and J. D. Simon, *Physical Chemistry A Molecular Approach*
- R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*
- R. J. Silbey, R. A. Alberty and M. G. Bawendi, *Physical Chemistry*
- I. N. Levine, *Physical Chemistry*

Exams (Spring 2017)

Quiz-1	[10%]	Take home assignments
Mid-Semester	[30%]	Will be fixed by DOAA [between Sept 24th to Oct 2nd, 2017]
Quiz-2	[10%]	Take home assignments and discussions
End-Semester	[50%]	Will be fixed by DOAA [between November 18th to 27th, 2017]

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