CHE-DSM
Credit: 04

Curriculum Framework Syllabus
B.Sc. (Chemistry) 2023-24
L-7 (V Semester)

Level / Semester	Nature of Course	Courses Code	Course Title	MM	L	T	P	C
L-7 V Semester	Discipline Specific: Major	CHE-DSM-511	d – Block Elements, Quantum Chemistry and Spectroscopy (Theory)	100	4	0	0	4
	Discipline Specific: Major	CHE-DSM-512	Chemistry Laboratory (Practical)	100	0	0	2	2
	Discipline Specific: Major	DSM-513	Other Department	100	6	0	0	6
	Multi Discipline Major	CHE-MDM-511	Medicinal Chemistry and Material Science (Theory)	100	4	0	0	4
	Multi Discipline Major	CHE-MDM-512	Medicinal Chemistry and Material Science (Practical)	100	0	0	2	2
	Ability Enhancement Course (AEC)	CHE-AEC-511	Basics of Pesticide Chemistry and Food Analysis (Theory)	100	2	0	0	2
	Value Enhancement Course	VEC-511	Other Department					Qualifying
Total Credits								**20**

10/10/23

11-10-23

Bachelor of Science – B.Sc.
Discipline Specific Major (DSM)
B.Sc. V Semester

CHE-DSM-511: d – Block Elements, Quantum Chemistry and Spectroscopy (Theory)

Credit: 04	Time: 60 Hrs

Course Objectives

1. To impact basic knowledge of d-Block elements and their structures among the students
2. To strengthen fundamental concepts of quantum chemistry and spectroscopy

Learning outcomes

1. To predict the theories behind the structures of complexes of d-block elements.
2. To determine the crystal field stabilization energy for different complexes
3. Importance of quantum chemistry and spectroscopy in chemistry
4. Fundamentals of Schrödinger equation and its applications rigid rotator and linear harmonic oscillator
5. Basics of photochemistry and different laws of photochemistry

Unit 1

Transition Elements (3d series) General group trends with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties, ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu. Lanthanoids and actinoids: Electronic configurations, oxidation states, colour, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only). Coordination Chemistry Valence Bond Theory (VBT): Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT. IUPAC system of nomenclature. 12h

Unit 2

Crystal Field Theory Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of D. Spectrochemical series. Comparison of CFSE for Oh and Td complexes, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, Square planar coordination.
12h

Unit 3

Quantum Chemistry & Spectroscopy Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter. Types of spectroscopy. Difference between atomic and molecular spectra. BornOppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components. Postulates of quantum mechanics, quantum mechanical operators. Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wavefunctions, concept of zero-point energy. 12h

Unit 4

Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels. Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy. Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels. Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen

bonding (inter- and intramolecular) and substitution on vibrational frequencies. Electronic Spectroscopy: Electronic excited states. Free Electron model and its application to electronic spectra of polyenes. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts. 12h

Unit 5

Photochemistry Laws of photochemistry. Lambert-Beer's law. Fluorescence and phosphorescence. Quantum efficiency and reasons for high and low quantum yields. Primary and secondary processes in photochemical reactions. Photochemical and thermal reactions. Photoelectric cells. 12h

Reference Books:

- G. M. Barrow: Physical Chemistry Tata McGraw Hill (2007).
- G. W. Castellan: Physical Chemistry 4th Edn. Narosa (2004).
- C. Kotz, P. M. Treichel & J. R. Townsend: General Chemistry, Cengage Lening India Pvt. Ltd., New Delhi (2009).
- B. H. Mahan: University Chemistry 3rd Ed. Narosa (1998).
- R. H. Petrucci: General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985).
- D. Lee: A New Concise Inorganic Chemistry, E.L.B.S.
- F.A. Cotton & G. Wilkinson: Basic Inorganic Chemistry, John Wiley.
- D. F. Shriver and P. W. Atkins: Inorganic Chemistry, Oxford University Press.
- Gary Wulfsberg: Inorganic Chemistry, Viva Books Pvt. Ltd.

Bachelor of Science – B.Sc.
Discipline Specific Major (DSM)
B.Sc. V Semester

CHE-DSM-512: Chemistry Laboratory (Practical)

Credit: 02	Time: 30 Hrs

Course Objective

1. To understand the gravimetric and volumetric analysis by the illustration of Ni estimation, magnesium estimation and hardness determination of water.
2. To strengthen the determination and better understanding of uv and visible spectroscopy.

Laboratory Work:

1. Estimation of the amount of nickel present in a given solution as bis(dimethylglyoximato) nickel(II) or aluminium as oxinate in a given solution gravimetrically.
2. Estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.
3. Estimation of total hardness of a given sample of water by complexometric titration.
4. To draw calibration curve (absorbance at λ_{max} vs. concentration) for various concentrations of a given coloured compound and estimate the concentration of the same in a given solution.
5. Determination of the composition of the Fe^{3+} - salicylic acid complex / Fe^{2+} - phenanthroline complex in solution by Job's method.
6. Determination of concentration of Na^+ and K^+ using Flame Photometry.
7. UV/Visible spectroscopy I. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule-1, kJ mol-1 , cm -1, eV).
8. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
9. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
10. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration.
11. Analyse the given vibration-rotation spectrum of HCl(g)

Reference Books:

A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
A.I. Vogel, Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

Bachelor of Science –B.Sc.
Multidisciplinary Major (MDM)
B.Sc. V Semester

CHE-MDM-511: Medicinal Chemistry and Material Science (Theory)

Credit: 04	Time: 60 Hrs

Course objectives

1. To provide basics knowledge of some drug molecules, concept of materials and soap and detergents

Learning outcomes

1. Concepts of drug receptors
2. Some important antineoplastic agents
3. Concept of amorphous, single and polycrystalline structures and non-crystalline materials
4. General introduction of Optical fiber, Laser glass, Superconductors etc.
5. To learn the definitions, classifications of nanomaterials, their properties and preparations.

UNIT I

Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physicochemical parameters; lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. 12h

UNIT II

Antineoplastic agents Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer, carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, and uracil. 12h

UNIT III

Concept of amorphous, single and polycrystalline structures, Nucleation and grain growth. Non-crystalline materials: silicate glasses, glass transition temperature, viscoelasticity. Imperfections in crystalline solids: point, line, surface and volume defects, non-stoichiometry. 12h

Unit IV

General introduction of Optical fiber, Laser glass, Superconductors, Piezoelectric, Ferroelectric, Optoelectric materials, Carbon-based materials, Polymer nanocomposites, Biomaterials, Shape memory alloys, Fuel cells, Sensors, Membranes, Liquid crystals and amphiphiles, Zeolites. 12h

Unit V

Overview of nanostructures and nanomaterials: classification. Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials. 12h

Books Suggested

1. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text Book of organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge.
3. An Introduction to Drug Design, S. S. Pandeya and J. R. Dimmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol. 1 (Chapter-9 and Ch-14), Ed. M. E.

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Wolff, John Wiley.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, Mc Graw-Hill.
6. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.
7. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.
8. Elements of Materials Science and Engineering – L. H. Van Vlack
9. Materials Science and Engineering: A First Course – V. Raghavan
10. Materials Science and Engineering: An Introduction – W. D. Callister and D. G. Rethwisch
11. Materials Science and Engineering – W. F. Smith, J. Hashemi and R. Prakash
12. The Science and Engineering of Materials – D. R. Askeland
13. Surface Active Agents and Detergents - Schwartz & Perry
14. Gemini Surfactants - Raoul Zana & Jiding Xia
15. Textbook of polymer science - Fred W. Billmeyer
16. Surfactants and Interfacial Phenomena - Milton J. Rosen & Joy T. Kunjappu
17. Macromolecules, an introduction to polymer science, F. A. Bovey and F. H. Winslow
18. Frank J. Ovens, Introduction to Nanotechnology

Bachelor of Science –B.Sc.
Multidisciplinary Major (MDM)
B.Sc. V Semester

CHE-MDM-512: Medicinal and Material Chemistry (Practical)

Credit: 02	Time: 30 Hrs

Course Objective

1. To provide the knowledge about synthesis of some basic drugs
2. To understanding the structure and imperfections of given crystals
3. To understand the process for the determination of Alkali Content & Total Fatty Matter in Cleansing Agents.

Lab work

1. Synthesis of paracetamol from p-aminophenol.
a. Synthesis of benzocaine from p-aminobenzoic acid.
b. To study crystal structures of a given specimen.
c. To study crystal imperfections in a given specimen.
d. To study microstructures of metals/ alloys.
e. To prepare solidification curve for a given specimen.
f. To study heat treatment processes (hardening and tempering) of.
g. Synthesis of silver and gold metal nanoparticles

Books Suggested

1. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.
2. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.
3. An Introduction to Drug Design, S. S. Pandeya and J. R. Dimmock, New Age International.

Bachelor of Science –B.Sc.
Ability Enhancement Course (AEC)
B.Sc. V Semester

CHE-AEC-511: Basics of Pesticide Chemistry and Food Analysis (Theory)

Credit: 02	Time: 30 Hrs

Course objectives

1. To introduce the basic applications of some significant pesticides among the students
2. To provide the basic knowledge of food analysis and its preservations

Learning outcomes

1. Introduction, benefits and adverse effects of pesticides
2. Learning of synthesis and important applications of some significant pesticides
3. Food Laws and Standards of India and International Food Laws
4. Standards of Quality and Safety of Food & Food Products laid down in the FSS Regulations, 2011
5. Principles of Food Preservation, Processing and Packaging

Unit - I

General introduction to pesticides (natural and synthetic), benefits and adverse effects, Changing concepts of pesticides, structure activity relationship. 6h

Unit – II

Synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,), Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl), Quinones (Chloranil), Anilides (Alachlor and Butachlor). 6h

Unit III

Food Laws and Standards of India and International Food Laws: Food Safety and Standards Act of India, 2006: Provision, definitions and different sections of the Act and implementation. FSS Rules and Regulations (2011) as amended from time to time - Licensing and registration: Central license, State license, Registration, Responsibilities of the FBO, Role of Designated officer, Food Safety Officer and Food Analyst. 6h

Unit IV

Standards of Quality and Safety of Food & Food Products laid down in the FSS Regulations, 2011. Regulations of food additive: What is an additive, various groups of additives and their technological functions, Packaging and labeling rules and regulations: List of ingredients, nutritional information, and special label declarations. 6h

Unit V

Principles of Food Preservation, Processing and Packaging: Food Processing Operations: Manufacturing processes, Food Preservation by Heat, Water Removal, Temperature Reduction, Radiation, Food Packaging, Effect of Environment on Food Stability, Different packaging materials used for food packaging and their properties. 6h

Reference Books:

1. R. Cremlyn: Pesticides, John Wiley.
2. Willard, H. H. Instrumental Methods of Analysis, CBS Publishers.
3. Skoog&Lerry. Instrumental Methods of Analysis, Saunders College Publications, New York.
4. Skoog, D.A.; West, D.M. & Holler, F.J. Fundamentals of Analytical Chemistry 6 th Ed., Saunders College Publishing, Fort Worth (1992).
5. Harris, D. C. Quantitative Chemical Analysis, W. H. Freeman.
6. Dean, J. A. Analytical Chemistry Notebook, McGraw Hill.

7. Day, R. A. & Underwood, A. L. Quantitative Analysis, Prentice Hall of India.
8. Freifelder, D. Physical Biochemistry 2ndEd., W.H. Freeman and Co., N.Y. USA (1982).
9. Cooper, T.G. The Tools of Biochemistry, John Wiley and Sons, N.Y. USA. 16 (1977).
10. Vogel, A. I. Vogel's Qualitative Inorganic Analysis 7thEd., Prentice Hall.
11. Vogel, A. I. Vogel's Quantitative Chemical Analysis 6thEd., Prentice Hall.
12. Robinson, J.W. Undergraduate Instrumental Analysis 5thEd., Marcel Dekker, Inc., New York (1995).