UNIVERSITY OF KERALA

Senate House Campus, Palayam
Thiruvananthapuram 34, Kerala, India

കേരള സർവകലാശാല

സെനറ്റ് ഹൗസ് കാമ്പസ്, പാളയം
തിരുവനന്തപുരം 34, കേരളം, ഇന്ത്യ

https://keralauniversity.ac.in

Department: Chemistry

Programme: MSc Chemistry with Specialization in Renewable Energy

FIRST SEMESTER

1.	Semester	**1**			
2.	Course Title	**Inorganic Chemistry I**			
3.	Course Code	**CHE-CC-511**			
4.	Credits	**3**			
5.	**CO:** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Describe the fundamentals of coordination chemistry and its significance		1-R, 2-Un, 3-Ap	FK	PSO1
	2. Describe the importance of inorganic chemistry in biological systems and process		2-Un, 3-Ap	FK, CK	PSO1, PSO2
	3. Explain the concept of acid strength and reactions in non-aqueous condition		2-Un, 3-AP, 4-An	FK, CK	PSO1, PSO3
	4. Memorize and explain the chemistry of noble gases and halogens		1-R, 2-Un, 3-Ap	FK, CK	PSO1, PSO3

MOD. No.	**COURSE CONTENT**	**CO No.**
I	Introduction to Coordination Chemistry: Types of ligands and complexes. Coordination number and geometry: Classification of complexes based on coordination numbers and possible geometries. Isomerism: Structural, geometrical and optical isomerism. Stability of complex ions in aqueous solution: Formation constants. Stepwise and overall formation constants. Factors affecting stability of complexes. Determination of stability constants. Irving William order of stability, Chelate and macrocyclic effects.	CO1
II	Theories of Structure and Bonding in Metal Complexes: Valence bond theory and its limitations. Ligand field theory: Splitting of d orbitals in different ligand fields such as octahedral, tetragonal, square planar, tetrahedral, trigonal bipyramidal and square pyramidal fields. Jahn Teller effect. LFSE and its calculation. Thermodynamic effects of LFSE. Factors affecting the splitting parameter. Spectrochemical series. Molecular orbital theory based on group theoretical approach and bonding in metal complexes. MO diagrams of complexes with and without π bonds. Effect of π bond on the stability of the complex. Sigma and pi bonding ligands such as CO, NO, CN-, R3P, and Ar3P. Nephelauxetic series.	CO1
III	Bioinorganic Chemistry: Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+. Photosynthesis-chlorophyll a, PS I and PS II. Z-scheme of photosynthesis. Role of manganese complex in oxygen evolution. Coordination compounds in medicine- Anticancer drugs: Platinum complexes- cisplatin. Various types of interaction of metal complexes with nucleic acids.	CO2
IV	Oxygen carriers and oxygen transport proteins-Hemoglobin, myoglobin and hemocyanin, hemerythrin and hemovanadin, Iron-Sulphur proteins.	CO2

	Nature of heme-dioxygen binding. cooperativity in hemoglobin. Iron storage and transport in biological systems-ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes, Carboxypeptidase A and Carbonic anhydrase – structure, function and mechanism of action. Nitrogen Fixation nitrogenase, vitamin B12 and the vitamin B12 coenzymes.	
V	Acid-Base Chemistry and Chemistry in Non-aqueous Solvents: Relative strength of acids, Pauling rules, Lux-Flood concept, Lewis concept, Measurement of acid base strength systematics of Lewis acid-base interactions steric and solvation effects acid – base anomalies , Pearson's HSAB concept, acid- base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness. Chemistry in non-aqueous solvents, reactions in NH3, liquid SO2, solvent character, reactions in SO2, acetic acid, solvent character, reactions in CH3COOH and some other solvents. Molten salts as non-aqueous solvents, solvent properties, room temperature molten salts, unreactivity of molten salts, solutions of metals.	CO3
VI	Chemistry of noble gases and halogens: Early chemistry, Xenon fluorides and oxofluorides; Synthesis, properties, structure and bonding. Xenon compounds with bonds to other elements. Chemistry of Krypton and Radon. Chemistry of halogens: Halogens in positive oxidation states. Interhalogen compounds, pseudohalogens and polyhalide ions including polyiodide anions.	CO4

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1. Coordination Chemistry (3rd Edn.), Banerjea, D., Asian books, 2009.
2. Advanced Inorganic Chemistry (6th Edn.), Cotton, F. A. and Wilkinson, G., Wiley Interscience, New York, 1999.
3. Inorganic Chemistry - Principles of Structure and Reactivity (4thEdn.), Huheey, J. E. Keiter, E. A. and Keiter, R. L., HarperCollins, New York., 1993.
4. Physical Inorganic Chemistry: A Coordination Chemistry approach, Kettle, S. F. A., Oxford University Press, 2000.
5. Principles of Bioinorganic Chemistry, Lippard, S. J. and Berg, J. M., University Science Books, 1994.
6. Inorganic Chemistry (5th Edn.), Atkins, P. W. and Shriver, D. F. ,OUP, 2009.
7. Bioinorganic Chemistry, Bertini, I, Gray, H. B., Lippard, S. J. and Valentine, J. S., University science books, 1994.
8. Inorganic Biochemistry - An Introduction (2nd Edn.), Cowan, J. A., Wiley-VCH, 1997.
9. Ligand Field Theory and its Applications, Figgis, B. N and Hitchman, M. A., Wiley-India, 2010.

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1. Inorganic Chemistry, Holleman, A. F. and Wiberg, E., Academic Press, 2001.
2. Concise Inorganic Chemistry (4th Edn.), Lee, J. D., Wiley-India, 2008.
3. Inorganic Chemistry, Purcell, K.F and Kotz, J. C., Holt-Saunders, 2010.
4. Concepts and Models of Inorganic Chemistry (3rd Edn.),Reddy, B. E. Douglas, D. H. McDanial and .Alexander, J. J, John Wiley, 2001.
5. Bioinorganic Chemistry, Reddy, K. H., New Age international, 2003

Model Question Paper

FIRST SEMESTER M.Sc. DEGREE EXAMINATION Month Year

Branch: CHEMISTRY

CHE-CC-511: INORGANIC CHEMISTRY I

Time: 3 hours **Max. Marks: 60**

SECTION-A

Answer **any 10** questions. **Each** question carries **2** marks

1. What is meant by step-wise formation constant of a complex? In the formation of the complex [ML_4] show that $\beta_4 = K_1.K_2.K_3.K_4$.
2. Give a note on Irving William order of stability.
3. Which ligand makes higher Δ_0 value; H_2O or OH^- ? Justify your answer.
4. Which one exhibits higher nephelauxetic effect; NH_3 or CN^- ? Substantiate your answer.
5. Give a short note on ionophores.
6. Trans-platin has no anticancer activity, though Cis-platin is a promising anticancer drug. Why ?
7. Distinguish between ferrintin and transferrin.
8. Discuss the role of P cluster in Nitrogenase.
9. Indicate the conjugate acids of the following : i) NH_3 ii) $NH2^-$ iii) H_2O iv) HI
10. 'Liquid ammonia is called a levelling solvent.' Justify the statement.
11. Why are the O-F bonds in O_2F_2 longer than OF_2 whereas the O-O bond in O_2F_2 is short compared with that in H_2O_2 ?
12. Draw the structure of XeF_2, XeF_4 and XeF_6.

SECTION-B

Answer **any 6** questions. **Each** question carries **4** marks

13. Draw the structure of Cis and trans – dichloro-bis(ethylene diamine)Cobalt(III) ion. Which isomer is optically active ? Justify your answer.
14. Chelate effect is an entropy effect. Justify the statement.
15. Discuss about the various factors affecting the magnitude of splitting parameter (Δ) in complexes.
16. What is valinomycin ? How can you explain that valinomycin binds K^+ more tightly than Na^+ ?
17. Discuss the structural features and function of Catalase.
18. Give a brief note on Iron-Sulphur proteins.
19. With suitable examples, explain the utility of molten salts as solvent in reactions.

20. Give the structure of IF_5. How does IF_5 reacts with XeF_2 and XeF_4 ? Liquid IF_5 conduct electricity. What is the reason behind it ?

SECTION-C

Answer **any 2** questions. **Each** question carries **8** marks

21. Discuss the merits of MOT over CFT and sketch the MO diagram for $[CoF_6]^{3-}$ and predict its magnetic behavior.

22. i) Describe the classification of complexes based on co-ordination numbers and geometry.

    ii) Compare the structure and function of any two zinc containing enzymes in mammals. (4 + 4)

23. Illustrate the z-scheme of photosynthesis.

24. i) Discuss the effect of substituents on the strength of Lewis acids and bases.

    ii) Give an account of polyhalide ions. (4 + 4)

1.	Semester	**1**			
2.	Course Title	**Organic Chemistry I**			
3.	Course Code	**CHE-CC-512**			
4.	Credits	**3**			
5.	CO On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Recognize and predict the nature and reactivity of organic molecules		1-R, 2-Un	FK, CK	I, III
	2. Assess the stability of various conformers of acyclic and cyclic systems		3-Ap, 4-An	FK, CK	I, II
	3. Identify and differentiate prochirality and chirality at centers, axis, planes and helices and designate the stereocenters and prochiral centers		3-Ap, 4-An	FK, CK	I, III
	4. Appreciate and apply the stereochemical implications on addition, substitution and elimination reactions		2-Un, 3-Ap	FK, CK	II, III
	5. Comprehend the reactivity of carbonyl groups towards base mediated condensation reactions		2-Un, 3-Ap	FK, CK	II, III
	6. Write the mechanisms of organic reactions involving reactive intermediates		5-E, 6-C	CK	III

MODULE No	**COURSE CONTENT**	**CO No.**
I	Structural Organic Chemistry - Aromaticity, Hückel's rule, criteria for aromaticity, annulenes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions, anti- and homo- aromatic systems, Fullerenes, Carbon nanotubes and graphenes, Physical organic chemistry - kinetic and thermodynamic control of reactions, Hammond's postulate, kinetic isotope effects with examples, linear free energy relationships, Hammett and Taft equations, Curtin-Hammett principle, Catalysis by acids and bases with examples like acetal, cyanohydrin, ester formations and hydrolysis reactions, Acidity and Basicity of organic compounds, pKa values, kinetic and thermodynamic acidity. Hard and soft acids and bases - HSAB principle and its applications.	1
II	Stereochemistry of Organic Molecules - Conformational analysis of alkanes and cycloalkanes, Effect of conformation on reactivity of cyclohexane and decalin derivatives. Anomeric effect, Sawhorse and Newmann projections, Geometrical isomers, E-Z nomenclature, Molecular symmetry and chirality, chiral centres – enantiomers and diastereomers, CIP rules. R and S, threo, erythro nomenclatures, non-carbon chiral centres, Axial and Planar chirality, Atropisomerism, Helicity, stereochemical descriptors for chiral axis and planes, Prostereoisomerism, topicity, Stereoselective and stereospecific reactions, regioselective and regiospecific reactions, calculation of enantiomeric excess and specific rotation, Chiral separation methods, Chiral shift reagents, non-carbon chirality.	2, 3
III	Reactions of sp3 Carbons - Stereochemical and mechanistic aspects of SN reactions, Effect of solvent, leaving group and substrate structure, Neighbouring group participation, Non-classical carbocations and ion pairs in SN reactions, Ambident nucleophiles and substrates, SN' and SNi reactions, Isotopic and salt effects, Formation and ring opening of epoxides in cyclohexyl systems (FürstPlattner rule). Elimination reactions leading to C=C bond formation. E1, E2 and E1CB mechanisms, Hoffman and Saytzeff modes of elimination, Effect of leaving group and substrate structure, Pyrolytic eliminations – Chugaev and Cope	3

	eliminations, Cis eliminations. Substitution vs elimination.	
IV	Reactions of sp2 Carbon and Aromatic Systems - Electrophilic addition to C=C - Mechanistic and stereochemical aspects of bromine addition, halolactonization, hydrogenations, hydroborations, epoxidation including Sharpless asymmetric epoxidation, hydroxylations including Woodward-Prevost hydroxylations, oxy-mercuration and de-mercuration and singlet carbene addition. Stereochemistry of addition to C=O systems. Cram, Cram-chelate, Felkin-Anhand Houk models. Zimmerman-Traxler transition states, Desymmetrization and kinetic resolution, Methods of determining absolute configuration, Aromatic electrophilic and nucleophilic substitutions, Electronic and steric effects of substituents. SN1, SNAr, Benzyne and SRN1 mechanism and their evidences.	4
V	Reactions of carbonyl compounds - Aldol and mixed-aldol condensations, Claisen, Reformatsky, Perkin, Stobbe, Darzens, Knoevenagel, Dieckmann, Thorpe, Henry and Mannich reactions, reductions of carbonyl group (Clemmenson and Wolff-Kishner), Addition of cyanide, ammonia, alcohol and Grignard reagents, Structure, synthesis and reactions of α,β – unsaturated carbonyl compounds, Michael addition and Robinson annulation, Prins reaction.	5
VI	Rearrangement Reactions - Structure, stability and formation of carbocations and carbanions, Classical and non-classical carbocations, Rearrangements including Wagner-Meerwein, Pinacol-Pinacolone, Dienone-Phenol, Beckmann and Benzidine, Baeyer-Villiger oxidation, Demjanov ring expansions, Favorskii and Benzilic acid rearrangements, Ramburg-Buckland reaction, Peterson and Julia olefinations, Structure and synthesis of phosphorus, sulphur and nitrogen ylides, Reactions of ylides including Wittig reaction. Structure, stability and formation of carbenes, nitrenes and benzynes. Bamford-Stevens reaction, Simmon-Smith reaction, Shapiro reaction, Wolff rearrangement, Arndt-Eistert homologation, Hofmann, Curtius, Lossen and Schmidt rearrangements. Addition and insertion reactions of carbenes and nitrenes, Nucleophilic aromatic substitutions and cycloadditions of benzynes.	6

References

1. Peter Sykes “A guidebook to mechanism in organic chemistry”, Longman, 6thEdn.
2. Smith, M. B. and March, J. "March’s Advanced Organic Chemistry", 6thEdn, Wiley. 2007.
3. Kalsi, P. S. "Stereochemistry and Reaction Mechanisms", Wiley Eastern, 2005
4. Nasipuri, D. "Stereochemistry of Organic Compounds – Principles and Applications", 3rd Edn, New Age International, 2018
5. ROC Norman and JM Coxon, “Principles of Organic Synthesis”, CRC Press, 3rd En, 1993.

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1. Clayden, J., Greeves, N and Warren, S. “Organic Chemistry”, OUP, 2001
2. Carey, F. A. and Sundberg, R J. “Advanced Organic Chemistry - Part A: Structure and Mechanisms”,5thEdn, Springer, 2007.
3. K. Peter, C. Vollhardt and NE Schore, “Organic Chemistry – Structure and Function”, Freeman, 2003
4. Lowry, T.H. and Richardson, K. S. “Mechanism and Theory in Organic Chemistry” 3rd Edn, Harper Row, 1987.
5. PS Kalsi “Stereochemistry and Mechanism Through Solved Problems” New Age International, 2001
6. Moody, C. J. and Whitham, W. H. "Reactive Intermediates", 1992, OUP.
7. McMurry, “Organic Chemistry”, Thomson Brooks/Cole, 1999.

Model Question Paper

FIRST SEMESTER M.Sc. DEGREE EXAMINATION 2020

Branch: CHEMISTRY

CHE-CC-512 :ORGANIC CHEMISTRY I

Time: 3 hours **Max. Marks: 60**

SECTION-A

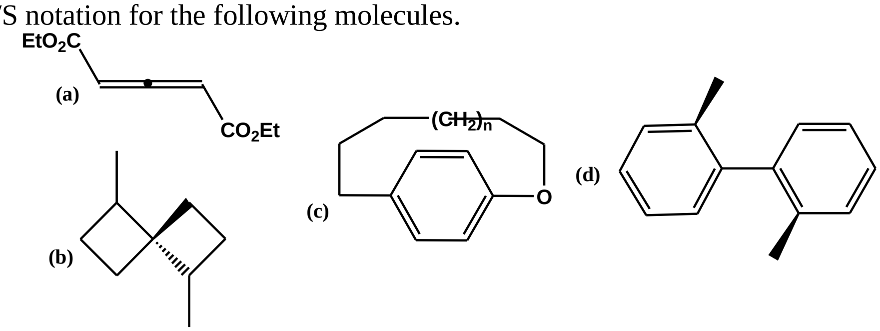
Answer **any 10** questions. **Each** question carries **2** marks

1. Arrange the following in the increasing order of aromaticity and justify: furan, pyridine, thiophene and pyrrole.
2. Depict the structure of the product formed when S-2-butanol is treated with thionyl chloride. Explain the mechanism of the reaction by providing suitable illustration.
3. "Hydroboration oxidation follows anti-Markownikov addition". Justify the statement providing suitable example.
4. Arrange the following in the increasing order of nucleophilicity and justify your answer: 4-nitro phenol, phenol, 3-chloro phenol and 4-methyl phenol
5. Predict the product/products with correct stereochemistry formed when bromine adds to cis-2-butene.
6. Compare the E1 and E1cB mechanisms providing suitable examples.
7. Depict the conformation of *cis*-4-*t*-butyl-1-methyl cyclohexane and *cis*-decalin
8. What is atropisomerism?. Illustrate with an example.
9. Suggest and illustrate a method to convert bromo benzene to biphenyl.
10. Suggest methods to convert cyclobutanone to γ-lactam and γ-lactone.
11. Predict the products when cyclohex-2,3-enone reacts separately with sulphoniumylide and sulphoxoniumylide.
12. Apply Cram's rule to identify the major product formed by the reaction of methyl magnexium bromide with (S)-2-phenyl propionaldehyde.

SECTION-B

Answer **any 6** questions. **Each** question carries **4** marks

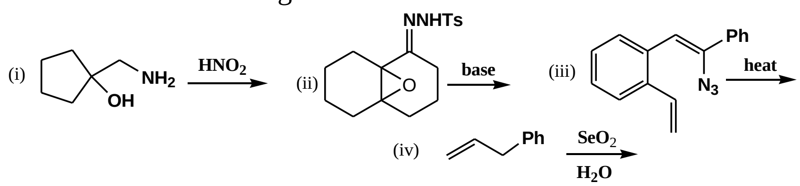
13. Provide R/S notation for the following molecules.



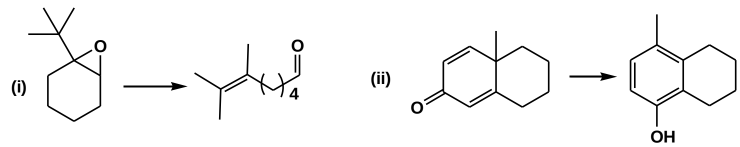
14. 2(R)-Hydroxy, 3(S) bromo butane when treated with a small amount of base yields compound **A**. Identify the structure of compound A and show the correct stereochemistry, reaction scheme and mechanism.
15. In each pair of similar substitution reactions below write the structures of the products of each; indicating which reaction is likely to have the faster rate and why.

i) Phenylmethyl chloride (benzyl chloride) or 2-phenylethyl chloride with silver acetate in methanol ii) Sodium cyanide in acetone with 1-methyl-1-idomethyl-cyclopentane or 2-cycopentylethyl iodide iii) 2-phenyl-2-propanol or 3-phenyl-2,4-dimethyl-3-pentanol on warming in concentrated HBr iv) Sodium salt of methyl malonate and ethyl iodide in methanol or in acetonitrile (CH_3CN)

16. Explain briefly Curtius, Hoffmann, Lossen and Schmidt rearrangements.
17. Predict the products from the following reactions



18. The following reactions take place in acid medium: Illustrate the mechanisms involved.



19. Predict the products when cyclohex-2,3-enone reacts separately with sulphonium ylide, sulphoxonium ylide, SeO_2 and CH_2I_2-Zn.
20. Explain the aromaticity in annulenes with examples.

SECTION-C

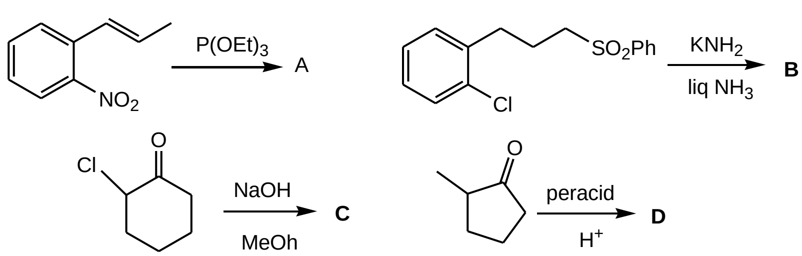
Answer **any 2** questions. **Each** question carries **8** marks

21 i) Distinguish between stereoselective and stereospecific reactions with suitable examples
ii) How can hyperconjugation explain the stability of substituted alkenes? (4 +4)

22. i) In the following reactions, decide whether it is likely to proceed by S_N1 or S_N2 mechanisms. Predict the products including the stereochemistry
    a) S-1-Pheny1-1-bromobutane + NaCN in dimethylformamide
    b) S-1-Pheny1-1-bromobutane + AgOAc in ethanol

    ii) Give 2 mechanisms for nucleophilic aromatic substitutions providing suitable examples. (4+4)

23. Identify **A** – **D** providing the mechanism for each reaction.



24. Depict the schemes with reagents and illustrate the mechanisms of Perkin, Stobbe, Dieckmann and Knoevenagel reactions.

1.	Semester	**1**			
2.	Course Title	**Physical Chemistry I**			
3.	Course Code	**CHE-CC-513**			
4.	Credits	**3**			
5.	**CO**: On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Describe and justify the importance of Quantum Mechanics		1-R; 5-E	FK,CK	I
	2. Understand and apply various postulates in deriving property operators and Schrodinger equation		2-Un;3-Ap	CK,PK	I, II
	3. Derive the Schrodinger equation of particle in a box, HO, RR and H-atom and interpret the results		1-R; 2-Un	FK,CK	I, II, III
	4. Identify the symmetry elements and operators and determine the correct point group		1-R; 5-E	CK,PK	I, II, III
	5. Construct the character table and apply this to characterize the molecular vibrations and hybrid orbitals.		3-Ap; 6-Cr	CK,PK	I, II, III
	6. Understand various adsorption isotherms and its use in surface area measurements		2-Un; 3-Ap	FK,CK	I, II
	7. Understand the concept of colloidal material and their stability for many practical use		2-Un	FK	I, II
	8. Explain various techniques to study the surfaces		2-Un	CK	I, II

MODULE No.	**COURSE CONTENT**	**CO No.**
I	Historic evolution of quantum mechanics: The wave nature of sub-atomic particles. The uncertainty principle and its consequences. The postulates of quantum mechanics. Wave functions, well-behavedness, Orthogonality theorem. Orthonormality. Concept of operators: Laplacian, Hamiltonian, linear and Hermitian operators. Angular momentum operators and their properties. Operator algebra, Commutators, Eigen function and eigen values. Expectation value. Time dependent and independent Schrodinger equation. Separation of variables.	1,2
II	Exactly solvable problems: Solutions of Schrodinger wave equations for: 1. A free particle in 1D. Particle in 1D box of infinite and finite potential wells. Tunnelling. Particle in 3D box. Zero point energy and significance. Applications in conjugated dyes. 2. 1D- Harmonic oscillator. Hermite equation and Hermite polynomials. Recurrence formula. 3D- harmonic oscillator. Oscillator model and Molecular vibrations. Selection rule for vibrational transitions.	3
III	Schrodinger equation in polar coordinates and exactly solvable problems: Solutions of Schrodinger wave equations for 1. Rigid rotator. Particle on a ring. Separation of variables. Real and Imaginary Wave functions. 2. Non-planar rigid rotator. Legendre and Associated Legende equations and polynomials. Rodrigue's formula. Spherical Harmonics. Polar Diagrams. Salient features. Space quantization. Hydrogen atom. Laguerre and Associated Laguerre equations and corresponding polynomials. Space quantization. Zeeman effect, Uhlenbeck and Goudsmith postulate of spin, Stern Gerlach experiment. Orbitals and Spin orbitals. Radial probability	3

	distribution function and graphs. Selection rules for spectral transitions.	
IV	Symmetry and character tables: Symmetry elements and symmetry operations. Point groups. Multiplication of operations. Conditions for a set of elements to form a group. Group multiplication table. Similarity transformation and classification of symmetry operations. Matrix representation of point group. Reducible and irreducible representations. Character of a matrix. Orthogonality theorem. Rules derived from orthogonality theorem (proof not required). Setting up of the character tables of simple groups - C2V, C2h, C3V and C4V on the basis of the rules. Reduction of reducible representations to irreducible representations. Molecular dissymmetry and optical activity. Applications of character tables to spectroscopy. Transition moment operators, vanishing integrals, determination of number of active IR and Raman lines. Application of character table to orbitals. Construction of hybrid orbitals. Construction of Symmetry adapted LCAO	4,5
V	Types of surfaces. Measurements of surface pressure and surface potential. Surfactants and micelles. The gas-solid interface. Types of adsorption. Heat of adsorption. Adsorption isotherms. Gibbs adsorption equation and its verification. Langmuir isotherm. Multilayer adsorption. Freundlich isotherm. BET isotherm. Solid-liquid interface. Influence of surface tension on adsorption. Measurements of surface area of solids.Harkin-Jure method. Entropy and point B methods. Use of Langmuir isotherm and BET method. Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism	6
VI	Colloids- zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium. Emulsions: macro- and micro-emulsions; aging and stabilization of emulsions; Phase behaviour of microemulsions. Surface Enhanced Raman Scattering, Surfaces for SERS studies, Chemical enhancement mechanism, Surface selection rules, Applications of SERS. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.	7,8

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1. Levine, I. N., "Quantum Chemistry", 7thEdition, Pearson Education Inc., 2014.
2. McQuarrie, D. A., "Quantum Chemistry", 2ndEdition,University Science Books, 2008.
3. Szabo, A.; Ostlund, N. S. “Modern Quantum Chemistry: Introduction to Advanced Electronic Structure theory”, Dover Publications, 1996.
4. Cotton, F. A., "Chemical Applications of Group Theory", 3rd Edition, Wiley-Interscience, 1990.
5. AlexanderA. andJohnsonP., “Colloid Science,” Oxford University Press, New York, 1996.
6. Raj, G. Surface Chemistry (Adsorption), 4th Edition, Goel Publishing House, 2002.
7. GreggS. J., “The Surface Chemistry of Solids”, 2nd Edition, Chapman Hall, 1961.
8. Jaffe, H.H.; Orchin, M., "Symmetry in Chemistry", Dover Publications, 2002.

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1. Pillar, F. L. “Elementary Quantum Chemistry”, 2nd Edition, Dover Publication, 2001.
2. Chandra, A. K., "Introduction to Quantum Mechanics", 4th Ed, Tata McGraw-Hill, New Delhi, 2003.
3. Prasad, R. K., “Quantum Chemistry”, 4thEdition, New Age International, 2009.
4. Gopinathan M. S.; Ramakrishnan, V., "Group Theory in Chemistry" 2nd Edition, Vishal Publications, 2013.
5. Somorjai, A., “Introduction to Surface Chemistry and Catalysis”, 2nd Edition, Wiley-Interscience, 2010.

Model Question Paper

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, Month Year
Branch: CHEMISTRY
CHE-C513: PHYSICAL CHEMISTRY-I

Times: 3 Hours Max. Marks: 60

SECTION- A

Answer **any 10** questions. Each question carries **2** marks.

1. Prove that the Hermitian operator always has real eigen values.
2. Normalize the function sin(kx) and e^{ikx} in the interval x = 0 and x = 2π.
3. Calculate the quantum number of a particle of mass of 1g in a 10cm length box having energy kT at room temperature.
4. Explain the term 'degeneracy'. Give a schematic sketch of the first three energy levels obtained in particle in 3D-cubic box indicating their degeneracy.
5. Prove that the nonexistence of zero point energy in planar rigid rotator is not in violation of Heisenberg's uncertainty principle.
6. Set up the Schrodinger equation for hydrogen atom in spherical polar coordinates.
7. What different point groups may the biphenyl molecule belong to depending on the rotational relationship of the two rings about the C-C bonds?
8. Explain with an example a) Symmetry Operation (b) Symmetry element.
9. Discuss the effect of temperature on chemisorption.
10. Find out the number of collisions that would occur on a catalyst surface when it is exposed to Helium gas at 100 micropascals and 200^0C.
11. What are the factors determining emulsion stability?
12. Enumerate two applications of Auger Electron Spectroscopy.

SECTION- B

Answer **any 6** questions. Each question carries **4** marks.

13. Explain the postulates of quantum mechanics.
14. Calculate the expectation value of the x-position of a particle in the state n=2 of a one-dimensional box of length L.
15. a) Write down the radial equation R(r) for H atom. Derive the general solution for R(r) when r is very large (r--> ∞) and very small (r-->0)?
16. For the D3h point group, classify each of the representation into Raman, IR active and both Raman and IR active.

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A1'	1	1	1	1	1	1		x^2+y^2,z^2
A2'	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x,y)	(x^2-y^2,xy)
A1"	1	1	1	-1	-1	-1		

A2”	1	1	-1	-1	-1	1	z
E”	2	-1	0	-2	1	0	(R_x,R_y) (xz,yz)

17. State the great orthogonality theorem. Explain how it is essential in constructing the character table?
18. A monolayer of N_2 is adsorbed on 1g of a catalyst powder at liquid nitrogentemperature. Upon warming N_2 occupied a volume of 3.86 cm^3 at 0^0C and 1 atmpressure. What is the surface area of the catalyst ? The effective area of N_2 molecule is 0.167 nm^2 (Given N = 6.023 E + 23)
19. Calculate adsorption enthalpy when a fixed volume of gas is adsorbed on a particular catalyst for following data ($R=8.31\ JK^{-1}\ mol^{-1}$)

P/torr	30	40
T(K)	200	240

20. How can you determine the type of emulsions? Explain one of the methods.

SECTION C

Answer **any two** questions. **Each** question carries **8** marks

21. a) Set up and solve the Schrodinger equation of motion for a SHO. Deduce the expressions for energy.
b) Find the hybridization of O in H_2O using the C_2v character table.

C_2v	E	C_2z	$\sigma_v(xy)$	$\sigma_v(yz)$		
A1	1	1	1	1	z	x^2,y^2,z^2
A2	1	1	-1	-1	Rz	xy
B1	1	-1	1	-1	x,Ry	xz
B2	1	-1	-1	1	y,Rx	yz

(4+4)

22. a) Write down the Schrodinger equation for H-atom in spherical polar coordinates and separate the variables.
b) What is the probability of finding the electron within radius of a_0 from the nucleus (Given ground state wave function of H-atom is $(1/\pi a_0^3)^{1/2}e^{-r/a_0}$) (4+4)

23. a) Discuss Gibbs adsorption equation.
b) Deduce the BET adsorption isotherm. (4+4)

24. a) Calculate the expectation values of Px and Px^2 for a particle in 1-dimensional box. Rationalize the results.
b) The 1s orbital of H-atom is given by the expression $1s= (1/\pi a_0^3)^{1/2}e^{-r/a_0}$, where a_0 is the Bohr radius. Show that the most probable radius at which the electron will be found in the 1s orbital is a_0. (4+4)

1.	Semester	**1**			
2.	Course Title	**Inorganic Chemistry Lab I**			
3.	Course Code	**CHE-CC-514**			
4.	Credits	**3**			
5.	**CO:** On completion of the course, students should be able to:		TL	KL	PSO No.
	1. Achieve hand on experience in inorganic experiments particularly separation of metal ions and identification from their binary mixture		3-Ap 4-An	CK, PK, MK	PSO5, PSO6
	2. Demonstrate various volumetric analysis independently		4-An 5-E	CK, PK, MK	PSO5, PSO6
	3. Describe the principles behind various volumetric analysis		2-Un	FK, CK	PSO1, PSO3
MOD. No.	**COURSE CONTENT**			**CO No.**	
I	Separation and identification of rare/less familiar metal ions such as Ti, W, Se, Mo, Ce, Th, Zr, V, U and Li in their binary mixtures. (A student must analyse at least 6 samples)			CO1	
II	Quantitative volumetric estimations of various metal ions using EDTA.			CO2, CO3	
III	Volumetric quantitative estimations using ammonium vanadate.			CO2, CO3	
IV	Volumetric quantitative estimations using cerium (IV) sulphate (Cerimetry).			CO2, CO3	
V	Quantitative volumetric estimations using chloramine-T.			CO2, CO3	
VI	Volumetric quatitative estimations using potassium iodate (A student must do a total of at least 8 volumetric estimations).			CO2, CO3	

References:

1. Skoog, D. A. and West, D. M. "Analytical Chemistry: An Introduction", Saunders.
2. Vogel, A. I. "A Text Book of Qualitative Inorganic Analysis", Longman.
3. Vogel, A. I. “A Text Book of Quantitative Inorganic Analysis", Longman.

1.	Semester	**1**			
2.	Course Title	**Organic Chemistry Lab I**			
3.	Course Code	**CHE-CC-515**			
4.	Credits	**3**			

5.	**CO** On completion of the course, students should be able to:	TL	KL	PSO No.
	1. Separate products formed in organic reactions using solvent extraction (if possible)	2-Un, 4-An	FK, PK	I, V
	2. Work-up organic reactions using suitable solvents	3-Ap	PK	I, V
	3. To do synthesis of solid derivatives of the compounds separated	1- R, 3-Ap	FK, PK	III, V
	4. Carry out distillation, sublimation and re-crystallization	3-Ap	PK	I, V
	5. Find out the Rf values of compounds by TLC analysis	4-An	FK, CK, PK	V, VI
	6. Purify compounds by simple column chromatography	3-Ap	FK, PK	I, V

MOD. No	**COURSE CONTENT**	**CO No.**
I	Quantitative wet chemistry separation of a mixture of two components by solvent extraction using ether. Separation of acidic component from basic component. Identification of the separated compounds	1, 2
II	Separation of acidic/basic component from neutral component. Identification of the separated compounds by functional group analysis,	1, 2
III	Preparation of derivatives for acidic, basic and neutral components like esters, anhydrides, amides, picrates, hydrazonesetc	3
IV	Separation by distillation method. Ordinary distillation and vacuum distillation, Separation by sublimation and crystallization methods.	4
V	Separation of binary mixtures of organic compounds using TLC. Identification using RF values, Identification of number of products in a reaction mixture, different methods for TLC visualization	5
VI	Separation of binary mixtures by column chromatography. Packing a column, loading of sample and elution. TLC visualization and removal of the solvent to collect the pure fraction, Demonstration of HPLC technique.	6

References:

1. S. P Bhutani, ArunaChhikara “Practical Organic Chemistry - Qualitative Analysis” ANE Books, New Delhi
2. Ahluwalia, V. K. and Aggarwal, R. “Comprehensive Practical Organic Chemistry” Vol 1 & 2, Universities Press.
3. Bell, C. E. Taber, D. F. and Clark, A. K. “Organic Chemistry Laboratory”, Thomson.
4. Pasto, D. J. Johnson, C. R. and Miller, M. J. “Experiments and Techniques in Organic Chemistry”, Prentice Hall.

1.	Semester	**1**			
2.	Course Title	**Physical Chemistry Lab I**			
3.	Course Code	**CHE-CC-516**			
4.	Credits	**3**			
5.	**CO:** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Understand the concept of solubility and apply it to calculate distribution coefficients and concentration of unknown.		2-Un; 3-Ap	CK,PK	IV; V
	2. Use refractometer to measure the refractive index		3-Ap	CK,PK	V; VI
	3. Measure the kinetic rate of hydrolysis of esters		5-Ev	CK,PK	V;VI
	4. Use calorimeter to determine heats of reactions		3-Ap;5-Ev	CK,PK	V; VI
	5. Use efficiently the polarimeter		3-Ap	CK,PK	V;VI
	6. Understand the basic principles of lab techniques adopted in physical Laboratories, monitor, record and present data in a scientific form		2-Un	FK	V, VII, VIII

MODULE No	**COURSE CONTENT**	**CO No.**
I	Distribution law: Partition of iodine, ammonia and aniline between water and organic solvents. Association of benzoic acid. Equilibrium constants of Tri-iodide and copper-ammonium complexes. Enthalpy change for tri-iodide formation.	1,6
II	Refractometry: Refractive index and molar refraction of liquids. Atomic refractions. Composition of solid solutes. Molecular and ionic radii from molar refraction. Study of the complex K2[HgI4].	2,6
III	Chemical kinetics: Acid hydrolysis of esters. Comparison of strengths of acids. Saponification of esters. Persulphate-iodide second order reaction. Activation energy. Arrhenius parameters. Primary salt effect.	3,6
IV	Thermochemistry: Determination of water equivalent. Heat of neutralization and heat of ionization. Integral and differential heats of solution. Thermometric titrations. Determination of concentrations of strong acids.	4,6
V	Polarimetry: Inversion of cane sugar. Velocity constants for different acid strengths. Comparison of strengths of two acids.	5,6
VI	Adsorption: Verification of Langmuir and Freundlich isotherms for solute adsorption on solids. Estimation of surface area. First order kinetics. Computation of adsorption thermodynamics. Exothermic and endothermic reactions.	6

References:

1. Daniels,F. and Mathews,J. H. "Experimental Physical Chemistry", McGraw Hill, 1970.
2. Finlay, A. and Kitchener,J. A. "Practical Physical Chemistry", Longman, 1977.
3. James,A. M. "Practical Physical Chemistry", Longman, 1981.
4. Shoemaker, D. P. and Garland,C. W. "Experiments in Physical Chemistry", McGraw Hill, 1998.
5. Willard,H. H. Merritt , L. L. and Dean,J. A. "Instrumental Methods of Analysis" 7th Edition, CBS Publishers, 2004..
6. Viswanathan, B.; Raghavan, P. S. “Practical Physical Chemistry,” Viva Books, 2004.

SECOND SEMESTER

1.	Semester	**2**			
2.	Course Title	**Inorganic Chemistry II**			
3.	Course Code	**CHE-CC-521**			
4.	Credits	**3**			
5.	**CO:** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Describe and compare the electronic, spectral and magnetic properties of metal complexes		2-Un, 4-An, 5-E	FK, CK	PSO1, PSO3
	2. Execute their fundamental knowledge in co-ordination chemistry to understand and evaluate properties of various metal complexes		3-Ap, 4-An, 5-E	FK, CK	PSO1, PSO3
	3. Classify and distinguish the stability and reactivity of metal complexes		4-An, 5-E	FK, CK	PSO1, PSO2
	4. Explain and demonstrate the coordination chemistry of lanthanides and actinides		4-An, 5-E	FK CK	PSO1, PSO2
	5. Describe, demonstrate and compare the fundamental concepts of organometallic chemistry		2-Un, 4-An, 5-E	FK CK	PSO1, PSO2
	6. Explain and examine the reactions of various organometallic complexes		3-Ap, 4-An 5-E	FK, CK	PSO1, PSO2 PSO3
	7. Evaluate the applications of organometallic complexes in various domains		4-An, 5-E	FK, CK	PSO2,PSO3
MOD No	**COURSE CONTENT**			**CO No.**	
I	Electronic Spectra of complexes-Term symbols of dn system. Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for dn and d10-n ions in octahedral and tetrahedral fields (qualitative approach), d-d transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling. Orgel diagrams. Tanabe Sugano diagrams. Effects of Jahn Teller distortion and spin orbit coupling on spectra. Charge transfer spectra. luminescence spectra.			CO1, CO2	
II	Magnetic properties of metal complexes: Types of magnetism shown by complexes- paramagnetic and diamagnetic complexes, molar susceptibility, Magnetic susceptibility measurements. Gouy method. Spin only value. Orbital contribution to magnetic moment. Temperature dependence of magnetism- Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Ferromagnetism and antiferromagnetism in complexes. Anomalous magnetic moments. Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.			CO1, CO2	
III	Reactions of Metal Complexes: Kinetics and mechanism of reactions involving complexes in solution. Inert and labile complexes. Kinetics and mechanism of nucleophilic substitution (Ligand displacement) reactions in square planar complexes. trans effect-theory and			CO3	

	applications. Kinetics and mechanism of octahedral substitution, Dissociative and associative mechanisms, Ligand field effects on reaction rate. Influence of acid and base on reaction rate. Racemization and isomerization. Redox reactions in complexes: Electron transfer and electron exchange reactions. Theories of Electron transfer reactions-outer sphere mechanism-Marcus theory, inner sphere mechanism, electron transfer in metalloproteins.	
IV	Coordination Chemistry of Lanthanides and Actinides: General characteristics of lanthanides-Electronic configuration, Term symbols for lanthanide ions, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents. General characteristics of actinides-difference between 4f and 5f orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.	CO4
V	Organometallic Compounds-Synthesis, Structure and Bonding: Compounds with transition metal to carbon bonds, classification of ligands, eighteen electron rule. Organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding. Complexes with cyclic pi donors-metallocenes and cyclic arene complexes structure and bonding. Carbene and carbyne complexes. Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging.	CO5
VI	Reactions of Organometallic Compounds: Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands. Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions. Catalysis by organometallic compounds: Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst. Reactions of carbon monoxide and hydrogen-the water gas shift reaction, the Fischer-Tropsch reaction (synthesis of gasoline). Hydroformylation of olefins using cobalt or rhodium catalyst. Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $Co_2(CO)_8$ catalyst in adipic ester synthesis. Palladium catalysed oxidation of ethylene-the Wacker process.	CO6, CO7

References:

1. Banerjea, D. “Coordination Chemistry”, 3rd Edn., Asian books, 2009.
2. Cotton, F. A. and Wilkinson, G. “Advanced Inorganic Chemistry”, 6th Edn, Wiley
3. Cotton, S. “Lanthanide and Actinide Chemistry”, John Wiley & Sons, 2007.
4. Dutta, R. L and Syamal, A. “Elements of Magnetochemistry”, 2nd Edn., East West press, 1993.
5. Huheey, J. E. Keiter, E. A. and Keiter, R. L. “Inorganic Chemistry - Principles of Structure and Reactivity”, 4th Edn, HarperCollins, New York., 1993.
6. Kettle, S. F. A. "Physical Inorganic Chemistry: A Coordination Chemistry approach", Oxford

University press, 2000.
7. Mehrotra, R. C. and Singh, A. “Organometallic Chemistry: A Unified Approach”, New age international, 2007.
8. Purcell, K. F. Kotz, J. C. ‘Inorganic Chemistry”, Holt-Saunders, 2010.
9. Sathyanarayana, D. N. “Electronic Absorption Spectroscopy and Related Techniques”, Universities press, 2001.
10. Miessler, G. L., Fischer, P. J and Tarr, D. A “ Inorganic Chemistry” 5thedn. Pearson, 2014.

Additional References

1. Bailar, J. C. "Chemistry of Coordination Compounds", Reinhold, 1956.
2. Basolo, F. Pearson, R. G. “Mechanisms of Inorganic Reaction”, John Wiley & Sons, 2006.
3. Crabtree, R. H. “The Organometallic Chemistry of Transition Metals”, 2Edn, Wiley.
4. Guptha, B. D. Elias, A. J “Basic Organometallic Chemistry”, Universities Press, 2010.
5. Holleman, A. F. and Wiberg, E. “Inorganic Chemistry”, Academic.
6. Lever, A. B. P. “Inorganic Electronic Spectroscopy”, 2nd Edn., Elsevier, 1984.
7. Lewi, E. s and Wilkins, R. G. (Eds.), "Modern Coordination Chemistry", Interscience, 1967.
8. Wilkins, R. G. “Kinetics &Mechanism of Reactions of Transition Metal Complexes”, 2Ed, VCH.

Model Question Paper

SECOND SEMESTER M.Sc. DEGREE EXAMINATION Month Year

Branch: CHEMISTRY

CHE-CC-521: INORGANIC CHEMISTRY II

Time: 3 hours **Max. Marks: 60**

SECTION-A

Answer **any 10** questions. **Each** question carries **2** marks

1. $[Ti\ Cl_6]^{3-}$ and $[Ti\ (CN)_6]^{3-}$ gives λ_{max} at 13,000 cm^{-1} and 22,300 cm^{-1} in their respective electronic spectra. Justify the statement.
2. The term symbols for d^3 and d^4 configuration is ^4F. Explain.
3. Predict the geometries and magnetic moments of $[Ni\ Cl_4]^{2-}$ and $[Ni\ (CN)_4]^{2-}$ on the basis of valence bond theory.
4. Calculate the magnetic moment for $[Co\ Cl_4]^{2-}$ taking into account the fact that there is angular momentum contribution to the magnetic moment. ($\Delta = 3100\ cm^{-1}$).
5. Which isomer of $[Pt\ (NH_3)_2\ Cl_2]$ is formed when $[Pt\ (NH_3)_4]^{2+}$ is reacted with 2 moles of HCl? Why?
6. 'The inert complexes are not necessarily thermodynamically stable'. Justify this statement with an example.
7. Lanthanides ions give rise to very sharp bands in their electronic spectra. Why?
8. Yttrium is concentrated along with lanthanides; why?
9. Draw the structures of the following 18 electron compounds and mention the hapticity of organic ligands:

   i) $[Mn\ (CO)_4\ (C_3H_5)]$ ii) $[Fe\ (CO)_2\ Cp\ (CH_3)]$
10. The IR stretching frequency of CO in metal carbonyls is lower than that for free CO molecule. Why?
11. What are oxidative addition and reductive elimination reactions, as applied to organometallic chemistry?
12. Write a catalytic cycle for the synthesis of acetic acid from methanol.

SECTION-B

Answer **any 6** questions. **Each** question carries **4** marks

13. Discuss the spectral consequence of Jahn- Teller distortion in transition metal complexes.
14. The electronic spectrum of $[Co\ (NH_3)_6]^{3+}$ has a weak band in the red – and two medium intensity bands in the visible to near UV region. Assign these transitions using Orgel diagram.

15. What is spin-only magnetic moment? How it is useful in the structural elucidation of transition metal complexes?
16. Illustrate the mechanism of inner-sphere electron transfer reactions using a specific example.
17. What is trans effect? What is its theoretical basis?
18. Discuss the bonding in metal nitrosyls.
19.) Exemplify and briefly discuss the structure and bonding in cyclic arene complexes.
20. Draw and discuss the catalytic cycle for hydroformylation of alkenes using rhodium complex as catalyst.

SECTION-C

Answer **any 2** questions. **Each** question carries **8** marks

21. Write briefly on Tanabe-Sugano diagrams with special reference to their construction and advantages in the interpretation of electronic spectra.
22. i) Discuss briefly about the temperature dependence on magnetism.
    ii) What is meant by aquation reaction? Using suitable examples, explain the mechanism of aquation reactions of octahedral complexes.
    (4 + 4)
23. Compare lanthanide and actinide complexes based on their oxidation state, electronic spectra and magnetic properties.
24. i) Discuss the general methods of preparation of metal carbonyls.

ii) Illustrate the mechanism of oxidation of ethylene using Wacker process.

(4 + 4)

1.	Semester	**2**		
2.	Course Title	**Organic Chemistry II**		
3.	Course Code	**CHE-CC-522**		
4.	Credits	**3**		
5.	**CO** On completion of the course, students should be able to:	TL	KL	PSO No.
	1. Comprehend the reactivity pattern of free-radicals	2-Un, 4-An	FK, CK	I
	2. Understand the orbital interactions and apply orbital symmetry correlations of various pericyclic reactions	2-Un, 3-Ap	FK, CK	I, III
	3. Understand photochemistry of molecules	2-Un, 3-Ap	FK	I, II, III
	4. Write the mechanisms of organic reactions involving free-radicals and concerted reactions	3-Ap, 5-E	CK, MK	III
	5. Apply NMR, IR, MS, UV-Vis spectroscopic techniques to solve structure of organic molecules and in determination of their stereochemistry.	3-Ap	CK, MK	III, VI
	6. Interpret the spectroscopic data of unknown compounds.	3-Ap, 5-E	CK, MK	VI

MODULE No	**COURSE CONTENT**	**CO No.**
I	Radicals in Organic Synthesis - Structure, stability and generation of free radicals, Baldwin's rules of ring closure, Inter and intramolecular additions of radicals to alkenes and alkynes, Radical chain reactions, Introduction to polymers and free-radical polymerizations, Named reactions – Pinacol, acyloin, McMurry, Hoffmann-Lofler-Freytag and Barton reactions, Use of NBS and tributyl tin hydrides, Ullmann coupling.	1, 4
II	Organic Photochemistry - Primary photoprocesses. Jablonski diagram, Photoreactions of C=O systems, enes, eneones, dienes and arenes. Photoisomerisations, Norrish type I and II reactions. Patterno-Buchi and Barton reactions. Di-π-methane and aromatic photo rearrangements. Photochemical remote functionalisation and hydrogen abstraction reactions. Introduction to PET, chemi and bioluminescent reactions. Chemistry of singlet oxygen. Photochemistry in nature. Photosynthesis. Introduction to organic applied photochemistry and femtochemistry, photochromism and thermochromism.	3, 4
III	Concerted Reactions - Symmetry properties of MOs. Principle of conservation of orbital symmetry. Pericyclic reactions - theory, mechanism and stereocourse of electrocyclic reactions, cycloaddition reactions and sigmatropic rearrangements, 1,3-dipolar cycloadditions, ene reactions, chelotropic reactions, Sommelet-Hauser, Cope, Claisen and Mislow-Evans rearrangements, thermal eliminations. Woodward-Hoffmann selection rules, secondary orbital interactions in [4+2] cycloadditons, factors affecting rates of cycloaddition reactions.	2, 4
IV	NMR Spectroscopy - Magnetic nuclei with emphasis on 1H and 13C,	5, 6

	shielding, de-shielding and chemical shifts, factors affecting chemical shifts - Field and anisotropic factors, relaxation processes, chemical and magnetic non-equivalence, 1H and 13C NMR scales, Spin-spin splitting – AX, AX2, AX3, A2X3, AB, ABC and AMX type coupling, Coupling constants.. Pascals triangle, first order and non-first order spectra, Karplus curve, Quadrapule broadening, virtual and long-range coupling, Shift reagents and their role, Decoupling and double resonance, Off-resonance decoupling, NOE. Introduction to 2D NMR. Correlation, NOE and quantum correlation spectroscopy techniques like COSY, HETCOR, HMQC, HMBC, NOESY and EXCY. Application of DEPT technique, Problems on spectral interpretation.	
V	UV-Vis and IR Techniques - UV-VIS spectra of enes, eneones, arenes and conjugated systems. Woodward-Fieser rules, Solvent effect on absorption spectra. Chiroptical properties – introduction to CD and ORD, Cotton effect, octant rule, axial haloketone rule. Characteristic IR bands of functional groups. Factors affecting the IR stretching frequency – vibrational coupling, hydrogen bonding, electronic, inductive and field effects, Identification of functional groups and other structural features by IR.	5
VI	MS in organic structure analysis. EI, CI, SIMS, FAB, ES and MALDI ion production methods. Characteristic EIMS fragmentation modes and MS rearrangements including McLafferty rearrangement, Spectral interpretation, structure identification and solving of structural problems using numerical and spectral data.	5, 6

References

1. ROC Norman and JM Coxon, "Principles of Organic Synthesis", CRC Press, 3rd En, 1993.
2. "Fundamentals of Photochemistry" – KK Rohatgi-Mukherjee, New Age International; 2017
3. Ian Fleming "Pericyclic Reactions", Oxford University Press, 2015
4. Williams, D. H. and Flemming, I. "Spectroscopic Methods in Organic Chemistry", 5th Edition, McGraw Hill. 2011
5. Kemp, W. " Organic Spectroscopy" Palgrave, 1991 (2008 reprint)

Additional References

1. Clayden, J., Greeves, N and Warren, S. "Organic Chemistry", OUP, 2001
2. Coxon, J. M. and Holton, B. "Organic Photochemistry", Paperback, 2015
3. Kagan, J. "Organic Photochemistry, Principles and Applications", Paperback, 1993
4. KC Majumdar and P. Biswas "Textbook of Pericyclic Reactions" MEDTECH, 2015
5. Kalsi, P. S. "Organic Spectroscopy", Wiley Eastern, 2014.
6. Pavia, D. L. Lampman, G.M. and Kriz, G. S. "Introduction to Spectroscopy" 3rd Edition, Brooks/Cole, 2001.
7. JR Dyer "Applications of absorption spectroscopy or organic compounds" PHI learning, 2015
8. Silverstein, R. M. *et sl*. "Spectrometric Identification of Organic Compounds" 8th Edn, Wiley.
9. Wayne, C. E. and Wayne, R. P. "Photochemistry", OU Primer 39, OUP.

Model Question Paper

SECOND SEMESTER M.Sc. DEGREE EXAMINATION 2020

Branch: CHEMISTRY

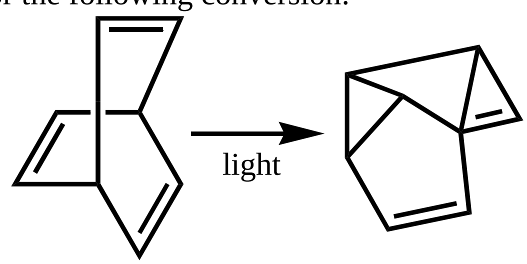
CHE-CC-522: ORGANIC CHEMISTRY II

Time: 3 hours **Max. Marks: 60**

SECTION-A

Answer **any 10** questions. **Each** question carries **2** marks

21. What is the product formed when $CO_2H(CH_2)_8CO_2H$ is treated with sodium in xylene followed by hydration?
22. Illustrate the polymerization mechanism of styrene.
23. Illustrate Di-pi-methane rearrangement.
24. Provide mechanism for the following conversion:

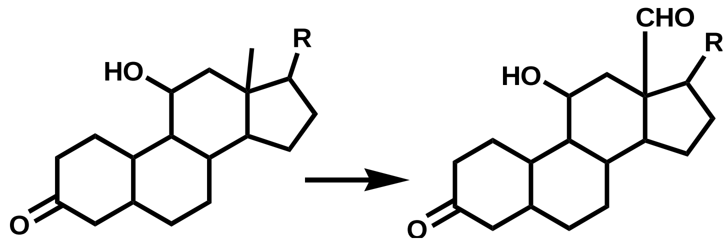


25. Predict the products formed when the following molecules are irradiated (i) (2Z, 4E)-hexadiene and (ii) (2Z, 4Z, 6E)-octatriene.
26. Depict the cycloaddition of tropone with butadiene.
27. Illustrate the product formed when benzyne undergoes cycloaddition to i) anthracene and ii) furan.
28. How many signals are present in the broadband decoupled ^{13}CNMR spectrum of i) catechol (ii) resorcinol and (iii) hydroquinone?
29. A compound shows the following ^{1}HNMR values: δ 9.2 (1H, s), 7.3-7.8 (5H, m), 6.8 (1H, d), 6.6 (1H, d). Identify the compound. What happens to the ^{1}HNMR if the compound is reduced?
30. Identify the structure of $C_8H_{10}O$ whose NMR spectra has 3 singlets at δ 2.1, 3.7 and 7.1 in the intensity ratio 3:2:5.
31. What is the characteristic feature in the MS of an organic compound containing (i) 3 Cl atoms and (ii) 2 Br atoms?
32. Determine the absorbance of a solution of an organic dye (0.0007moldm^{-3}) in a cell with a 2cm pathlength if its absorptivity is 650mol^{-1}dm^{3}cm^{-1}.

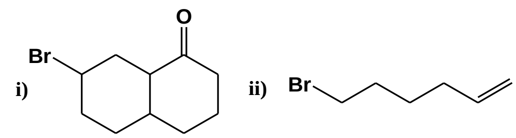
SECTION-B

Answer **any 6** questions. **Each** question carries **4** marks

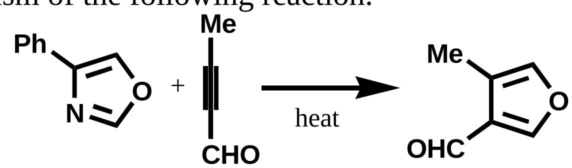
33. How can the following conversion be effected? Give the reagents and mechanism.



34. What are the products formed when the following molecules are treated with Bu_3SnH and AIBN



35. Explain the mechanism of the following reaction.



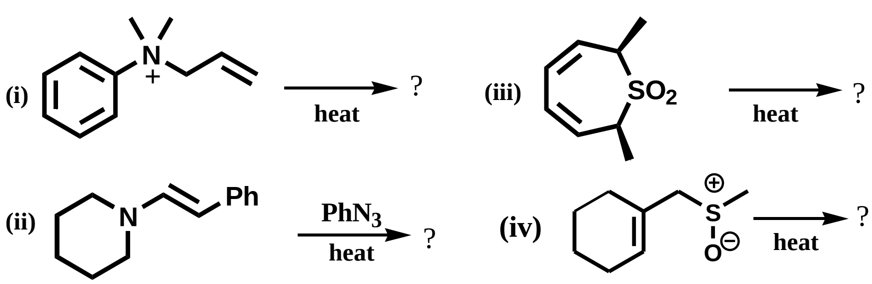
36. Based on the FMO theory predict and explain the product formation when (2E, 4Z, 6E)-octatriene electrocyclizes a) thermally and b) photochemically
37. A compound with molecular formula $C_4H_6O_2$ shows an IR band at 1770 cm^{-1}. The ^{13}CNMR peaks are at 178, 68, 28 and 22 ppm. The compound is either five-membered or a four-membered lactone with a side chain. Deduce the correct structure.
38. Arrange the following in the order of increasing IR stretching frequencies i) cyclobutene-1,2-dione, cyclohex-2-enone, cyclopent – 2-enone and tropone ii) benzophenone, 4-chloro-benzaldehyde, anisaldehyde and benzaldehyde.
39. What is the intensity ratio of the molecular ion cluster in (i) CH_2Br_2 and (ii)CH_2Cl_2?
40. What is the mass of metastable ion produced due to decomposition of fragment ion (m/z: 177) in the sequence: Diethyl phthalate (M^+: 222) to (fragment 1)$^+$ (177) to (fragment 2)$^+$ + CO.

SECTION-C

Answer **any 2** questions. **Each** question carries **8** marks

41. a) Explain the orbital correlation diagram for an electrocyclic reaction.
    b) Predict the major product formed from the following pericyclic reactions

[4+4]



22. a) How can *cis*-2-butene be differentiated from *trans*-2-butene using i) IR spectroscopy and ii) NMR spectroscopy?
    b) Depict and explain the ^{1}H-^{1}H COSY spectrum of *iso*-butyl acetate [4+4]

23. a) Identify the structure of the two isomers A and B of molecular formula $C_8H_7BrO_2$

	IR cm^{-1}	**^{1}H NMR chemical shift**
Isomer A	1698	2.8, s; 3 sets of Ar H's at 7.2-7.4 (2 sets of soublets), 7.44-7.48 (dd), 7.52-7.6 (dd)
Isomer B	1688	2.6, s; Symmetric aromatic H's at 7.6, d and 7.8, d

b) Explain NOE with an example [4+4]

24. a) Explain why [4+2] cycloaddition is thermally allowed whereas [2+2] is forbidden using FMO theory.

b) Illustrate the synthesis of i) oxetanes and ii) cyclobutanes by photochemical reactions.

1.	Semester	**2**			
2.	Course Title	**Physical Chemistry II**			
3.	Course Code	**CHE-CC-523**			
4.	Credits	**3**			
5.	**CO** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Understand and apply approximation methods to solve for many body problems.		2-Un;3-Ap	CK,PK	I,II,III
	2. Derive the various atomic and diatomic molecular term symbols		4-An	CK	I, II, III
	3. Explain and differentiate molecular orbital and valence bond theories		3-Ap; 4-An	CK	I, II, III
	4.Explain HartreeFock Theory and semiempiricalHuckel MO treatment and its application to conjugated molecules		3-Ap	CK,PK	II, III, IV, VI
	5. Understand the principles of the rotational, vibrational, electronic, and magnetic resonance spectroscopic techniques		2-Un	FK,CK	I, II
	6. Apply the principles of spectroscopy and interpret the data to understand the structure of compounds		2-Un, 4-An,5-Ev	CK,PK	II, III, IV, VI

MODULE No	**COURSE CONTENT**	**CO No.**
I	Many electron atoms- Approximations. Independent particle model. Variational method. Theorem and proof. Variational treatment of hydrogen and helium atom. Secular determinant. Perturbation method – 1st and 2nd order perturbation to energy and wave function. Application to particle in 1-D box of increasing potential, Helium atom. self-consistent field method. Pauli's exclusion principle. Symmetry and antisymmetry wave functions. Slater determinants. Vector atom model. Spin orbit coupling. Spectroscopic Term symbols and spectral lines.	1,2
II	Molecular problems. Born-Oppenheimer approximation. Molecular Orbital Theory. MO theory of hydrogen molecule ion. Valence Bond theory (H2). MO theory of H2 and other homonuclear diatomic molecules. Molecular orbital diagrams, Bond order and stability. MO theory of simple heterogeneous diatomic molecules like HF, LiH, CO and NO. Defects in simple MO and VB theories.Semi empirical MO treatment of planar conjugated molecules. HuckelMO theory and calculation of energy and MO of ethylene, butadiene and allylic anion and cyclic systems – cyclobutadiene and benezene. Calculation of charge distribution, bond order and free valency.	2,3
III	Ab initio methods. Hartree equations and Hartree-Fock equations for molecular problems. Roothaan modification. Hartree Fock Roothan equations.Basis sets andBasis functions. Slater type orbital (STO) and Gaussian type orbital (GTO). Contracted and primitive. Basis sets and classification. Minimal, multiple zeta, split-valence, polarized and diffused. Pople style basis sets. Electron correlation and relativistic effects, Configuration interaction. Z-matrtix.	4
IV	Spectra of diatomic molecules: Microwave spectroscopy. Rotation of diatomic molecules. Rotational spectrum. Intensity of spectral lines. Calculation of internuclear distance. Nonrigid rotors and centrifugal distortion. Introduction to instrumentation. Infrared spectroscopy: Rotational spectra of polyatomic	5,6

	molecules. Linear and symmetric top molecules. Vibrational spectra of harmonic and anharmonic diatomic molecules. Fundamental and overtones. Determination of force constants. Vibrational rotational couplings. Different branches of spectrum. Symmetry of vibrational-rotation spectrum. Vibrational spectra of polyatomic molecules. Normal modes. Classification of vibrations. Overtones, combination and Fermi resonance. Group frequencies.Introduction to instrumentation and FT IR.	
V	Raman spectra: Scattering of light. Raman scattering. Polarizability and classical theory of Raman spectrum. Quantum theory of Raman spectrum. Rotational and vibrational Raman spectrum. Introduction to instrumentation. Laser Raman spectrum. Raman spectra of polyatomic molecules. Complementarity of Raman and IR spectra.Electronic spectra: Term symbols of molecules. Electronic spectra of diatomic molecules. Vibrational coarse structure and rotational fine structure of electronic spectrum. Franck-Condon principle. Herzberg-Teller vibronic coupling, KHD equation, Fermi Golden rule. Types of electronic transitions. Fortrat diagram. Predissociation. Morse function. Calculation of heat of dissociation. Introduction to instrumentation.Electronic spectra of polyatomic molecules: Electronic transitions and absorption frequencies. Effect of conjugation.	5,6
VI	Resonance spectroscopy: Nuclear spin and interaction with an applied magnetic field. Nuclear resonance. Population of energy levels. 1H NMR spectrum. Chemical shift. Relaxation, Spin-spin coupling, Fine structure; Fourier transform NMR spectroscopy, Nuclear overhauser effect, NMR spectra of other nuclei. Introduction to instrumentation. Electron spin in molecules and its interaction with magnetic field. ESR spectrum. The g factor and its determination. Fine structure and hyperfine structure. Mossbauer spectroscopy: Doppler effect. Chemical shift. Quadrupole effect.	5,6

References:

1. Levine, I. N., "Quantum Chemistry", 7thEdition, Pearson Education Inc., 2014.
2. McQuarrie, D. A., "Quantum Chemistry", 2ndEdition,University Science Books, 2008.
3. Banwell, C. N.; McCash, E.M., “Fundamentals of Molecular Spectroscopy", 4th Edition, McGraw-Hill, 1999.
4. Barrow, G. M., " Introduction to Molecular Spectroscopy", McGraw Hill, 1962.
5. Daniels, F. and Alberty, R. A., "Physical Chemistry",4th Edition, Wiley Eastern, 1976.

A**dditional** R**eferences:**

1. Atkins, P. W., "Physical Chemistry", 9th Edition, OUP, 2010.
2. Chandra, A. K., "Introduction to Quantum Mechanics", 4th Ed, Tata McGraw-Hill, New Delhi, 2003.
3. Prasad, R. K., “Quantum Chemistry”, 4th Edition, New Age International, 2009.
4. Drago, R. S., "Physical Methods in Inorganic Chemistry", East West, 2012.
5. Moelwyn Hughes, E. A., "Physical Chemistry", 2nd Revised Edition, Pergamon, 1965.

Model Question Paper

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, Month Year
Branch: CHEMISTRY
CHE-CC-523: PHYSICAL CHEMISTRY II

Times: 3 Hours Max. Marks: 60

SECTION- A

Answer **any 10** questions. Each question carries **2** marks.

1. Write down the perturbation term in the Hamiltonian of Helium atom.
2. Write down the Slater determinant of Li atom.
3. What is Born-Oppenheimer approximation? Why is it important?
4. Write down the ground state term symbol for a) O_2 b) CO
5. Write down the Huckel determinant for benzene and cyclobutadiene.
6. Differentiate between *ab initio* and semiempirical MO treatments.
7. The microwave spectrum of CN shows a series of lines separated by 3.8 cm^{-1}.Calculate the internuclear distance between C and N.
8. Homonuclear diatomic molecules are IR inactive, but Raman active. Why?
9. What are polarized Raman lines? How is it important in the structure elucidation?
10. What is the significance of Franck Condon principle?
11. What is 'g factor'? Explain its significance.
12. Which is the commonly used reference standard in ^{1}H NMR? Why is it preferred?

SECTION- B

Answer **any 6** questions. Each question carries **4** marks.

13. State and Prove variational theorem.
14. Explain various steps to solve H_2 by VB method.
15. Define Coulomb and Exchange integrals. Justify their sign and magnitude.
16. The fundamental and first overtone transitions of NO are centered at 1876 cm^{-1} and 3724 cm^{-1} respectively. Calculate the equilibrium vibration frequency and anharmonicity constant.
17. Give a brief note on FTIR.
18. Explain Fortrat diagram.
19. Explain the quantum theory of Raman spectrum.
20. Explain the ESR spectrum of methyl radical.

SECTION- C

Answer any ***two*** question. Each question carries **8** marks

21. a) Set up first order perturbation equation for a non-degenerate system
    b) Solve this to get the expression for first order correction to energy and wave function.
    (3+5)

22. a) Briefly explain the approximations involved in the Hückel MO method.
    b) Calculate the delocalization energy of benzene using HMO method. (3+5)

23. a) Write a note on anisotropic effect in ^{1}H NMR.
    b) Explain in detail the factors that govern the chemical shift values. (4+4)

24. a) Explain the factors that affect the intensity of spectral lines
    b) Distinguish between pure rotational spectrum and vibrational rotational spectrum of molecule. How are these different from electronic spectrum? (3+5)

1.	Semester	**2**			
2.	Course Title	**Inorganic Chemistry Lab II**			
3.	Course Code	**CHE-CC-524**			
4.	Credits	**3**			
5.	**CO:** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Perform colorimetric experiments for the quantitative determination of various metals		3-Ap 4-An	CK, PK	PSO5 PSO6
	2. Perform simple inorganic synthesis and conduct characterization techniques such as IR, UV-Vis absorption and NMR spectroscopy		3-Ap 4-An	PK, MK	PSO4 PSO5 PSO6
	3. Discuss coordination chemistry of Ni complexes		2-Un 4-An	CK	PSO1 PSO2

MOD. No	**COURSE CONTENT**	**CO No.**
I	Colorimetric estimation of Iron after plotting calibration graph.	CO1
II	Quantitative estimation of Chromium by colorimetry.	CO1
III	Quantitative estimation of Manganese by colorimetry.	CO1
IV	Colorimetric estimations of Ti, W and Cu., after plotting calibration graph.	CO1
V	Synthesis and Characterization of Ni(II) Complexes a. The preparation of [Ni(en)3]Cl2 2H2O b. The preparation of [Ni(NH3)6]Cl2 c. The preparation of [Ni(en)2]Cl2 . 2H2O	CO2, CO3
VI	Synthesis and characterization of tetraphenylporphyrin and its Zn(II) complex	CO2

References:

1. Furman and Welcher, "Standard Methods of Inorganic Analysis", Van Nostrand.
2. Kolthoff, I. M. Elving, V. J. and Sandell, “Treatise on Analytical Chemistry”, Interscience.
3. Skoog, D. A. and West, D. M. "Analytical Chemistry: An Introduction", Saunders.
4. Vogel, I. “A Textbook of Quantitative Inorganic Analysis”, Longman.

1.	Semester	**2**			
2.	Course Title	**Organic Chemistry Lab II**			
3.	Course Code	**CHE-CC-525**			
4.	Credits	**3**			
5.	**CO** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Set-up organic reactions - single-step and double-step		3-Ap	PK	I, V
	2. Prepare certain heterocyclic compounds		I-R, 3-Ap	FK, PK	V
	3. Purify the products by filtration or chromatography		3-Ap	PK	V
	4. Record the melting point of compounds		3-Ap	PK	V
	5. Apply spectroscopic techniques to characterize compounds		3-Ap, 4-An	FK, CK	IV, VI
	6. Record IR and UV data of compounds		3-Ap	CK, PK	IV

MODULE No	**COURSE CONTENT**	**CO No.**
I	Preparation of organic compounds by single step reactions – benzoylation, esterification, nitration, sulphonation, halogenation and hydrolysis	1, 2
II	Preparation of compounds by double-stage synthesis – nitration followed by hydrolysis, bromination followed by hydrolysis etc	1
III	Reactions of carbonyl compounds – aldol condensation – preparation of chalcones and oximes	1, 2
IV	Preparation of heterocyclic compounds - benzimidazoles, thiazoles and N-alkylated isatins.	2
V	Spectral interpretation of organic compounds [simple as well as those prepared in lab as above} using UV-VIS and IR, NMR analysis of compounds	5
VI	Recording the UV-Vis and IR spectra of synthesized compounds	6

References:

1. Ahluwalia, V. K. and Aggarwal, R. " Comprehensive Practical Organic Chemistry", Vol 1 & 2, Universities Press.
2. Furniss, B. S and others, "Vogel's Textbook of Practical Organic Chemistry", ELBS.
3. Silverstein, R. M. et al., "Spectrometric Identification of Organic Compounds", 8th Edn, Wiley.

1.	Semester	**2**
2.	Course Title	**Physical Chemistry Lab II**
3.	Course Code	**CHE-CC-526**
4.	Credits	**3**

6.	**CO** On completion of the course, students should be able to:	**TL**	**KL**	**PSO No.**
	1. Use the viscometer to measure the viscosity of solutions	2-Un; 3-Ap	CK,PK	IV; V
	2. Measure surface tension of liquids	3-Ap	CK	IV; V
	3. Measure the freezing points of mixtures and apply it to study depression constant, association and dissociation and eutectic diagrams	3-Ap; 5-Ev	CK,PK	V;VI
	4. Determine the miscibility temperatures to construct the phase diagram	3-Ap;5-Ev	CK,PK	V; VI
	5. Determine the transition temperature.	3-Ap	CK	V;VI
	6. Understand the principles of lab techniques adopted in physical Laboratories,monitor, record and present data in a scientific form	2-Un	FK	V, VII, VIII

MODULE No	**COURSE CONTENT**	**CO No.**
I	Viscosity: Viscosities of liquids and mixtures of liquids. Verification of Kendall's equation and Jones-Dole equation. Viscosity of polymer solutions. Variation of viscosity with temperature.	1,6
II	Surface tension: Surface tension and parachor of liquids by differential capillary and stalagmometer methods. Variation of surface tension with concentration. Determination of atomic parachor.	2,6
III	Cryoscopy: Determination of molar freezing points. Depression constant and molecular mass using solid and liquid solvents. Study of dissociation and association of solutes. Atomicity of substances like sulphur.	3,6
IV	Phase equilibria I: CST of phenol-water system. Determination of unknown concentrations of NaCl, acetic and oxalic acid. Construction of phase diagrams of unknown mixtures.	4,6
V	Phase equilibria II: Construction of Two component eutectic diagrams, determination of unknown concentration of given mixture. Three component systems with one pair of partially miscible liquids. Construction of phase diagrams and tielines.Composition of homogeneous mixtures.	3,6
VI	Transition temperature: Transition temperature of sodium acetate. Kf of sodium acetate. Molecular mass of urea. Transition temperature of sodium thiosulphate.	5,6

References:

1. Daniels,F. and Mathews,J. H. "Experimental Physical Chemistry", McGraw Hill, 1970.
2. Finlay, A. and Kitchener,J. A. "Practical Physical Chemistry", Longman, 1977.
3. James,A. M. "Practical Physical Chemistry", Longman, 1981.
4. Shoemaker, D. P. and Garland,C. W. "Experiments in Physical Chemistry", McGraw Hill, 1998.
5. Willard,H. H. Merritt , L. L. and Dean,J. A. "Instrumental Methods of Analysis" 7th Edition, CBS Publishers, 2004..
6. Viswanathan, B.; Raghavan, P. S. "Practical Physical Chemistry," Viva Books, 2004.
7. YadavJ. B., "Advanced Practical Chemistry", Krishna Prakashan Media, 2015.

Model Question Paper

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, Month Year
Branch: CHEMISTRY
CHE-DE-527: ADVANCED PHYSICAL CHEMISTRY

Times: 3 Hours Max. Marks: 60

SECTION- A

Answer **any 10** questions. Each question carries **2** marks.

1. Write an example for Grubb's second generation catalyst.
2. How does the reaction of MeCOOMe with CO under conditions of the Monsanto ethanoic acid process can lead to ethanoic anhydride.
3. What do you understand by electrochemical series? How is it useful in determination of corrosion of metals?
4. What is sacrificial anode? Mention its role in control.
5. What is a vehicle or drying oil? Mention their functions.
6. What is phosphate coatings and why it is employed?
7. What is meant by electrochemical cell? Explain the functioning of Daniel cell?
8. What is dry cell? Explain.
9. What is singlet oxygen? Write one method for its generation.
10. Discuss the working of a solar cell?
11. What is the difference between 6-31G* and 6-31+G?
12. What are contracted and primitive basis functions?

SECTION- B

Answer **any 6**questions. Each question carries **4** marks.

13. Explain the mechanism of olefin metathesis reaction.
14. Explain the corrosion of iron by dilute mineral acids.
15. Explain in detail electroless nickel plating.
16. What are fuel cells? Explain the hydrogen-oxygen fuel cell and its advantages.
17. What is photoinduced electron transfer process. Explain Marcus theory to interpret the process in solution.
18. Explain the applications of semiconductor photocatalysis.
19. Distinguish between semi empirical and ab initio methods in computational chemistry.
20. Differentiate between STO and GTO.

SECTION- C

Answer any ***two*** question. Each question carries **8** marks

21. a) Explain the principle and application of femtosecond pump-probe spectroscopy.
    b) What are the catalysts employed in olefin metathesis? Discuss. (4+4)

22. a) Explain the term corrosion? Describe the different theories to explain. How can you prevent a metal from corrosion?

b) What are paints? What are their constituents and uses? (4+4)

23. a) Illustrate photosensitized decomposition of water.
    b) Discuss the photodynamic therapy for cancer treatment. (4+4)

24. a) Write the z-matrix of ammonia and staggered ethane
    b) What are the basic approximations in HF theory? Explain, how the energy in HF limit differ from exact energy? (3+5)

THIRD SEMESTER

1.	Semester	**3**
2.	Course Title	**Inorganic Chemistry III**
3.	Course Code	**CHE-CC-531**
4.	Credits	**3**

5.	**CO:** On completion of the course, students should be able to:	**TL**	**KL**	**PSO No.**
	1. Describe the fundamentals of solid state chemistry and X-ray diffraction	2-Un, 4-An	FK	PSO1, PSO3
	2. Explain and compare solid properties based various binding forces and imperfections in solids	2-Un, 4-An	FK, CK	PSO1, PSO3
	3. Describe and apply the basics of electrical and magnetic properties of solids	2-Un, 3-Ap, 4-An	FK, CK	PSO1, PSO3
	4. Examine and correlate the solid state properties with real life materials	2-Un, 3-AP	FK, CK	PSO1, PSO2
	5. Get an insight about the chemistry of open and closed structure compounds of important non-metallic elements	2-Un, 4-An	FK	PSO1, PSO3
	6. Describe and examine the structure and properties of various metallic clusters	2-Un, 4-An	FK, CK	PSO1, PSO3

MOD No	**COURSE CONTENT**	**CO No.**
I	Introduction to Solid State: Crystal systems and lattice types. Bravais lattices. Crystal symmetry. Point groups and space groups. Miller indices. Reciprocal lattice concept. Close packed structures: BCC, FCC and HCP. Voids. Coordination number. X Ray diffraction by crystals: Functions of crystals. Transmission and reflection grating. Braggs equation. Diffraction methods. Powder, rotating crystal, oscillation and Weisenberg methods. Indexing and determination of lattice type and unit cell dimensions of cubic crystals. Structure factor. Crystal defects: Point, line and plane defects.	CO1
II	Solid State Theories and Properties: Binding forces in solids: Ionic bonding and potential energy field. Lattice energy. Born theory and Born Haber cycle. Molecular, ionic, covalent, metallic and hydrogen bonded crystals. Free electron theory and band theory of solids. Conductors, insulators and semiconductors. Mobility of charge carriers. Hall effect. Electrons and holes. Imperfections and nonstoichiometry (oxides and sulphides). Techniques of introducing imperfections in solids.Electrical properties of solids: Conductivity of pure metals. Superconductivity. Photoconductivity. Photovoltaic effect. Dielectric properties. Piezoelectricity and ferroelectricity. Magnetic properties of solids: Diamagnetism, paramagnetism, ferromagnetism, ferrimagnetism and antiferromagnetism. Lasers and their applications.	CO2,CO3,CO4
III	Inorganic nanomaterials and applications: Popular and scientific perspective of nanotechnology; Fabrication of nanomaterials-top-down and bottom-up methods; Different types of nanostructures- 0D, 1D and 2D materials- nanoparticles, nanorods, nanocombs, nanotubes,	CO5

	nanowires and quantum dots, semiconductor nanoparticles; Carbon based nanomaterials and applications-Fullerene, graphene, carbon nanotubes and diamondoidnanomaterials; Nonocomposites- natural, organic polymer, metal and ceramic nanocomposite; Nanomaterials in various applications-Magnetic nanoparticle for information storage applications, Light-emitting devices based on direct band gap semiconductor nanoparticles. Nanomaterials for energy applications-fuel cell, photovoltaic and rechargeable batteries. Nanometerials in biomedical applications.	
IV	Structures of Sulphur, Nitrogen, Phosphorus and Silicone Compounds: Sulphur Nitrogen compounds: Tetrasulphurtetranitride, disulphurdinitride and polythiazyl. SxNy compounds. S-N cations and anions. Other S-N compounds. Sulphur phosphorus compounds: Molecular sulphides such as P4S3, P4S7, P4S9 and P4S10. Phosphorus-nitrogen compounds: Phosphazines. Cyclo and linear phosphazines. Other P-N compounds. Silanes, silicon halides, silicates; Classification and structure, silicones.	CO6
V	Structure of Boron Compounds: Boron hydrides: Reactions of diborane, and its structure and bonding. Polyhedral boranes: Preparation, properties, structure and bonding. The topological approach to boron hydride structure. Styx numbers. Wade's rules. Carboranes: Closo, nido and arachnocarboranes. Metalloboranes and metallocarboranes. Organoboron compounds and hydroboration. Boron-nitrogen compounds: Borazine, substituted borazines and boron nitride.	CO6
VI	Other Metal clusters: Factors favouring metal-metal bonds, Dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in (Re2X8)2-trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons. Polyatomic zintl anion and cations. Infinite metal chains. Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W.	CO7

References:

1. Adams, D, M. Inorganic Solids: An Introduction to Concepts in Solid State Structural
2. Azaroff, L. V. "Introduction to Solids", McGraw Hill.
3. Chakrabarty, D. K. "Solid State Chemistry," New Age Pub., 2010.
4. Cotton, F. A. and Wilkinson, G. "Advanced Inorganic Chemistry", 6th Edn, Wiley.
5. Galway, A. K"Chemistry of Solids", Chapman Hall.
6. Huheey, J. E. Keiter, E. A. and Keiter, R. L. "Inorganic Chemistry - Principles of Interscience, New York, 1999.
7. Phillips, F. C. "An Introduction to Crystallography", Longman.
8. West, A. R. "Solid State Chemistry and its Applications", Wiley.
9. Atkins, P. W. and Shriver, D. F. "Inorganic Chemistry", 5th Edn, OUP, 2009.
10. Douglas, B. E. McDanial, D. H. and Alexander, J. J. "Concepts and Models of Inorganic Chemistry", 3rd Edn, John Wiley, 2001.
11. L. H. Gabor, H. F. Tibbals, J. Dutta, J. J.Moore, Intoduction to nanoscience and nanotechnology, CRC press, 2009.
12. M. S. RamachandraRao and S. Singh, Nanoscience and nanotechnology: Fundamentals to frontiers, Wiley, 2014.

Additional References

1. Emeleus, H. J. Sharpe, A. G. “Modern Aspects of Inorganic Chemistry”, 4th Edn., ELBS, 1973.
2. Holleman, A. F. and Wiberg, E. “Inorganic Chemistry”, Academic press, 2001.
3. Kittel, C. “Introduction to Solid State Physics”, Wiley.
4. Lee, J. D. “Concise Inorganic Chemistry,” 4th Edn., Wiley-India, 2008.
5. Purcell, K.FandKotz, J. C. “Inorganic Chemistry,” Holt-Saunders, 2010.

Model Question Paper

THIRD SEMESTER M.Sc. DEGREE EXAMINATION Month Year

Branch: CHEMISTRY

CHE-CC-531: INORGANIC CHEMISTRY III

Time: 3 hours **Max. Marks: 60**

SECTION-A

Answer **any 10** questions. **Each** question carries **2** marks

1. Explain the basis for classification of lattices into 7 crystal systems and 14 Bravais lattices.
2. Calculate the number of atom in a unit cell of BCC and FCC crystal structure.
3. Discuss the defect structure in non-stoichiometric sulphides.
4. What are the similarities and differences between ferrimagnetism and antiferromagnetism ?
5. What is meant by a 2D nanomaterial ? Give example.
6. Explain with example ‘quantum confinement’.
7. Discuss the structure of S_4N_4.
8. Describe the structure of P_4S_9 and P_4S_{10}.
9. Find styx numbers forB_6H_{10}.
10. Even though borazine is isoelectronic with benzene, borazine is far more reactive than benzene. Why ?
11. Predict the number of metal-metal bonds in $Co_2(CO)_8$.
12. Establish the isolobal analogy between CH_3 and $Mn(CO)_5$.

SECTION-B

Answer **any 6** questions. **Each** question carries **4** marks

13. Differentiate between FCC and HCP close packed structures.
14. What are intrinsic and extrinsic semiconductors ?
15. What is superconductivity and critical transition temperature ?
16. Explain with example ‘bottom-up’ approach of nanomaerial synthesis.
17. Discuss the bonding and aromaticity in cyclic phosphazenes.
18. Differentiate closo and nido carboranes with examples.
19. Compare the stability of o- and p- Dicarbadodecarborane.
20. Discuss the different types of bonding modes of carbonyl ligands in LNCCs.

SECTION-C

Answer **any 2** questions. **Each** question carries **8** marks

21. Differentiate between conductors, insulators and semiconductors based on band theory of solids.
22. i) Derive Bragg's equation.
    ii) Discuss about the classification of silicates based on their structures.
    (4 + 4)
23. Discuss the energy and biomedical applications of nanomaterials.
24. i) Write a note on the application of Wade's rules in predicting the structures of boranes.
    ii) Discuss the bonding in $[Re_2Cl_8]^{2-}$.
    (4 + 4)

<table>
<tr><td>1.</td><td>Semester</td><td colspan="4">3</td></tr>
<tr><td>2.</td><td>Course Title</td><td colspan="4">Organic Chemistry III</td></tr>
<tr><td>3.</td><td>Course Code</td><td colspan="4">CHE-CC-532</td></tr>
<tr><td>4.</td><td>Credits</td><td colspan="4">3</td></tr>
<tr><td rowspan="7">5.</td><td colspan="2">CO
On completion of the course, students should be able to:</td><td>TL</td><td>KL</td><td>PSO No.</td></tr>
<tr><td colspan="2">1. Use various reagents and organic reactions in a logical manner for synthesis of heterocycles and carbocycles</td><td>1-R,
3-Ap</td><td>FK, CK</td><td>I, II</td></tr>
<tr><td colspan="2">2. Use retrosynthetic method for the logical dissection of complex organic molecules and devise synthetic methods</td><td>4-An,
5-E,
6-C</td><td>FK, CK,
MK</td><td>I, III</td></tr>
<tr><td colspan="2">3. Choose appropriate oxidation/reduction reagent as needed for the substrate</td><td>3-Ap,
4-An</td><td>FK, CK</td><td>II, III, VI</td></tr>
<tr><td colspan="2">4. Identify the class of natural product and predict the biosynthetic pathway</td><td>1-R,
4-An,
6-C</td><td>FK</td><td>II, III</td></tr>
<tr><td colspan="2">5. Elucidate the structure of some natural products by retrosynthesis and chemical degradation</td><td>3-Ap,
4-An</td><td>FK, CK</td><td>I, VI</td></tr>
<tr><td colspan="2">6. Comprehend the chemistry of amino acids, nucleic acids, proteins and peptides</td><td>1-R,
2-Un</td><td>FK, CK</td><td>I, II</td></tr>
</table>

<table>
<tr><td>MODULE No</td><td>COURSE CONTENT</td><td>CO No.</td></tr>
<tr><td>I</td><td>Construction of Carbocyclic and Heterocyclic Rings - Importance of heterocyclic compounds, Structure and aromaticity of heterocycles, Trivial and Systematic Hantzsch Widman Nomenclature of heterocyclic compounds, Different methods of ring synthesis, Three and four membered heterocycles, Named reactions for synthesis of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline including Paal-Knorr, Feist-Benary, Fischer indole, Hantzsch, Skraup, Pictet-Spengler and Bischler-Napieralski methods, Electrophilic and nucleophilic substitutions of 5-membered, 6-membered, indole, quinoline and isoquinoline rings, Heterocycles with more than one heteroatom – synthesis and reactivity. Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Olefin metathesis.</td><td>1</td></tr>
<tr><td>II</td><td>Organic Synthetic Strategies - Introduction to retrosynthetic analysis. Linear and convergent synthesis, Synthons, functional group interconversions (FGI), Role of protecting groups in organic synthesis, Enolate and enamine alkylation reactions including Stork-enamine reaction, Dipole inversion - Umpolung. Organometallic reagents like Grignard, alkyl lithium and Gilman Reagents and their utility, Organocuprates, DABCO and Baylis-Hilman reaction, Role of palladium in organic synthesis, Heck, Sonogashira, Suzuki, Stille and Negishi coupling reactions. Glaser coupling, Tebbe olefination, Sakurai reaction, Brook rearrangement, Mitsunobu reaction, PPh_3-CBr_4 reagent.</td><td>1, 2</td></tr>
</table>

III	Reagents for oxidation - Oxidations using manganese and chromium reagents, PCC, PDC Collins and Jones reagents, Etard reaction, Use of SeO_2, MnO_2, Ag_2CO_3 and lead tetraacetate, DMSO based reagents - Swern oxidation, Oppenauer oxidation. Oxidation of alkenes - OsO_4, RuO_4, HIO_4, ozone and peracids. Sharpless asymmetric epoxidation, Woodward and Prevost hydroxylations, Dehydrogenation to aromatic compounds. Baeyer-Villiger oxidation, Dakin reaction.	3
IV	Reagents for reduction - Catalytic hydrogenation and stereochemistry. Hydrogenation catalysts and their selectivity. Adam's catalyst, Rosenmund reduction, Lindlar catalyst, Wilkinson's catalyst, Homogeneous hydrogenations. Fe, Zn, Na and Li reductions. Dissolving metal reductions – Clemmenson reduction, metal-alcohol reductions, Birch reduction, Hydride transfer reductions – MPV reduction, Reduction using $NaBH_4$, LAH, LAH-$AlCl_3$, DIBAL-H and $NaCNBH_3$, selectrides. Reductions using borane reagents, hydroboration, Luche reduction, Wolff Kishner and diimide reductions..	3
V	Natural Products Chemistry - Classification, Isolation, identification, typical examples and structures of secondary metabolites - Alkaloids, Terpenoids, Steroids, Prostaglandins, Coumarins and flavones. Degradation methods for structural elucidation – Hoffmann and Emde methods, examples of alkaloids, Total synthesis of reserpine, Classification of terpenes, Cationic rearrangements and formation of cyclic terpenes, Structural elucidation of santonin, Structure and importance of quercetin; β-carotene and ascorbic acid. Synthesis of Vitamin C from glucose, Biosynthesis of fatty acids and polyketides by acetate pathway, monoterpenes by mevalonic acid pathway and alkaloids by shikimic acid pathway, biosynthesis of higher terpenes and steroids. Structure of cholesterol and other important steroids, Barbier Wielander degradation and Blanc rule	4, 5
VI	Chemistry of nucleic acids and proteins - Amino acids, proteins and peptides: Structures and synthesis of amino acids – Strecker synthesis, Azlactone synthesis and enantioselective synthesis. Reactions of amino acids due to the NH_2 group, COOH group and its reaction with ninhydrin, Structure of proteins, Introduction to enzyme and co-enzymes, structure and relevance of NAD, chymotrypsin, pyridoxal and thiamine, Peptide bond formation methods, amino and carboxy protection in SPPS. ADP and ATP. Automated polypeptide and oligonucleotide synthesis. Structure of polysaccharides including starch, cellulose, glycogen and chitin.	6

References:

1. Thomas L. Gilchrist "Heterocyclic Chemistry" Pearson, 2013
2. P. S. Kalsi "Organic Synthesis through Disconnection Approach" MEDTEC, 2014
3. Carruthers, W. "Some Modern Methods of Organic Synthesis", Cambridge University Press, 2004.
4. Hanson, J. R. "Natural Products: Secondary Metabolites", RSC
5. Mann, J and others, "Natural Products: Chemistry and Biological Significance". Longman 2006

Additional References:

1. Harbourne, J. B. “Phytochemical Methods” Chapman Hall. 1998
2. Warren, S. “Organic Synthesis: The Disconnection Approach”, John Wiley, 2004.
3. Hanson, J. R “Organic Synthetic Methods” RSC , 2002.
4. Norman, R. O. C. and Coxon, A. "Modern Synthetic Reactions", Chapman Hall, 1993
5. Mackie, R. K., Smith, D. M. and Aitken, R. A. “Guidebook to Organic Synthesis”, 3 Edn, Longman.1990
6. Krishnaswamy, N. K. “The Chemistry of Natural Products,” Universities Press 2010
7. Mann, J. “Chemical Aspects of Biosynthesis”, Oxford primer 20, OUP.1994
8. Simmonds, R. J. "Chemistry of Biomolecules", RSC. 1992
9. Smith, M. B. "Organic Synthesis", 2 Edn, McGraw Hill. 1994.

Model Question Paper

THIRD SEMESTER M.Sc. DEGREE EXAMINATION 2020

Branch: CHEMISTRY

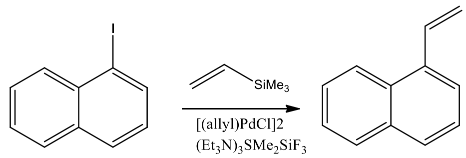
CHE-CC-532 : ORGANIC CHEMISTRY III

Time: 3 hours **Max. Marks: 60**

SECTION-A

Answer **any 10** questions.**Each** question carries **2** marks

1. Illustrate mechanism for the conversion of pyrrole to 3-chloro pyridine.
2. Illustrate the product formed when 2-ethoxy-1,4-pentadiene-3-one is treated with aluminium chloride at room temperature in acetonitrile.
3. Explain the mechanism of the reaction

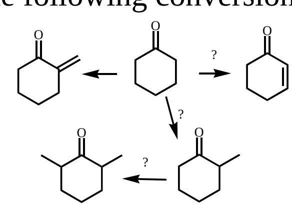


4. Illustrate the retrosynthetic analysis for paracetamol.
5. How do you convert 2-butyne to (i) *cis*-2-butene and (ii) *trans*-2-butene
6. What product is formed when trans-2-butene is treated with iodine and silver acetate under anhydrous conditions?
7. An aldehyde can be coupled with ethyl acrylate in presence of DMAP. Illustrate the reaction with mechanism.
8. What reagents are used for conversion of i) ethyl cinnamate to cinnamyl alcohol and ii) ethyl benzoate to benzaldehyde?
9. Suggest and illustrate a method to convert bromo benzene to biphenyl.
10. How are fatty acids biosynthesized in living cells?
11. Illustrate formation of shikimic acid in cells.
12. Depict the Strecker synthesis of aminoacids.

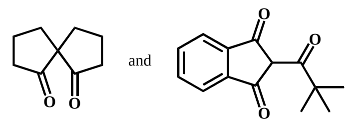
SECTION-B

Answer **any 6** questions. **Each** question carries **4** marks

13. What reagents are required to convert cyclohexanone to i) cyclohexane-1,2-dione ii) cyclohexane iii) cyclohexanol iv) cyclohexyl amine?
14. Illustrate a method each for the synthesis of indole and isoquinoline
15. What reagents are required for the following conversions?



16. Give a retrosynthetic analysis and suggest a synthetic strategy for the following molecules

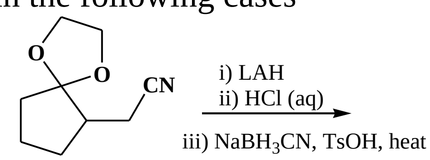


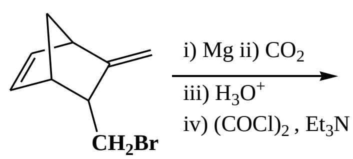
17. Illustrate biosynthesis of monoterpene.
18. Explain the secondary and tertiary structure of proteins.
19. Explain Barbier Wielander degradation and Blanc rule
20. Predict the product formed when isoquinoline is treated with lithium in liquid ammonia.

SECTION-C

Answer **any 2** questions. **Each** question carries **8** marks

21. Predict the product formed i) dibenzoyl methane reacts with hydroxylamine and ii) N-chloro-N-methylpentamine is exposed to light in acid medium.
22. Illustrate i) Mitsunobu reaction ii) Glaser coupling iii) Heck reaction and iv) Suzuki polymerization.
23. What products are formed in the following cases

a) 

b) 

24. Illustrate the retrosynthetic approach and major synthetic strategies adopted for synthesis of reserpine by Woodward.

1.	Semester	**3**		
2.	Course Title	**Physical Chemistry III**		
3.	Course Code	**CHE-CC-533**		
4.	Credits	**3**		
5.	**CO** On completion of the course, students should be able to:	**TL**	**KL**	**PSO No.**
	1. Understand and apply the laws of thermodynamics and thermodynamics of irreversible process	2-Un;3-Ap	CK,PK	I, II, III
	2. Explain partition functions and its relationship with thermodynamic properties	3-Ap; 5-Ev	CK	II,III, VI
	3. Explain and differentiate Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac Statistics	3-Ap; 4-An	CK	II, III
	4. Explain the kinetics of unimolecular, chain and fast reactions.	2-Un	CK,PK	I,II
	5. Understand the theories of reaction rates	2-Un	FK,CK	I, II
	6. Explain the mechanism and theories of homogeneous and heterogeneous catalysis	2-Un	CK	I, II
	7. Understand and explain the concepts and theories of electrolytes and electrodes	2-Un; 3-Ap	FK,CK	I, II, III

MODULE No	**COURSE CONTENT**	**CO No.**
I	First and second laws of thermodynamics. Thermodynamic criteria for equilibrium and spontaneity. The Clausius inequality, Maxwell relations. The third law of thermodynamics. Need for the third law. Nernst heat theorem. Apparent exceptions to third law. Applications of third law. Thermodynamics of irreversible processes: Simple examples of irreversible processes. General theory of nonequilibrium processes. Entropy production. The phenomenological relations. Onsager reciprocal relations. Application to the theory of diffusion, thermal diffusion, thermoosmosis and thermomolecular pressure difference. Electrokinetic effects. The Glansdorf-Pregogine equation.	1
II	Statistical thermodynamics: Mechanical description of molecular systems. Thermodynamic property and entropy. Microstates. Canonical and grand canonical ensembles. Equation of state for ideal quantum gases. Maxwell-Boltzman distribution. The partition functions. Partition function for free linear motion, for free motion in a shared space, for linear harmonic vibration. Complex partition functions and partition functions for particles in different force fields. Langevins partition function and its use for the determination of dipole moments. Electrostatic energies. Molecular partition functions. Translational, rotational, vibrational and electronic partition functions. Total partition functions. Partition functions and thermodynamic properties. Heat capacity of gases. Equipartition principle and quantum theory of heat capacity.	2
III	Quantum statistics: Bose-Einstein statistics. Examples of particles. Theory of paramagnetism. Bose-Einstein condensation. Liquid helium. Super cooled liquid. Fermi-Dirac statistics. Thermionic emission. Relations between Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac statistics. Heat capacity of solids. The vibrational properties of solids. Einstein theory of heat capacity. The spectrum of normal modes. The Debye theory. The electronic specific heat.	3

	Structure of liquids, X-ray diffraction studies, Short range order, radial distribution function, configurational partition function for liquids. Theories of liquids state. Free space and van der Waals theories. Lennard-Jones theory of melting. Specific heats and communal entropy of liquids.	
IV	Order and molecularity of reactions. Time dependency of order. Complex reactions: Reversible, consecutive, concurrent and branching reactions. Free radical and chain reactions. Steady state treatment. Reactions like H2-Cl2 and H2-Br2. Decomposition of ethane, acetaldehyde and N2O5. Rice-Herzfeld mechanism. Unimolecular reaction. Lindemann treatment. Semenoff-Hinshelword mechanism of chain reactions and explosion. Kinetics of fast reactions: Relaxation method. Relaxation spectrometry. Flow method, Stopped-flow technique. Shock method. Pulse method. Flash photolysis. Factors influencing reaction rates in solution. Salt effects. Curtin-Hammett equation, kinetic isotope effect. Theories of reaction rates. Arrhenius equation, Collision theory, potential energy surfaces and reaction coordinate, TransitionState theory, comparative study of the theories. Kinetics of reactions in solution. Diffusion controlled reactions. Ionic reactions and effect of ionic strength, Effect of solvents, effects of pressure on velocity of gas reactions.	4,5
V	Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Acid-base catalysis. Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanisms, acidity function. Enzyme catalysis. Michaelis-Menton equation, effect of pH and temperature on enzyme catalysis. Mechanism of heterogeneous catalysis- Unimolecular and Bimolecular surface reactions. Langmuir-Hinshelwood mechanism. Introduction to photochemistry: Laws of photochemistry. Quantum yield. Radiative and non-radiative transitions. Fluorescence and phosphorescence. Intensity and concentration. Fluorescence indicators. Quenching of fluorescence. Chemiluminescence. Explosion reaction. Kinetics of photochemical reaction of H2and Cl2, and H2and Br2.	6
VI	Ionic activity. Ion-solvent interaction. Strong electrolytes. Ion transport. Debye-Huckel theory of strong electrolytes, Debye-Huckel limiting law. Mean ionic activity coefficient. Debye-Huckel- Onsagar equation and its derivation. Debye-Falkenhagen effect. Wein effect. Types of electrodes. Electrochemical cells. Liquid junction potential and its determination. Evaluation of thermodynamic properties and activities. Electrical double layer, and its various models. Electrode-electrolyte interface. Electrokinetic phenomena. Current-potential curves. Over potential and its theories. Butler-Volmer equation. Tafel and Nernst equations. Corrosion and methods for prevention. Porbaux diagram and Evans diagram. Introduction to polarography, cyclic voltammetry. Theory and working of Fuel Cells.	7

References:

1. Engel T. and Reid, P. Thermodynamics, Statistical Thermodynamics, & Kinetics, 3rd edition, 2013, Pearson Education.
2. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3rd edition, 2006, Springer.
3. Houston, P. A., "Chemical Kinetics and Reaction Dynamics", Dover, 2006.
4. Panchenkov, G. M. and Labadev, V.P., "Chemical Kinetics and Catalysis", MIR Publishing.

5. Laidler, K. J. “Chemical Kinetics” 3rd Edition, Prentice Hall, 1987.
6. Moore, J. W. and Pearson, R. G. “Kinetics and Mechanism”, 3rdedition, 1981, John Wiley and Sons.
7. Bokris, J. O. M.; Reddy, A. K. N., “Modern Electrochemistry”, Wiley-Interscience, 1972.
8. Glasstone, S., “Introduction to Electrochemistry”, East West Press Pvt Ltd. 1965.

Additional References:

1. Daniels, F. and Alberty, R. A., "Physical Chemistry",4th Edition, Wiley Eastern, 1976.
2. Atkins, P. W., "Physical Chemistry", 9th Edition, OUP, 2010.
3. Berry, R. S.; Rice, S. A. and Ross, J. “Physical Chemistry”, Oxford University Press, Oxford, 2000.
4. Sears, F. W., “Introduction to Thermodynamics, Kinetic Theory of Gases and Statistical mechanics”, 2nd Edition, Addison Wesley, 1972.

Model Question Paper

THIRD SEMESTER M.Sc. DEGREE EXAMINATION, Month Year
Branch: CHEMISTRY
CHE-CC-533: PHYSICAL CHEMISTRY III

Times: 3 Hours Max. Marks: 60

SECTION- A

Answer **any 10** questions. Each question carries **2** marks.

1. Define active transport. Explain its significance.
2. State and explain Onsager reciprocal relations.
3. Distinguish between microstate and macrostate.
4. Show that molecular partition function is the product of the partition functions for various degrees of freedom.
5. Compare the free space and van der waals theories of liquid state.
6. Calculate the pressure and the energy of a 3D non-interacting Boson gas below its BEC critical temperature?
7. Explain primary salt effect.
8. Radioactivity of a sample (z=22) decreases 90% after 10 years. What will be the half life of the sample.
9. What is the effect of pH on the rate of an enzyme catalyzed reactions.
10. Differentiate between inter system crossing and internal conversion.
11. Calculate the thickness of ionic atmosphere in 0.01 molal aqueous KCl at 25^{o}C. Dielectric constant of water is 78.5.
12. Distinguish between inner and outer Helmholtz plane.

SECTION- B

Answer **any 6** questions. Each question carries **4** marks.

13. a) Define phenomenological coefficient. Show that direct coefficients always dominate indirect coefficients.
14. Use third law of thermodynamics, show that absolute zero of temperature is unattainable.
15. Explain the term dilute system. Show that all particles follow Maxwell-Boltzmann statistics under dilute system conditions.
16. Calculate the heat capacity of diamond at 1000 K. Its characteristic temperature is 1860 K.
17. Explain Lennard Jones theory of melting.
18. Derive the distribution law for velocity of gases in two dimensions.
19. Give the steady state treatment for the reaction H_2+Br_2 ---> 2HBr
20. The emf of the cell $Pt\left|\begin{matrix}H_{2(g)}\\1b\end{matrix}\right|\begin{matrix}HCl\\0.01m\end{matrix}\left|\right|AgCl_{(S)}\left|Ag\right.$ was found to be 0.3524 V at 25^{o}C. Calculate the activity coefficient of 0.01m HCl. The standard electrode potential of $\bar{Cl}\left|AgCl_{(S)}\right|Ag$ is 0.2224 V.

SECTION- C

Answer any ***two*** question. Each question carries **8** marks

21. a) Rationalize thermal osmosis and thermal diffusion using irreversible thermodynamics.
    b) Discuss briefly Bose-Einstein condensation. (4+4)

22. a) Explain the Lindemann theory for unimolecular reactions.
    b) Give the kinetics for the following reaction $2H_2$ (g)+O_2 (g) ---> $2H_2O$ (g) (4+4)

23. a) Compare the postulates of Maxwell-Boltzmann and Fermi-Dirac statistics.
    b)Derive Butler-Volmer equation. Discuss. (4+4)

24. a) Discuss the application of Porbaux diagram in predicting the stability of metals.

    b) Provide a comparison of the free space and vander Waals theories of liquid state.

    (4+4)

1.	Semester	**3**
2.	Course Title	**Inorganic Chemistry Lab III**
3.	Course Code	**CHE-CC-534**
4.	Credits	**3**

5.	**CO:** On completion of the course, students should be able to:	**TL**	**KL**	**PSO No.**
	1. Implement the analytical techniques learned earlier to the real cases	3-AP 5-E	CK,PK MK	PSO4, PSO5 PSO6
	2. Describe and execute ion-exchange separation technique	2-Un 4-An	CK, PK MK	PSO4, PSO5 PSO6
	3. Execute inorganic synthesis of model coordination complexes	4-An 5-E	PK	PSO5 PSO6
	4. Interpret and compare the electronic properties of complexes based on the given experimental results	3-Ap 4-An 5-E	PK, MK	PSO3 PSO4 PSO5
	5. Describe and operate analytical and spectroscopic tools to characterize and analyse various inorganic complexes	3-AP 4-An 5-E	PK, MK	PSO4 PSO5 PSO6

MOD. No	**COURSE CONTENT**	**CO No.**
I	Analysis of some typical ores: Carbonate ore, sulfate ore, ilmenite and monazite.	CO1
II	Analysis of fertilizers: Estimation of nitrogen in ammonium compounds. NPK estimations in synthetic fertilizers	CO1
III	Ion exchange separation of binary mixtures: Zn & Mg and Co & Ni.	CO2
IV	Synthesis of $[Ti(urea)_6]I_3$: An air stable d^1 Complex. Compare the electronic property with $[Ti(H_2O)_6]^{3+}$	CO3, CO4, CO5
V	Preparation of various transition metal complexes	CO3
VI	Characterizations of prepared metal complexes by UV-VIS, IR, magnetic susceptibility and electrical conductivity	CO4, CO5

References:

1. Drago, R. S. "Physical Methods in Inorganic Chemistry", Affiliated East West.
2. Furman and Welcher, "Standard Methods of Inorganic Analysis", Van Nostrand.
3. Kolthoff, I. M. and Strenger, "Volumetric Analysis", Interscience.
4. Kolthoff, I. M., Elving, V. J. and Sandell, "Treatise on Analytical Chemistry", Interscience.
5. Palmer, W. G. "Experimental Inorganic Chemistry", CUP.
6. Schoder, W. R. and Powell, A. R. "Analysis of Minerals and Ores of Rare Elements".
7. Weining, I. and Schoder, W. P. "Technical Methods of Ore Analysis".

1.	Semester	**3**
2.	Course Title	**Organic Chemistry Lab III**
3.	Course Code	**CHE-CC-535**
4.	Credits	**3**

5.	**CO** On completion of the course, students should be able to:	**TL**	**KL**	**PSO No.**
	1. To estimate the various functional groups present in organic molecules	3-Ap, 4-An	CK, PK	II, III, V
	2. To apply volumetry for organic analysis	3-Ap	FK, PK	V
	3. To apply UV-Vis spectrophotometry to analyze certain functional groups	3-Ap,	CK, PK	III, IV

MODULE No	**COURSE CONTENT**	**CO No.**
I	Estimation of esters and acids using acid - base titration method.	1, 2
II	Estimation of reducing sugars by using freshly prepared Fehling\s solution	1, 2
III	Estimation of phenols, amines and ketones using iodometric titration method	1, 2
IV	Estimation of acid value, iodine value and sap value of oils	1, 2
V	Spectrophotometric estimation of total ascorbic acid content in various fruits and vegetables	3
VI	Spectrophotometric estimation of glucose	3

References:

1. Agarwala, A. C. and Sharma, R. M. "A Laboratory Manual of Milk Inspection", Asia Publishing
2. Ahluwalia, V. K. and Aggarwal, R. “Comprehensive Practical Organic Chemistry”, Vol 1 & 2, Universities Press.
3. Vishnoi, A. K. “Advanced Practical Organic Chemistry” Vikas Publishing, 2009

1.	Semester	**3**			
2.	Course Title	**Physical Chemistry Lab III**			
3.	Course Code	**CHE-CC-536**			
4.	Credits	**3**			
5.	**CO** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Use conductometer to perform conductometric titrations, and to measure equivalent conductance		2-Un; 3-Ap	CK,PK	IV; V; VI
	2. Perform potentiometric titrations		3-Ap	CK,PK	IV; V; VI
	3. Perform polarographic estimations		3-Ap; 5-Ev	CK,PK	IV; V;VI
	4. Perform flame photometry or Karl-Fischertitrator estimations		3-Ap;5-Ev	CK,PK	V; VI
	5. Have a basic understanding on photocatalysis and redox potential determination		3-Ap; 6-Cr	PK,MK	V;VI
	6. Understand the basic principles of lab techniques adopted in physical Laboratories, monitor, record and present data in a scientific form		2-Un	FK	V, VII, VIII

MODULE No	**COURSE CONTENT**	**CO No.**
I	Conductance: Verification of Onsagar equation. Solubility of sparingly soluble substances. Oswald's dilution law. Basicity of acids. Dissociation constants of acids and bases. Conductometric titrations involving acid-base and precipitation reactions. Equivalent conductance of solutions of strong electrolytes and weak electrolytes.	1,6
II	Potentiometry: Single electrode potentials of hydrogen and glass electrodes. Quinhydrone electrode. Potentiometric titrations involving acid-base, redox and precipitation reactions. pH of buffer solutions. Solubility of AgCl. Determination of dissociation constant.	2,6
III	Polarography: Polarographic estimation of cadmium, zinc and lead. Composition of mixtures.	3,6
IV	Flame photometry: Estimation of Na^+, K^+, Li^+, Ca^{2+} and Mg^{2+}. Composition of the mixtures.	4,6
V	Karl-Fischer titrator: Estimation of water contents in pharmaceuticals, oils, fats and paints.	4,6
VI	Non-Evaluative experiments: 1. Preliminary Characterization of Battery- Charging Discharging efficiency 2. Preliminary Fuel cell characteristics 3. Photocatalysis-Dye degradation (Preliminary studies) 4. Redox potential Determination (Preliminary studies)	5,6

References:

1. Kanetkar Y. P., "Let us C++" 2nd Edition, BPB Publications, Delhi, 2003.
2. VogelA.I., "A Text Book of Quantitative Inorganic Analysis", Longman.
3. WillardH. H., Merritt L. L. and DeanJ. A., "Instrumental Methods of Analysis", Affiliated East -West.
4. Daniels,F. and Mathews,J. H. "Experimental Physical Chemistry", McGraw Hill, 1970.
5. YadavJ. B., "Advanced Practical Chemistry", Krishna Prakashan Media, 2015.

1.	Semester	**3**			
2.	Course Title	**Renewable Energy Materials**			
3.	Course Code	**REC-DE-531**			
4.	Credits	**4**			
5.	**CO** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Understand solar thermal power technology.		2-Un;3-Ap	CK,PK	II,III
	2. Describe biomass production and utilization		3-Ap; 4-An	PK,MK	II, III
	3. Illustrate energy systems modeling and analysis		3-Ap; 4-An; 5-Ev	CK,PK	II, III, VI
	4. Understand advanced materials for energy applications		2-Un	CK,PK	II,III
	5. Illustrate materials characterization techniques for energy applications		2-Un;3-Ap	FK,CK	II, III

MODULE No	**COURSE CONTENT**	**CO No.**
I	Solar Thermal Power Technology: Solar radiation, Solar angles, classifications of Solar thermal collectors, Non-concentrating and concentrating collectors, Heat transfer fluids, Tracking mechanisms, Emerging solar thermal technologies, Application of solar thermal technologies: Power generation, Industrial process heating, Water distillation, Refrigeration, Building heating and cooling, Cooking, Drying, Thermal energy storage systems: Sensible, Latent and Thermochemical energy storage, Integration of thermal energy systems with various end use applications, Economic analyses of solar thermal energy systems, Life cycle assessment of solar thermal energy systems.	1
II	Bioenergy: Introduction to bioenergy; biomass harvesting; characterization of biomass feedstock (physico-chemical properties, ultimate, proximate, compositional, calorific value, thermogravimetric, differential thermal and ash fusion temperature analyses); classification of biomass feedstock: first, second and third generation biofuels; Different pre-treatment processes of biomass; different production routes for biomass conversion to biofuels: biochemical methods (anaerobic, enzymatic- saccharification and fermentation process, and dark fermentation, ABE fermentation); chemical processes (transesterification, hydro-processing, micro-emulsification); thermochemical methods (combustion, gasification, pyrolysis, partial oxidation, auto-thermal reforming) for biofuels production including synthesis gas, bio-hydrogen, ethanol, butanol, biogas, methanol, dimethyl ether and paraffinic fuels.	2
III	Energy Systems Modeling and Analysis: Energy Chain, Primary energy analysis. Modelling overview- levels of analysis, steps in model development, examples of models. Quantitative Techniques: Interpolation- polynomial, lagrangian, curve fitting, regression analysis, solution of transcendental equations. Systems Simulation- information flow diagram, solution of set of nonlinear algebraic equations, successive substitution, Newton Raphson. Examples of energy systems simulation Optimisation: Objectives/constraints, problem formulation. Unconstrained problems- Necessary & Sufficiency conditions. Constrained	3

	Optimisationlagrange multipliers, constrained variations, Kuhn-Tucker conditions. Linear Programming - Simplex tableau, pivoting, sensitivity analysis. Dynamic Programming. Search Techniques-Univariate/Multivariate.	
IV	Carbon Based Materials for Energy Applications: Introduction –Carbon molecules-nature of the carbon bond-new carbon structures-discovery of C60-structure of C60 and its crystal-From a Graphene Sheet to a Nanotube – Single wall and Multi-walled Nanotubes - Zigzag and Armchair Nanotubes - Euler's Theorem in Cylindrical and Defective Nanotubes, Structure and Bonding. Fullerenes: Structure and Bonding- Nomenclature, The Structure of C60, Structure of Higher Fullerenes - Growth Mechanisms; Production and Purification, Physical and Chemical Properties. Carbon nanotubes: Structure and Nomenclature of Carbon Nanotubes (SWCNT and MWCNT). Structure and production of other tubular carbon materials. Graphene: Structure of graphene; Preparation of graphene – synthesis of graphene by various physical and chemical methods and Purification; Electronic Properties - Band Structure of Graphene - Mobility and Density of Carriers - Quantum Hall Effect. Applications of carbon nanomaterials: Application of Fullerene, CNT, Graphene and other carbon nanomaterials - Mechanical, Thermal, Electronic and biological Applications.	4
V	Other Advanced Materials for Energy Applications: Microporous and Mesoporous Materials: Introduction of nanoscale porosity in organic and inorganic materials, surface acidity and basicity measurements. Impact of nanoscale porosity and surface acidity/basicity in the energy and environmental research. Nanomaterials: Size effect and properties of nanostructures- Top down and Bottom up approach. Quantum dots: Excitons and excitonic Bohr radius – difference between nanoparticles and quantum dots. Applications of nanoparticles, quantum dots, nanotubes and nanowires for nanodevice fabrication. Thin Film: Overview of physical and chemical methods of preparation, Applications of thin films. Ceramics: Oxide ceramics, Ferroelectric ceramics, Magnetic ceramics, Superconducting ceramics. Composites: Metal matrix composites, Polymer matrix composites, Ceramic matrix composites, Hybrid composites, Applications of composites.	4
VI	Materials Characterization Techniques for Energy Applications: Introduction to materials characterization Techniques, Structure analysis tool: X-ray diffraction, Phase identification, indexing and lattice parameter determination. Microscopy techniques: Introduction to Microscopes, Optical microscopy (OM), Transmission Electron Microscopy (TEM); Basic Electron scattering, Concepts of resolution, TEM instruments, Various imaging modes, Analysis of micrographs. Scanning Electron Microscopy, Rutherford backscattering spectrometry. Atomic Force Microscopy, Scanning Probe Microscopy. Thermal analysis techniques: Differential thermal analysis (DTA), Differential Scanning Calorimetry (DSC), Thermo-gravimetric analysis (TGA). Electrical characterization techniques: Electrical resistivity in bulk and thin films, Hall effect, Magnetoresistance. Optical characterization techniques: UV-VIS spectroscopy, Fourier transform infrared spectroscopy, Raman spectroscopy, X-ray photoelectron spectroscopy.	5

References:

1. Large-scale solar thermal power: technologies, costs and development, W. Vogel, H. Kalb, John Wiley & Sons, 2010.
2. Advances in concentrating solar thermal research and technology, M. Blanco, L.R. Santigosa,

Woodhead Publishing, 2016.
3. Biomass to renewable energy processes, J. Cheng, CRC press, 2017.
4. Recent Advancements in Biofuels and Bioenergy Utilization, P.K. Sarangi, S. Nanda, P. Mohanty, Springer, 2018.
5. Optimization of energy systems, I. Dincer, M.A. Rosen, P. Ahmadi, Wiley Online Library, 2017.
6. Intelligent renewable energy systems: modelling and control, G. Rigatos, Springer, 2016.
7. Innovative Advanced Materials for Energy Storage and Beyond: Synthesis, Characterisation and Applications, V.K. Thakur, Multidisciplinary Digital Publishing Institute, 2020.
8. Handbook of Materials Characterization, S.K. Sharma, D.S. Verma, L.U. Khan, S. Kumar, S.B. Khan, Springer, 2018.
9. Materials characterization techniques, S. Zhang, L. Li, A. Kumar, CRC press, 2008.

Additional References:

1. Solar energy technology handbook, E.W. Dickinson, CRC Press, 2018.
2. Biomass and bioenergy, K.R. Hakeem, M. Jawaid, U. Rashid, Springer, 2016.
3. Modeling Power electronics and interfacing energy conversion systems, M.G. Simões, F.A. Farret, John Wiley & Sons, 2016.
4. Rational design of carbon-rich materials for energy storage and conversion, D. Kong, Y. Gao, Z. Xiao, X. Xu, X. Li, L. Zhi, Advanced Materials. 31 (2019) 1804973.
5. Electrochemical energy: advanced materials and technologies, P.K. Shen, C.-Y. Wang, X. Sun, J. Zhang, CRC Press, 2018.
6. Materials characterization: introduction to microscopic and spectroscopic methods, Y. Leng, John Wiley & Sons, 2009.

1.	Semester	**3**			
2.	Course Title	**Electronic Structure Theory And Applications**			
3.	Course Code	**CHE-DE-537**			
4.	Credits	**4**			
5.	**CO** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1.Understand and apply the theories of molecular mechanics and dynamics		2-Un;3-Ap	CK,PK	II,III
	2. Distinguish and apply various MO treatments for polyatomic molecules		3-Ap; 4-An	PK,MK	II, III
	3. Classify various basis sets and justify its use for a specific problem		3-Ap; 4-An; 5-Ev	CK,PK	II, III, VI
	4. Understand the post HF methods		2-Un	CK,PK	II,III
	5. Explain the basic theories and classification of density functional theory		2-Un;3-Ap	FK,CK	II, III
	6. Construct the structure of polyatomic molecule in terms of internal coordinates		6-Cr	CK,PK	III, VI
	7. Understand the theories of computing properties of structure and charge		2-Un	CK,PK	II, III

MODULE No	**COURSE CONTENT**	**CO No.**
I	Molecular dynamics: Brief description of computational methods: abinitio, semi empirical, and empirical methods. Molecular mechanics. Potential energy functions. Force fields. Geometry minimization, Molecular dynamics. Periodic boundary conditions, Propagation of Newton's equation using Verlet, Velocity verlet and Leap-Frog algorithm.	1
II	Ab initio Methods: Approximations. HartreeFock method. Self consistent field. Slater determinants. Roothan approximation. Restricted HartreeFock (RHF), Restricted open HF (ROHF), and Unrestricted HF (UHF) methods. Semi empirical treatments: Extended Hückel theory. Introduction to CNDO, INDO, NDDO. Applications. Computing the matrix elements. Slater's rules for matrix elements. Convergence. Optimization.	2
III	Basis sets andBasis functions. Slater type orbital (STO) and Gaussian type orbital (GTO). Contracted and primitive. Basis sets. Minimal, multiple zeta, split-valence, polarized and diffused. Pople style basis sets, designation of basis set size – Dunnings correlation consistent basis sets Relativistic effects - Effective core potential, ECP.	3
IV	Post HF methods-Exchange and Correlation energy. Static and dynamic electron correlation, Avoided crossings and configuration mixing. Configuration Interaction (CI). Couple cluster, Multi-Configuration and Complete active space SCF (MCSCF, and CASSCF), Moller-Plesset Perturbation methods (MPn). Pros and Cons of these methods.	4
V	Density Functional Theory: Development of density function theory (DFT). Density matrices. Thomas-Fermi model. Hohenberg-Kohn existence and variational theorems. Chemical potential. Kohn-Sham self consistent field method. Exchange correlation functionals. Local density approximation (LDA), density Gradient corrections (GGA). Hybrid and meta–GGA functionals. Advantages and	5

	applications of DFT.	
VI	Specifying the molecule in Cartesian and internal coordinates: Writing the Z-matrix of H2O, CH4, ethane, Cyclopentadiene, and benzene with suitable point group. Dummy atoms and Ghost atoms. Influence of point group in computations. Illustration by taking H2O, and NH3. Computing the quantities- structure, potential energy surface, and chemical properties such as Mulliken and natural charges. Dipole moments.SCF orbital energies. Koopmann's theorem and Brillouin theorem.	6,7

References:

1. Cramer, C. J., "Essentials of Computational Chemistry- Theories and Models", 2nd Edition, Wiley, 2004.
2. Foresman, J. and Frisch, A.," Exploring chemistry with electronic structure methods", GuassianInc, 2000.
3. Jensen, F., "Introduction to Computational Chemistry", 3rdEdition, Wiley, 2017.
4. Leach, A. R., "Molecular Modeling – Principles and Applications", Addison Wesley Longman, 2001
5. Levine, I. N., "Quantum Chemistry", 7thEdition, Pearson Education Inc., 2014.
6. McQuarrie, D. A., "Quantum Chemistry", 2ndEdition,University Science Books, 2008.
7. Young, D., "Computational Chemistry – A Practical Guide", Wiley, 2001.

Model Question Paper

FOURTH SEMESTER M.Sc. DEGREE EXAMINATION, MONTHYEAR
Branch: CHEMISTRY
CHE-DE-538 ELECTRONIC STRUCTURE THEORY AND APPLICATIONS

Times: 3 Hours Max. Marks: 60

SECTION- A

Answer **any 10** questions. Each question carries **2** marks.

1. What is a stochastic process? Which simulation method is most suitable for this process?
2. Which method among these is computationally least expensive for a particular problem and why?
   i) molecular mechanics, ii) Semi-empirical methods and iii) *ab initio* methods.
3. State Koopmanns theorem. Is it applicable to open shell systems in ROHF calculations?
4. What is the major difference between single point energy calculation and geometry optimization?
5. Calculate the number of contracted and primitive basis functions for carbon if you are using 6-311+G(d,p).
6. What are the advantages of adding polarization and diffusion functions in a basis set?
7. What is correlation energy? Differentiate between Coulomb correlation and Fermi correlation.
8. Write down the form of exchange integral and its effect on total electronic energy.
9. Why density functional theory is named so instead of density function theory?
10. Differentiate between LDA and GGA.
11. What type of computation will be performed to verify if the molecule is indeed a minimum on the potential energy surface.
12. Differentiate dummy and ghost atoms.

SECTION- B

Answer **any 6** questions. Each question carries **4** marks.

13. What is boundary condition and why these are necessary for dynamic simulation?Give an account of Monte Carlo simulations
14. Briefly explain semi empirical method giving emphasis to CNDO.
15. Explain the concept of PES? How will you identify the global minima?
16. Explain correlation consistent basis sets and the advantage of using this in computations.
17. Give an account of configuration interaction
18. Compare and contrast DFT and HF methods.
19. Write a note on the influence of point groups in calculations?
20. What is meant by geometry optimization? Explain the steps.

SECTION- C

Answer **any two** questions. **Each** question carries **8** marks

21. a) Explain ‘Force Fields’
    b) What are Pople style basis sets? Briefly explain the classification and its relevance. (4+4)
22. Explain and differentiate with examples the various approximations employed under density functional theory methods.
23. Explain in detail the various steps involved in HF methods. Also, differentiate RHF and UHF methods.
24. Explain Kohn-Sham theorem and applications

1.	Semester	**3**			
2.	Course Title	**Photophysical Processes And Applications**			
3.	Course Code	**CHE-DE-538**			
4.	Credits	**4**			
5.	**CO** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Summarize and differentiate various photophysical processes in molecular systems		1-R; 2-U; 4-An	FK, CK	01, 02
	2. Exemplifies and distinguish diverse absorption and emission phenomenon observed in molecular systems		4-An; 5-E	FK, CK	01, 02
	3. Explain the concepts and demonstrate the applications associated with photoinduced electron transfer and energy transfer		2-U; 3-Ap	CK	01, 02
	4. Illustrate the techniques and instrumentation of fluorescence and other fast light induced processes / reactions		2-U; 3-Ap	FK, CK	01, 02
	5. Identify and design molecular sensors for metal ions, anions and neutral molecules based on various photo-chemical/-physical processes		4-An; 6-Cr	CK, MK	02, 03
	6. Describe and compare the properties and applications of light active semiconductor nanoparticles and lanthanide based systems		2-U; 3-Ap; 5-E	FK, CK	01, 02
	7. Comprehend the properties and applications of metal-ligand complexes and AIE luminogens		2-U; 4-An	CK, MK	01, 02
	8. Appreciate the processes happening in natural photosyntheitic systems		2-Un; 4-An	FK, CK	01, 02
	9. Elaborate reactions happening in artificial solar energy converting systems and compare it to those in natural photosynthetic systems		4-An; 5-E	CK, MK	01, 02, 03

MODULE No	**COURSE CONTENT**	**CO No.**
I	Photophysical Properties of the Electronically Excited Molecules:Basic principles of photochemistry: Absorption of radiation-Beer Lambert's law. Electronic transitions. Frank Condon principle. Jablonski diagrams. Nonradiative transitions. Internal conversion and inter system crossing. Radiative transitions: Fluorescence emission, triplet states and phosphorescence. Absorption complexes. Charge transfer absorption. Excimers. Exciplexes. Delayed fluorescence. Chemiluminescence.	1, 2
II	Bimolecular Processes: Fluorescence quenching. Collisional quenching. Stern-Volmer equation. Static quenching Photoinduced electron transfer (PET): Concepts and theories, electron donors and acceptors, quantum yield, efficiencies and lifetimes, intermolecular, intramolecular and supramolecular PET. Fluorescence resonance energy transfer (FRET): Trivial or radiative mechanism; Forster and Dexter type energy transfer. Energy transfer versus electron transfer. Applications of electron transfer and energy transfer.	3
III	Techniques and Instrumentation:Light sources, filters and monochromators: Incandescent lamps and arc lamps, optical filters, spectrographs and monochromators. Lasers as excitation sources: General principles, Two, three and four level lasers, Solid state lasers (Ruby and Nd/YAG) and gas lasers. Luminescence measurements: Steady-state fluorescence spectroscopy.	4

	Luminescence quantum yield measurements, Time-resolved fluorescence spectroscopy, single photon counting, Detection and kinetics of reactive intermediates, Transient absorption spectroscopy: Nanosecond laser flash photolysis and Picosecond laser flash photolysis.	
IV	Application of fluorescence in chemical sensing: Various approaches of fluorescence sensing, Fluorescent pH indicators, Fluorescent molecular sensors based on ion or molecular recognition: Recognition units and topology, recognition based on photoinduced electron transfer(PET), photoinduced charge transfer (PCT), Excimer formation and disappearance and Forster resonance energy transfer (FRET). Fluorescent sensors for Metal ions (based on all above mentioned recognition mechanisms), Fluorescent sensors for anions and neutral molecules.	5
V	Novel Fluorophores:Semiconductor Nanoparticles: Spectral properties of quantum dots, Labeling cells with quantum dots, Quatum dots and Resonance Energy Transfer (RET), Lanthanides: RET with lanthanides, Lanthanide nanoparticles, Near-infrared emitting lanthanides, Long-lifetime metal–ligand complexes: Introduction to metal–ligand probes, Spectral properties of MLC probes, Metal-ligand complex sensors, Aggregation induced emissive (AIE) fluorophores: Mechanism of AIE and applications.	6,7
VI	Solar Energy Conversion:Natural photosynthetic system: Light dependant reactions, photosynthetic reaction centre, Z-scheme of photosynthesis. Artificial photosynthesis, conversion of solar energy to chemical and other forms of energies. Solar water splitting. Photocatalytic hydrogen production, Photocatalytic carbon dioxide reduction. Photovoltaic cells: Polymer solar cells and dye sensitized solar cells. Photo-biochemical energy production.	8,9

References:

1. Lakowicz, J. R. “Principles of Fluorescence Spectroscopy”, 3rd Ed., Springer, New York, 2006.
2. Valeur, B B. “Molecular Fluorescence: Principles and Applications”, Wiley-VCH Verlag
3. Kavarnos,G. J. “Fundamentals of Photoinduced Electron Transfer”, VCH publishers
4. Rohatgi-Mukherjee, K. K. “Fundamental of Photochemistry”, New Age International (P) Ltd.,New Delhi, 1986.
5. Turro, N. Ramamurthy,J. V. Scaiano, J. C. “Principles of Molecular Photochemistry”, University Science, Books, CA, 2009.
6. Gratzel, M. “Energy Resources through photochemistry and catalysis, Academic Press, 1983.Inc., New York, 1993.

Additional References:

1. Barber J, Tran PD. “From natural to artificial photosynthesis”, J R Soc Interface 10:20120984. http://dx.doi.org/10.1098/rsif.2012.0984, 2013
2. Depuy C. H. and Chapman,O. L. “Molecular Reactions and Photochemistry”,
3. Feng,G. Kwok, R. T. K. Tang, B. Z. and Liu,B. “Functionality and versatility of aggregation-Induced Emission Luminogens”, Appl. Phys. Rev., 4, 021307 (2017)GmbH, Weinheim, 2002.
4. Mei, J. Leung, N. L. C.Kwok, R. T. K. Lam, J. W. Y. and Tang, B. Z. “Aggregation-Induced Emission: Together We shine, United We Soar” Chem Rev., 115, 11718-11940 (2015). Prentice Hall of India Pvt. Ltd., 1988.
5. Serpone N. and Pelizzetti, E. “Photocatalysis,” Wiley, New York, 1989.
6. Suppan, P. “ Chemistry and light”, Royal Society of Chemistry, Cambridge, 1994.

Model Question Paper

THIRD SEMESTER M.Sc. DEGREE EXAMINATION Month Year

Branch: CHEMISTRY

CHE-DE-539: PHOTOPHYSICAL PROCESSES AND APPLICATIONS

Time: 3 hours **Max. Marks: 60**

SECTION-A

Answer **any 10** questions. **Each** question carries **2** marks

1. State and Explain Frank Condon principle.
2. Guanosine has a maximum absorbance of 275 nm. $\varepsilon_{275} = 8400\ M^{-1}\ cm^{-1}$ and the path length is 1 cm. Using a spectrophotometer, you find that the absorbance at 275 nm is 0.70. What is the concentration of guanosine?
3. What is Stern-Volmer equation? How it is useful in distinguishing static and dynamic quenching?
4. Explain the concept of donor and acceptor in photoinduced electron transfer (PET) with suitable examples.
5. Which are the light sources used in the UV-Vis absorption spectrophotomerter?
6. Experimentally how can you characterise the triplet state of an organic chromophore?
7. What is a fluorescent pH indicator? Explain with an example.
8. Exemplify the concept of excimer based fluorescence sensor.
9. Luminescence lifetimes of metal-ligand complexes are usually high compared to that of pure organic fluorophores. Why?
10. How luminescence originates in quatum dots?
11. What is the function of redox couple in dye sensitized solar cell?
12. Write a note on photocatalytic carbon dioxide reduction.

SECTION-B

Answer **any 6** questions. **Each** question carries **4** marks

13. Exemplify the concept of delayed fluorescence.
14. Briefly discuss about the phenomenon of chemiluminescence with suitable examples.
15. What is Fluorescence resonance energy transfer (FRET)? Briefly explain the Foster type energy transfer.
16. Briefly explain the principle of working of lasers.
17. Portrait the working of metal ion sensors based on any two different recognition mechanisms.
18. Briefly represent the mechanism of aggregation induced emission.
19. Quantum dots are useful candidates in bio-medical field. Justify the statement.

20. Briefly discuss about dye sensitised solar cells.

SECTION-C

Answer **any 2** questions. **Each** question carries **8** marks

21. Write note on Photoinduced electron transfer (PET) in molecular systems. How can we make use of PET in designing molecular sensors?
22. i) Illustrate and explain various radiative and non-radiative transitions in molecular systems with the help of Jablonski diagram.
    ii) Explain the principle and instrumentation of Transient absorption spectroscopy.
    (4 + 4)
23. Discuss the photochemistry of metal-ligand complexes. Exemplify their use in solar water splitting.
24. i) Illustrate the instrumentation of steady-state fluorescence spectroscopy.

ii) Illustrate the light-dependent reactions in natural photosynthesis.

(4 + 4)

FOURTH SEMESTER

1.	Semester	**4**			
2.	Course Title	**Dissertation**			
3.	Course Code	**REC-CC- 541**			
4.	Credits	**10**			
5.	**CO** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Conduct a literature survey		3-Ap, 5-E	PK	VI, VII,VIII
	2. Design and execute small reaction schemes		5-E, 6-C	PK, MK	VI,VII,VIII
	3. Independently write scientific reports		6-C	CK,PK	VII, VIII
	4. Communicate through various forms of presentation		3-Ap	CK	VIII

1.	Semester	**4**		
2.	Course Title	**Renewable Energy Generation and Storage**		
3.	Course Code	**REC-DE-542**		
4.	Credits	**3**		
5.	**CO** On completion of the course, students should be able to:	**TL**	**KL**	**PSO No.**
	1. Understand Hydrogen energy Systems	2-Un;3-Ap	CK,PK	II,III
	2. Appraise Hydrogen energy utilization, storage and safety	3-Ap; 4-An	PK,MK	II, III
	3. Illustrate energy storage technologies	3-Ap; 4-An; 5-Ev	CK,PK	II, III, VI
	4. Describe battery storage mechanism	2-Un	CK,PK	II,III
	5. Appraise super capacitors	2-Un;3-Ap	FK,CK	II, III
	6. Comprehend electrochemistry and electroanalytical techniques	6-Cr	CK,PK	III, VI

MODULE No	**COURSE CONTENT**	**CO No.**
I	Introduction of Hydrogen Energy Systems: Properties of hydrogen as fuel, Hydrogen pathways introduction – current uses, General introduction to infrastructure requirement for hydrogen production, storage, dispensing and utilization, and Hydrogen production power plants. Hydrogen Production Processes: Thermal Steam Reformation – Thermo chemical Water Splitting – Gasification – Pyrolysis, Nuclear thermo catalytic and partial oxidation methods. Electrochemical – Electrolysis – Photo electro chemical. Biological – Photo Biological – Anaerobic Digestion – Fermentative Micro-organisms.	1
II	Hydrogen Storage & Safety: Physical and chemical properties – General storage methods, compressed storage – Composite cylinders – Glass micro sphere storage - Zeolites, Metal hydride storage, chemical hydride storage and cryogenic storage. Hydrogen Safety: Safety barrier diagram, risk analysis, safety in handling and refueling station, safety in vehicular and stationary applications, fire detecting system, safety management, and simulation of crash tests.	2
III	Energy Storage: Introduction to electrochemical energy storage, Need for energy storage, Classifications of energy storage technologies based on the form of energy stored: Mechanical energy storage, Electrochemical energy storage, Chemical energy storage, Electrical energy storage, Thermal energy storage. Comparison of different energy storage technologies, Challenges and future prospects. Sensible Thermal Energy Storage, Latent Energy Storage, Thermal Management System design using Latent Thermal Energy Storage, Optimization of Thermal Energy Systems, Thermochemical heat storage system, Battery Electrical Energy Storage Systems, Pumped storage systems, Other electrical energy storage systems, Integration of energy storage systems, energy storage system optimization.	3
IV	Battery Storage: Primary Batteries, Secondary Batteries, Stationary Systems: Flow Batteries and Thermal Batteries. Rechargeable batteries and their Fundamental electrochemistry, Lithium batteries, Nickel metal hydride battery, Lead-acid battery, High temperature batteries for back-up applications, Flow batteries for load levelling and large scale grid application,	4

	Ni-Hydrogen batteries for space and marine applications, Manufacturing technologies of batteries, Sustainable design of batteries, Hybridization of battery, Battery recycling technologies, Battery applications for stationary and secondary use, Battery chargers and battery testing procedures, Battery management, Regulations and safety aspects of high voltage batteries.	
V	Supercapacitors : Energy Storage in Supercapacitors, Significance of electrochemical energy storage, Plot of Energy Vs Power Density, Different types of supercapacitors (Electrochemical double layer capacitor, pseudocapacitor and hybrid capacitor), Components of supercapacitors, Asymmetric capacitors, Different models of electric double layer, Comparison of the performance of supercapacitors and batteries, Different applications.	5
VI (Non-Evaluative)	Introduction to Electrochemistry and Electroanalytical Techniques: Dynamic electrochemistry, Butler-Volmer and Tafel equations. Overpotentials. Kinetically and mass transport controlled electrochemical processes. Mass transport (migration, convection and diffusion), Solid state electrochemistry, Potentiostatic and galvanostatic methods. Electroanalytical techniques: Theoretical principles of electroanalytical chemistry, electrodes, polarization and depolarization, electrochemical cell, Electrode reactions, kinetics, reversibility and irreversibility. Electrochemical methods: ion-selective potentiometry, chronoamperometry, chronocoulometry, cyclic voltammetry, pulse voltammetry, ion-transfer voltammetry, impedance spectroscopy, Charge/ discharge cycles. Instrumentation: rotating disk electrodes, microelectrodes, chemically modified electrodes, scanning electrochemical microscopy (SECM), EC-STM, and quartz crystal microbalance.	6

References:

1. The hydrogen economy: opportunities and challenges, M. Ball, M. Wietschel, Cambridge University Press, 2009.
2. Hydrogen energy: challenges and prospects, D.A.J. Rand, R.M. Dell, Royal Society of Chemistry, 2007.
3. Alternative transportation fuels: utilisation in combustion engines, M.G. Babu, K.A. Subramanian, CRC Press, 2013.
4. Electrochemical energy storage, J.-M. Tarascon, P. Simon, John Wiley & Sons, 2015.
5. Energy storage devices for electronic systems: rechargeable batteries and supercapacitors, N. Kularatna, Academic Press, 2014.
6. Instrumental methods in electrochemistry, D. Pletcher, R. Greff, R. Peat, L.M. Peter, J. Robinson, Elsevier, 2001.
7. Electrochemical methods fundamentals and applications, J.B. Allen, R.F. Larry, John Wiley & Sons, 2001.

ADDITIONAL REFERENCES

1. Handbook of hydrogen energy, S.A. Sherif, D.Y. Goswami, E.L. Stefanakos, A. Steinfeld, CRC Press, 2014.
2. Nanostructured materials for electrochemical energy production and storage, E.R. Leite, Springer Science & Business Media, 2010.
3. Advances in thermal energy storage systems: Methods and applications, L.F. Cabeza, Elsevier, 2014.
4. Handbook of electrochemistry, C.G. Zoski, Elsevier, 2006.
5. Electrochemical techniques in battery research: a tutorial for nonelectrochemists, X. Yang, A.L. Rogach, Advanced Energy Materials. 9 (2019) 1900747.

1.	Semester	**4**			
2.	Course Title	**Data Analysis / Case study**			
3.	Course Code	**REC-DE- 543**			
4.	Credits	**2**			
5.	CO: On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Conduct a literature survey		3-Ap; 4-An; 5-Ev	CK, PK	II, III, VI
	2. Design an Industrial unit		2-Un	CK, PK	II,III
	3. Independently write analysis reports		2-Un; 3-Ap	FK,CK	II, III
	4. Communicate through various forms of presentation		6-Cr	CK, PK	III, VI

MOD. No	**COURSE CONTENT**	**CO No.**
I	Case study to be undertaken-Illustrative/Exploratory/ Critical Instance/ Program Implementation/Program Effects/Cumulative	1, 2
II	Report on case study analysis - Introduction, Background, Evaluation of the case, Proposed solution/changes, recommendations.	3, 4

1.	Semester	**4**
2.	Course Title	**Renewable Energy Lab**
3.	Course Code	**REC-DE- 544**
4.	Credits	**4**

5.	**CO:** On completion of the course, students should be able to:	**TL**	**KL**	**PSO No.**
	1. Understand the working of solid-state energy generation and storage devices	3-Ap;5-Ev	CK, PK	V; VI
	2. Evaluate the properties of semiconductors for the application in the energy field.	3-Ap; 6-Cr	PK, MK	V;VI
	3. Comprehend the use of electroanalytical techniques for energy applications.	2-Un	FK	V, VII, VIII
	4. Understand the characteristics of energy conversion and storage systems.	2-Un	FK	V, VII, VIII

EXP. No	**COURSE CONTENT**	**CO No.**
1	Evaluate the properties of semiconductors for the application in the energy field.	1, 2
2	Hall Effect	1
3	Elemental characterization of a fuel using CHNS(O) analyser	3
4	Solar radiation measurement	4
5	Wavelength dependent energy conversions efficiency from solar cell	4
6	Determination of first and second figures of merit (F1 and F2) of a box type solar cooker.	1, 4
7	Numerical simulation training for modelling a Solar cell	4
8	Identify the defects and ionization energy in CuInGaSe2 thin film using temperature dependent I-V measurement.	2, 3
9	Evaluation of HOMO-LUMO levels of organic energy material using cyclic voltammetry.	2, 3
10	Determine the characteristics of a supercapacitor	4
11	Characterization of a Photo-electrochemical cell	3, 4
12	Characterization of Battery- Charging Discharging efficiency	3, 4
13	Fuel cell characteristics	3, 4
14	Photocatalysis-Dye degradation	2, 4
15	Redox potential Determination	3

References:

1. Instrumental methods in electrochemistry, D. Pletcher, R. Greff, R. Peat, L.M. Peter, J. Robinson, Elsevier, 2001.
2. Electrochemical techniques in battery research: a tutorial for nonelectrochemists, X. Yang, A.L. Rogach, Advanced Energy Materials. 9 (2019) 1900747.
3. Practical Physics, 4^{th} ed., G.L. Squires, Cambridge University Press, Cambridge, 2001.
4. Practical Physics for Engineers, A.K. Mishra, Firewall Media, 2006.
5. Advanced Physics Practicals: With 3D Simulations, R. Lucas, CreateSpace Independent Publishing Platform, 2017.

Generic Course:

1.	Semester	**1**			
2.	Course Title	**Analytical and Environmental Chemistry**			
3.	Course Code	**CHE-GC-501**			
4.	Credits	**2**			
5.	**CO:** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Understand the basics of data analysis and titrations		1-R, 2-Un, 3-Ap	FK, CK	I, II
	2. To understand the practice of titrations and volumetry		2-Un, 3-Ap 4-An	FK, CK	I, II, III
	3. Comprehend the theory of chromatography and understand the various chromatographic methods		1-R, 2-Un	FK, CK	I, III
	4. To know the science behind the various environment phenomena like greenhouse effect, acid rain etc		2-Un, 5-E	FK, CK	I, II, III
	5. To know about various types of pollution		2-Un, 3-Ap	FK, CK	II, III
	6. To understand solid waste management issues		2-Un, 3-Ap	CK	III

MODULE No.	**COURSE CONTENT**	**CO No.**
I	Data Analysis - Accuracy and precision. Evaluation of analytical data, The mean and median. Standard deviation, variance and coefficient of variation. Classification of errors. Minimization of errors. Significant figures and computations. Statistical methods in analysis. Students T test, Rejection of suspected value, Q test.	1
II	Volumetric Analysis and Precipitation Methods - Classification of reactions in volumetry (titrimetry). Acid-base equilibria in water. Buffers. Titration curves. Theories of indicators. Theory of complexometric titrations and applications, Solubility product. Common ion effect. Super saturation and precipitate formation. Precipitation from homogeneous solutions. The purity of precipitate. Co-precipitation and post precipitation. Contamination of precipitates. Washing of precipitate. Ignition of precipitate. Organic reagents used in gravimetry	1, 2
III	Chromatographic Methods: Principles, instrumentation and applications of column chromatography, paper chromatography, thinlayer chromatography, ion-exchange chromatography, Gas chromatography and HPLC. Detectors, Hyphenated techniques, Introduction to Chiral Chromatography, Molecular Exclusion Chromatography, Introduction to Method development and Analysis of samples using the above techniques.	3
IV	Introduction to Environmental Chemistry - Components of Environment. Earth's atmosphere, Stratosphere chemistry, Ozone formation and depletion, Protection of ozone layer, Chlorofluorocarbons, Chemistry of photochemical smog, Acid rain, Atmospheric production of nitric acid, sulphuric acid, Rain, snow and fog chemistry, Aerosols, Adverse effects of	4

	acid rain, Green house effect. Impact of greenhouse effect on global climate.	
V	Air and Water Pollution - Air pollution incidents. Control measures for air pollution. Water pollution, Incidents of water pollution in India – examples – causes, effects and remedial measures, Case studies, Humic material, Metal complexes of ligands of anthropogenic origin, Soaps and detergents. Eutrophication.	5
VI	Solid Waste Management - Heavy metals. Industrial waste water treatment: Solid wastes from mining and metal production, Organic wastes, Mixed urban wastes, Solid waste management, Pollutants in soil. Radioactive pollutants. Pollutants from industries and agriculture. Chemical toxicology. Biochemical effects of pesticides and heavy metals.	6

References:

1. Bailey, R. A. Clark, H. M. Perris, J. P. Krause, S. and Strong, R. L. “Chemistry of the Environment”,Academic.
2. De, A. K. “Environmental Chemistry”,Wiley Eastern.
3. Manjooran,K. B. “Modern Engineering Chemistry”, Kannatheri Publications, Kochi.
4. Skoog,D. A. West, D. M. and Holler,F. J. "Fundamentals of Analytical Chemistry", Saunders
5. Sodhi,G. S. “Fundamental Concepts of Environmental Chemistry”, Narosa.
6. van Loon, G. W. “Environmental Chemistry”, OUP.
7. Vogel, I. "A Textbook of Quantitative Inorganic Analysis", Longman.
8. Wilson, C. L. and Wilson,D. W. “Comprehensive Analytical Chemistry”, Vol. IB

Model Question Paper

FIRST SEMESTER M.Sc. DEGREE EXAMINATION 2020

Branch: CHEMISTRY

CHE-GC-501: ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

Time: 3 hours **Max. Marks: 60**

SECTION-A

Answer **any 10** questions. **Each** question carries **2** marks

1. Write down significant figures of i)0.0009 Kg ii) 9.50 mm iii) 85000 iv) 4.5600×10^4
2. Calculate the mean and median for the data: 17.4; 17.5; 17.6; 17.8; 18.1; 18.3
3. Exemplify the concept of common ion effect.
4. Plot a titration curve for the titration between a strong acid *vs* strong base. Which indicator can be used for this titration?
5. Explain a method to separate polymers according to their size.
6. How can two stereoisomers of a compound be separated?
7. Explain the photochemical smog phenomenon.
8. What are the chief greenhouse gases present in our atmosphere?
9. What are the control measures for air pollution?
10. Differentiate between soaps and detergents
11. What are the main sources of heavy metal pollution?
12. Explain the term “chemical toxicology”.

SECTION-B

Answer **any 6** questions. **Each** question carries **4** marks

13. What is meant by distribution of random errors? Explain.
14. Write a note on any three organic reagents used in gravimetry.
15. Briefly mention the theory of acid-base indicator.
16. What are hyphenated techniques? Give the principle of any two.
17. How can thin layer chromatography be carried out? Explain.
18. Explain how ozone is formed and decomposed in the atmosphere.
19. What are the causes, effects and remedial measures for water pollution?
20. What are the major solid waste management strategies?

SECTION-C

Answer **any 2** questions. **Each** question carries **8** marks

21. Explain various ways to minimize the errors encountered during an analysis.
22. What are the organic precipitants generally employed in gravimetry ? Discuss.
23. Explain greenhouse effect and acid rain.
24. Explain the biochemical effects of pesticides and heavy metals.

Programme Structure of M.Sc. Physics / Chemistry (Specialization in Renewable Energy)

<u>Courses to be offered at Center for Renewable Energy and Materials</u>

1.	Semester	**1**
2.	Course Title	**Renewable Energy-Perspectives**
3.	Course Code	**REC-GC-501**
4.	Credits	**2**

5.	**CO** On completion of the course, students should be able to:	**TL**	**KL**	**PSO No.**
	1. Describe various conventional and non-conventional energy sources.	1-R; 5-E	FK,CK	I
	2. Understand energy policy perspectives	2-Un;3-Ap	CK,PK	I, II
	3. Understand basic techniques for energy and environmental analysis of industrial processes.	1-R; 2-Un	FK,CK	I, II, III

MODULE No.	**COURSE CONTENT**	**CO No.**
I	Energy Source: Energy Sectors: Domestic, Transportation, Agriculture and Industry. Availability of Conventional & Non-Conventional Energy Resources. Conventional Energy Sources : Fossil Fuel, Hydro Resources, Nuclear Resources, Coal, Oil, Gas, Thermal Power Stations. Comparison of various conventional energy systems, their prospects and limitations. Advantages and Disadvantages of Conventional Energy Sources. Non-Conventional Energy Sources: Solar Energy, Wind Energy, Energy from Biomass & Biogas, Ocean Thermal Energy Conversion, Tidal Energy, Geothermal Energy, Hydrogen Energy, Fuel Cell, Magneto Hydro-Dynamics Generator. Advantages & Limitations of Non-Conventional Energy Sources	1
II	Energy Policy: Overview of world energy scenario; Energy Demand- present and future energy requirements. Importance of energy management. Relevance of economic and financial viability evaluation of renewable energy technologies. Concepts of pollution and climate change, Global warming; Green House Gas emissions, impacts, mitigation; sustainability; United Nations Framework Convention on Climate Change (UNFCC); Sustainable development; Kyoto Protocol; Conference of Parties (COP); Clean Development Mechanism (CDM); Prototype Carbon Fund (PCF).	2
III	Energy and environmental analysis of industrial processes: Industrial energy use and its disaggregation (in terms of production dependent, weather dependent and independent etc. components), Energy intensity, Pinch analysis, Lean energy analysis, Thermodynamics and energy analysis, Life cycle energy analysis, Energy analysis and energy management, Energy audits, Managing energy efficiency in the industry, Identifying opportunities for improving energy efficiency in industrial energy systems. Basic approaches and tools for environment analysis, life cycle analysis and environmental impact assessment of industrial products and processes, Inventory of materials and energy inputs and environmental emissions, Emission factors, Relevant ISO standards (such as ISO 14040 and ISO 14044), Potential of energy and materials recovery.	3

References:

1. Energy for the 21st century: a comprehensive guide to conventional and alternative sources, (2nd Edition), R. Nersesian, Routledge, Taylor & Francis Group, New York, 2014.

2. Renewable energy: sources and methods, A.E. Maczulak, Infobase Publishing, 2010.
3. Renewable Energy Sources and Climate Change Mitigation: Special Report of the Intergovernmental Panel on Climate Change, O. Edenhofer, R. Pichs-Madruga, Y. Sokona, K. Seyboth, S. Kadner, T. Zwickel, P. Eickemeier, G. Hansen, S. Schlömer, C. von Stechow, P. Matschoss, Cambridge University Press, 2011.
4. Non-conventional energy resources, B.H. Khan, Tata McGraw-Hill Education, 2006.
5. Z. Morvay, D. Gvozdenac, Applied Industrial Energy and Environmental Management, John Wiley & Sons, 2008.

Additional References

1. Energy management and conservation handbook, F. Kreith, D.Y. Goswami, CRC Press, 2007.
2. Industrial ecology and global change, R. Socolow, C. Andrews, F. Berkhout, V. Thomas, Cambridge University Press, 1997.
3. Energy Security: Policy challenges and solutions for resource efficiency, N. Mouraviev, A. Koulouri, Springer, 2018.
4. A dynamic analysis of financing conditions for renewable energy technologies, F. Egli, B. Steffen, T.S. Schmidt, Nature Energy. 3 (2018) 1084–1092.
5. Comprehensive review on India's growth in renewable energy technologies in comparison with other prominent renewable energy based countries, R.M. Elavarasan, Journal of Solar Energy Engineering. 142, 2020.

1.	Semester	**2**			
2.	Course Title	**Renewable Energy Technology**			
3.	Course Code	**REC-GC-502**			
4.	Credits	**2**			
6.	**CO** On completion of the course, students should be able to:		**TL**	**KL**	**PSO No.**
	1. Understand combustion and combustion generated air pollution		3-Ap	CK,PK	II, III
	2. Appraise wind, hydro and ocean energy conversion		2-Un	FK	I, II
	3. Illustrate photovoltaic conversion mechanism		2-Un; 5-Ev	FK,CK	I, II, III

MODULE No.	**COURSE CONTENT**	**CO No.**
I	Combustion and air pollution: Fuels, Basics of flames and Flammability limits. Ideal gases and mass conservation, Basics of thermodynamics, Combustion stoichiometry. Thermochemical calculations- Enthalpy and Enthalpy of formation, Internal Energy, Entropy. Kinetic theory of gases, Chemical Kinetics, Reaction kinetics. Chemical equilibrium- Basic equations, Equilibrium modelling, Equilibrium composition and temperature, Conservation, energy and equilibrium equations. Air quality and air pollution. Pollutant formation and oxidation kinetics. Pollutant emission reduction techniques- Combustion modification for NOx reduction, Post combustion technique for NOx reduction, Sulphur compounds reduction techniques.	1
II	Wind, Hydro and Ocean Energies: Wind Energy: General introduction; Power, torque and speed characteristics. Atmospheric circulations; factors influencing wind, wind shear, turbulence, wind speed monitoring; Betz limit; Types and classification of WECS, characteristics and applications. Hydro-electricity: Overview of micro mini and small hydro systems, Basic criteria, Penstocks and turbines, Speed and voltage regulation, Investment issues, load management and tariff collection, Distribution and marketing issues, Wind and hydro based stand-alone / hybrid power systems, Control of hybrid power systems. Ocean Energy: Ocean energy resources, Ocean energy routes; principles of ocean thermal energy conversion systems; ocean thermal power plants; Principles of ocean wave energy conversion and tidal energy conversion.	2
III	Solar Energy & Photovoltaic Conversion: Solar radiation, its measurements and prediction; Solar thermal collectors- flat plate collectors, concentrating collectors; solar heating of buildings; solar still; solar water heaters; solar driers; conversion of heat energy in to mechanical energy, solar thermal power generation systems. Photovoltaic Conversion -Intrinsic, extrinsic and compound semiconductor; Absorption of light; Recombination process; p-n junction: homo and hetero junctions; Dark and illumination characteristics; Principle of photovoltaic conversion of solar energy, Figure of merits of solar cell; First, Second and Third Generation PV Devices, Basics of Design and Fabrication, Energy Losses and Efficiency	3

References:

1. Fundamentals and technology of combustion, F. El-Mahallawy, S.-D. Habik, Elsevier, 2002.
2. Renewable energy: sources and methods, A.E. Maczulak, Infobase Publishing, 2010.
3. Non-conventional energy resources, B.H. Khan, Tata McGraw-Hill Education, 2006.

4. Solar photovoltaics: fundamentals, technologies and applications, C.S. Solanki, PHI Learning Pvt. Ltd., 2015.

Additional References

1. Green Energy Advances, D. Enescu, Intech Open, 2019.
2. Challenges and solution technologies for the integration of variable renewable energy sources—a review, S.R. Sinsel, R.L. Riemke, V.H. Hoffmann, Renewable Energy. 145 (2020) 2271–2285.
3. Review on recent trend of solar photovoltaic technology, M. Gul, Y. Kotak, T. Muneer, Energy Exploration & Exploitation. 34 (2016) 485–526.
4. Fundamentals of Photovoltaic Generation: A Review, in: Solar Photovoltaics, N.D. Kaushika, A. Mishra, A.K. Rai, Springer, 2018.