DISCIPLINE SPECIFIC CORE COURSE - 19 (DSC-19): Chemistry of d- and f-Block Elements, Advanced Organic Spectroscopy and 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 Quantum Chemistry **(DSC-19)**	**04**	**03**	**-**	**01**	**Class 12th with Physics, Chemistry and Maths**	**--**

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 explain the concept of linear Hermitian operators and commutation of operators and applications.
- To apply the postulates for deriving equations of various models and extend it to hydrogen atom and hydrogen like atoms.
- To explain the valence bond and molecular orbital theories and their applications to simple molecules

Learning outcomes

By studying this course, students will be able to:

- Analyse the important properties of transition metals, lanthanoids, and actinoids
- Understand Latimer diagrams to predict and identify species which are reducing, oxidizing and tend to disproportionate and calculate skip step potentials.

- Apply the principles of synthesis of Inorganic compounds and chromatographic separation of metal ions.
- Develop an 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 wavefunctions 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 EMF (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 ^{1}H NMR)

Carbon-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 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: Properties of operators, Particle in a Box, Harmonic Oscillator and Hydrogen Atom **(6 Hours)**

Linear and Hermitian operators, Turn-over rule, Commutation of operators, and Uncertainty principle. Angular momentum operators, Eigenvalues and eigenfunctions, Particle in a box (3-D) and ring, and the concept of degeneracy.

Calculation of various average values ($\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$ and $\langle p^2 \rangle$) for simple harmonic oscillator. Calculation of the probabilities and most probable values of hydrogen 1*s* wavefunction.

Unit-4: Approximation Methods, Many Electrons Atom and Chemical Bonding (9 Hours)

First order time-independent perturbation theory for non-degenerate states, Variation theorem and variational methods. Use of these methods illustrated with some examples (particle in a box with a finite barrier, He atom).

Indistinguishability of the electrons and their intrinsic spin, spatial and spin wavefunctions, Pauli's Exclusion principle. Many-electron atom (Qualitative discussion).

Chemical bonding: Born-Oppenheimer approximation. Setting up of wavefunction of $\boldsymbol{H_2^+}$ using Valence bond theory approach and qualitative discussion of solutions. Linear Combination of Atomic Orbitals (LCAO), salient features of MO theory and setting up of wavefunction of $\boldsymbol{H_2}$,

Practical: Credits: 01
(Laboratory periods: 15 classes of 2 hours each)

PART A : INORGANIC CHEMISTRY

Inorganic Preparations

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

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

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

PART B: ORGANIC CHEMISTRY
(Note: 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*-nitro benzaldehyde) 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 orbital 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 correlate them with the correspondence principle.

    (ii) Calculate the bond length of conjugated dye molecules (i.e., cyanine/β-carotene) using particle in 1D box model.

13. (i) Setting up of Schrödinger equation of Many-electron atoms and cite limitations to carry out exact solution of the problem.

(ii) Carry out calculation of various average values ($\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$ and $\langle p^2 \rangle$) for simple harmonic oscillator using MS-EXCEL.

14. Demonstrate the variational treatment of hydrogen molecule ion and also exhibit Valence bond and Molecular orbital (LCAO) treatment of hydrogen molecule. Calculation of HOMO and LUMO energies using computational software; Comparison of HOMO and LUMO energies relative to H-atom.

15. Demonstration of shapes and electronic features of bonding and antibonding $\boldsymbol{\sigma}$ and $\boldsymbol{\pi}$ orbitals on a visualization software.

Essential/recommended readings

Theory

1. Lee, J. D. (2010), Concise lnorganic Chemistry, Wiley lndia.
2. Huheey, J.E.; Keiter, E.A.; Keiter; R. L.; Medhi, O. K.(2009), lnorganic 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. Chandrashekhar,V. (2005}, Inorganic and Organometallic Polymers, 5^{th} Edition, Springer Publications.
10. Kemp, W. Organic Spectroscopy 3^{rd} 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) (ISBN: 9788196225107).
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. (2008) Mathematics for Physical Chemistry University Science Books.
12. Mortimer, R. (2005) Mathematics for Physical Chemistry. 3rd Ed. Elsevier.
13. Steiner, E. (1996) The Chemical Maths Book Oxford University Press.

14. Yates, P. (2007) Chemical Calculations. 2nd Ed. CRC Press.
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.