DISCIPLINE-SPECIFIC CORE COURSE - 19 (DSC-19)

Advanced Chemistry-I

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Chemistry-I (DSC-19)	**04**	**03**	—	**01**	--	--

Learning Objectives

- The course is designed to provide the fundamental understanding of the principles of operation and interpretation of spectra of inorganic and organic compounds for their structural characterization relevant to real-world applications. The students will acquire knowledge of solving structural problems based on UV-VIS, IR, ^{1}HNMR, ^{13}CNMR, and Mass spectral data.
- To introduce fundamental concepts of quantum mechanics, including vector spaces, operator algebra, angular momentum, spin, and the application of these concepts to atomic and molecular systems.
- To develop a quantitative understanding of Dirac notation, commutation relations, the Heisenberg Uncertainty Principle, and spin eigenfunctions.
- To provide a foundational understanding of molecular symmetry through symmetry elements, point groups, and character tables.
- To apply group theory to interpret spectroscopic data, derive selection rules, and understand molecular vibrations in infrared and Raman spectroscopy.

Learning Outcomes

The students will learn to:

1. To analyze and interpret experimental data collected of inorganic materials using different spectroscopic techniques
2. To be able to learn and analyze the theory and principle of mass spectroscopy, various ionization techniques involved and different types of detectors used and to implement the theory to interpret the mass spectra.

- Understanding spectroscopic techniques and their application in the structural elucidation of organic molecules.

- Understand the basic concepts and quantitative aspects of chemical phenomena, which require knowledge of both quantum chemistry and mathematics.
- Apply relevant mathematical methods essential for solving problems in quantum chemistry.
- Interpret symmetry elements and operations in molecules using the principles of group theory.
- Predict spectroscopic transitions using symmetry considerations and selection rules.
- Demonstrate an integrated understanding of how quantum chemistry and group theory together contribute to the interpretation of molecular spectroscopy.

SYLLABUS OF DSC 19

Unit-1: Spectroscopy for Inorganic Materials & Basics of Mass Spectrometry (Hours: 15)

ATR-IR, and Solid state or multinuclear NMR Spectroscopy of inorganic materials: Basics and applications of IR spectra in inorganic materials, total internal reflectance of inorganic materials, diffuse reflectance spectroscopy (DRS), Kubelka-Munk equation. ^{1}H, ^{13}C NMR spectra of metal complexes, dipolar and contact shifts. Basics of Magic angle spinning NMR spectroscopy (MAS NMR).Example of solid-state NMR with ^{10}B, ^{11}B, ^{17}O, ^{19}F, ^{27}Al, ^{29}Si, ^{31}P nuclei.

Mass spectrometry: Experimental arrangements, Ion sources, Mass analysers and detectors, Data analysis, Molecular ions, Fragmentation, Ion reactions, combined mass spectrometry methods, Tandem mass spectrometry (MS/MS), Chromatography-coupled mass spectrometry.

Unit-2: Organic Spectroscopy (Hours: 15)

Recapitulation of the Spectroscopic Techniques (UV- VIS, IR, and $^{1}HNMR$)
13-CNMR and 2D NMR Spectroscopy: Resolution and multiplicity of ^{13}C NMR, ^{1}H-decoupling, noise decoupling, broadband decoupling; Deuterium, fluorine, and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR. DEPT and general introduction about 2D NMR.
MASS: Theory, Fourier transform mass spectrometry instrumentation (FTMS); Unit mass and molecular ions; Important terms singly, doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity; Recognition of M^{+} ion peak; Nitrogen rule; Rule of 13; Ionization methods (EI and ESI). General fragmentation rules: McLafferty rearrangement, ortho effect.
ESR: Basic Principles and applications for organic Compounds
Structure elucidation of organic compounds using UV, IR, NMR, and Mass Spectra**.**

Unit 3: Quantum Chemistry (Hours: 7)

Introduction to vector spaces (Particle in 1-D box), Dirac's Bra-ket notation, Turn-over rule, Commutation of operators Heisenberg's Uncertainty principle (derivation and physical significance), Angular momentum: definitions, creation and annihilation operators; spherical harmonics, Spin operators and eigenfunctions; two-electron systems (qualitative).

Unit 4: Molecular Symmetry (Hours: 8)

Symmetry elements and operations; Point groups (BF_3, NH_3, H_2O), Classes, reducible and irreducible representations, Similarity transformation, Character table & Great Orthogonality Theorem (without proof)), Transition moment integrals, Selection Rules, IR and Raman activity: Group theoretical approach, examples predicting vibrational activity using character tables.

Practical component

1. Synthesis of substituted ferrocene and its mass-spectrometry analysis.
2. Synthesis of substituted Metal acetylacetonate and its mass-spectrometry analysis.
3. ATR-IR, NMR analysis of metal complexes acetylacetonate complexes of Iron, Manganese and Copper.
4. Diels-Alder reaction between maleic anhydride and anthracene and identification of the product using IR and NMR Spectroscopy.
5. Knoevenagel condensation between aromatic aldehydes (benzaldehyde/*p*-nitrobenzaldehyde) and active methylene compounds (malononitrile/ethylcyanoacetate/diethylmalonate) and identification of the product using IR and NMR Spectroscopy.
6. Differentiate between maleic and fumaric acid solutions by UV spectroscopy.
7. Determination of the effect of pH on absorbance maximum (UV-Vis spectra) of the organic compounds. (Aniline, Benzoic acid, phenol etc.)
8. Demonstration of the separation of the mixture of *p*-nitrophenol and *o*-nitrophenol by column chromatography and their characterization by melting point and spectroscopic techniques.
9. Determine the specific reaction rate of the potassium persulphate-iodide reaction by the Initial Rate Method.
10. Titrate a moderately strong acid (Salicylic/Mandelic acid) by the (a) salt-line method (b) double alkali method.
11. Titrate a tribasic acid (phosphoric acid) against NaOH potentiometrically.
12. Plotting of atomic orbitals (Spherical Harmonics S(θ) versus θ using polar graph paper. Student will be provided with the *p*-, *d*- and *f*- functions.
13. Plotting of $\psi_n(x)$, and $|\psi_n(x)|^2$ for wavefunctions of 1D harmonic oscillator in different energy levels within the domain of x, $-\infty < x < +\infty$.
14. Calculate the bond length of conjugated dye molecules (i.e., cyanine/β-carotene) using particle in 1D box model.
15. Simulated IR Spectra: assign bands using symmetry and selection rules.

(Spectra to be provided wherever required and may be obtained using the following link: https://webbook.nist.gov/chemistry

Note: A minimum of 4 to be done from 9-15

Recommended References and Textbooks (For Theory)

1. Banwell, C.N.; McCash, E.M. (2006), Fundamentals of Molecular Spectroscopy, Tata McGraw- Hill.
2. Springsteen, A. (1998), Reflectance Spectroscopy: an overview of classification and techniques. In Applied Spectroscopy; Workman, J., Springsteen, A., Eds.; Academic Press 193–224. DOI: 10.1016/B978-012764070-9/50008-1.
3. Fitzgerald, J.J. and DePaul, S. M. (1999), Solid-State NMR Spectroscopy of Inorganic Materials: An Overview, 2-133, DOI: 10.1021/bk-1999-0717.ch001.
4. Brevard, C. and Granger, P. Handbook of high resolution multinuclear NMR, A Wiley publisher, 1981 and Brevard, C. The multinuclear approach to NMR spectroscopy, Springer Netherlands, 1983.
5. Nielsen, NielsChr, Strassø, Lasse A, and Nielsen, Anders B. Solid state NMR, Springer-Verlag Berlin Heidelberg, 2012.
6. D. W. Rankin, N. Mitzel, and C. Morrison, Structural methods in molecular inorganic chemistry. John Wiley & Sons, 2013.
7. E. A. V. Ebsworth, D. W. Rankin, and S. Cradock, Structural methods in inorganic chemistry. Blackwell Scientific Publications, Oxford, 1987.
8. William Henderson and J. Scott McIndoe, Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds: Tools – Techniques – Tips, John Wiley and Sons, Ltd, 2005, ISBN 0-470-85015-9
9. J.M. Modern spectroscopy, Hollas, 4th edition John Wiley and sons Ltd., 2004.
10. Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (1991).
11. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. Spectroscopic Identification of Organic Compounds. John Wiley & Sons (1981).
12. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. Introduction to Spectroscopy. Cengage Learning (2014).
13. Organic Structures from spectra; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., 2007.
14. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).
15. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).
16. Mortimer, R. G. Mathematics for Physical Chemistry 2nd Ed. Elsevier (2005).
17. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).
18. Atkins, P. W. &Friedman, R.S.,Molecular Quantum Mechanics 3rd Ed., Oxford University Press (2004).
19. Kakkar R., *Atomic and Molecular Spectroscopy*, Cambridge University Press, (2015).
20. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
21. Bakhshi, A. K., and Thakral P., Quantum Chemistry Simplified, Vidyavani Foundation, New Delhi, ISBN: 9788196225107 (2023).
22. Cotton, F. A. Chemical Applications of Group Theory Wiley Interscience: N.Y (1990).
23. Bishop, D. M. Group Theory and Chemistry, Clarendon Press: Oxford, U.K. (1973)

Supplementary readings

1 Quantum Chemistry and Group Theory, MCH-018, IGNOU Self Learning Material, egyankosh, Indira Gandhi National Open University (2025) https://egyankosh.ac.in/handle/123456789/107771

2 Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley (2004)

3 Rakshit, S. C.; Atomic & Molecular Symmetry Groups and Chemistry, CRC Press, Taylor and Francis Group.

Recommended Reference and Textbooks (For Practical)

1. Vogel, A. I. (**2012**). Quantitative Organic Analysis, Part 3, Pearson Education.

2. Mann, F. G., Saunders, B.C. (**2009**), Practical Organic Chemistry, Pearson Education.

3. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (**2012**), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.

4. Ahluwalia, V.K., Dhingra, S. (**2004**), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.

5 Morrill, L. A., Kammeyer, J. K., & Garg, N. K. (**2017**). Spectroscopy 101: A practical introduction to spectroscopy and analysis for undergraduate organic chemistry laboratories.*J. Chem. Educ.*94(10), 1584-1586.

6 McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).

7 Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.

8 Kapoor, K.L., A Textbook of Physical Chemistry, Vol. IV, fifth Edition, McGraw Hill Education.

9 Atkins, P. W. & Paula, J. de Atkin’s Physical Chemistry 8th Ed., Oxford University Press (2006).