

Course Code	Course Title	C	H	I	E	T
17P3CMC9	PHYSICAL CHEMISTRY-III	4	4	25	75	100

UNIT I MOLECULAR SPECTROSCOPY - I 12 Hrs

Electromagnetic radiation – interaction of electromagnetic radiation with matter – types of molecular spectroscopy – molecular energy levels – Einstein’s transition probability – spectral line intensity – emission and absorption spectroscopy - Microwave spectroscopy: rotation of molecules – rotational spectra of rigid rotator – selection rule - intensities of rotational lines - effect of isotopic substitution - – rotational spectra of non rigid rotator - Applications : Calculation of moment of inertia, bond length and atomic mass from microwave spectra- classification of molecules based on moment of inertia.

Infrared spectroscopy: Spectra of diatomic molecules – instrumentation – selection rule – harmonic and an harmonic oscillator - fundamental bands – P,Q and R branches – overtones – hot bands- fundamental vibrational modes of H₂O and CO₂.

UNIT II MOLECULAR SPECTROSCOPY - II 12 Hrs

Raman spectroscopy: classical and quantum theory of Raman effect - Stokes and antistokes line – experimental aspects – polarisability – selection rule – diatomic molecules – pure rotational Raman spectrum – s-branch – application – determination of internuclear distance – mutual exclusion principle – Fermi resonance – Laser Raman Spectra.

Electronic spectra of diatomic molecules- Born-Oppenheimer approximation - coarse structure – Frank-Condon principle - dissociation energy - calculation - Birge- Sponer extrapolation technique, pre-dissociation spectra- Fortrat diagram- Electronic spectra of molecules.

UNIT III NMR SPECTROSCOPY 12 Hrs

Nuclear magnetic moment – nuclear spin states and nmr active nuclei, mechanism of resonance absorption applied field and its interaction -chemical shift and shielding.Nuclear spins in a magnetic field– Zeeman effect -Larmor precession - resonance – bloch equation – spin-lattice and spin-spin relaxation times – nuclear shielding and chemical shift - spin-spin coupling - line width - MRI basic concept - basic principle of FT-NMR spectroscopy – ¹³C NMR – basic principle and experimental techniques.

UNIT IV ELECTRON SPIN RESONANCE AND PHOTOELECTRON SPECTROSCOPY 12 Hrs

ESR – principle – presentation of spectrum- EPR spectrum of hydrogen atom -g-factor-hyperfine splitting; nuclear spin ($I = \frac{1}{2}, 1, \frac{3}{2}, \frac{5}{2}$)interaction with electron – epr spectra of organic radicals (Hydrogen atom, methyl radical, 1,4-benzosemiquinone radical anion, naphthalene negative ion, triphenyl methyl radical) zero field splitting - Kramer’s degeneracy-applications.

Photoelectron spectroscopy- basic principles, spectrum, X-ray PES, ESCA- Vibrational structure- Koopman's theorem- PES of argon, oxygen and nitrogen.

UNIT V PHOTOCHEMISTRY

12 Hrs

Introduction – Physical properties in electronically excited molecules - Jablonski diagram -. Photophysical processes in electronically excited molecules: Intersystem crossing, internal conversion, fluorescence, phosphorescence and other deactivation processes – determination of excited state dipole moment, acidity constant - Photophysical kinetics of unimolecular and bimolecular processes – delayed fluorescence – Stern-Volmer equation and its applications – photosensitisation – chemiluminescence – bioluminescence - experimental techniques – actinometry – elementary idea of photosynthesis - Laser .

Text Book(s):

1. Banwell, C.N. and Mc Cash, E.M. “Fundamental of Molecular Spectroscopy”, Fifth Edition, Mc Graw Hill Education (India) Pvt., Ltd., New Delhi, 2013.
2. Atkins, P. and de Paula, J., “Physical Chemistry”, Ninth Edition, Oxford University Press, New Delhi, 2011.
3. Ball, D. W., “Physical Chemistry”, First Indian Edition, Cengage Rearing India Pvt., Ltd., New Delhi, 2009.
4. Mortimer, R.G. “Physical Chemistry”, Third Edition, Academic Press – An imprint of Elsevier, London, 2009.
5. Engel, T. and Reid, P., “Physical Chemistry”, Second South Asian Edition, Pearson Publication, New Delhi, 2011.
6. Berry, R.S., Rice, S.A and Ross. J, “Physical Chemistry”, Second Edition, Oxford University Press, New York, 2007.
7. Rohatgi - Mukerjee, K.K. “Fundamentals of Photochemistry”, Second Edition, Wiley Eastern Ltd, New York, 2011.

Reference Books:

1. Aruldas, G. “Molecular Structure and Spectroscopy”, First Edition, Prentice-Hall of India Pvt. Ltd., New Delhi, 2005.
2. Puri, B.R., Sharma, L.R. and Pathania, M.S., “Principles of Physical Chemistry”, Forty sixth Edition, Vishal Publishing Co., Jalandhar, 2013.
3. Bhal, A., Bhal, B.S. and Tuli, G.D., “Essentials of Physical Chemistry”, First Edition, S.Chand & Company Ltd., New Delhi, 2012.