ST.JOSEPH'S COLLEGE FOR WOMEN (AUTONOMOUS), VISAKHAPATNAM

VIII SEMESTER B.Sc. HONOURS CHEMISTRY Time:4hrs/week

Code CH8203(3) Revised Syllabus Under CBCS 2020-21 Marks: 100

Physical Chemistry: Quantum and Molecular Spectroscopy

I

Course objective: To introduce students to the basic concepts of quantum chemistry and fundamental aspects of molecular spectroscopy and FORTRAN 77

Course outcomes:

- Students learn the basic non-relativistic quantum mechanics.
- Understand the time-dependent and time-independent Schrödinger equation for simple potentials like for instance the harmonic oscillator and hydrogen like atoms, as well as the interaction of an electron with the electromagnetic field.
- 3)Understand the principles and theories of rotational, vibrational and vibrational spectroscopy methods.
- Interpret the molecular spectra and find molecular properties from molecular spectra.

II. Syllabus:

Unit – I Basic Quantum Chemistry-I: 12 Hours

Wave equation-interpretation of wave function-properties of wave function-normalization and orthogonalisation, Operators- linear and non-linear- commutators of operators. Postulates of quantum mechanics; setting up of operators to observables; Hermitian operator- Eigen values AndEigen functions of Hermitian operator; Expansion theorems. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.

UNIT-II

Basic Quantum Chemistry-II: 12 Hours

Wave mechanics of simple systems with constant potential energy, particle in one-dimensionalboxfactors influencing color transition- dipole integral, Symmetry arguments in deriving the selection rules, the concept of tunneling- particle in three-dimensional box. Calculations using wave functions of the particle in a box-

Orthogonality, measurability of energy, position and momentum, average values and probabilities. Rigid rotor, Wave mechanics of systems with variable potential energy- simple harmonic oscillator- solution of wave equation- selection rules.

UNIT-III

Fundamentals of Molecular Spectroscopy-I: 12 Hours

Microwave and IR- Spectroscopy- Rotational spectra of diatomic molecules-Rigid rotor-Selection rules- Calculations of bond length- Isotopic effect, Second order stark effect and itsapplications. Infrared spectra of diatomic molecules- harmonic and anharmonic oscillators-Selection rulesOvertones- Combination bands- Calculation of force constant, anharmonicityconstant and zero point energy. Fermi resonance, simultaneous vibrational-rotational spectra ofdiatomic molecules.

UNIT- IV

Fundamentals of Molecular Spectroscopy-II: 12 Hours

Raman and Electronic Spectra- Classical and quantum mechanical explanations-RotationalRamanand Vibrational Raman spectra. Electronic spectra of diatomic molecules- Vibrational Coarse structure- intensities of spectral lines- Franck-Condon principle- applications, Rotational Fine structure- band head and band shading. Charge transfer spectra

UNIT- V

Introduction to computer programming- FORTRAN 77: 12 Hours

Basic structures and functioning of computer with P.C. as an illustrative example-Main memorySecondary storage memory- input/output devices- computer languages-operating systems- principles of algorithms-and flow charts-constants and variables-Arithmetic expressionsArithmetic statements-Replacement statement- IF statement-logical IF and BLOCK IF statements- GOTO statements-subscripted variable and DIMENSION statement. DO statementRules for DO statement- Functions and subroutines- Development of FORTRAN statements for simple formulae in chemistry such as Vander Waals equation- pH of a solution- First order rate equation- Cell constant-Electrode potential. Flowcharts and computer programs for

a) Program for the calculation of Cell Constant, Specific Conductance and Equivalence.

b) Rate Constant of First order reaction or Beer’s law by linear least square method.

c) Hydrogen ion concentration of a strong acid solution/Quadratic equation.

d) Solution for Vander Waals equation or Hydrogen ion concentration of a monoprotic weak acid

e) Standard deviation and Variance of univariant data.

III. Co-Curricular Activities :

1. Training of students by related industrial experts.
2. Assignments, Seminars and Quiz (on related topics), collection of relevant videos and material.
3. Visits of abilities, firms, research organizations etc.
4. Invited lectures and presentations on related topics by field/industrial experts

IV. List of Reference books:

1. Fundamentals of Molecular spectroscopy: by C.N. Banwell
2. Molecular spectroscopy: by B.K.Sharma
3. Molecular spectroscopy: by Aruldas
4. Introductory quantum mechanics: by A.K. Chandra
1. Quantum chemistry: by R.K. Prasad
2. Principles of computer programming (FORTRAN 77 IBM PC): by V.Rajaraman
3. Basics of computers for chemists: by P.C. Jurs