

**Subject Code: 02CY0401****Subject Name: Physical Chemistry-I****M.Sc. Sem - I****Objectives:**

- The course presents advanced quantum chemistry in order to provide a soiled foundation for students.
- The course provides an introduction to molecular spectroscopy. Some of the fundamental concepts used in understanding molecular spectroscopy will be discussed in detail.
- Basic knowledge of physical and chemical phenomena taking place at solid surfaces and techniques that are used in modern surface science which reveals information of the surface and adsorbates.
- Describe the self association of surfactants.

**Credits Earned: 5 Credits****Course Outcomes:** After completion of this course, student will be able to

- Identify, select and explain which concepts are involved and the way of theoretical framework of quantum mechanics.
- Identify, describe and explain the quantum mechanical behaviour of simple systems, such as the harmonic oscillator and the rigid rotor.
- Understand the application of molecular spectroscopy to different areas of science.
- Solve problems related to physical and chemical aspects of solid surfaces.

**Pre-requisite of course: NA.****Teaching and Examination Scheme**

Teaching Scheme (Hours)			Credits	Theory Marks			Tutorial/ Practical Marks		Total Marks
Theory	Tutorial	Practical		ESE (E)	Mid Sem (M)	Internal (I)	Viva (V)	Term work (TW)	
4	0	3	6	50	30	20	25	25	150

**Contents:**

Unit	Topics	Contact Hours
1	<p><b>Quantum Mechanics :</b></p> <p>Time independent Schrödinger equation. Properties of the Hermitian operator, canonical commutation relations, Ehrenfest theorem.</p> <p>Applications: Particle-in-a-box (1-, 2-, 3- dimensional), different potential functions and barrier problems, degeneracy, density of states.</p> <p>Simple harmonic oscillator: Ladder operator, properties of the eigenfunctions.</p> <p>Rigid rotor: Angular momentum operator, spherical harmonics.</p> <p>Hydrogen atom: Details of the solution, shapes of the orbitals.</p>	20
2	<p><b>Molecular Spectroscopy :</b></p> <p>Region of spectra, microwave spectroscopy, rigid rotor, selection rule, non-rigid rotor, Infrared spectroscopy, harmonic and anharmonic oscillator, selection rule, Diatomic vibrating rotor, Electronic spectroscopy, Frank-Condon principle, Raman spectroscopy, condition of Raman activity, Vibrational Raman spectra of A-B<sub>2</sub> type molecule.</p>	20
3	<p><b>Surface Phenomena :</b></p> <p>Thermodynamics of surfaces, adsorption phenomena (mono- and multi layer). Langmuir and B.E.T. isotherms.</p> <p>Classification and properties of surfactants. Hydrophobic interactions. Micellization. Thermodynamics of micellization, 'phase separation' and 'mass action' models. Emulsion and 'reverse micelles'. Effect of micellization on the rate of chemical reactions.</p> <p>Characterization of the surface of a solid by different experimental techniques, including spectroscopy. Langmuir-Blodgett films.</p>	20
	<b>Total Hours</b>	<b>60</b>

**References:**

1. Quantum Chemistry (7th Edition) - I. N. Levine.
2. Introduction to Quantum Mechanics (2nd Edition) - D. J. Griffith.
3. Introduction to Molecular Spectroscopy-G. M. Barrow.
4. Fundamentals of Molecular Spectroscopy (4th Edition) - C.W. Banwell.
5. Physical Chemistry: A Molecular Approach-D. A. McQuarrie& J. D. Simon.
6. A Textbook of Physical Chemistry(5<sup>th</sup> Edition) - K L Kapoor,Macmillan India Ltd.
7. Atkin's Physical Chemistry (9th Edition) - P. W. Atkins & J. de Paula, Oxford University Press.

**Suggested Theory distribution:**

The suggested theory distribution as per Bloom's taxonomy is as per follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery and evaluation					
Remember	Understand	Apply	Analyze	Evaluate	Create
30%	25%	15%	15%	10%	5%

**Suggested List of Experiments: (Any Six)**

Experiments involving-

**A. Conductometric method**

- (i) To determine the cell constant of a given conductivity cell.
- (ii) To determine the concentration of Acetic acid and Oxalic acid in a given mixture conductometrically.

**B. Spectrophotometry**

- (iii) To examine Lambert-Beer law in concentrated solution.
- (iv) To determine  $p^K_{In}$  value of an acid-base indicator by colorimetric method.

**C. pH metric method**

- (v) To determine the concentration and dissociation constant of Oxalic acid by pHmetry.
- (vi) To determine the dissociation constant of Acetic acid with the help of Henderson-Hasselbalch equation.

**D. Kinetic study**

- (vii) To determine the rate constant for the inversion of cane sugar.

**E. Partition coefficient**

(viii) To study the distribution of Benzoic acid between toluene and water.

❖ **Reference Books:**

1. An Advanced Course in Practical Chemistry, A. K. Nad, B. Mahapatra and A. Ghoshal, New Central Book Agency (P) Ltd.
2. Practicals in Physical Chemistry, P S Sindhu, Macmillan.
3. Experimental Physical Chemistry: A Laboratory Textbook, Arthur Halpern, George McBane, W. H. Freeman, 2006.

**Instructional Method:**

- a. The course delivery method will depend upon the requirement of content and need of students. The teacher in addition to conventional teaching method by black board, may also use any of tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.
- b. The internal evaluation will be done on the basis of continuous evaluation of students in the laboratory and class-room.
- c. Practical examination will be conducted at the end of semester for evaluation of performance of students in laboratory.
- d. Students will use supplementary resources such as online videos, NPTEL videos, e-courses, Virtual Laboratory.
- e. Use of hazardous/toxic chemicals should be avoided as far as possible in laboratory.
- f. All students in the laboratory must wear safety goggles and lab coats during lab session.

**Supplementary Resources:**

1. <http://www.nptel.ac.in/courses/104103069/#>
2. <http://ocw.mit.edu/courses/chemistry/>
3. <http://vlab.amrita.edu/index.php?sub=2>
4. [http://www.vlab.co.in/ba\\_labs\\_all.php?id=9](http://www.vlab.co.in/ba_labs_all.php?id=9)