DEPARTMENT OF CHEMISTRY
INDIAN INSTITUTE OF TECHNOLOGY PALAKKAD, KERALA

COURSE & EVALUATION PLAN

1) Course Code: CY 1020 **2) Course Title:** Chemistry Theory **3) L-P-T:** 2-0-1 (3) **4) Credit:** Three

5) Pre-Requisite: Nil **6) Course Catagory:** B.Sc **7) Teaching Department:** Chemistry

8) Course For: 2nd Semester B.Tech

9) Objectives of the Course:

Appreciation and basic understanding of the theoretical principles of chemical interactions at the atomistic and molecular level and their relationship to the thermodynamics and kinetics of chemical changes.

10) Course Coverage: 42 Classes

S.No	Topic	Blow up Syllabus	Classes
1.	**Basic Concepts of Quantum Chemistry**	The Schrodinger wave equation; Born interpretation; Uncertainty principle; Motion of a quantum mechanical particle in one, two and three dimensions, degeneracy; Tunneling, Spectroscopic models-Rotational motion (rigid rotor) and Vibrational motion (harmonic oscillator); The Schrodinger wave equation for the hydrogen atom; physical meaning of wave function, radial wave functions and probability densities, quantum numbers, wave function and orbital shapes, electron spin.	15
2.	**Molecular Spectroscopy**	Rotational and vibrational spectroscopy of diatomic molecules; vibrational spectroscopy of polyatomic molecules (normal modes of CO_2 and H_2O); Electronic spectroscopy of molecules, Beer-Lambert law, different types of electronic transitions, UV spectra of π-electron systems (conjugated C-chains in dyes and polyenes-shift of absorption maximum with chain length)	6
3.	**The Chemical Bond**	Born-Oppenheimer approximation; LCAO-MO; H^{2+} molecule; Bonding and antibonding orbitals; Electronic structure of homonuclear diatomic molecule, bond order, paramagnetism (B_2 and O_2 molecules)and diamagnetism (C_2, N_2 and F_2 molecules); Hereronuclear diatomic molecules (HF); Formation of bands in solids-metals, semiconductors and insulators.	5
4.	**Chemical Thermodynamics**	Second Law of Thermodynamics-Entropy change accompanying various processes (isothermal expansion, phase transition, heating, entropy of mixing of perfect gases); Absolute entropy and the Third Law of thermodynamics; Statistical entropy; Spontaneity of a chemical reaction and Gibbs energy; Standard Gibbs energies of formation and reactions; Thermodynamic functions (A, G, U & H) and four fundamental equations, Maxwell relationships; variation of G with T and P, Gibbs-Helmholtz equation, Chemical potential; G versus extent of reaction, Equilibrium constant through chemical potential (gas equilibria), reaction between K_p & K_c; Phase equilibria; Gibbs phase rule, phase diagrams of water and carbon dioxide (supercritical H2O & CO_2), Clausius-Clapeyron equation; Liquid-solid phase diagrams-two-component eutectic systems and cooling curves.	9
5.	**Chemical Kinetics**	Parallel, opposing and consecutive reactions; Mechanism of complex chemical reactions; Analysing mechanisms using the steady-state approximation, Chain reactions (hydrogen-bromine reaction); Unimolecular reactions (thermodynamic approach); Transition State Theory for bimolecular reactions (thermodynamic approach); Enzyme catalysis (Michaelis-Menten Mechanism). Chemisorption and Langmuir Isotherm.	7

11) Reference Books:

a) Elements of Physical Chemistry by P W Atkins and J de Paula, 5th Ed., Oxford.
b) Atkin's Physical Chemistry by P W Atkins and J de Paula, 10th Ed., Oxford University Press.
c) Physcial Chemistry: A Molecular Approach by Donald A. McQuarrie, John D Simon, University Science Books.
d) Principles of Physical Chemistry bu Hans Kuhn, Horst-Dieter Foersterling and David H. Waldeck, Wiley.
e) Fundamentals of Molecular Spectroscopy by C N Banwell and E M McCash, 4th Ed., Tata McGraw-Hill.
f) Chemical Kinetics by K J Laidler, 3rd Ed., Tata McGraw-Hill.

12) Evaluation Plan

a) Course is evaluated in 2 components: Continuous Evaluation and End Sem Exam
b) The weightage for two components are as follows:

Continuous Evaluation: 40 marks
End Sem Exam: 60 marks

c) As part of the continuous evaluation

i) Two quiz Tests will be conducted each fro 20 Marks.
ii) Regular Assignments will be given during the semester, which will be solved in the tutorial hours.

d) The 2 Quiz tests and the End Sem Exam will be scheduled as follows:

Quiz Test 1: 2nd week of Feburary 2017
Quiz Test 2: 2nd week of March 2017
End Sem Exam: 3rd week of April 2017

e) The End-Sem test will be a comprehensive test including the entire syllabus of the course.
f) The Question papers of the Quiz tests and End-Sem tests **will not have any Choice.**