Shri Vaishnav Vidyapeeth Vishwavidyalaya, Indore

P.G. Program M.Sc. (Chemistry) CBCS
BATCH 2018-19

Semester-II (M.Sc.)

SUBJECT CODE	Category	SUBJECT NAME	TEACHING & EVALUATION SCHEME								
			THEORY			PRACTICAL		Th	T	P	CREDITS
			END SEM University Exam	Two Term Exam	Teachers Assessment *	END SEM University Exam	Teachers Assessment *				
MSCHE 201	PGDC	**Main Group Chemistry and Inorganic Photochemistry**	60	20	20	60	40	4	0	4	6

Legends: L-Lecture; T-Tutorial/Teacher Guided Student Activity; P–Practical; C-Credit; Q/A–Quiz /Assignment/Attendance, MST Mid Sem Test.

Teacher Assessment shall be based following components: Quiz/ Assignment / Project / Participation in Class, given that no component shall exceed more than 10 marks.

Paper - Main Group Chemistry and Inorganic Photochemistry

Course Objectives:-

To give knowledge of Main group elements.
To develop the understanding of Kinetics and photochemistry.

Course Outcomes:-

After completion of this course the students are expected to be able to demonstrate following knowledge, skills and attitudes. The student will demonstrate capability of

CO1. Theoretical understanding of main group elements.
CO2. Became aware of Kinetics and photochemistry.
CO2. Became aware of Kinetics and photochemistry.

Syllabus

UNIT-I Main group elements

General characteristics, allotropes, structure and reactions of simple and industrially important compounds: boranes, carboranes, silicones, silicates, boron nitride, borazines and phosphazenes. Hydrides, oxides and oxoacids of pnictogens (N, P), chalcogens (S, Se & Te) and halogens, xenon compounds, pseudo halogens and interhalogen compounds. Shapes of molecules and hard-soft acid base concept. Structure and Bonding(VBT) of B, Al, Si, N, P, S, Cl compounds. Allotropes of carbon: graphite, diamond, C60. Synthesis and reactivity of inorganic polymers of Si and P.

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UNIT-II Transition Elements

General characteristics of d and f block elements; coordination chemistry: structure and isomerism, stability, theories of metal- ligand bonding (CFT and LFT), mechanisms of substitution and electron transfer reactions of coordination complexes. Electronic spectra and magnetic properties of transition metal complexes, lanthanides and actinides. Metal carbonyls, metal-metal bonds and metal atom clusters, metallocenes; tranition metal complexes with bonds to hydrogen, alkyls, alkenes and arenes; metal carbenes; use of organometallic compounds as catalysts in organic synthesis. Bioinorganic chemistry of Na, K. Mg, Ca, Fe, Co, Zn, Cu and Mo.

UNIT-III Solids

Crystal systems and lattices, miller planes, crystal packing, crystal defects; Bragg's Law, ionic crystals, band theory, metals and semiconductors, Different structures of AX, AX2, ABX3 compounds, spinels.

UNIT-IV Kinetics

Collision theory (detailed treatment); outline of Transition State theory. Primary kinetic salt effect. Lindemann theory of unimolecular reaction. Potential energy curves (diatomic molecules), Frank-Condon principle and vibrational structure of electronic spectra. Bond dissociation and principle of determination of dissociation energy (ground state). Decay of excited states by radiative and non-radiative paths. Fluorescence and phosphorescence, Jablonsky diagram.

UNIT-V Photochemistry

Laws of photochemistry: Grotthus-Draper law, Stark-Einstein law of photochemical equivalence and Lambert-Beer's law; quantum yield and its measurement for a photochemical process, actinometry. Photo stationary state. Photosensitized reactions. Kinetics of HI decomposition, H_2-Br_2 reaction, dimerisation of anthracene

Recommended Texts:

1. Lee, J. D. Concise Inorganic Chemistry, ELBS, 1991.
2. Douglas, B.E. and McDaniel, D.H., Concepts & Models of Inorganic Chemistry, Oxford, 1970
3. Atkins, P.W. & Paula, J. Physical Chemistry, Oxford Press, 2006.
4. Day, M.C. and Selbin, J.Theoretical Inorganic Chemistry, ACS Publications 1962.
5. Laidler, K.J. Chemical Kinetics, Pearson Education:New Delhi 2004

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Semester - II (M.Sc.)

SUBJECT CODE	Category	SUBJECT NAME	TEACHING & EVALUATION SCHEME								
			THEORY			PRACTICAL		Th	T	P	CREDITS
			End Sem. Univ. Exam	Two Term Exam	Teachers Assessment*	End Sem University Exam	Teachers Assessment*				
MSCHE202	PG	Physical Organic Chemistry	60	20	20	60	40	4	0	4	6

Legends: L - Lecture; T - Tutorial/Teacher Guided Student Activity; P – Practical; C - Credit; Q/A – Quiz/Assignment/Attendance, MST Mid Sem Test.
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Paper- Physical Organic Chemistry

Course Objectives:-
To give basic knowledge of concept of physical chemistry and organic chemistry.
To develop the understanding of organic reaction mechanism with physical aspect.

Course Outcomes:-
After completion of this course the students are expected to be able to demonstrate following knowledge, skills and attitudes. The student will demonstrate capability of the following, CO1. This course on Physical Organic Chemistry will provide the conceptual understanding of chemical bonding, aromaticity, anti- and homo aromaticity, structure and stereochemistry, steric and conformational properties, CO2. The influence of stereoelectronic properties of molecule on its reactivity and became aware of mechanistic aspect of organic chemistry and thermodynamic, kinetic aspect of physical chemistry.

Unit I: Chemical kinetics and its significance
Recapitulation. Complex Reactions : Reactions approaching equilibrium, steady state approximation, Rate laws for consecutive, opposing and parallel reactions, explosive reactions. Techniques to study gas phase reactions. Fast reactions; relaxation, stop flow and flash photolysis. Kinetics of enzyme reactions. Harpoon mechanism (Molecular Beam method). Activated complex theory: Reaction coordinate and the transition state, potential energy surface, concentration of activated complex and rate constant.

Unit II: Surface phenomena and catalysis
Heat of adsorption, Langmuir and BET isotherms, estimation of surface thermodynamics of chemisorption. Adsorption in liquid systems and surface films. General features of homogeneous and heterogeneous catalysis, catalytic activity and strength of

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chemisorption, sticking probability, kinetics of adsorption and desorption, promoters and poisons, catalyst support, methods of preparation of heterogeneous catalysts, catalyst characterization, Important industrial catalysts (three), phase transfer catalysis.

Unit III: Coordination chemistry, structure and reactions

Coordination Chemistry–Reaction Mechanism: Kinetics and mechanism of reactions in solution– labile and inert complexes, Ligand displacement reactions in octahedral and square planar complexes ,acid hydrolysis, base hydrolysis and anation reactions , trans effect , theory and applications. Electron transfer reactions, electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes, isomerization and racemization reactions of complexes.

Unit IV: Structure, conformations of organic molecules and concept of aromaticity

Structure and reactivity of organic molecules with respect to chemical bonding, and correlation of structure with reactivity. Concept of aromaticity, antiaromaticity example and structure of molecules. Different types of reactive intermediates and their importance in different reactions, fundamental concepts of chemical and biochemical catalysis. Conformational analysis, introduction to molecular mechanics and quantum chemical calculations. Symmetry operations, stereochemisry and Stereoelectronic effects. Non-covalent interactions and solvent effects.

Unit V: Huckel theory and LFE

Hückel theory for conjugated hydrocarbons, Different forms of conjugation and aromaticity. Construction of molecular orbitals for important organic molecules and functional groups. Molecular recognition and supramolecular chemistry. Kinetic isotope effects. Linear free energy relationships. Acidity, nucleophilicity, electrophilicity. Reactive intermediates (cationic, anionic, radical, carbene and nitrene) and reaction mechanisms. Apply different techniques for the determination of mechanisms of organic reactions.

Recommended Texts:

1. Chakrabarty, D. K. (Reprint 2007), Adsorption and Catalysis by Solids, New Age International Publishers, New Delhi.
2. Bond, G. C. (1974), Heterogeneous catalysis: Principles and applications Clarendon Press, Oxford .
3. Laidler,K. J., (1987)Chemical Kinetics, Third Edition, Pearson Education, Noida (India).
4. Levine, R.D., Molecular reaction Dynamics, (2009), Cambridge University Press, NY. (Paperback Edition)
5. Raja Ram J. and Kuriacose J.C., (1993).Kinetics and Mechanism of Chemical Transformations, MacMillan Indian Ltd., New Delhi
6. Rakshit,P.C.,(2004) Physical Chemistry, 7th Edition, Sarat Book Distributors, Kolkata.
7. Day, M.C and Selbin,J (1985): Theoretical Inorganic Chemistry, 2nd Edition , Affiliated East West Press Pvt.Ltd.
8. Basolo, F. and Pearson, R.G (1967): Mechanism of Inorganic Reactions, John Wiley, New York.
9. Carey F.A., and Sundberg R.A., (2007): Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edition, Springer, New York.
10. Isaacs N., Physical Organic Chemistry, 2nd Edition, Addison-Wesley-Longman, 1995.
11. March J., and Smith B. M., (2013): Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Edition; John-WileyISBN: 978-0-470-46259-1; April, 2080 pages.
12. Eliel, E. L.; Wilen, S. H. (1994): Stereochemistry of Organic Compounds. Wiley.

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Semester-II (M.Sc.)

SUBJECT CODE	Category	SUBJECT NAME	TEACHING & EVALUATION SCHEME								
			THEORY			PRACTICAL		Th	T	P	CREDITS
			END SEM University Exam	Two Term Exam	Teachers Assessment*	END SEM University Exam	Teachers Assessment*				
MSCHE 203	PG	Medicinal Chemistry	60	20	20	60	40	4	0	4	6

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PAPER – MEDICINAL CHEMISTRY

Unit: 1
Introduction to Medicinal Chemistry, History of Medicinal Chemistry, Classification of drugs, Important Terminology used in Medicinal Chemistry,

Pharmacokinetics: Introduction to drug absorption, disposition, drug metabolism, elimination , important pharmacokinetic parameters in defining drug disposition and in therapeutics, mention of uses of pharmacokinetics in drug development process, concept of pro drug and soft drug.

Pharmacodynamics: Introduction, principles of drug action,mechanisms of drug action, introduction to the concept of receptors and drug receptor interactions, Dose-response relationships, drug potency and efficacy, combined effect of drugs.

Unit: 2
Drug Design & Development, History and development of SAR and QSAR, Physiochemical parameters, Lipophilicity, electronic parameters, steric parameters, Shelton and surface activity parameters and redox potentials, Free Wilson and Hansch analysis, other statistical methods.

Unit: 3
Introduction, classification, synthesis and SAR of old and new drugs I:
Antibiotics: Introduction, classification.

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a) β-lactam antibiotics: penicillin, Classification (early, resistant, broad spectrum, broad spectrum,adverse effects of penicillins.SAR of penicillin, Synthesis: ampicillin, mode of action
b) Cephalosporin: introduction, classification, SAR, mode of action
c) Tetracyclines: introduction, classification, SAR, mode of action
d) Sulphonamide: introduction, classification, SAR, mode of action
e) Quinolones: introduction, classification, SAR, mode of action

Anasthetics, Antidipressants, Oral anticoagulants.(Introduction, classification, SAR.)

Unit: 4

Introduction, classification, synthesis and SAR of old and new drugs II:

Antihistamines and anti ulcer drugs, Diuretics, Antihypertensive, Cholinergic drugs, Narcotic Analgesics, Sedatives, Hypnotics, Anxiolytics, Antianginal, Oral Hypoglycemic (Introduction, classification & SAR).

Unit: 5

Combinatorial Chemistry: Including automation, solid supported and solution phase of synthesis (SPPS & SPOS concept) and related other methodologies, preparation and study of targeted or focused libraries.

Reference Books:

1. Medicinal Chemistry, A. Burger Vols. I to V Ed. M. E. Wolff, John Wiley.
2. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-Hill .
3. S. S. Pandeya & J. R. Dimmock. Introduction to Drug Design,New Age International.
4. D. Lednicer. Strategies for Organic Drug Synthesis and Design,John Wiley .
5. Graham & Patrick. Introduction to Medicinal Chemistry (3rd edn.), OUP
6. Medicinal Chemistry — A molecular and Biochemical Approach,Thomas Nogrady and Donald F. Weaver
7. Principles of Medicinal Chemistry, W. O. Foye
8. Wilson and Gisvolds Text book of Medicinal Chemistry
9. The Organic Chemistry of the Drug Design and Drug Action,Richard B. SilvermanS
10. Analogue based Drug Discovery, János Fischer and C. Robin Ganellin
11. Goodman and Gilmans Text book of Pharmacology.
12. Chemoinformatics - Concepts, Methods, and Tools for Drug Discovery,Jürgen Bajorath
13. A Kar, Textbook of Medicinal Chemistry; Asian Age Publication.
14. Sriram D and Yogeshwari P, Medicinal Chemistry; Pearson Education.
15. Ahluwalia V K, Chopra Madhu, Medicinal Chemistry; Ane Books India.

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Semester-II (M.Sc.)

SUBJECT CODE	Category	SUBJECT NAME	TEACHING & EVALUATION SCHEME								
			THEORY			PRACTICAL		Th	T	P	CREDITS
			END SEM University Exam	Two Term Exam	Teachers Assessment *	END SEM University Exam	Teachers Assessment *				
MSCHE204	PGDC	Leather Chemistry & Technology	60	20	20	60	40	4	0	4	6

Paper - Leather Chemistry & Technology

Legends: L-Lecture; T-Tutorial/Teacher Guided Student Activity; P–Practical; C-Credit; Q/A–Quiz /Assignment/Attendance, MST Mid Sem Test.

Teacher Assessment shall be based following components: Quiz/ Assignment / Project / Participation in Class, given that no component shall exceed more than 10 marks.

Course Objectives:-

To give knowledge of Leather Chemistry .

Course Outcomes:-

After completion of this course the students are expected to be able to demonstrate following knowledge, skills and attitudes. The student will demonstrate capability of

CO1. Theoretical understanding of Leather Chemistry.

SYLLABUS

UNIT I LEATHER CHEMISTRY

Introduction - Constituents of Animal Skin - Preparing skins and hides - leaning and soaking - Liming and degreasing- Manufacture of Leather - Leather Tanning - Vegetable Tanning – Chrome Tanning and Mineral Tanning- Dyeing and Fat liquoring – Leather finishing – oil tanning - byproducts.

UNIT II VEGETABLE TANNING

Classification, identification, physical and chemical properties. Study of vegetable tanning materials, preparation of tanning liquors by leaching and preparation of extracts, types of extracts, sulponation of tan liquors, factors involved in vegetable tanning mechanism of vegetable tanning.

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UNIT III OIL TANNING

Types of oils and fats, their properties, mechanism of oil tanning

UNIT IV CHEMICALS INTANNING

Reactions of formaldehyde with proteins, mechanism of aldehyde tanning, use of glutaraldehyde and dialdehyde in leather manufacture. Alum Tanning – Chemistry of aluminium salts (chlorides, sulphates) hydrolysis, olation, oxolation, basification effect of masking salts, mechanism of Alum tanning. Zirconium Tanning – Zirconium sulphates, chlorides, hydrolysis basification, mechanism of zirconium tanning, use of zirconium salts in tanning

UNIT V COMBINATIONTANNAGES

Application of vegetable oils and syntans in combination in the production of semichrome, Alum, chrome, Alum retan, sulphur -oil-vegetable tannage, chrome zirconium tannage, oil aldehyde tannage – their mechanism, application of iron salts and sodium silicate salts in tanning processes

REFERENCE

1. An Introduction to Principles of Leather Manufacture by SS Dutta, Indian Leather Technologists Association, Kolkota
2. Theory and Practice of Leather Manufacture by KT Sarkar
3. Leather Technicians Handbook by JH Sharp house, Lather Producers Association, Northampton, UK
4. Chemistry and Technology of Leather by O'Flaherty, Roddy and Lollar, Vol.I and II, Robert E. Krieger Publishing Company, USA
5. Vegetable Tanning Materials of India by VS Sundara Rao
6. Practical Leather Technology by TC Thorstensen, Robert E. Krieger Publishing Co., Florida

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SEMESTER II

SUBJECT CODE	Category	SUBJECT NAME	TEACHING &EVALUATION SCHEME								
			THEORY			PRACTICAL		Th	T	P	CREDITS
			END SEM University Exam	Two Term Exam	Teachers Assessment	END SEM University Exam	Teachers Assessment				
MSCHE 205	PGDC	**NANOMATERIALS**	60	20	20	60	40	4	0	4	6

Legends: **L** - Lecture; **T** - Tutorial/Teacher Guided Student Activity; **P**- Practical; **C** - Credit; **Q/A**- Quiz/Assignment/Attendance, **MST** - Mid Semester Test.

Course Objectives:

To give knowledge of Nanomaterials.
To develop the understanding of chemical approaches.

Course Outcomes:

1. Student after successful completion of course must possess skills to think critically and analyze chemicalproblems.
2. They must also feel confident to work in teams as well as independently.
3. Students are also expected to learn solving chemistry problems with an technical purview.
4. Laboratory work is intended for students to learn conducting experiments, and analyze experimental data.

Syllabus

UNIT 1

BASICS OF CARBON NANOTUBES

Carbon materials – Allotropes of carbon – Structure of carbon nanotubes – Types of CNTs – Electronic properties of CNTs – Band structure of Graphene – Band structure of SWNT from graphene – Electron transport properties of SWNTs – Scattering in SWNTs – Carrier mobility in SWNTs.

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UNIT - II
SYNTHESIS AND INTEGRATION OF SWNT DEVICES

Introduction – CVD synthesis – Method – Direct incorporation with device fabrication process – SWNT synthesis on metal electrodes – Lowering the synthesis temperature – Controlling the SWNT growth – Location, Orientation, Chirality – Narrowing diameter distributions – Chirality distribution analysis for different CVD processes – Selective removal of the metallic nanotubes in FET devices – Integration.

UNIT – III
CARBON NANOTUBE FIELD-EFFECT TRANSISTORS

Schottky barrier heights of metal S/D contacts – High k-gate dielectric integration – Quantum capacitance – Chemical doping – Hysteresis and device passivation – Near ideal, Metal-contaced MOSFETs – SWNT MOSFETs – SWNT band-to-band tunneling FETs.
UNIT - IV AC RESPONSE AND DEVICE SIMULATION OF SWNT FETs Assessing the AC response of Top gated SWNT FETs – Power measurement using a spectrum analyzer – Homodyne detection using SWNT FETs – RF characterization using a two tone measurement – AC gain from a SWNT FET common source amplifier – Device simulation of SWNT FETs – SWNT FET simulation using NEGF –Device characteristics at the Ballistic limit – Role of Phonon scattering – High frequency performance limits – Optoelectronic phenomena.

UNIT - V
CARBON NANOTUBE DEVICE MODELING AND CIRCUIT SIMULATION

Schottky barrier SWNT-FET modeling – Compact model for circuit simulation – Model of the intrinsic SWNT channel region – Full SWNT-FET model – Applications of the SWNT-FET compact model – Performance modeling for carbon nanotube interconnects – Circuit models for SWNTs – Circuit models for SWNT bundles – Circuit models for MWNTs – Carbon nanotube interconnects – Applications.

REFERENCES:

1.Ali Javey and Jing Kong, —Carbon Nanotube Electronics‖ Springer Science media, (2009).
2. Michael J. O'Connell, —Carbon nanotubes: Properties and Applications‖, CRC/Taylor & Francis, (2006).
3. Francois Leonard, —The Physics of Carbon Nanotube Devices‖, William Andrew Inc., (2009).
4. R. Saito and M. S. Drbselmus, —Physical properties of Carbon Nanotubes‖ Imperial College Press, (1998).

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