SIDDAGANGA INSTITUTE OF TECHNOLOGY, TUMKUR-572 103.
(An Autonomous Institution affiliated to VTU, Belgaum)

Syllabus from the academic year 2025-26 onwards

III Sem. B.E. (Chemical Engineering)

TECHNICAL CHEMISTRY

Course name	**Technical Chemistry**	**Course credits**	**4.0**
Course code	**S3CHI02**	**L+T+P**	**3+0+2**
Total No. of Contact Hours	**Theory: 39 hrs Lab classes: 26 hrs**	**CIE Marks**	**50**
Contact Hours / Week	**03**	**SEE Marks**	**50**

Course Learning Objectives (CLO): (Based on Bloom's Taxonomy)

CO1: Introduce to the principles of electronic spectroscopy, infrared spectroscopy and NMR spectroscopy techniques and instruments, UV-Visible spectra, FTIR spectra and its interpretation, for identification of molecules

CO2: Learn about different kinds of reactive intermediates, attacking reagents and various Electronic displacement effects on organic reactions.

CO3: Acquire knowledge on fundamental of quantum mechanics, structure and stability of the molecules.

CO4: Describe the estimation of different organic compounds by standard methods.

CO5: Acquire skills to determine using analytical instruments, amount of nitrates, transition temperature of salts, concentration of a given solute in a given mixture, and rate kinetics of a reaction.

CO6: Learn about analyzing the results obtained, validate and communicate the same through report writing.

UNIT – I

GENERAL INTRODUCTION TO SPECTROSCOPY

Introduction, Types of spectroscopy - atomic and molecular spectroscopy, nature and interaction of electromagnetic radiations with matter, energies corresponding to various kinds of radiations,

spectral band width – definition and factors contributing spectral width , factors influencing positions and intensity of spectral lines. **4 Hours**

ELECTRONIC SPECTROSCOPY

Principles of electronic spectroscopy - Types of electronic transitions in organic molecules. Chromophores and auxochromes. Bathochromic shift or Red shift, hypsochromic shift or blue shift. Hyperchromic effect and hypochromic effect. Effect of solvent and extent of conjugation on λ_{max} and on the energies of n $-\pi^*$ and $\pi - \pi^*$ transitions. Instrumentation, qualitative and quantitative analysis. **4 Hours**

UNIT – II

INFRARED SPECTROSCOPY

Principles of IR spectroscopy. Requirements for IR absorption. Types of vibrations - Stretching vibrations and bending vibrations. Fundamental modes of vibrations for linear and non linear molecules. Characteristic group frequencies for infrared absorption of organic molecules. Factors affecting the group frequencies – coupled interactions (Fermi resonance, aldehyde) electronic effects (carbonyl compounds) and hydrogen bonding (alcohols, carboxylic acids). Numerical problems on vibrational frequencies. Instrumentation - FTIR instrument and its advantages. Sample handling techniques – Nujol mull and KBr pellet. **8 Hours**

UNIT - III

NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

The nuclear spin, Larmor precession, the NMR isotopes, energy levels for a nucleus with spin quantum number I = ½ , $^3/_2$ and $^5/_2$, theory of population of nuclear spin levels, spin-spin and spin-lattice relaxation, chemical shift – definition, causes, measurement. TMS as a reference compound and its advantages, factors affecting chemical shift, shielding and deshielding mechanisms, spin – spin coupling, spin – spin splitting, intensity ratio of multiplet- Pascal's triangle method, chemical exchange, effect of deuteration, classification of spin systems (AX, AMX, AB, ABC), first order spectra, low and high resolution spectra, determination of peak areas, coupling constants-short and long range couplings, Instrumentation of NMR.

8 Hours

UNIT – IV

FUNDAMENTALS OF ORGANIC CHEMISTRY

i) Bond cleavage: Homolytic and heterolytic bond cleavage. Attacking reagents – electrophiles and nucleophiles. Reactive intermediates - carbocations, carbanions and free radicals, their types, structure, formation, and stability.

ii) Nucleophilic aliphatic substitution reactions: Meaning of SN1 and SN2 reaction. Mechanism of hydrolysis of alkyl halides of SN1 and SN2 reactions, SN2 versus SN1 reactions. Effect of nature of alkyl groups, leaving groups, nucleophiles and solvents on SN1 and SN2 mechanisms.

iii) Elimination reactions: Meaning of E1 and E2 reactions. Mechanism of dehydrohalogenation of alkyl halides of E1 and E2 reactions. E1 versus E2 mechanism.

iv) Nucleophilic and electrophilic aromatic substitution reactions: Electrophilic aromatic substitution reactions. Meaning and reactions of electrophilic aromatic substitution. Nitration, sulphonation, halogenation, Friedel-Craft alkyl and acylation reactions of benzene.

v) Nucleophilic addition and rearrangement reactions: Condensation Reactions: Reaction of Aldol and Claisen condensation. Rearrangement Reactions: Reaction of Reimer-Tiemann and Pinacol-pinacolone rearrangement. **8 Hours**

UNIT – V

Fundamentals of Quantum Mechanics:

Introduction to Quantum Mechanics, Classical Mechanics and its limitations, blackbody radiation, photoelectric effect, Compton effect, Schrödinger equation (time-dependent and time-independent), Postulates of Quantum Mechanics: Operators, wave functions, Eigenvalue equations, expectation values, Applications to model systems: particle in a box, harmonic oscillator, hydrogen atom, rigid rotor. Approximation methods, perturbation theory, variational method, Chemical Bonding: Hydrogen molecular ion, linear combination of atomic orbitals (LCAO), molecular orbitals, valence bond theory, molecular orbital theory, modern density-functional theory (DFT), description of molecules: Valence bond treatment and stability of bonds, molecular orbital theory and its applications in simple systems, molecular orbital theory of polyatomic molecules, the concept of delocalization, conjugated systems, butadiene. Molecular orbitals of homonuclear and heteronuclear diatomic molecules. VSEPR. Molecular orbital and valence bond approaches to polyatomic molecules. Hybrid orbitals and Huckel theory

8 Hours

Course Outcomes / Programme Outcomes (POs):

On successful completion of this course, the graduate will be able to:

CO1: Demonstrate knowledge about the principles of electronic spectroscopy, infrared spectroscopy and NMR spectroscopy techniques and instruments, UV-Visible spectra, FTIR spectra and its interpretation, for identification of molecules

CO2: Predict about different kinds of reactive intermediates, involved in a reaction.

CO3: Predicting the structure, bonds and stability of the atom or molecules.

CO4: Estimate organic compound present in a solution by adopting standard methods (L2).

CO5: Demonstrate skills to use analytical instruments, to estimate chemical and physical parameters of a solution/mixture.

CO6: Exhibit skill to analyze obtained results, validate and submit a technical report.

Program Articulation Matrix:

	POs											
	1	2	3	4	5	6	7	8	9	10	11	12
CO1		√										
CO2	√											
CO3	√											
CO4				√								
CO5				√								
CO6				√								

Course Articulation Matrix:

	POs											
	1	2	3	4	5	6	7	8	9	10	11	12
CO1		2										
CO2	1											
CO3	1											
CO4				4								
CO5			3									

[1]High association, [2]Moderate association, [3]Low association

TEXT BOOKS:

1. Spectrometric Identification of organic compounds, R.M. Silverstein and W.P. Webster, Wiley & Sons, 1999.
2. Organic Chemistry, Morrison B.R. and Boyd L.L., 6th Edition, ELBS, New Delhi, 1999
3. A Textbook of Chromatography, Rajbir Singh 2016, Mittal Publications
4. The Essence of Chromatography, Colin F. Poole, 2003, , Elsevier publications.

REFERENCE BOOKS:

1. Instrumental methods of Chemical Analysis, G.W. Ewing, 5th Edition, McGraw-Hill, New York, 1988.

2. Principles of Instrumental Analysis, Skoog, D.A, S.J. Holler, T.A. Nilman, 5th Edn., Saunders college publishing, London, 1998.
3. Instrumental Methods of Chemical Analysis, Chatwal Anand, Himalaya Publishing House.
4. Principles of Electroanalytical Methods, T. Riley and C. Tomilinsom, John Wiley and Sons.
5. Instrumental Methods of Chemical Analysis, K. Sharma, Goel Publishing House, Meerut 2000.
6. Organic Reactions Mechanism, Peter Sykes, ULBS Publishers, New Delhi.
7. Organic Chemistry Vol I and II, I L Finar, ULBS Publishers, New Delhi.
8. Organic Chemistry, Tiwari Melhrotra and Vishnoi, 7th edition, Chand S. and Co., New Delhi, 1996.
9. A Text Book of Organic Chemistry, Arun Bahl and Bahl B.S., 15th Edition. S. Chand and Company, New Delhi, 1998.
10. Engineering Chemistry, Fundamental and applications, Shikha Agarwal, Second Edition Cambridge University Press, United Kingdom, 2019
11. A Handbook of Chromatography, Verlag Omniscriptam 2017, Scholar's Press publication.
12. Chromatography and Separation Science, Satinder Ahuja, (2002), Academic Press
13. Chromatography: Principles and Instrumentation, Mark F. Vitha (2016) Wiley Publications