

## INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **Department of Chemistry**

1. Subject Code: **CYN-001**                      Course Title: **Physical Chemistry**

2. Contact Hours:        **L: 3**    **T: 0**    **P: 2**

3. Examination Duration (Hrs.):                      **Theory**                       **Practical**

4. Relative Weightage: **CWS**     **PRS**     **MTE**     **ETE**     **PRE**

5. Credits:                       6. Semester: **Autumn**                      7. Subject Area: **BSC**

8. Pre-requisite:        **Nil**

9. Objective: To provide a theoretical and experimental knowledge of fundamental physical chemistry to engineering students.

10. Details of Course:

S. No.	Contents	Contact Hours
<b>1.</b>	<b>Quantum Chemistry:</b> Postulates, commuting and non-commuting operators, Schrödinger equation, particle in a one-, two- and three dimensional box and their implications, H-atom - radial and angular wave functions, shapes of orbitals (s, p and d), application of quantum chemistry concepts to hydrogen-like atoms and their atomic spectra.	<b>7</b>
<b>2.</b>	<b>Chemical Equilibria and Reaction Dynamics:</b> Description of equilibrium, feasibility of chemical reaction, Gibbs-Helmholtz equation, phase transition - Clapeyron equation, Clapeyron-Clausius equation, free energy changes in reversible processes, chemical potential, partial molar quantities, activity coefficient and fugacity, basic concepts of statistical thermodynamics.	<b>6</b>
<b>3</b>	<b>Reaction Dynamics:</b> Collision theory of bimolecular reactions and its drawbacks, potential energy surfaces, transition state theory using partition functions, thermodynamic formulation of transition state theory, mapping of transition states using ultrafast processes.	<b>6</b>
<b>4.</b>	<b>Photochemistry:</b> Laws of photochemistry, photophysical and photochemical processes and their quantum efficiencies, spontaneous and stimulated processes. Franck-Condon principle, photosensitizers - photosynthesis and solar cells.	<b>6</b>

5.	<b>Catalysis:</b> Homogeneous catalysis – kinetics of acid, base and enzyme catalyzed reactions with suitable examples. Heterogeneous catalysis – surface phenomenon, porosity, derivation of Langmuir adsorption isotherm, Langmuir-Hinshelwood and Rideal-Eley mechanisms, comparison of rates of homogeneous and heterogeneous reactions based on activated complex theory.	6
6.	<b>Spectroscopy:</b> Interaction of electromagnetic radiation with matter, instrumental spectroscopic techniques (AAS, ICP, UV-Vis and IR spectroscopy), application of spectroscopy techniques to atomic and molecular systems.	6
7.	<b>Solid-State Chemistry:</b> Bonding in solids, diffraction methods – scattering of X-rays from a crystal, structure factor and systematic absences, methods of synthesis of solids–ceramic, sol-gel, hydrothermal, microwave and sonochemical.	5
	<b>Total</b>	<b>42</b>

### List of Experiments:

i)	Determination of iron in iron ore using potassium dichromate (internal indicator method).
ii)	Heat of neutralization of a strong base by a strong acid.
iii)	Determination of surface excess concentration of 1-butanol in aqueous solution.
iv)	To study the kinetic of a redox reaction.
v)	Blue Printing using sunlight.
vi)	pH metry/ potentiometry titrations a) Strong acid – strong base;    b) Strong acid – weak base c) Weak acid – strong base;    d) Redox titration: Fe <sup>2+</sup> or Mn <sup>2+</sup>
vii)	Acid-base titrations using conductivity meter. a) Strong acid – strong base;    b) Strong acid – weak base c) Weak acid – strong base;
viii)	Spectrophotometry: Determination of [Fe (III)] by colorimetry.
ix)	Determination of hardness of water by EDTA- complexometry titration.
x)	Determination of the composition of mixtures of liquids using viscometry.

### 11.Suggested Books:

S. No.	Authors/ Title/ Publisher	Year of Publication
1.	Silbey R.J. and Alberty R.A., “Physical Chemistry”, 3 <sup>rd</sup> Ed., John Wiley &	2003

	Sons, Inc.	
<b>2.</b>	Atkins P.W., Physical Chemistry, 8 <sup>th</sup> Ed., Oxford University Press.	<b>2006</b>
<b>3.</b>	West A.R., Solid State Chemistry and its Applications, Wiley-India Edition	<b>2003</b>
<b>4.</b>	Levine, I. N., Quantum Chemistry, Pearson Education.	<b>2000</b>
<b>5.</b>	Turro N.J., Ramamurthy V. and Scaiano J.C., Modern Molecular Photochemistry of Organic Molecules, University Science Books.	<b>2008</b>
<b>6.</b>	Skoog D.A., Holler F.J. and Crouch SR, "Principles of Instrumental Analysis", 6th Ed., Thomson Brooks.	<b>2006</b>