

Semester VII

DISCIPLINE-SPECIFIC CORE COURSE - 19 (DSC-19): Chemistry of d- and f- block elements, Advanced Organic Spectroscopy and Elements of Quantum Chemistry

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/ Practice		
Chemistry of d- and f- block elements, Advanced Organic Spectroscopy and Elements of Quantum Chemistry (DSC-19)	04	03	-	01	Class 12 th with Physics, Chemistry	--

Course Objectives

The objectives of this course are as follows:

- To provide thorough knowledge about the d- and f- block elements with respect to the general group trends, physical and chemical properties of these elements.
- To impart the knowledge about synthetic methods and principles of chromatography.
- Understanding spectroscopic techniques and their application in the structural elucidation of organic molecules.
- To familiarize the students with the postulates of quantum chemistry
- To explain how to apply the postulates to derive equations for various models and extend to the hydrogen atom and hydrogen-like atoms.
- To provide an insight into the MO approach of chemical bonding.

Learning outcomes

By studying this course, students will be able to:

- Understand the important properties of transition metals, lanthanoids, and actinoids
- Use Latimer diagrams to predict and identify species which are reducing, oxidizing and tend to disproportionate and calculate skip step potentials.
- Develop understanding on the principles of synthesis of Inorganic compounds and chromatographic separation of metal ions.

- Develop understanding of the basic principles of NMR spectroscopy, such as chemical shift, coupling constant, and anisotropy, and describe how they are affected by molecular structure, and identify organic compounds by analysis and interpretation of spectral data.
- Develop an understanding of quantum mechanical operators, quantization, probability distribution, uncertainty principle
- Understand Schrodinger equations for different types of systems
- Analyse different wave functions and probability distribution curves.

UNIT- 1: Chemistry of Transition Elements

(15 Hours)

General group trends with special reference to electronic configuration, colour, variable valency, magnetic properties, catalytic properties, and ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer diagrams), Frost diagrams of Mn and Cr. A brief discussion of differences between the first, second and third transition series

A brief discussion of electronic configuration, oxidation states, colour, spectral and magnetic properties. Lanthanoid contraction (causes and effects), separation of lanthanoids by ion exchange method.

UNIT-2: Spectroscopic Techniques in Organic Chemistry

(15 Hours)

Recapitulation of the Spectroscopic Techniques (UV- VIS, IR, and ^1H NMR)

Carbon-NMR Spectroscopy

Resolution and multiplicity of ^{13}C NMR, ^1H -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 Spectrometry

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 Spectroscopy

Basic Principles and applications for organic Compounds.

Structure Elucidation

Structure elucidation of Organic Compounds Using UV, IR, NMR, and Mass Spectra.

UNIT -3: Quantum Mechanics: An overview

(6 Hours)

Recapitulation of postulates of quantum mechanics and quantum mechanical operators; Linear and Hermitian operators, commutation rules and Uncertainty principle.

Particle in a 1-D box, quantization of energy levels, zero-point energy, wave functions, probability distribution functions, nodal properties, and qualitative extension to 3-D box (Final Energy expression only) and the concept of degeneracy.

UNIT -4: Quantum Mechanical treatment: Atoms and Molecules (9 Hours)

Vibrational and Rotational Motion: Schrödinger equation of a linear harmonic oscillator and brief qualitative discussion of its results. Schrödinger equation of a rigid rotator and brief qualitative discussion of its results.

Qualitative treatment of hydrogen atom; setting up of Schrödinger equation in spherical polar coordinates, radial part and quantization of energy (only final energy expression). Qualitative idea of indistinguishability of the electrons and their intrinsic spin, spatial and spin wavefunctions, Pauli's Exclusion principle.

Linear Combination of Atomic Orbitals (LCAO), salient features of MO theory and setting up of wavefunction of H_2 molecule.

Practical:
(Laboratory periods: 15 classes of 2 hours each)

Credits: 01

PART A: INORGANIC CHEMISTRY

Inorganic Preparations

1. Potassium aluminium sulphate $KAl(SO_4)_2 \cdot 12H_2O$ (potash alum} or Potassium chromium sulphate $KCr(SO_4)_2 \cdot 12H_2O$ (chrome alum}.
2. Manganese phosphate and
3. Sodium peroxoborate

Paper chromatographic separation of following metal ions (minimum two exercise to be done):

4. Ni(II) and Co(II)
5. Cu(II) and Cd(II)
6. Fe(III) and Al(III)

PART B: ORGANIC CHEMISTRY

(Spectra to be provided wherever required)

7. Diels-Alder reaction between maleic anhydride and anthracene and identification of the product using IR and NMR Spectroscopy.
8. Knoevenagel condensation between aromatic aldehydes (benzaldehyde/*p*-nitrobenzaldehyde) and active methylene compounds (malononitrile/ethyl cyanoacetate/ diethylmalonate) and identification of the product using IR and NMR Spectroscopy.
9. Differentiate between maleic and fumaric acid solutions by UV spectroscopy.
10. 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.

PART C: PHYSICAL CHEMISTRY

11. Plot the radial wavefunctions and probability distribution for H atom's 1s, 2s, 2p orbitals using software, i.e. MS-EXCEL.
12. (i) Draw probability plots for a particle in a 1-dimensional box for different values of quantum number n- commenting on the number of points of zero probability and then correlating them with the correspondence principle.
(ii) Calculation of the bond length of conjugated dye molecules (i.e., cyanine/ β -carotene) using a particle in 1D box model using MS-EXCEL.

Hands-on/ Instruction Mode:

13. (i) Carry out the calculation of various average values ($\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$ and $\langle p^2 \rangle$) for the simple harmonic oscillator.
(ii) Setting up of Schrödinger equation of Many-electron atoms and cite limitations to carry out an exact solution of the problem.
14. Demonstrate the variational treatment of the hydrogen molecule ion and also exhibit Valence bond and Molecular orbital (LCAO) treatment of the hydrogen molecule.

Essential/recommended readings

Theory

1. Lee, J.D.(2010), Concise Inorganic Chemistry, Wiley India.
2. Huheey, J.E.; Keiter, E.A.; Keiter, R.L.; Medhi, O.K.(2009), Inorganic Chemistry- Principles of Structure and Reactivity, Pearson Education.
3. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), Shriver and Atkins Inorganic Chemistry, 5th Edition, Oxford University Press.
4. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), Inorganic Chemistry, 5th Edition, Pearson.
5. Pfennig, B. W. (2015), Principles of Inorganic Chemistry. John Wiley & Sons.
6. Cotton, F.A.; Wilkinson, G. (1999), Advanced Inorganic Chemistry, Wiley-VCH.
7. Das, A. K.; Das, M. (2014), Fundamental Concepts of Inorganic Chemistry, 1st Edition, Volume 1-3, CBS Publishers & Distributors Pvt. Ltd.
8. S. K. Ghuman, A. Sakthivel, D. T. Masram, M. Sathiyendiran, (2017) Electronic and Magnetic properties of transition and inner transition elements and their complexes, Nova Science Publishers, New York.
9. Chandrashekar, V. (2005), Inorganic and Organometallic Polymers, 5th Edition, Springer Publications.
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. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, McGraw Hill Education, Vol 4, 5th Edition, McGraw Hill Education.
15. Bakhshi, A. K. & Thakral P., Quantum Chemistry Simplified Vidyavani Foundation: New Delhi (2025).
16. House, J.E. (2004), Fundamentals of Quantum Chemistry, 2nd Edition, Elsevier.
17. McQuarrie, D.A. (2016), Quantum Chemistry, Viva Books.

18. Atkins, P.W.; Paula, J.de. (2014), Atkin's Physical Chemistry Ed., 10th Edition, Oxford University Press.
19. Atkins, P.W.; Friedman, R. (2010), Molecular Quantum Mechanics, 5th Edition, Oxford University Press.

Practical:

1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989), Vogel's Textbook of Quantitative Chemical Analysis, John Wiley and Sons,
2. Harris, D. C.; Lucy, C. A. (2016), Quantitative Chemical Analysis, 9th Edition, Freeman and Company.
3. Day, R. A.; Underwood, A. L. (2012), Quantitative Analysis, Sixth Edition, PHI Learning Private Limited.
4. Marr, G.; Rockett, B.W. (1972), Practical Inorganic Chemistry, Van Nostrand Reinhold.
5. Vogel, A. I. (2012). Quantitative Organic Analysis, Part 3, Pearson Education.
6. Mann, F. G., Saunders, B.C. (2009), Practical Organic Chemistry, Pearson Education.
7. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A. R. (2012), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
8. Ahluwalia, V.K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
9. 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.
10. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, McGraw Hill Education, Vol 4, 5th Edition, McGraw Hill Education.
11. McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books(2008).
12. Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
13. Steiner, E. The Chemical Maths Book Oxford University Press (1996).
14. Yates, P. Chemical Calculations. 2nd Ed. CRC Press (2007).
15. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001) 487 pages.
16. Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985).

Assessment Methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.