DEPARTMENT OF CHEMISTRY

ISLAMIC UNIVERSITY OF SCIENCE AND TECHNOLOGY, AWANTIPORA-192122, J&K, India

Semester-IV

Fourth Semester

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credits	Total Credits
				Internal*	Final	Total	L	T	P		
IV	CHM651C	Advanced Inorganic Chemistry	Core	50	50	100	3	1	0	4	22
	CHM652C	Advanced Organic Chemistry	Core	50	50	100	3	1	0	4	
	CHM653C	Advanced Physical Chemistry	Core	50	50	100	3	1	0	4	
	CHM654C	Polymers and Nanotechnology	Core	50	50	100	3	1	0	4	
	CHM655C	Project and Dissertation	Core	50	50	100				4	
		Choose from the list of Open Elective courses of other Departments	Open Elective	25**	25	50	2	0	0	2	

*(Midterm 30 marks + Assignment 10 marks + Attendance 10 marks)
**(Midterm 15 marks + Assignment 5 marks + Attendance 5 marks)

A total of 22 credits to be taken by students with following breakup:
Core =20 Credits
Open Elective=2 Credits

Forth Semester
Core Course
Course Title: Advanced Inorganic Chemistry
Course Code: CHM651C

Credits = 4
M.M. = 100

Unit I: Symmetry Aspects of Molecular Vibrations

Construction of character tables for C_4v, D_{3h}, D_3v and T_d. Application of group theory to IR and Raman spectroscopy, Symmetry of IR and Raman active normal vibrational modes of AB_2, AB_3, AB_4 type molecules. Determining the symmetry types of the normal modes (Normal mode analyses of water molecule, carbonate ion and N_2F_2), Contribution of particular internal coordinates to normal modes, Symmetry selection rules for fundamental vibrational transitions (qualitative treatment), Use of symmetry considerations to determine the number of active infrared and Raman lines (example SF_4).

Unit II: Symmetry Aspects of Hybrid and Molecular Orbitals

Transformations properties of atomic orbitals. Hybrid orbitals for sigma bonds in trigonal planar (BCl_3), Tetrahedral (CH_4), Square planar $[PtCl_4]^{2-}$ and trigonal bipyramidal (PF_5), Hybridization scheme for pi bonding in trigonal planar (AB_3) and tetrahedral (AB_4) systems, Mathematical form of equivalent hybrid orbitals, Trigonal planar sp^2 equivalent hybrid orbitals in BCl_3, Tetrahedral sp^3 equivalent hybrid orbitals in CH_4, Molecular orbitals for sigma bonding in trigonal planar and tetrahedral systems.

Unit III: Atomic Absorption and Emission Spectroscopy

Atomic Absorption Spectroscopy: Principle of atomic absorption spectroscopy, Instrumentation and applications of atomic absorption spectroscopy, Sensitivity, detection limit and spectral interferences in atomic absorption spectroscopy.
Atomic Emission Spectroscopy and Flame Photometry
Principle of emission spectroscopy, source of excitation, instrumentation for AES, Flame emission spectroscopy, Qualitative and quantitative analysis, Limitations of Flame emission spectroscopy, Principle of plasma emission spectroscopy, inductively coupled plasma source, ICP-AES instrumentation, applications and comparison of ICP-AES with AAS.

Unit IV: Inorganic Polymers

Boron nitrides: Carboranes, Metallocarboranes and Fluorocarbons: Introduction, preparation, properties, structure, bonding and uses, Polymeric Sulfur and Sulfur nitrides: Preparation, properties, structure, bonding and uses. Polyphosphates: preparation, reactions, properties, structure, bonding and uses. Silicates: Classification, properties, structure and uses. Silicones: Preparation, reactions, properties, structure, bonding and uses.

Books Recommended:

1. Chemical Applications of Group Theory: by F.A. Cotton.
2. Group Theory and Symmetry in Chemistry: by Lowell H. Hall.
3. Symmetry, Orbitals and Spectra: by Milton Orchin and H.H. Jaffe.
4. Physical Methods in Chemistry: by R.S. Drago. 5. Molecular Spectroscopy: by G.M. Barrow, McGraw-Hill.
5. Introduction to chemical Analysis, R. D.Braun, Mc. Graw-Hill, International Book Co., 1988
6. Inorganic Polymers NJLRay; Academic Press; 1978.
7. Inorganic Porymers James. E.Mark, HarryAllock & Roberta West; Prentice Hall.
8. Inorganic Porymers F.G-A-Stone & W. A. Graham; Academic Press.
9. Instrumental methods of Chemical Analysis, 5th edn., G.W. Ewig, McGraw Hill Book Co., 1985.
10. Instrumental Methods of Analysis by G.D. Christian and C.N. Reilly.
11. Basic Concepts of Analytical Chemistry, S. M. Khopkar, New Age International Publishers, 2nd Edition, 2005.
12. Analytical Chemistry, G. L. David Krupadanam, D Vijaya Prasad, K. Varaprasad Rao, K.
13. L. N. Reddy, C. Sudhakar, University Press(india) Limited, 2001.
14. Analytical Chemistry, H. Kaur, Pragati Prakashan, 2008

Fourth Semester
Core Course
Course Title: Advanced Organic Chemistry
Course Code: CHM652C

Credits = 4
M.M. = 100

Unit I: Retrosynthetic Analysis

An introduction to synthons and synthetic equivalents, The importance of order of events in organic synthesis, Functional group interconversions, The disconnection approach. One group, Two group and electrocyclic disconnections, Examples involving connections and rearrangements.
Protection of functional groups: Principle of protection of carbon-hydrogen bonds (in terminal alkynes and hydrogens of aldehydes), Carbon-carbon double bonds, Alcoholic hydroxyl groups, Amine groups, Carbonyl and carboxyl groups.

Unit II: Natural Products

Terpenoids: Isoprene rule, Classification, Nomenclature, General methods of structure determination, Stereochemistry and synthesis of α-Pinene, Menthol, Farnesol. Biosynthetic routes to mono and sesquiterpenoids. Essential oils, their chemical composition, Extraction, Methods of analysis.
Alkaloids and flavonoids: Introduction, classification, nomenclature and general methods of structure determination, biosynthesis of flavonoids. Medicinal applications of flavonoids and alkaloids.

Unit III: Medicinal Chemistry

Classification and sources of drugs, concept of lead compounds and lead modification, Analogues, Structure activity relationship (SAR): isosterism, bioisosterism, changing the size and shape, number of methylene groups in chain, degree of unsaturation, Effect of introduction of methyl groups, Halogens, Hydroxyl, Carbonyl, Thiols sulphides groups and introduction/removal of ring systems on pharmacological activity. Prodrugs and types of prodrugs.

Unit IV: Heterocyclic Chemistry

Nomenclature of heterocycles (Hantzsch-Widman nomenclature, Replacement nomenclature), Non-aromatic and aromatic heterocycles. Structure of five membered, six membered and bicyclic heteroatomic systems, Aromaticity of various heterocyclic systems, Resonance energies. Mesoionic systems. UV/Visible and NMR spectroscopy of heterocycles. Reactivity of aromatic heterocycles. Synthesis of aromatic heterocycles, Reaction types most frequently used in heterocyclic ring synthesis, Cyclisation, Cycloaddition, Electrocyclic processes in heterocyclic ring synthesis.

Books Recommended:

1. Heterocyclic Chemistry, 4th Ed., J.A.Joule and K. Mills (Black Well Science. 2000).
2. Medicinal Chemistry- An Introduction, Gareth Thomas (Wiley-2000). 3rd Edition.
3. Medicinal Chemistry, Ashutosh Kar. (Wiley Eastern-1993).
4. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin (Verlag VCH-1986).
5. Designing Organic Synthesis, S. Warren (Wiley-1978).
6. Some Modern Methods of Organic Synthesis, 3rd Ed., W. Carruthers (Cambridge University Press-1986).
7. Modern Synthesis Reactions, 2nd Ed. H.O. House (W.A.Benjamin, NY-1972).
8. Principles of Organic Synthesis 2nd, R.O.C.Norman (Chapman and Hall-1978).
9. Heterocyclic Chemistry, Thomas. L. Gilchrist, Prentice Hall; 3 Edition April 14, 1997.
10. Introduction to strategies for organic synthesis, Laurie S. Starkey, First Edition, John Wiley & Sons, 2018.

Forth Semester
Core Course
Course Title: Advanced Physical Chemistry
Course code: CHM653C

Credits = 4
M.M. = 100

Unit I: Quantum Chemistry-IV

Huckel's Pi-MO theory, Application to linear and cyclic polyenes, Aromaticity, Pi-electron charge and pi-bond-order. Alternant hydrocarbons, Naphthalene. Limitations of Huckel theory, Extended Huckel-method (basic idea).
Self-Consistent field method: Hamiltonian and wave function for multi-electron systems, Electronic hamiltonian, Antisymmetrized wave function, Slater-determinant, Hartree-Fock self-consistent field method in the light of minimal basis H_2 molecule system ; one and two electron integrals. General polyelectronic system, Coulomb and exchange operators and integrals.

Unit II: Statistical Thermodynamics-II

Thermodynamic properties of a diatomic gas**.** Calculation of equilibrium constant using partition functions; examples of : isotope exchange reaction, $H_2 + O_2$ reaction, reaction between C_2H_4 and H_2.
Concept of ensembles, ensemble average and postulate of equal a priori probability. Canonical, Grand-canonical and Micro-canonical ensembles. Perfect gas in canonical ensemble, Entropy and free energy. Grand partition function and its characteristic equation.
Einstein model of energy and heat capacity of a solid using canonical partition function. Limitations of Einstein model, Debye model of heat capacity.

Unit III: Irreversible Thermodynamics

Basic principles of non-equilibrium thermodynamics: Second law of thermodynamics for open systems, law of conservation of mass, charge and energy. Irreversible processes and uncompensated heat, degree of advancement, reaction rate & affinity of a reaction. Relation of uncompensated heat to other thermodynamic functions. Entropy production, entropy production due to matter flow, heat flow, charge flow and chemical reactions; entropy production and efficiency of galvanic cells.
Concept of forces and fluxes, Onsager‘s theory of irreversible processes, phenomenological laws, their domain of validity. Principle of microscopic reversibility and Onsager relations, Chemical reactions near equilibrium. Curie–Prigogine principle. Transformation properties of forces and fluxes.

Unit IV: Micelles, Solubilization and Micellar Catalysis

Surfactants: Classification , Kraft temperature and cloud point. Micellization : Critical micelle concentration (cmc), Aggregation number (N), Counterion binding. Factors affecting cmc and N in aqueous media, Structure and shape of micelles: Chain packing, Variation of micellar size and shape with surfactant concentration and organic additives. Thermodynamics of micellization: Pseudophase and mass action models.
Mixed Micelle formation (two components): Clint equation, Rubing equation.
Solubilization and factors affecting solubilization, Nature of surfactant/solubilizate, Additive and temperature, Solubilization of drugs into micelles and its importance in drug delivery systems and controlled release.
Micelles as reaction media: Theoretical consideration of reactions in micellar media, Examples of micellar catalysis for hydrolysis, Oxidation and reduction reactions.

Books Recommended:

1. Quantum Chemistry, D. A. McQuarie, Viva Books Pvt Ltd,Student edn.
2. Quantum Chemistry- Ira. N. Levine, Prentice Hall, 7th Edn.; 2013.
3. Quantum Chemistry, Prasad, New Age Publishers, 4th Edn.; 2010.
4. Norman, O, Smith, Elementary Statistical Thermodynamics, , Plenum Press.
5. R.P.H. Gasser and W.G. Richards, Introduction of Statistical Thermodynamics, World Scientific, Singapore (1995).
6. D. A. McQuarie, Statistical Mechanics, Viva Books Pvt Ltd,Student edn
7. T.L. Hill, An Introduction to Statistical Thermodynamics, Dover, New York (1986).
8. Thermodynamics of IrreversibleProcesses;DeGroot,Mazur;Dover;1986.
9. Introduction to Thermodynamics of Irreversible Processes; I.Prigogine; Wiley Interscience; 1967.
10. Thermodynamics for students of Chemsitry, Kuriacose, Rajaram, (S. ChandandCo., 1996).
11. Modern Thermodynamics, D Kondipodi & I Prigogine, John Wiley.& Sons, 2002
12. Robert J. Hunter, ―Foundations of Colloid Science‖, Oxford University Press, New York, 2007.
13. P.C. Heimenz, ―Principles of Colloid and Surface Chemistry‖, Marcel Dekker Inc. New York, 1986.
14. M. J. Rosen, ―Surfactants and Interfacial Phenomena‖, John Wiley & Sons, New York, 2004.
15. D. Y. Meyer, ―Surfaces, Interfaces and Colloids‖, VCH Publishers, Inc. 1991.

Fourth Semester
Core Course
Course Title: Polymers and Nanotechnology
Course code: CHM654C

Credits = 4
M.M. = 100

Unit I: Chemistry of Polymerization

Review and recapitulation (Importance of polymers, Basic concepts, Monomers, Repeat units, Degree of polymerization) Classification of polymers: skeletal structures, Isotactic polymers, Atactic polymers, Syndiotactic polymers, Graft polymers, Polymerization mechanism: Chain polymerization (Free radical, ionic, coordination), Step polymerization, Copolymerization, Miscellaneous polymerization reactions, Polymerization techniques (Bulk, Solution, Suspension, Emulsion polymerization), Polymer Reactivity, Engineering and specialty polymer; Polyamides, ABS, polycarbonates, Polysulphones.

Unit II: Polymer Characterization and Properties

Polydispersion and average molecular weight concept: Number, Weight and viscosity average molecular weights, Measurement of molecular weights: End-group, Membrane osmometry, light scattering and viscometry, Polymer crystallization, Morphology and chain tacticity; Melting (T_m) and glass transition (T_g) temperature, Effects of molecular weight, chemical structure, branching and cross linking on T_m and T_g, Relationship between T_m and T_g, Thermal analysis and Visco-elastic properties.

Unit III: Nanotechnology-I

Nanoscience and nanotechnology, Nanostructures in nature, Surface effects of nanomaterials, Surface plasmon resonance, Quantum size effects, Effect of size on properties; reactivity, optical, electrical, and magnetic properties.
Application of nanomaterials in medicine, Nanomaterials for energy sector, Nanomaterials in food, Nanomaterials for the environment, Nanomaterials in automobiles.

Unit IV: Nanotechnology-II

Nanomaterials synthesis, Top-down and bottom-up approaches, Mechanical attrition (Ball Milling and Tube milling), Lithography, Co-precipitation, Sol-Gel Method. Solvothermal synthesis, Hydrothermal synthesis, Reverse micellar/Micro-emulsion method, Reverse micelles as nano reactors.
Brief introduction to characterization techniques for Nano-materials

Books Recommended:

1. Textbook of Polymer Science, F.W. Billmeyer Jr., John Wiley & Sons, Inc., 2000.
2. An Introduction to Polymer Chemistry, W.R. Moore, University of London Press Ltd., London.
3. Introduction to Polymers, R.J. Young and P.A. Lovel, Chapman & Hall, London.
4. Polymer Chemistry-An Introduction, R.B.Seymour & C.E. Carraher, Jr., Marcel Dekker, Inc., New York.
5. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedahr, New Age International(P) Ltd. Publishers, 2001.
6. Sperling LH, *Introduction to Physical Polymer Science*, Fourth Edition, Wiley-Inter science (2005)
7. Chanda M, *Introduction to Polymer Science and Chemistry, A Problem Solving Approach*, CRS Press (2006)
8. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad, Narosa Publications, 2010.
9. Nano Materials, B. Viswanathan, Narosa Publications, 2009.
10. Nano: The Essentials, T. Pradeep, Tata Mcgraw Hill, 2009.
11. Chemistry of Nanomaterials: Synthesis, Properties and Applications by C.N.R. Rao, A.Muller and A. K. Cheetham (eds.), Wiley-VCH, Weinheim, 2004.
12. Nanoscale Materials by Luis M. Liz-Marzan and Prashant V.Kamat, Kluwer Academi Publishers (Boston), 2003.
13. Physical Principles of Electron Microscopy: An introduction to TEM, SEM and AFM by R.F. Eqerton, Springer, 2008.

Forth Semester
Core Course
Course Title: Project and Dissertation
Course Code: CHM655C

Credits = 4
M.M. = 100

- In this course, the student will choose a lab oriented problem and perform theoretical and practical work after reviewing literature from different sources.
- The student will be guided by a faculty during this course and will have to submit a short synopsis, duly verified by the faculty, project coordinator and Head of the Department.
- The student will have to submit a dissertation based on the problem chosen by him/her (after consultation with the guide) during this course to the Department for evaluation.
- The student will also have to give a seminar about the literature surveyed and work done during this course.