

INDIAN INSTITUTE OF TECHNOLOGY TIRUPATI
PROFORMA FOR NEW COURSE

1.	Title of the Course	Physical and Theoretical Chemistry
2.	Course Number	CY1101
3.	Status of the Course	Core
4.	Structure of Credits	2-1-0-3
5.	Offered To	UG
6.	New Course/Modification to	New
7.	To be Offered by	Department of Chemistry
8.	To take effect from	July 2018
9.	Prerequisite	NIL
10.	Whether approved by the Department	Yes
11.	Course Objective: This course is designed to give an exposure to build a strong foundation of fundamental physical and theoretical chemistry to provide microscopic understandings of chemical bonding, molecular spectroscopy, thermodynamics and chemical kinetics. Potential industrial applications of these topics will also be addressed briefly.	
12.	Course Content: Quantum chemistry: Schrödinger wave equation; Born interpretation; uncertainty principle; particle in a box; symmetry and degeneracy; tunnelling; rigid rotor, harmonic oscillator; hydrogen atom; quantum numbers, orbital shapes and electron spin. Chemical bonding and spectroscopy: Born-Oppenheimer approximation; LCAO-MO; bonding and anti-bonding orbitals; bond order; magnetism; electronic structure of diatomic molecules; molecular spectroscopy. Thermodynamics: Laws of thermodynamics; Carnot Cycle; condition of spontaneity; fundamental equations, Maxwell relationships; Gibbs-Helmholtz equation; chemical potential; phase equilibria, phase diagrams of water, Clausius-Clapeyron equation. Chemical Kinetics: First, second and third order reactions; mechanism of parallel, opposing, chain and consecutive reactions; steady-state approximations, unimolecular reactions mechanism; Michaelis-Menten mechanism.	
13.	Text book(s): 1. P. W. Atkins and J. de Paula, <i>Atkin's Physical Chemistry</i> , Oxford University Press, (2010). 2. D. A. McQuarrie and J. D. Simon, <i>Physical Chemistry: A Molecular Approach</i> , University Science Books, (1997).	
14.	Reference(s): 1. G. W. Castellan, , <i>Physical Chemistry</i> , Narosa Publishing House, (2004).	