

MAR IVANIOS COLLEGE (AUTONOMOUS)
THIRUVANANTHAPURAM
(Affiliated to the University of Kerala)



SYLLABUS & GUIDELINES
POSTGRADUATE PROGRAMME IN CHEMISTRY

**(Revised Syllabus under Semester System
with effect from 2025 Admissions)**

POSTGRADUATE PROGRAMME IN CHEMISTRY

PREAMBLE

The PG programme in M.Sc Chemistry shall extend over a period of two academic years comprising of four semesters, each of 450 hours in 18 weeks duration. The syllabus and scheme of examinations of the programme are detailed below. The syllabus is effective from 2025 admission.

1. Evaluation

1.1 Evaluation of each course shall be done in two parts – Continuous Evaluation [CE] or Continuous Assessment (CA) and End Semester Evaluation [ESE] or End Semester Assessment (ESA)

1.2 The distribution of marks for the above two shall be as follows:

Continuous Evaluation CE /CA - 25% of the total marks for each paper, End Semester Evaluation ESE/ESA - 75% of the total marks for the paper.

1.3 All records of Continuous Evaluation shall be kept in the Department and shall be made available for verification by any competent authority, if and when necessary.

2. Continuous Evaluation

2.1 The allocation of marks for each component under Continuous Evaluation shall be as given below:

Theory courses				Practical courses			
1	Attendance	5 marks		1	Attendance	5 marks	
2	Assignment	5 marks		2	Record	5 marks	
3	Seminar	5 marks		3	Practical viva	5 marks	
4	Internal test(s)	10 marks		4	Internal test(s)	10 marks	
Total		25 marks		Total		25 marks	

2.2 There shall be no Continuous Evaluation for the dissertation/project work.

3. Attendance

3.1 Students have to secure a minimum of 75% attendance for each course within a

semester to become eligible to register for each End Semester Examination. The attendance percentage will be calculated from the day of commencement of the semester to the last working day of

that semester as specified in the semester schedule. Periodic evaluation of each student's attendance shall be done by the respective Class Teacher within each semester [i.e., at least twice within each semester].

3.2 There will be no provision for condonation.

3.3 Reappearance of course(s) will be distinctly indicated in the final mark/grade sheet.

3.4 Allotment of marks

The allotment of marks for attendance shall be as follows:

Less than 75%	0 mark
75%	1 mark
76 to 80%	2 marks
81 to 85%	3 marks
86 to 90%	4 marks
Above 90%	5 marks

4. Assignments

4.1 Each student shall be required to do one assignment for each course in each semester.

4.2 The Class teacher shall explain to the students the expected quality of an assignment in terms of its structure, content, presentation etc.

4.3 Valued assignments must be returned to the students.

5. Tests

5.1 For each course there shall be two internal tests during a semester conducted by the department. The tentative dates of the Internals shall be announced at the beginning of each semester. Internal marks shall be awarded on the basis of the best mark scored in either of the two tests for each course.

It is mandatory that all students must appear for both tests. There will be provision for

retest if a student is absent in any one test. The scheme and question paper pattern for the test papers as well as for the End Semester Examination will be prepared by the Boards of Studies.

5.2 Valued answer scripts must be made available to the students for perusal in 10 working days from the date of the tests.

6. Seminar

6.1 Each student shall present a seminar in each course in each semester on a topic/area allotted.

6.2 Seminar presentations shall be done in the respective class room itself so as to benefit all the students. The interaction of the entire class is expected during the seminar presentations.

6.3 Seminars shall be evaluated on the basis of the quality of the presentation, content, interaction etc. The evaluation shall be done by the concerned teacher of the faculty who handles the topic/course.

NB: All the records of the continuous assessment must be kept in the department and be made available for verification by the concerned authorities, if necessary.

7. Comprehensive viva, R&D visit and Dissertation/Project Evaluation*

Dissertation/Project submitted at the end of the fourth semester will be valued by a Board of Examiners appointed and constituted by the Controller of Examinations. The maximum marks for the project/dissertation shall be **70**, of which **10** marks shall be allotted to the project-based viva-voce, which shall be conducted along with the comprehensive viva-voce examination. Detailed mark distribution is given below.

1	Comprehensive viva-voce	25 marks
2	Visit to R&D Centre	5 marks
3	*Project evaluation	
(i)	Introduction to the work/ Statement of the Problem	5 marks
(ii)	Review of Literature	5 marks
(iii)	Objectives	5 marks
(iv)	Materials and Methods	5 marks
(v)	Results and Discussion	15 marks
(vi)	Quality and Innovation	10 marks
(vii)	Language and style of presentation	5 marks
(viii)	References	5 marks
(ix)	Conclusions and future recommendations	5 marks
(x)	Dissertation viva-voce	10 marks
	Total	100 marks

SYLLABUS AND SCHEME OF EXAMINATION

(Revised syllabus under semester system with effect from 2025 admissions)

Course No and Title		Hours per week		Duration of ESA	Marks for CA	Marks for ESA	Total Marks
		L	P				
SEMESTER I*							
APCH121	Inorganic Chemistry I	5		3	25	75	100
APCH122	Organic Chemistry I	5		3	25	75	100
APCH123	Physical Chemistry I	5		3	25	75	100
APCH2PI	Inorganic Chemistry Practical I		3	(To be continued in Semester II)			
APCH2PII	Organic Chemistry Practical I		3	(To be continued in Semester II)			
APCH2PIII	Physical Chemistry Practical I		4	(To be continued in Semester II)			
Total marks for Semester I							300
*Distribution of teaching hours/week: Theory–15 hours, Practical's –10 hours							
SEMESTER II*							
APCH221	Inorganic Chemistry II	5		3	25	75	100
APCH222	Organic Chemistry II	5		3	25	75	100
APCH223	Physical Chemistry II	5		3	25	75	100
APCH2PI	Inorganic Chemistry Practical II		3	6	25	75	100
APCH2PII	Organic Chemistry Practical II		3	6	25	75	100
APCH2PIII	Physical Chemistry Practical II		4	6	25	75	100
Total marks for Semester II							600
*Distribution of teaching hours/week: Theory–15 hours, Practical's –10 hours							
SEMESTER III*							
APCH321	Inorganic Chemistry III	5		3	25	75	100
APCH322	Organic Chemistry III	5		3	25	75	100

APCH323	Physical Chemistry III	5		3	25	75	100
APCH4PIV	Inorganic Chemistry Practical II		3	(To be continued in Semester IV)			
APCH4PV	Organic Chemistry Practical II		3	(To be continued in Semester IV)			
APCH4PVI	Physical Chemistry Practical II		4	(To be continued in Semester IV)			
Total marks for Semester III							300
*Distribution of teaching hours/week: Theory–15 hours, Practical's –10 hours							
SEMESTER IV*							
APCH421	Chemistry of Advanced Materials and Research Methodology	5		3	25	75	100
APCH422a	Advanced Inorganic Chemistry	5		3	25	75	100
APCH422b	Advanced Organic Chemistry						
APCH422c	Advanced Physical Chemistry						
APCH4PIV	Inorganic Chemistry Practical II		3	6	25	75	100
APCH4PV	Organic Chemistry Practical II		3	6	25	75	100
APCH4PVI	Physical Chemistry Practical II		4	6	25	75	100
APCH423	Dissertation**					70	70
APCH424	Comprehensive viva-voce					25	25
	Visit to R&D Centre					5	5
Total marks for Semester IV							600
Grand Total (for semesters I – IV)							1800
*Distribution of teaching hours/week: Theory–10 hours, Practical's –10 hours, 5 hours for discussion on project.							

** 10 marks out of the 70 marks for dissertation will be for dissertation viva-voce.

Programme Specific Outcomes

- PSO 1 Develop a better understanding of the current chemical principles, methods and theories with the ability to critically analyse at an advanced level.

- PSO 2 Acquire solid knowledge of classical and modern experimental techniques and interpretation of results; thereby acquire the ability to plan and carry out independent projects.
- PSO 3 Develop the qualities of time management and organization, planning and executing experiments.
- PSO 4 Have a good level of awareness of the problems associated with health, safety and environment.
- PSO 5 Understand how chemistry relates to the real world and be able to communicate their understanding of chemical principles to a lay audience and as well apply the knowledge when situation warrants.
- PSO 6 Learn to search scientific literature and databases, extract and retrieve the required information and apply it in an appropriate manner.
- PSO 7 Demonstrate proficiency in undertaking individual and/or team-based laboratory investigations using appropriate apparatus and safe laboratory practices.
- PSO 8 Develop analytical solutions to a diversity of chemical problems identified from application contexts; critically analyse and interpret qualitative & quantitative chemical information's.
- PSO 9 Set the stage to make use of the wide range of career options open to chemistry graduates.

SEMESTER - I

APCH121: INORGANIC CHEMISTRY I

cO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	explain the functioning of the frontier materials in inorganic chemistry like Solid Electrolytes, Magnetic materials, Photocatalysts, Molecular materials and fullerides.	U	1,4, 6
2.	explain the preparation, properties and structure of isopoly acids of Mo, W and V and heteropoly acids of Mo and W.	U	1
3.	explain the unusual structure of certain inorganic molecules of Be, Cu and Ce.	U	1
4.	explain the preparation and properties of xenon fluorides, and identifying their utility as fluorinating agents.	U, Ap	1
5.	employ crystal field theory in analysing the splitting of d orbitals in octahedral, tetragonal, square planar, tetrahedral, trigonal bipyramidal and square pyramidal fields, calculate Crystal Field Stabilization Energy and Interpret Octahedral Site Stabilization Energy.	Ap, An u	1
6.	apply Jahn-Teller theorem and demonstrate evidence for J T effect, static and dynamic J T effect.	Ap	1
7.	illustrate MOT for octahedral and tetrahedral complexes with and without pi bonds and construct MO diagrams.	An C	1
8.	critically evaluate data from a variety of analytical chemistry techniques and apply knowledge of the statistical analysis of data.	Ap, E	1, 2
9.	interpret complexometric titrations, redox titrations, gravimetric titrimetric and titrations in non-aqueous solvents.	E, U	1, 2
10.	apply TG, DTA and DSC in the study of metal complexes.	Ap, An	1, 2
11.	identify the chemical processes occurring naturally in earth's atmospheric, aquatic and soil environments and evaluates the impacts of human perturbations to these processes.	An, E	4

PSO—Programme Specific Outcome

CO—Course Outcome

Cognitive Level:

R—Remember

U—Understanding

Ap—Apply

An—Analyse

E—Evaluate

C—Create

Module	Course Description	No. of Hrs	CO No.
1.0	Frontiers in Inorganic Chemistry	18	
1.1	Solid Electrolytes: Mixed oxides, cationic, anionic solid electrolytes, mixed ionic-electronic conductors.	4	1
1.2	Giant and colossal magnetoresistance by perovskite materials, Superparamagnetic materials	2	1
1.3	Solid state chemistry of metal nitrides and fluorides, chalcogenides, intercalation chemistry and metal-rich phases.	4	1
1.4	Inorganic pigments, Inorganic phosphors, Photocatalysts	4	1
1.5	Molecular materials and fullerides, basic idea of molecular materials chemistry like One dimensional metals, Molecular magnets and Inorganic liquid crystals.	4	1

2.0	Compounds with Special Structures	18	
2.1	Isopoly acids: Preparation, properties and structure of isopoly acids of Mo, W and V.	4	2
2.2	Heteropoly acids: Heteropoly acids of Mo and W. Keggin Structure, Keggin anions, Polyoxometalates.	4	2
2.3	Basic Beryllium nitrate $[\text{Be}_4\text{O}(\text{NO}_3)_6]$. Basic Beryllium acetate $[\text{Be}_4\text{O}(\text{OAc})_6]$, Beryllium oxalate $[\text{Be}(\text{ox})_2]^{2-}$ Copper acetate, $\text{Re}_2\text{Cl}_8^{2-}$, $[\text{Ce}(\text{NO}_3)_6]^{3-}$ Chevrel Phases,	4	3
2.4	Xenon fluorides, Structure of XeF_2 (MO theory only), Perxenate ion, Organo xenon compounds, Coordination compounds of Xenon. Xenon compounds as Fluorinating agents	6	4
3.0	Coordination Chemistry-I: Theories of Metal Complexes	18	
3.1	Crystal field theory: Splitting of d orbitals in octahedral, tetragonal, square planar, tetrahedral, trigonal bipyramidal and square pyramidal fields.	4	5
3.2	Jahn-Teller theorem, evidence for J T effect, static and dynamic J T effect.	2	6
3.3	Crystal Field Stabilization Energy. CFSE for d^1 to d^{10} systems. Octahedral Site Stabilization Energy. Factors affecting the splitting parameter.	4	5
3.4	Spectrochemical series. Evidence of covalency in Metal-Ligand bond, introduction to Ligand field theory.	2	5
3.5	Molecular Orbital Theory, Sigma and pi bonding in complexes. MO diagrams of octahedral and tetrahedral complexes with and without pi bonds.	4	7
3.6	Experimental evidence of pi bond on the stability of sigma bond. Nephelauxetic effect.	2	7
4.0	Analytical Principles	18	
4.1	Evaluation of analytical data: Accuracy and precision. Standard deviation, variance and coefficient of variation. Student 't' test, 'Q' test, and 'F' test. Confidence limits.	2	8
4.2	Errors: Classification, distribution, propagation, causes and minimization of errors. Significant figures and computation rules.	2	8
4.3	Correlation analysis: Scatter diagram. Correlation coefficient, r. Calculation of r by the method of least squares.	2	8
4.4	Volumetric methods: Classification of reactions in volumetry. Theory of indicators.	2	8
4.5	Complexometric titrations: Titration using EDTA-direct and back titration methods. Precipitation titrations. Redox titrations.	4	9
4.6	Titration in non-aqueous solvents. Organic reagents used in gravimetry: Oxine, dimethylglyoxime and cupferron.	2	9
4.7	Applications of TG, DTA and DSC in the study of metal complexes.	4	10
5.0	Chemistry of Natural Environmental Processes	18	
5.1	Chemistry of processes in atmosphere: Composition of the	3	11

	atmosphere. Automobile pollutants and the catalytic converter. Photochemical smog.		
5.2	Chemistry of the stratosphere. Catalytic destruction of ozone. Depletion of the ozone layer. Hazards of common air pollutants on the human health.	3	11
5.3	Chemistry of processes in hydrosphere: The hydrologic cycle. Cycling and purification. The unique properties of water. Acid-base properties.	4	11
5.4	Other natural cycles of the environment: Oxygen Cycle and Nitrogen Cycle	2	11
55	Chemistry of processes in Lithosphere: Redox status in soil. pE, pH predominance diagrams for redox sensitive elements Fe and Cr. Acidity in soil materials. Acid neutralization capacity and the quantification of the soil acidity. Ion speciation in soil solution. Cation exchange capacity and exchange phase composition.	6	11

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9. H.V. Jadhav, Elements of Environmental Chemistry, Himalaya Publication House, 2010.
10. E. Michael Essington, Soil and water Chemistry, CRC Press, 2nd edition, 2015.

Further Reading

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2. D. A. Skoog and D. M. West, Principles of Instrumental Analysis, Saunders College Publishing, 5th edition, 1998.
3. S. F. A. Kettle, Physical Inorganic Chemistry, Oxford University Press, 1st edition, 1998.
4. E. James Girard, Principles of Environmental Chemistry, Jones and Bartlett Publishers, 3rd Edition, 2013

APCH122: ORGANIC CHEMISTRY I

co No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	determine E and Z configurations of alkene system, R and S configuration for compounds with one or more chiral centers, biphenyls, allenes, spiranes and catenanes. P and M configuration for helical chiral compound.	U	1
2.	explain the conformations of open chain and ring systems and the factors affecting the same and understands how the conformation controls the reactivity of disubstituted cyclohexane system, fragmentation and intramolecular reactions.	U, Ap, An	1, 8
3.	explain stereoselective reactions and asymmetric synthesis	U, Ap, An	1
4.	explain the relation between optical activity and chirality	Ap, An	1
5.	identify Homotopic, Enantiotopic and diastereotopic ligands	An	1
6.	apply Cram's rule and Felkin — Ahn model	Ap, An	1
7.	identify the reactive intermediates involved in organic reactions and explain their structure and stability	Ap, An, E	1, 8
8.	identify C-C bond formation reactions by base and acid catalysed reaction	Ap, An, E	1, 8
9.	identify nucleophilic substitution reactions, electrophilic substitution reactions and explain their mechanism	U, Ap	1, 8
10.	explain electrophilic substitution on aromatic substrates	Ap, An	1
11.	explain C=C bond formation reactions and their mechanism	Ap, An	1

Module	Course Description	No. of Hrs	CO No.
1.0	Stereochemistry	18	
1.1	Cis — Trans isomerism — Resulting from Double bonds-E-Z Nomenclature, Mono cyclic compounds, fused and Bridged ring system, out-in isomerism. R-S configuration for one or more chiral centres.	2	1
1.2	Conformational analysis: Conformation in open chain systems — factors affecting conformations such as hydrogen bonding, steric hindrance, dipole moment. Conformation in six membered rings — cyclohexane and six membered rings containing hetero atoms, factors such as diaxial interaction, flag-pole interaction, anomeric effect. Conformation in fused systems such as decalin and 9-methyl decalin.	3	2
1.3	Effect of Conformation on the reactivity of substituted cyclohexane systems, stereochemical control in intramolecular reactions and Fragmentation reactions	2	2
1.4	Stereo selective reactions — Stereo selectivity of bromine addition across alkyne, Iodolactonization and epoxide ring opening reaction by nucleophile with acid catalyst and without acid catalyst	2	3
1.5	Optical activity and Chirality-Stereogenic carbon atom, quadrivalent stereogenic atom, trivalent stereogenic atom, adamantanes. Chirality in mono and disubstituted	3	4

	cyclohexane system. Chiral axis — biphenyls, allenes, spiranes, catenanes and their R-S configuration. Planar chirality — cyclophanes, Ansa compounds, trans cyclo alkenes and their R-S configuration. Helical chirality — P and M Nomenclature.		
1.6	Homotopic, Enantiotopic and diastereotopic ligands Identification by substitution addition criteria, symmetry criterion. prochiral faces — Pro R and Pro S, Re face and Si face attack.	2	5
1.7	Asymmetric synthesis — Enantiomeric excess or optical purity. Enantioselective synthesis by using chiral auxiliaries, alkylation of chiral enolates, chiral reagents and chiral catalysts such as [(S)][BINAP]Ru(OAc) ₂ , [R][BINAP]Ru(OAc) ₂ [DIPAMP] RhL ₂ ⁺ . OSQ ₄ With hydroquinidine and hydroquinine for asymmetric dihydroxylation, Bakers yeast and R-[BINAP] RuCl ₂ .	3	3
1.8	Diastereo selective synthesis Cram's rule and Felkin — Ahn model	1	6
2.0	Reactive Intermediates	18	
2.1	Carbenes — stabilité and structure — Formation of singlet and triplet carbenes, Reactions of carbenes, Rearrangement reactions in carbenes, Reimer-Tiemann reaction, Simmons-Smith reaction, Stereo and Regio selectivity of carbene addition across C—C.	2	7
2.2	Nitrenes — Stability and structure, formation of nitrenes — Reactions — Insertion, addition across C-C bond, rearrangement, abstraction, and dimerization.	3	7
2.3	Free radical — Structure and stability, Captodative effect, Applications of Bu ₃ SnH/AIBN, TEMPO, NBS and Sml ₂ .	3	7
2.4	Free radical reactions — Chlorination of alkane, addition of HX, SRN ¹ mechanism, Iodo decarboxylation, polymerisation, homolytic aromatic substitution, coupling of alkynes.	3	7
2.5	Kolbes electrolytic reaction, Ullman reaction, Hunsdieckers reaction, Acyloin condensation, McMurray reaction.	3	7
2.6	Barton reaction, Hofmann—Löffler—Freytag reaction, pinacol coupling reactions	2	7
2.7	Structure, formation and stability of carbocations and carbanions	2	7
3.0	C-C Bond Formation by Base and Acid Catalysed Reactions	18	
3.1	Common bases in organic reactions, Kinetic and thermodynamic deprotonating agents. — LDA, potassium tert-butoxide, cyclic amines and alkoxide.	3	8
3.2	Cannizaro reaction, Reformatsky reaction, Claisen ester condensation, Claisen reaction, Perkin reaction, Darzen reaction, Stobbe condensation, Henry reaction, Knoevenagel reaction	4	8
3.3	Thorpe reaction, Dieckmann reaction, Stork Enamine reaction, regio selectivity in enamine formation and Benzoin	2	8

	condensation.		
3.4	Aldol condensation, intramolecular aldol condensation, diastereoselectivity in aldol condensation, directed aldol condensation, Michael addition, 1,4 conjugated addition reactions by enolates, CN^- , RS^- and enamine, Robinson annulation	5	8
3.5	Alkylation of 1,3 diketones, β -ketoesters by using various bases, use of thiazolium ring in C—C bond formation	2	8
3.6	Prins reaction, Mannich reaction, acid catalysed aldol condensation.	2	8
4.0	Nucleophilic and Electrophilic Substitution Reactions	18	
4.1	Nucleophilic substitution at sp^3 carbon- SN^1 and SN^2 mechanism, competition between SN^1 and SN^2 reaction, Walden inversion, stereochemistry, effects of solvent, leaving group, and substrate structure on rates of SN^1 and SN^2 substitutions	4	9
4.2	Neighbouring group mechanism — a group with an unshared pair, n and a bonds (non-classical carbo cations), cyclopropyl, and phenyl. SN^1 mechanism, tetrahedral mechanism, ester hydrolysis. Nucleophilic substitution at vinylic carbon.	5	9
4.3	Phase transfer catalyst and its application to nucleophilic substitution reaction	1	9
4.4	Nucleophilic substitution on aromatic substrates — $\text{S}_{\text{N}}\text{Ar}$ mechanism on activated benzene system, pyridine and Quinoline system. Benzyne mechanism, $\text{S}_{\text{N}}1$ mechanism and Chichibabin reaction.	3	9
4.5	Electrophilic substitution on aromatic substrates— alkylation, nitration, nitrosation, sulphonation halogenation Vilsmeier-Haack reaction, Gattermann formylation, Gattermann-Koch formylation, orientation in disubstituted benzene, orientation in naphthalene and five membered, six membered heterocyclic systems containing one hetero atom and fused heterocyclic systems quinoline and iso quinoline.	5	10
5.0	C=C Bond Forming Reactions	18	
5.1	Elimination reaction leading to C=C bond formation and their mechanism, E1 , E2 and E1cB mechanism	5	11
5.2	Stereo aspects of C=C bond formation in cyclic and acyclic systems — Bredt's rule — Regio selectivity in elimination, Hoffmann and Saytzeff elimination, Effect of basicity, temperature, leaving group and substrate structure.	5	11
5.3	Cis elimination — esters, sulfoxides, selenoxides, Chugaev reaction, Cope elimination. Stereo aspects of cis elimination in cyclic and bicyclic system	4	11
5.4	Alkenes from — hydrazones -Shapiro reaction — 1,2 diols, alkynes, Lindlars catalyst, $\text{Na}/\text{NH}_3/\text{C}_2\text{H}_5\text{OH}$ [$\text{Cp}_2\text{Zr}(\text{H})\text{Cl}$]	4	11

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8. R. K. Mackie, D. M. Smith and R. A. Aitken, Guide Book to Organic Synthesis, 2nd edition, Longman.
9. Jerry March, Advanced Organic Chemistry-Reactions, Mechanism and Structure, Wiley Interscience, 2004.
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APCH123: PHYSICAL CHEMISTRY I

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able</i>	Cognitive Level	PSO No.
1.	outline the development of quantum mechanics and its tools and apply them in determining the wave functions and energies of moving particles.	U, Ap, An	1
2.	recognize the nature of adsorption and propose theories and choose theoretical and instrumental methods of measurements of surface property.	U, Ap, An	1
3.	understand theory and mechanism of catalytic action.	U	1
4.	understand and appraise the mechanism and kinetics of enzyme catalysis	U, An	1
5.	correlate thermodynamic properties and apply them in systems.	U, Ap, An	1
6.	understand theories, mechanism and, kinetics of reactions and solve numerical problems.	U, Ap, An	1
7.	identify point groups and construct character table and predict hybridization and spectral properties of molecules.	U, Ap, C	1

Module	Course Description	No. of Hrs	CO No.
1.0	Quantum Chemistry I	18	
1.1	Postulates of quantum mechanics: State function postulate: Born interpretation of the wave function, well behaved functions, normalization, orthonormality of wave functions, Kronecker delta symbol.	1	1
1.2	Operator postulate: Operator algebra, linear and nonlinear operators, Laplacian operator, commuting and non-commuting operators, Hermitian operators and their properties. Non-commuting property of operators, the uncertainty principle	2	1
1.3	Eigen value postulate: eigen value equation, Schrodinger wave equation as an eigen value equation, eigen functions of commuting operators.	2	1
1.4	Expectation value postulate. Postulate of time-dependent Schrödinger equation, Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (L_x L_y L_z and L^2) and their commuting properties (derivation not required).	2	1
1.5	Application of Quantum mechanics to Exactly Solvable Model Problems. Translational motion: free particle in one-dimension, particle in one dimensional box its application to conjugated systems, two-dimensional box (rectangular and square box), three-dimensional box and cubical box, concept of degeneracy	3	1
1.6	Particle with finite potential barriers, one potential barrier, two finite barriers. Quantum mechanical tunnelling, Applications in Scanning Tunnelling Microscopy (STM)	3	1
1.7	Vibrational motion: one-dimensional harmonic oscillator	3	1

	(complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features of wave Functions.		
1.8	Schrödinger wave equation for 3D-harmonic oscillator, expressions for energy and wave function, degeneracy of energy levels (derivation not required).	2	1
2.0	Surface Chemistry and Catalysis	18	
2.1	Types of adsorptions. Heat of adsorption-integral differential and isosteric heat of adsorption and their determination.	1	2
2.2	Adsorption isotherms - Freundlich and Langmuir isotherms. Statistical derivation of Langmuir adsorption isotherm. Multilayer adsorption- classification, the BET theory and Harkins-Jura theory.	3	2
2.3	Determination of surface area of solids-Harkins-Jura absolute method, point B method, Langmuir method and BET method. Determination of surface acidity-TPD method	4	2
2.4	Adsorption from solutions: Gibb's adsorption equation and its verification. Adsorption with dissociation. Adsorption with interaction between adsorbate molecules.	2	2
2.5	Different types of surfaces, properties of surface phase. Thermodynamics of surface.	1	2
2.6	Selected Surface characterization methods: PES, XPES, Auger electron spectroscopy. Low Energy Electron Diffraction (LEED) and Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy.	3	2
2.7	Surface films-different types, surface pressure and its measurement.	2	3
2.8	Catalysts: Mechanism and theories of homogeneous and heterogeneous catalysis. Bimolecular surface reactions. Langmuir-Hinshelwood mechanism. Enzyme catalysis-Michaelis-Menten theory, Lineweaver-Burk plot. Eadie-Hofstee method.	2	4
3.0	Classical Thermodynamics	18	
3.1	Laws of Thermodynamics and its concepts. Concept of Entropy - Dependence of entropy on variables of a system (S, T and V; S, T and P). Entropy of mixing, Thermodynamic equations of state. Criteria for equilibrium and spontaneity, Gibbs and Helmholtz free energy.	2	5
3.2	Euler's relation. Maxwell relations and significance, temperature dependence of free energy, Gibbs-Helmholtz equation and its applications.	2	5
3.3	Partial molar quantities - Chemical potential, Gibbs Duhem equations, determination of partial molar properties-partial molar volume and partial molar enthalpy.	2	5
3.4	Fugacity – relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Fugacity of liquid mixtures, fugacity of mixture of gases, Lewis-Randall rule.	3	5
3.5	Activity, activity coefficients, dependence of activity on temperature and pressure. Determination of activity and activity coefficients of electrolytes and non-electrolytes.	2	5

3.6	Thermodynamics of mixing, Duhem-Margules equation, Konowaloff's first and second laws, Henry's law, excess thermodynamic functions-determination of excess enthalpy and volume.	4	5
3.7	Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium-van't Hoff reaction isochore and isotherm.	3	5
4.0	Chemical Kinetics	18	
4.1	Theories of reaction rates: Collision theory and its derivation, limitations. Transition state theory: Eyring equation-derivation, Comparison of the two theories. Thermodynamic formulation of the reaction rates.	3	6
4.2	Theories of unimolecular reactions - Lindemann theory. Lindemann-Hinshelwood mechanism, qualitative idea of RRK and RRKM theory.	2	6
4.3	Kinetics of complex reactions- Parallel reactions, opposing reactions, consecutive reactions and chain reactions, steady state treatment, kinetics of $\text{H}_2\text{-Cl}_2$ and $\text{H}_2\text{-Br}_2$ reactions, decompositions of ethane, acetaldehyde and N_2O_5 . Rice-Herzfeld mechanism, branching chain reactions, Hinshelwood mechanism of chain reactions and explosion.	4	6
4.4	Kinetics of fast reactions: Relaxation method-temperature, pressure and field jump methods, flow method-continuous, stopped and quenched flow methods, shock method and flash photolysis. Introduction to femtosecond methods. Molecular beams: Principle of crossed-molecular beams; Potential energy surfaces - attractive and repulsive surfaces, London Equation.	3	6
4.5	Reactions in solution: Factors affecting reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation.	3	6
4.6	Kinetic effects: Primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship. Hammett equation and Taft equation.	3	6
5.0	Molecular Symmetry and Group Theory	18	
5.1	Symmetry elements and symmetry operation. Matrix representation Block factored matrices, Character of a matrix. Conditions for a set of elements to form a mathematical group. Point groups and their systematic identification.	2	7
5.2	Multiplication of operations. Group multiplication table (C_{2v} , C_{3v} , C_{2h} , C_3 and C_6). Similarity transformation and classification of symmetry operation, Reducible and Irreducible representations.	3	7
5.3	The Great Orthogonality Theorem. Rules derived from GOT (proof not required).	1	7
5.4	Setting up of character table of C_{2v} , C_{3v} . and C_{2h} groups. Reduction formula, reduction of reducible representation to IRs. Importance of IRs. Transformation properties of atomic orbitals.	4	7

5.5	Applications of character tables: Hybridisation- identification of atomic orbitals taking part in hybridisation of BF_3 and CH_4 molecules. Inverse transformation and construction of hybrid orbitals	4	7
5.6	Spectroscopy: Direct product representations, vanishing and non-vanishing integral, transition moment integral. Determination of number of IR-active and Raman active vibrations by taking simple molecules belongs to C_{2v} , C_{3v} and C_{2h} point groups as example. Rationalization of rule of mutual exclusion principle using group theory.	4	7

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6. T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006.
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8. W. D. Harkins, The Physical Chemistry of Surface Films, Reinhold.
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12. S. Glasstone, Thermodynamics for Chemists, East —West Press Private Ltd., New Delhi.
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16. J. Rajaram and J. C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.
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20. A Salahuddin Xunju, G Krishnan, Group Theory and Its Applications In Chemistry, Second Edition, PHI Learning Pvt. Ltd, Delhi 2015.
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Further Reading

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2. P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, 5th Edn., Oxford University Press, 2010.
3. R. A. Albert and R. J . Silby, Physical Chemistry, Wiley Eastern
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6. L.H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill, 1969.
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APCH2PI: INORGANIC CHEMISTRY PRACTICALS I

Total 125 h

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	interpret data from an experiment, including the construction of appropriate graphs and the evaluation of errors.	U, E	3, 7, 8
2.	estimate volumetrically the concentration of Zn, Mg and Ni using EDTA and the volumetric estimation of Fe.	Ap, An	7, 8
3.	estimate volumetrically the hardness of water and concentration of Ca in water samples using EDTA.	Ap, An	7, 8
4.	estimate colorimetrically the concentration of Chromium - (using Diphenyl carbazide), Iron (using thioglycollic acid), Iron (using thiocyanate), Manganese (using potassium periodate), Nickel (using dimethyl glyoxime).	Ap, An	7, 8
5.	carry out the preparation of the metal complexes Potassium trioxalatochromate(III), Tetraammoniumcopper (II) sulphate, Hexamminecobalt(III) chloride.	Ap	7, 8
6.	record the UV spectra, IR spectra, magnetic susceptibility, TG, DTA and XRD of the complexes prepared.	Ap, An	2, 7, 8

Module	Course Description	No. of Hrs	CO No.
1.	Volumetric estimation using EDTA - Zn, Mg, Ni (back titration), Hardness of water, Ca (using murexide).	25	1, 2, 3
2.	Determine the hardness of water and the concentration of Ca in water samples using EDTA.	20	1, 2, 4
3.	Volumetric estimation of Fe.	10	1, 2, 3
4.	Colorimetric estimation of Chromium — (Diphenyl carbazide), Iron (thioglycollic acid), Iron (thiocyanate), Manganese (potassium periodate), Nickel (dimethyl glyoxime).	35	1, 2, 5
5.	Preparation of metal complexes - Record UV, IR, magnetic susceptibility, TG, DTA and XRD of the complexes prepared (a) Potassium trioxalatochromate (III) (b) Tetraammoniumcopper (II) sulphate (c) Hexamminecobalt (III) chloride	35	1, 2, 6, 7

References

1. A. I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 4th edition, 1978.
2. A. I. Vogel, A Text Book of Qualitative Inorganic Analysis, Longman 5th edition, 1979.
3. D. A. Skoog and D. M. West, Analytical Chemistry: An Introduction, Saunders College Publishing, 4th edition, 1986.
4. W. G. Palmer, Experimental Inorganic Chemistry, Cambridge University,

APCH2PII: ORGANIC CHEMISTRY PRACTICALS I

Total 125 h

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	interpret data from an experiment, including the construction of appropriate graphs and the evaluation of errors.	U, E	3, 7, 8
2.	determine the correct method for separation of a binary mixture and make the separated compounds in pure form.	An, E	2, 7, 8
3.	develop thin layer chromatogram of a compound and determine its purity.	C	2, 7, 8
4.	separate two compounds by column chromatography.	An	2, 7, 8
5.	utilize the synthetic procedures and reagents to convert a compound into another. Differentiate the products by spectroscopic methods.	An	2, 7, 8
6.	use green chemical principles in the synthesis.	Ap	2, 4
7.	solve GC MS and LC MS of a compound to ascertain purity and identity, apply the basic principles	Ap, E	2, 7

Module	Course Description	No. of Hrs	CO No.
1.	Separation and identification of organic compounds- a. Quantitative wet chemistry separation of a mixture of two components by solvent extraction. b. TLC of the purified samples along with the mixture in same TLC plates (component 1 with mixture and component 2 with mixture on separate TLC plate) and calculation of R _f values- Reporting and recording TLC in standard formats- preparation of sample solution, adsorbent, dimensions of the plate, saturation time, developing time, visualization and detection, R _f Value, Drawing - in the form of a table.	30	1, 4, 5
2.	Separation of a mixture by column chromatography (not for end semester evaluation) a. Malachite green and methylene blue, b. o-nitroaniline and p-nitroaniline.	20	1, 4
3.	Preparation of compounds by two stages. • Recording UV, IR, ¹ H—NMR and ¹³ C—NMR and EI mass spectra of synthesized compounds. • Record and interpret GC—MS and LC—MS of the purified compound. • TLC analysis-Stage 1 reactants and products on TLC plate 1 and stage 2 reactants and products on plate 2). • Record TLC in standard format as in separation. <i>All preparations must restricted to 1 g level</i> I. Nitration (1) Acetanilide → p-nitroacetanilide → p-nitroaniline (2) (2-Methylbenzoate → methyl m-nitrobenzoate → m-nitrobenzoic acid) II. Bromination (3) Acetanilide → p-bromoacetanilide → p-bromoaniline	75 <i>(average 12.5 hrs for preparation and analysis of each)</i>	1, 5, 6, 7

	<i>using CAN for bromination</i> III. Aldol condensation- Synthesis of heterocycles. (4) Benzaldehyde → Dibenzylideneacetone → 1,5-Diphenyl-3-styryl-2-pyrazoline IV. Diazocoupling (5) Aniline → Diazoaminobenzene → p-aminoazobenzene V. Rearrangement (6) Pthalic anhydride → Pthalimide → Anthranilic acid VI. Synthesis of Dyes (7) N,N-Dimethylaniline → N,N-dimethyl-4-nitrosoaniline → methylene blue	
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The board of examiners have to select either TLC of separated components OR TLC of preparation for an examination. But both TLC examinations are to be practiced and entered in the record of experiments.

References

1. B. S. Furniss, Vogel's text book of practical organic chemistry, 5th Edition, Longman, 1989.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz and R. G. Engel, A microscale approach to organic laboratory techniques, Wadsworth Publishing, 5th Edition, 2012.
3. R. K. Bansal, Laboratory manual of organic Chemistry, Wiley Eastern, 1994.
4. N. K. Vishnoi, Advanced Practical Organic Chemistry, 3rd Edition, Vikas
5. F. G. Mann and B. C. Saunders, Practical Organic Chemistry, Pearson Education, 2009.
6. J. B. Cohen, Practical organic chemistry, Forgotten Books, 2015
7. P. F Shalz, Journal of Chemical Education, 1996, 173: 267.
8. Monograph on green laboratory experiments, DST, Govt. of India, pp 1-79.
9. For spectral data of organic compounds, see: http://sdb.sriodb.aist.go.jp/sdb/cgi-bin/directframe_top.cgi.

APCH2PIII: PHYSICAL CHEMISTRY PRACTICALS I

Total 125 h

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	interpret data from an experiment, including the construction of appropriate graphs and the evaluation of errors.	U, E	3, 7, 8
2.	construct Freundlich & Langmuir isotherms for adsorption of acetic/oxalic acid on active charcoal/ alumina & determine the concentration of acetic/ oxalic acid	C, Ap, An	7, 8
3.	determine the rate constant, Arrhenius parameters, rate constant and concentration using kinetics	Ap	7, 8
4.	construct the phase diagram and determine the composition of an unknown mixture	Ap, An	7, 8
5.	construct the ternary phase diagram of acetic acid chloroform-water system and outline the procedure in an unfamiliar situation to find out the composition of given homogeneous mixture.	C, Ap, An	7, 8
6.	Construct the tie-line in the ternary phase diagram of acetic	C, Ap,	7, 8

	acid chloroform-water system	An	
7.	determine distribution coefficient using distribution law.	Ap	7, 8
8.	determine the equilibrium constant employing the distribution law.	Ap	7, 8
9.	determine the coordination number of Cu^{2+} in copper-ammonia complex.	Ap	7, 8
10.	determine the viscosity of liquid mixtures and use this in determining the concentration of a component in a mixture	Ap, An	7, 8
11.	determine surface tension and parachor of liquids.	Ap	7, 8
12.	ascertain the relationship between surface tension with concentration of a liquid and use this to find out the composition of given homogeneous mixture.	Ap, An	7, 8
13.	determine the concentration of given strong acid/alkali.	Ap, An	7,8
14.	determine the heat of ionisation of acetic acid.	Ap, An	7,8
15.	determine the heat of displacement of Cu^{2+} by Zn.	Ap, An	7, 8

Module	Course Description	No. of Hrs	CO No.
1	Adsorption a) Freundlich and Langmuir isotherms for adsorption of acetic/oxalic acid on active charcoal/ alumina. b) Determination of concentration of acetic/ oxalic acid.	15	1, 2,
2	Kinetics a) Determination of rate constant of acid hydrolysis of methyl acetate. b) Determination of Arrhenius parameters. c) Determination of concentration of given acid. d) Determination of rate constant of the saponification of ethyl acetate and evaluation of Arrhenius parameters. e) Determination of rate constant of reaction between $\text{K}_2\text{S}_2\text{O}_8$ and KI.	20	1, 3
3	Phase rule I. Solid-liquid equilibria a) Construction of phase diagram and determination of the composition of unknown mixture (naphthalene/ biphenyl, naphthalene/ benzophenone, naphthalene/ diphenyl amine). b) Construction of phase diagram with simple eutectic - naphthalene/ metadinitrobenzene. II. Partially miscible liquid pairs a) CST of phenol-water system. b) Three component system - Construction of ternary phase diagram of acetic acid chloroform- water system and hence the composition of given homogeneous mixture. Construction of tie-line.	20	1, 4, 5, 6
4	Distribution law a) Distribution coefficient of ammonia between hexane and water. Determination of equilibrium constant of copper - ammonia complex by partition method or coordination number of Cu^{2+} in copper-ammonia complex.	20	1, 7, 8, 9

	b) Distribution coefficient of benzoic acid between toluene and water. c) Distribution coefficient of iodine between hexane and water. d) Determination of the equilibrium constant of the reaction $KI + I_2 \rightleftharpoons KI_3$ and hence the concentration of given KI in hexane and water.		
5.	Viscosity a) Viscosity of liquids and mixtures of liquids. b) Verification of Kendall's equation. c) Composition of unknown mixtures. d) Determination of molecular masses of polymers by viscosity measurements (Mark-Houwink equation)	15	1, 10
6.	Surface tension a) Determination of surface tension of various liquids (water - ethanol, water - glycerol, water - sorbitol, nitrobenzene-toluene) by Stalagmometric method (drop number/ drop weight) and by Capillary rise method. b) Determination of parachors of molecules and various groups. c) Determination of concentration of a mixture. d) Determination of surface tension and parachor of liquids using double capillary method. e) Variation of surface tension with concentration. Unknown concentration of a mixture. Interfacial tension. f) Determination of surface excess and area per molecule.	20	1, 11, 12
7.	Thermochemistry a) Determination of the concentration of given strong acid/alkali. b) Thermometric titration of NaOH vs standard HCl. c) Heat of displacement of Cu^{2+} by Zn. d) Determination of the heat of ionisation of acetic acid.	15	1, 13, 14, 15

References

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2. B. P. Levitt and J. A. Kitchener, Findlay's Practical Physical Chemistry, Longmans, London, 9th Edn., 1973.
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4. A. M. James and F. E. Pichard, Practical Physical Chemistry, Longman.
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6. B. Viswanathan, Practical Physical Chemistry, Viva Publications, 2012.
7. P. S. Sindhu, Practicals in Physical Chemistry-A Modern Approach, McMillan India, 2005.
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First Semester M.Sc. Degree Examination - Model question paper
APCH121: INORGANIC CHEMISTRY I
(2025 admission Onwards)

Time: 3 Hrs

Max. Marks: 75

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) What are inorganic phosphors?
(b) List any two advantages of solid electrolytes over conventional electrolytes.
(c) What are single molecule magnets?
2. (a) Give one method for preparation of polysiloxanes.
(b) Complete the reactions
(i) $\text{C}_6\text{F}_5\text{XeF} + \text{Cd}(\text{CLF})_2$ (ii) $\text{C}_6\text{F}_5\text{XeF} + (\text{CH}_3)_3\text{SiCN}$
(c) On the basis of VSEPR theory, determine the probable structure of perxenate ion.
3. (a) Sketch the splitting of d orbitals in a trigonal bipyramidal complex.
(b) Which among CN^- and NH_3 have a higher nephelauxetic effect? Why?
(c) Calculate the CFSE for a d^4 ion.
4. (a) Differentiate accuracy from precision.
(b) What are metallochromic indicators? Give an example.
(c) What is a Student's t test used for?
5. (a) List two conditions that favour the formation of photochemical smog.
(b) Discuss briefly a method to quantify soil acidity.
(c) How do chlorine free radicals tamper the ozone layer?

(2 x 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) Give an account of cationic SSE's.
(b) Discuss the structural aspects of metal nitrides.
7. (a) Discuss the uniqueness of the structure of BBN.
(b) Briefly explain about the Chevrel phase.
8. (a) State and illustrate Jahn-Teller distortion.
(b) Discuss the factors affecting the magnitude of A_o .
9. (a) What is a scatter diagram? What is its significance?
(b) Discuss briefly the principle behind EDTA titrations.
10. (a) Name any two common air pollutants. What are their hazards?
(b) Give a brief account of hydrological cycle.

[5 x 5 = 25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. What are molmats? What are their advantages? Discuss any two categories of Molmats.

12. Write a note on preparation and properties of heteropoly acids of Mo and W.
13. Explain molecular orbital theory of bonding in the complex $[\text{Co}(\text{NH}_3)_6]^{3+}$.
14. (a) Differentiate between co-precipitation and post-precipitation. How do they affect quantitative analysis? How they can be avoided?
(b) Describe the use of oxine as precipitant in gravimetry. [7+3]
15. What are pourbaix diagrams? Outline its role in explaining the chemistry of processes in lithosphere.

[10 3 = 30]

First Semester M.Sc. Degree Examination - Model question paper
APCH122: ORGANIC CHEMISTRY I
 (2025 admission Onwards)

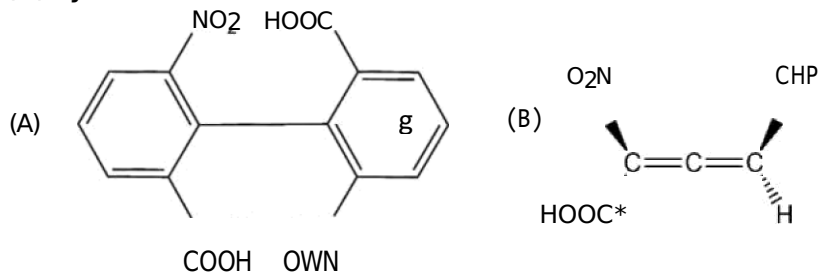
Time: 3 Hrs

Max. Marks: 75

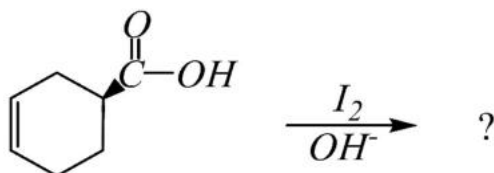
SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

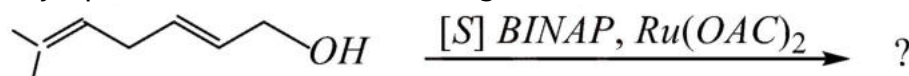
1. (a) Identify the 'R' or 'S' configuration for the following biphenyl (A) and allene (B) systems?



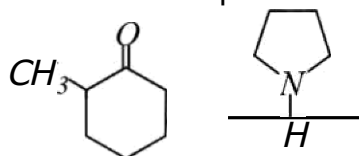
- (b) The major product formed in the following reaction is



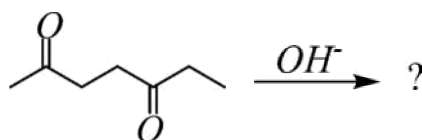
- (c) The major product formed in the following reaction is



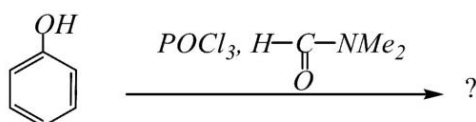
2. (a) What is the application of NBS?
 (b) What is Mc Murray reaction?
 (c) What is the application of Samarium Iodide?
3. (a) What is the basic difference between LDA and potassium tertiary butoxide?
 (b) What will be the product formed in the following reaction?



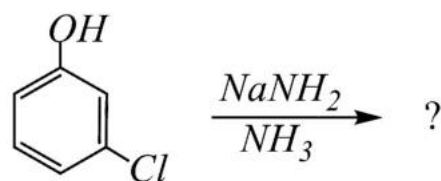
- (c) What will be the major product formed in the following reaction?



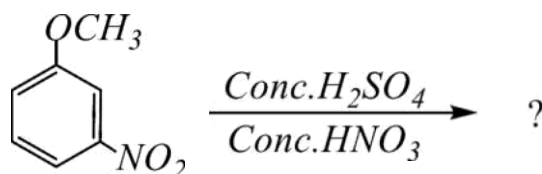
4. (a) What will be the major product formed in the following reaction?



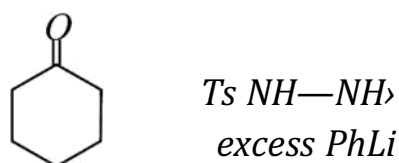
- (b) What will be the major product formed in the following reaction?



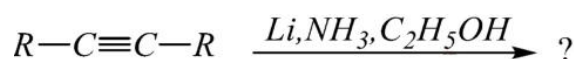
(c) What will be the major product formed in the following reaction?



5. (a) What is Bredt's rule?
 (b) What will be the major product formed in the following reaction?



(c) What will be the major product formed in the following reaction?

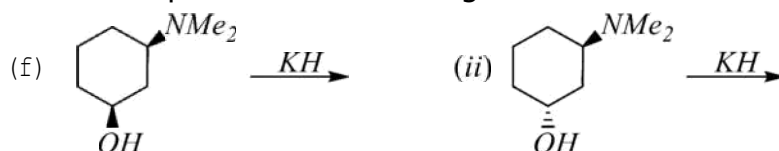


[2 x 10 = 20]

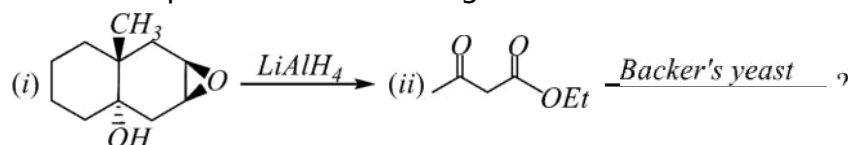
SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

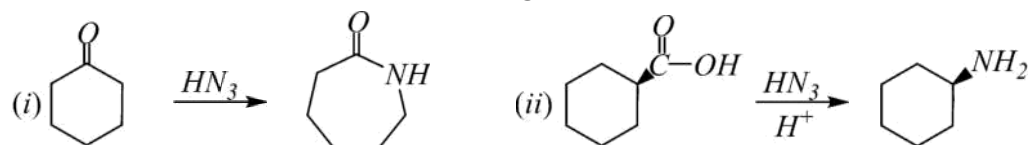
6. (a) Predict the product of the following reaction



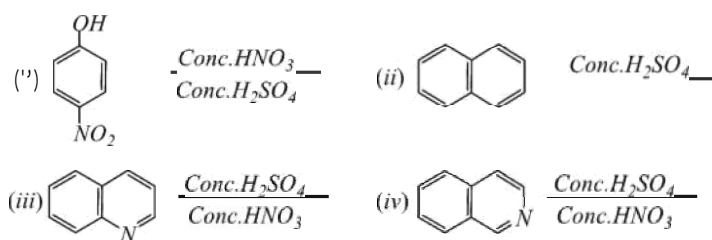
- (b) Predict the product of the following reaction



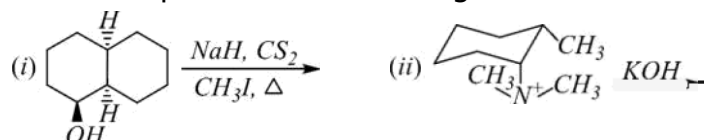
7. (a) Write a note on Barton reaction with mechanism?
 (b) Predict the mechanism for the following?



8. (a) Write a note on Benzoin condensation?
 (b) Write a note on Robinson annulation?
9. (a) Explain how the cyclopropyl and phenyl group acting as an anchimeric assistance?
 (b) Predict the major product in the following reaction.



10. (a) Write down the application of the Zirconium compound $[\text{Cp}_2\text{Zr}(\text{H})\text{Cl}]$?
 (b) Predict the product in the following reaction?



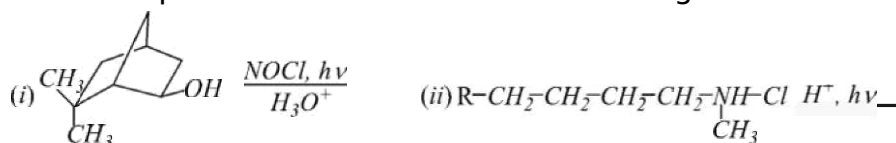
[5 5 =25]

SECTION C

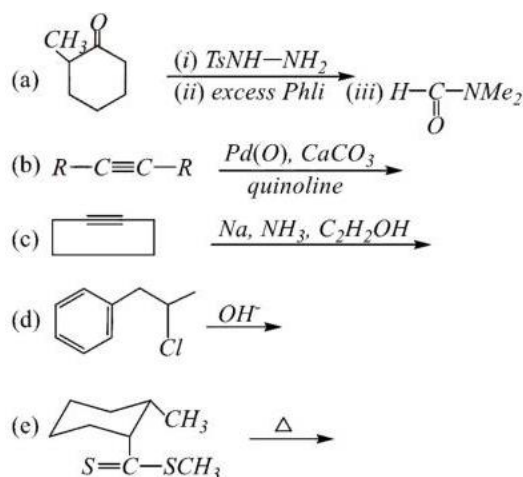
Answer any three questions. Each question carries 10 marks

11. (a) Explain how the conformation controls the reactivity of disubstituted cyclohexane system with examples.
 (b) Explain the optical activity exhibited by biphenyl, allene and spiro system.

12. Predict the product and mechanism of the following reaction.



13. (a) Write a note on diastereoselectivity in aldol reaction?
 (b) Write a note on Prins and Mannich reaction?
14. (a) Write a note on Neighbouring group mechanism in aliphatic nucleophilic substitution reaction?
 (b) Write the mechanism involved in Reimer-Tiemann formylation and Vilsmeier formylation?
15. Write down the products of the following?



[30]

[10 × 3 = 30]

First Semester M.Sc. Degree Examination — Model question paper
APCH123: PHYSICAL CHEMISTRY I
(2025 admission Onwards)

Time: 3 Hrs

Max. Marks: 75

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) Normalize the function e^{-n} within the limit 0 to n
(b) Show that the time-independent Schrodinger wave equation is an eigen value equation.
(c) Explain the concept of degeneracy with reference to particle in a cubic box problem.
2. (a) Distinguish between associative and dissociative chemisorption.
(b) Outline the principle of EXAFS.
(c) Explain one method of determination of surface pressure.
3. (a) Calculate entropy of mixing when 2 moles of Xe, 3 moles of He and 2 moles of H_2 are mixed at fixed temperature assuming ideal behaviour and no chemical change.
(b) Write any two Maxwell's relations and give their significance.
(c) State and explain Lewis- Randall rule.
4. (a) Explain the flash photolysis method for the study of kinetics of fast reactions.
(b) Explain steady state principle?
(c) How volume of activation affects the reaction rate?
5. (a) Identify the symmetry elements present in the following and assign the point group
(i) H_2 (ii) CO
(b) Explain improper axis of symmetry with an example
(c) Why cyclic groups are abelian?

[2 × 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) Discuss quantum tunnelling? How quantum tunnelling is applied in STM?
(b) Prove that the position and momentum operators by evaluating the commutator.
7. (a) Write any two methods for the determination of surface area of a solid.
(b) Discuss the Lineweaver-Burk method in enzyme catalysis.
8. (a) Derive Van't Hoff isotherm. How is this useful in the study of chemical equilibria?
(b) Derive Gibbs-Duhem equation.
9. (a) Discuss the kinetics of unimolecular reactions based on the Lindemann theory.
(b) Derive the rate law for the decomposition of N_2O_5 .

10. (a) Construct the group multiplication table for the symmetry operations of NHS molecule.
 (b) Determine the number of active IR and Raman lines in the vibrational spectrum of CH Cl.

[5 x 5 = 25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. Discuss the postulates of quantum mechanics.
 12. Explain any two instrumental techniques used for surface characterization.
 13. Write a brief account of the methods for the determination of activity coefficient of electrolytes and non-electrolytes.
 14. Derive expression for collision theory of reaction rate. Compare collision theory and transition state theory.
 15. (a) Explain the hybridization scheme in BF₃ molecule using group theory.
 (b) Show that the four elements of C_{2v} point groups forms 4 classes?

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1		R_z	
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)

[10 x 3 = 30]

SEMESTER - II

APCH221: INORGANIC CHEMISTRY II

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	obtain the term symbols of d^n system and determine the splitting of terms in weak and strong octahedral and tetrahedral fields.	E	1
2.	explain the correlation diagrams for d^n and d^{0-n} ions in octahedral and tetrahedral fields and interprets electronic spectra of complexes.	U, E	1
3.	applies magnetic measurements in the determination of structure of transition metal complexes.	Ap	1
4.	relates crystalline structure to X-ray diffraction data and the reciprocal lattice and explains the diffraction methods	U	1
5.	explains crystal defects.	U	1
6.	elaborates the structure of selected compounds of AX, AX ₂ , A ₂ X ₃ and spinels.	C	1
7.	explains the electronic structure of solids using free electron theory and band theory.	E	1
8.	understands the differences in semiconductor and dielectric materials and their electrical and optical properties	U, E	1
9.	explain the structure and reactions of S—N, P—N, B—N, S—P, Se compounds and boron hydrides.	U, E	1
10.	analyse the topological approach to boron hydride structure and estimates styx numbers and apply Wade's and Jemmis rules in borane and carboranes.	Ap, An, E	1
11.	explain the characteristic properties of lanthanides and actinides.	Ap	1
12.	sketches the shapes of f orbital and shows their splitting in cubic ligand field.	U	1
13.	elaborates the importance of the beach sands of Kerala and their important components.	C	1

PSO—Programme Specific Outcome

CO—Course Outcome

Cognitive Level:

R—Remember

U—Understanding

Ap—Apply

An—Analyse

E—Evaluate

C—Create

Module	Course Description	No. of Hrs	CO No.
1.0	Coordination Chemistry-II: Spectral and Magnetic Properties of Transition Metal Complexes	18	
1.1	Electronic spectra of metal complexes-Term symbols of d^n system, splitting of terms in weak and strong octahedral and tetrahedral fields.	4	1
1.2	Correlation diagrams for d^n and d^{0-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.	3	2
1.3	Interpretation of electronic spectra of complexes- Orgel diagrams, Tanabe-Sugano diagrams, Racah parameters, calculation of Dq , B and β (Nephelauxetic ratio) values, charge transfer spectra. Charge-Transfer and Energy	3	2

	Applications		
1.4	Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy's method for the determination of magnetic moment of complexes, spin only magnetic moment.	4	3
1.5	Temperature dependence of magnetism. Temperature Independent Paramagnetism (TIP). Spin state crossover, Antiferromagnetism - inter and intra molecular interaction.	2	3
1.6	Application of magnetic measurements in the determination of structure of transition metal complexes.	2	3
2.0	Crystalline State	18	
2.1	Crystal symmetry- Introduction to point groups and space groups. Miller indices. Reciprocal lattice concept.	2	4
2.2	X-ray diffraction by crystals: Function of crystals. Transmission grating and reflection grating. Bragg's equation.	2	4
2.3	Diffraction methods: Powder and rotating crystal. Indexing and determination of lattice type and unit cell dimensions of cubic crystals.	3	4
2.4	Crystal defects: Perfect and imperfect crystals. Point, line and plane defects. Thermodynamics of Schottky and Frenkel defects.	3	5
2.5	Colour centers in alkali halide crystals. Defect clusters. Extended defects: Crystallographic shear structure and stacking faults. Dislocations and crystal structure.	3	5
2.6	Structure of compounds of AX (Zinc blende, Wurtzite), AX ₂ (Rutile, fluorite, antiferite), A _m X ₂ (Nickel arsenide), ABX ₃ (Perovskite, Ilmenite), Spinel. Inverse spinel structures. Pyrochlore (A ₂ B ₂ O ₇)	5	6
3.0	Solid State Chemistry	18	
3.1	Electronic structure of solids. Free electron theory, band theory. Refinements to simple band theory, k space and Brillouin zones. Fermi levels	4	7
3.2	Conductors, insulators and semiconductors. Band structure of conductors, insulators and semiconductors and their applications.	3	7
3.3	Intrinsic & extrinsic semiconductors, doping of semiconductors & conduction mechanism, the band gap.	3	7
3.4	Temperature dependence of conductivity, carrier density and carrier mobility in semiconductors.	2	7
3.5	Superconductivity, Type I and Type II superconductors. Low temperature superconducting alloys, High Temperature Superconductors (YBa ₂ Cu ₃ O ₇ and Related Compounds) Photoconductivity, Photovoltaic effect.	3	7
3.6	Dielectric properties. Dielectric materials. Ferroelectricity, pyroelectricity, piezoelectricity and ionic conductivity. Applications of ferro, piezo and pyroelectrics.	3	8
4.0	Compounds of S, N, P, B, Se	18	
4.1	Sulphur-Nitrogen compounds: S ₄ N ₄ , S ₂ N ₂ , S ₄ N ₂ , (SN) _x and	2	9

	S _x N _y Compounds. S-N cations and anions. S ₃ N ₃ Cl ₃		
4.2	Sulphur-Phosphorus compounds: Molecular sulphides such as P ₄ S ₃ , P ₄ S ₄ , P ₄ S ₇ , P ₄ S ₉ and P ₄ S ₁₀	2	9
4.3	Phosphorous-Nitrogen compounds: 6 and 8 membered cyclophosphazines, linear polyphosphazines. Craig-Paddock and Dewar model	2	9
4.4	Boron-Nitrogen compounds: Borazine, substituted borazines and boron nitride.	2	9
4.5	Compounds of Selenium: Selenium Oxide, Selenium halides, Selenium oxoacid, Selenium compounds in Xerox	1	9
4.6	Boron hydrides: Reactions of diborane. Structure and bonding in boron hydrides. Polyhedral boranes: Preparation, properties, structure and bonding.	3	10
4.7	The topological approach to boron hydride structure. Styx numbers. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures.	4	10
4.8	Carboranes and metallocarboranes. Wade Mingos and Jemmis rules	2	10
5.0	Lanthanides and Actinides	18	
5.1	Lanthanides: Characteristic properties. Electronic configurations and term symbols. Occurrence and extraction (solvent extraction and ion—exchange methods). Separation techniques.	4	11
5.2	Oxidation states of lanthanides. Spectral and magnetic properties of lanthanides. Lanthanide complexes as shift reagents, luminescent materials, and magnetic materials. Gd complexes as T ₁ MRI contrast agents: Gd-DTPA and Gd-DOTA.	4	11
5.3	Shapes of f orbital and their splitting in cubic ligand field.	2	12
5.4	Actinides: Occurrence and general properties. Extraction of thorium and uranium. Electronic configuration and term symbol. Oxidation states. Spectral and magnetic properties.	4	11
5.5	Comparative properties of lanthanides and actinides. Trans-uranium elements and their stabilities.	2	11
5.6	Comprehensive study of the beach sands of Kerala and their important components such as monazite, ilmenite, zircon and sillimanite.	2	13

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2. B. N. Figgins and M. A. Hitchman, Ligand Field Theory and its Applications, Wiley-VCH, 2000.
3. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.

APCH222: ORGANIC CHEMISTRY II

co No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	To explain the fundamentals, operating principles and instrumentation of separation techniques.	U	1,2
2.	To explain the underlying principles involved in normal and ultra centrifugation and solvent extraction	U, Ap	1, 2
3.	To describe the various methods of determining reaction mechanisms and basic thermodynamic principles of organic reactions.	U, An	1
4.	To explain the Hammett parameters of reaction and design an experiment to confirm the mechanism of a reaction.	An, E	1
5.	To identify different types of rearrangement reactions, determine the product of the reaction applying migratory aptitude, and reproduce the evidences for the mechanism of the reaction.	E	1
6.	To understand that the outcomes of pericyclic reactions may be understood in terms of frontier orbital interactions, correlation diagram, Mobius and Huckel approach.	U, An	1
7.	To recall and define the various types of pericyclic reaction; define such terms as 'conrotatory', 'suprafacial'.	Ap	1
8.	To predict and rationalise the outcomes of pericyclic reactions including stereospecificity, regioselectivity, and stereoselectivity.	An	1, 8
9.	To describe the fate of excited molecule based on Jablonski diagram, predict the course of an organic photochemical reaction and identify the product with the type of functional group.	C	1
10.	To explain the photoreactions of vitamin D and the photochemistry of vision	Ap, An	1, 4

Module	Course Description	No. of Hrs	CO No.
1.0	Separation Techniques	18	
1.1	Classification of chromatographic methods. Theory of chromatography. Applications of chromatographic methods. Adsorption and partition chromatography. Paper, thin layer and column chromatographic methods.	4	1, 2
1.2	Common Spray reagents and Developing agents in chromatography.	2	1, 2
1.3	Centrifugal TLC, pressure column chromatography, HPLC and GC-column matrices, detectors. Affinity and chiral separations using HPLC.	4	1, 2
1.4	GC MS and LC MS Principle. Instrumentation and applications.	4	1, 2
1.5	Normal and ultra-centrifugation. Gel and capillary electrophoresis and their applications.	2	1, 2
1.6	Solvent extraction. Extraction using supercritical liquid CO ₂ . Craig's technique of liquid-liquid extraction.	2	1, 2

2.0	Physical Organic Chemistry	18	
2.1	Kinetic and thermodynamic control of reactions with examples	1	3, 4
2.2	Kinetics requirements for reaction, Baldwin rules for ring closure, Hammond postulate, microscopic reversibility, Marcus theory	4	3, 4
2.3	Solvent polarity and parameters Y, Z and E parameters and their applications. Kinetic isotopic effect in aromatic electrophilic substitution, salt effects and special salt effects in S _N reactions.	4	3, 4
2.4	Methods of determining reaction mechanism. Identification of product, determination of the presence of intermediate isotopic labelling, stereo chemical evidence, kinetic evidence, isotopic effects	5	3, 4
2.5	Linear free energy relations, The Hammett equation and its applications. Hammett plot and its deviation. Significance of sigma (σ) and rho (ρ) reactions with negative and positive ρ , low and high ρ , Taft equation.	4	3, 4
3.0	Molecular Rearrangements and Transformation Reactions	18	
3.1	Base catalysed rearrangements: Favorskii rearrangement, rearrangement in 1,2 dicarbonyl compounds — (benzil-benzilic acid) and Dakin reaction.	2	5
3.2	Acid catalysed rearrangements: Wagner Meerwein, Dienone phenol, pinacol-pinacolone, semi pinacolone, Demjanov rearrangements	2	5
3.3	Carbon to nitrogen rearrangements: Hoffmann, Lossen, Curtius, Schmidt, Stieglitz, and Beckmann rearrangements.	3	5
3.4	Fries, Fischer-Hepp, Hofmann-Martius, Von Richter, Orton, Bamberger, and Smiles.	4	5
3.5	Bucherer reaction, Rupe, Stevens, rearrangement	4	5
3.6	Rearrangement involving diazomethane-Arndt Eistert reaction, Wolf rearrangement.	3	5
4.0	Aromaticity and Pericyclic Reactions	18	
4.1	Concept of aromaticity, antiaromaticity, homoaromatic, bis homo aromatic and non- aromatic — concepts to charged rings, completely conjugated exocyclic double bonded systems, annulenes, fused hydrocarbon, heterocyclic compounds, meso-ionic compounds and tropolone systems.	2	6, 7, 8
4.2	Electro cyclic ring closure and ring opening reactions — selection Rule — FMO, Correlation diagram and Mobius Huckel theory of electro cyclic reaction.	4	6, 7, 8
4.3	Thermal $2\pi+2\pi$, $4\pi+2\pi$ and higher cyclo addition reactions photochemical $2\pi+2\pi$ cyclo addition reactions — FMO, correlation diagram and Mobius Huckel theory of cycloaddition reactions; Diels Alder reactions — regioselectivity, stereospecificity — Effect of substituent on the diene and dienophile reactivity — Retro Diels Alder reaction, and Intramolecular Diels Alder reaction Industrial	6	6, 7, 8

	application Aldrin, Dieldrin, endosulfan and anti-stroke drugs.		
4.4	1,3 dipolar cycloaddition reactions: Dipoles derived from aziridine, azide, diazo alkane, nitrile oxide, nitrile imine, nitrile ylide, azomethine ylide, azomethine imine and nitron and their reactions with alkene with stereo specificity. Preparation of nitrite oxide.	2	6, 7, 8
4.5	Sigmatropic rearrangement: classification of [i,j] sigmatropic rearrangements — [1,3], [1,5], [1,7], [3,3], [2,3] and [5,5] rearrangements. Ene reaction, Sommelet Hauser rearrangement, Benzidine rearrangement, Fischer indole synthesis, Claisen and Cope arrangement with stereochemistry - Johnson Claisen rearrangement Ireland Claisen rearrangement. FMO theory of sigmatropic rearrangement for carbon and hydrogen migration.	4	6, 7, 8
5.0	Organic Photochemistry	18	
5.1	Photochemical process singlet and triplet states and their reactivity Jablonski diagram, energy transfer, sensitization and quenching	3	9
5.2	Photo reactions of simple carbonyl compounds — Norrish type (I) and Norrish type (II) reactions, photo reductions of aromatic ketones, photochemistry of cyclic α , β - unsaturated ketones, photo enolisation and hydrogen abstraction	5	9
5.3	Photoaddition: Photoaddition of alkenes to aromatic compounds, dimerization of alkenes, conjugated dienes and aromatic compounds.	2	9
5.4	Photo oxidation, Intramolecular photo cyclisation and photo rearrangements, di- π methane rearrangement, oxa di- π methane rearrangement and photo Fries rearrangement.	4	9
SS	Cis Trans isomerisation, photo Oxidation of diene and alkenes — photochemical reactions of dienone, photo reactions of aromatic compounds	2	9
5.6	Photoreactions of vitamin D, photochemistry of vision	2	10

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10. Rohatgi-Mukherjee, Fundamentals of Photochemistry, New Age International Publishers, 2nd edition, 2006.

APCH223: PHYSICAL CHEMISTRY II

co No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	apply quantum mechanical principles in solving both real and imaginary spherical harmonics systems-multi electron systems and analyse spectral lines.	U,Ap,An	1
2.	describe and explain the physical and chemical principles that underlie molecular structure determination techniques like microwave, vibrational, Raman and electronic spectroscopy.	R, U	1
3.	predict likely spectral characteristics of given molecular species, and be able to rationalise those characteristics on the basis of structural and electronic arguments.	Ap, An	1
4.	acquire knowledge of basics of statistical mechanics and compare statistical methods.	U, Ap	1
5.	understand and apply of theories of heat capacity.	U,Ap	1
6.	understand theories of electrolytes and electrochemical reactions.	R,U, Ap, An	1
7.	ascertain the application of electrochemistry in energy storage and in industrial fields	An	1
8.	understand the theories and applications behind various types of analytical techniques in electrochemistry.	U	1
9.	acquire skill in solving numerical problems.	Ap	1

Module	Course Description	No. of Hrs	CO No.
1.0	Quantum Chemistry II	18	
1.1	Rotational motion: The wave equation in spherical polar coordinates-particle on a ring, the phi equation and its solution, wave functions in the real form.	3	1, 9
1.2	Non-planar rigid rotor and particle on a sphere- separation of variables, the phi and the theta equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Rodrigue's formula, Spherical harmonics (imaginary and real forms)- polar diagrams of spherical harmonics.	5	1, 9
1.3	Quantum Mechanics of Hydrogen-like systems: The wave equation in spherical polar coordinates: separation of variables — r , θ and ϕ equations and their solutions, wave functions and energies of hydrogen-like systems.	4	1, 9
1.4	Radial distribution functions, angular functions and their plots.	2	1
1.5	Wave functions for multi electron systems, wave equation for multi electron systems, symmetric and anti- symmetric wave functions, Pauli's anti-symmetry principle, postulate of spin by Uhlenbeck and Goudsmith, Spin orbitals. Spin- orbit coupling. Term symbols-Hunds rule for determination of ground term, selection rules and explanation of spectral lines of hydrogen atom.	4	1

2.0	Spectroscopy I	18	
2.1	Rotational spectroscopy. Diatomic molecule as a rigid rotator, selection rules, Derivation for maximum populated rotational level, effect of isotopic substitution on rotation spectra, factors affecting the width and intensity of spectral lines, calculation of bond length. Non-rigid rotors and centrifugal distortion. Instrumentation	3	2, 3
2.2	Vibrational spectra of harmonic and anharmonic oscillator. Selection rules. Morse curve, fundamentals and overtones. Fermi resonance, combination band and difference bands. Hot bands, Determination of force constant.	3	2, 3, 9
2.3	Rotational fine structure, P, Q, R branches of spectra.	1	2, 3
2.4	Vibrational spectra of polyatomic molecules: Normal modes of vibration, skeletal and group frequency vibration. Principle of fourier transformation, Introduction to FTIR, instrumentation.	3	2, 3
2.5	Raman scattering, polarizability and quantum theory of Raman effect. Stokes and anti-Stokes lines.	1	2, 3
2.6	Rotational and vibrational Raman spectrum. Raman spectra of polyatomic molecules. Complementarity of IR and Raman spectra. Mutual exclusion principle.	2	2, 3
2.7	Introduction to Laser Raman spectroscopy, CARS and SERS (qualitative idea only).	1	2, 3
2.8	Electronic spectra of diatomic molecules. Vibrational coarse structure and rotational fine structure of electronic spectrum. Franck-Condon principle.	2	2, 3, 9
2.9	Types of electronic transitions. Format diagram. Dissociation energy and dissociation spectra Predissociation.	2	2, 3
3.0	Statistical Thermodynamics-I	18	
3.1	Fundamentals: Microstates and macro state, Stirling's approximation, statistical weight factor (g), thermodynamic probability and entropy-Statistical Distribution of Particles.	3	4
3.2	Concept of ensembles- canonical, microcanonical, canonical and grandcanonical ensembles. Types of statistics	3	4
3.3	Maxwell-Boltzmann statistics (concept and derivation of partition function).	2	4
3.4	Bose-Einstein statistics, Thermodynamic probability, Bose Einstein distribution function. Examples of Bosons. Application: Bose Einstein Condensates and Liquid Helium	4	4
3.5	Fermi-Dirac statistics. Examples of fermions- Fermi- Dirac distribution function. Application: Electrons in metals (thermionic emissions).	4	4
3.6	Comparison between Maxwell Boltzmann, Bose Einstein and Fermi-Dirac statistics. Dilute systems-relation between three statistics	2	4
4.0	Statistical Thermodynamics-II	18	
4.1	Molecular partition functions - Translational (1D, 2D and 3D), vibrational, rotational and electronic partition functions. Total partition functions. Relation between molecular and molar partition functions	4	4

4.2	Relation between partition function and thermodynamic properties (U , C_v , C_p , S , G , A , P , H), Translational thermodynamic properties of monoatomic gas, Sackur-Tetrode equation. The contributions of partition functions (translational, rotational, vibrational and electronic) to the thermodynamic properties.	4	4
4.3	Relationship between Equilibrium constant and Partition Function. Concept of Equipartition Principle and its use for calculation of heat capacity of molecules from partition function.	2	4
4.4	Quantum theory of heat capacity - calculation of heat capacity of gases; limitation of the method.	2	5
4.5	Heat capacity of solids. Dulong and Petit's law, Kopp's law; and its limitations.	2	5
4.6	Einstein theory of heat capacity; limitations.	2	5
4.7	The Debye theory of specific heat capacity of solids.	2	5
5.0	Electrochemistry	18	
5.1	Ionics: Activity and activity coefficient of electrolytes, determination of activity coefficient.	1	6
5.2	Debye-Huckel theory of strong electrolytes, Debye-Huckel-Onsager equation and its derivation, limitation of the model, conductance at high frequencies and high potentials —Wein effect and Debye - Falkenhagen effect.	4	6
5.3	Ionic strength, Debye - Huckel limiting law, mean ionic activity coefficient.	1	6, 9
5.4	Electrode: Different type of electrodes. Electrochemical cells, liquid junction potential and its determination,	1	6, 9
5.5	Over potentials: Butler-Volmer equation. Tafel and Nernst equation, Tafel plot and its significance.	4	6, 7
5.6	Fuel cells: H_2 - O_2 , hydrocarbon oxygen, and solid oxide fuel cells. Batteries: Ni-Cd, Ni- H_2 , Li ion	3	7
5.7	Electro analytical methods: Coulometric titrations. Voltammetry: principle and method of polarography, cyclic voltammetry, stripping voltammetry and amperometry.	4	8

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Model Question Papers

General Instruction to question paper setters

- There will be a 15 main questions in each question paper divided into 3 sections A, B and C
- Each of the sections A, B and C will have 5 questions each, 1 **from each module**.
- Each question in Section A will have 3 sub questions (a), (b) and (c), of which the candidate has to answer any two (2 marks each).
- Each question in Section B will have 2 sub questions (a) and (b), of which the candidate has to answer any one (5 marks each).
- Candidate should answer any three out of the five questions in Section C (10 marks each).
- Section A carries a total of 20 marks, Section B carries 25 marks, and Section 3 carries 30 marks.
- The maximum marks will be 75 and the duration of the exam will be 3 hrs.

Second Semester M.Sc. Degree Examination - Model question paper

APCH221: INORGANIC CHEMISTRY — II

(2025 admission Onwards)

Time: 3 Hrs

Max. Marks: 75

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

- What is meant by spin state cross over?
 - What is difference between Orgel diagram and Tanabe Sugano diagram?
 - What is the reason for narrow line obtained from solution spectra of Mn^{2+} ion complexes?
- What are inverse spinels? Give examples.
 - What is Schottky defect?
 - Differentiate H-centre from V-centre in NaCl crystals.
- What is photovoltaic effect? What are its uses?
 - What is the effect of temperature on the conductance of metals. Why?
 - What are pyroelectric and ferroelectric effects?
- Predict the products formed when borazine react with HCl and $NaBH_4$.
 - Which undergoes addition reactions faster — Benzene or Borazine? Why?
 - Classify the following into closo, nido and arachno.
 B_2H_6 , $C_2B_5H_{11}$, $B_3H_{12}^{3-}$, B_5H_{11} ,
- What is misch metal?
 - Actinides form oxocations but lanthanides don't. Give reason?
 - Which among lanthanides and actinides has a higher tendency to form complexes? Why?

(2 × 10 = 20)

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

- State Laporte rule. Why Laporte rule is not obeyed by octahedral complexes.
 - Briefly explain the temperature dependence of magnetism of metal complexes.
- What are crystal defects? Discuss about point, line and plane defects.
 - Explain the rotating crystal method of X-ray diffraction method to determine the structure of a crystal.

8. (a) Discuss the doping of semiconductors and its conduction mechanism
(b) Explain superconductivity with examples.
9. (a) How is polythiazyl synthesized? Describe its structure. Why is it treated as a one dimensional conductor?
(b) Suggest a probable structure for B₃H₃ after finding out its *styx* number.
10. (a) Discuss the separation of the lanthanide elements by ion exchange methods.
(b) Briefly describe the industrial importance of the beach sands of Kerala.

[5 x 5 = 25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. Explain the Guoy's methods used to determine magnetic susceptibility. How is it important in structure determination?
12. Discuss in detail the perovskite structure by taking SrTiO₃ as the example.
13. Discuss the salient features of the band theory of solids and compare it with the free electron theory of solids.
14. What are carboranes and metallocarboranes? Discuss with examples.
15. Compare the spectral and magnetic properties of lanthanides and actinides.

[10 x 3 = 30]

Second Semester M.Sc. Degree Examination — Model question paper
APCH222: ORGANIC CHEMISTRY — II
 (2025 admission Onwards)

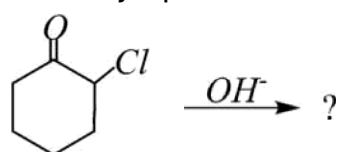
Time: 3 Hrs

Max. Marks: 75

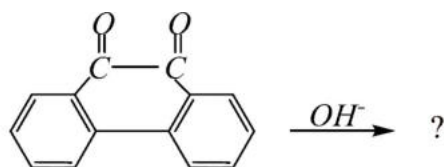
SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

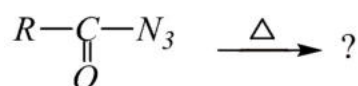
- What are the advantages of HPLC technique?
 - What is the principle involved in GC-MS?
 - What is the basic principle of solvent extraction?
- What is Baldwin's rule for ring closure reaction?
 - What is inverse kinetic Isotopic effect?
 - What is Hammond postulate?
- The major product formed in the following reaction is



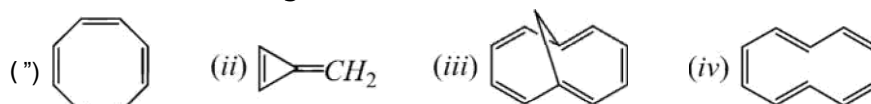
- The major product formed in the following reaction is



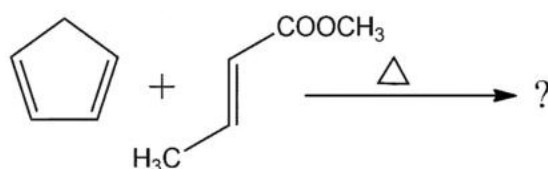
- The major product formed in the following reaction is



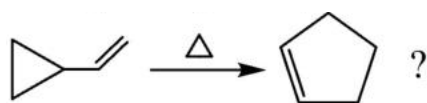
- Which of the following are Aromatic?



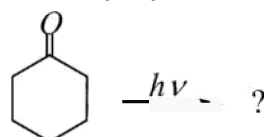
- The major product formed in the following reaction.



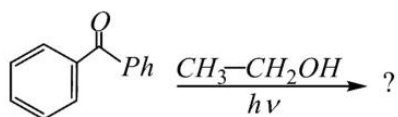
- Identify the sigma tropic shift involved in the following reaction.



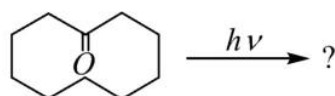
- The major product formed in the following reaction is



- The major product formed in the following reaction is



(c) The major product formed in the following reaction is



[2 x 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

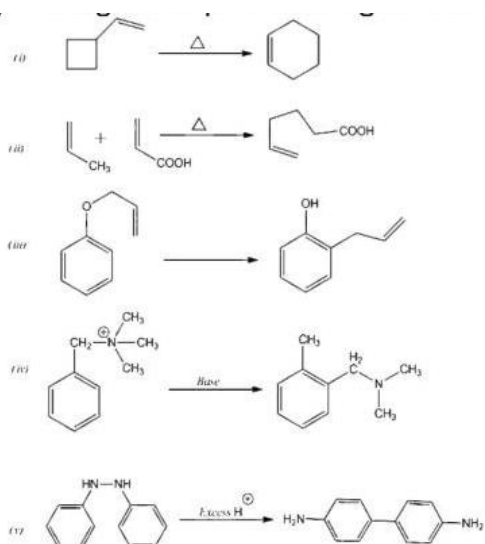
6. (a) Write note on solvent extraction using super critical liquid CO₂?
(b) Describe the various types of detectors used in GC?
7. (a) Write a note on Marcus theory?
(b) Write a note on primary and secondary kinetic isotopic effect?
8. (a) Write a note on Dienone-Phenol rearrangement?
(b) Write a note on Bucherer reaction?
9. (a) Write a note on 1,3 dipolar cycloaddition reaction with respect to nitrile oxide and nitrile ylide?
(b) Write a note on aromaticity in metallocenes and Tropolone systems?
10. (a) Write a note on N (1) and N (11) reactions?
(b) Write a note on photo oxidation of conjugated dienes and alkenes?

[5 x 5 = 25]

SECTION C

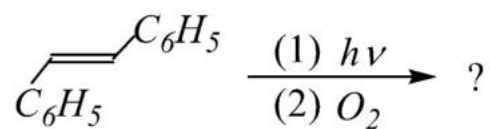
Answer any three questions. Each question carries 10 marks

11. (a) Write a note on craig's technique of liquid-liquid extraction.
(b) Write a note on the application of gel chromatography.
12. Write a note on Hammett equation, Hammett plot and their deviation.
13. Write a note on favorskii rearrangement (at least four applications).
14. Identify the sigma tropic rearrangement involved in the following cases.



[8]

15. (a) Predict the product and explain the mechanism involved in the following reaction.



- (b) Write a note on oxa di-n methane rearrangement.

[10 x 3 = 30]

Second Semester M.Sc. Degree Examination - Model question paper

APCH223: PHYSICAL CHEMISTRY - II

(2025 admission Onwards)

Time: 3 Hrs

Max. Marks: 75

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) Write the determinantal form of wave function for lithium atom.
(b) Explain spherical harmonics.
(c) Sketch the radial probability distribution of 2s and 2p orbitals.
2. (a) How would one determine the theoretical force constant of the C—C bond?
(b) Anti-stokes lines are usually weak. Why?
(c) Explain the effect of isotopic substitution on rotation spectra.
3. (a) Differentiate Bosons and Fermions.
(b) Explain the concept of ensembles and give the difference in properties of each category.
(c) Obtain the relation between thermodynamic probability and entropy.
4. (a) Calculate the value of C_v for any element when its temperature is equal to the Debye characteristics temperature.
(b) Give the limitations of Einstein's theory of specific heat capacity
(c) Distinguish between Dulong Pettit law and Kopps law.
5. (a) What are solid oxide fuel cells?
(b) What is the significance of half-wave potential?
(c) Calculate the mean activity coefficient of 0.01 M BaCl_2 in water at 25°C .
[2 x 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) Obtain the term symbols for hydrogen atom and explain the spectral lines based on selection rules.
(b) Give the Schrodinger equation for hydrogen atom in polar coordinates and separate the variables.
7. (a) Spacing between adjacent lines in HCl molecule is 10 cm^{-1} . Force constant is $1.38 \times 10^{-2} \text{ J K}^{-1}$, Calculate maximum population at room temperature.
(b) Outline the principle and applications of CARS and SERS
8. (a) Explain Maxwell-Boltzman distribution law.
(b) Apply Fermi-Dirac statistics to electrons in metals.
9. (a) Deduce Sackur-Tetrode relation using partition function.
(b) Calculate the translational partition function for methane in a volume of 1 m^3 at 25°C .
10. (a) What is over potential? Derive Butler-Volmer equation.
(b) The exchange current density of a $\text{Pt}/\text{H}_2, \text{H}^+(\text{aq})$ electrode is 0.79 mA cm^{-2} . What current flows through a standard electrode of total area 5 cm^2 when

the potential difference across the electrode is 5 mV, the temperature 25°C and the proton activity unity?

[5 x 5 =25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. Apply Schrodinger equation to a rigid rotator, separate variables and solve the separated equations. Give expression for energy.
 12. (i) Explain the origin of P and R branches in rotational-vibrational spectrum.
(ii) Discuss the instrumentation of FT-IR spectroscopy. [5+5]
 13. (i) Explain Bose-Einstein distribution, obtain expression for thermodynamic probability and number of particles
(ii) Write short note on Bose-Einstein condensation [7+3]
 14. (i) Derive the relation between partition function and thermodynamic properties internal energy, entropy and specific heat capacity
(ii) Discuss the Debye theory of specific heat capacity of solids. [7+3]
 15. (i) Discuss briefly about the Ni-Cd and Li-ion batteries.
(ii) Describe the theory and application of cyclic voltammetry. [5+5]
- [10 x 3 =30]

SEMESTER - III

APCH321: INORGANIC CHEMISTRY III

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	demonstrate knowledge of advanced content in the areas of inorganic chemistry such as in organometallic compounds, bioinorganic compounds, spectroscopic methods in inorganic Chemistry and nuclear chemistry.	U	1
2.	examine the bonding in simple and polynuclear carbonyls with and without bridging and complexes with linear n donor ligands.	U, An	1
3.	explain the concept of fluxionality and carbonyl scrambling and the utility of NMR in studying the structure of organometallic compounds.	U, An	1
4.	explain the structure and bonding of ferrocene and dibenzenechromium with the help of MO theory	U, An, C	1
5.	understand fundamental reaction types and mechanisms in organometallics and to employ them to understand selected catalytic processes in industry.	U, An, C	1
6.	Illustrate the steps in catalytic cycles using Tolman Loop	A, C	1, 5
7.	contrasts the thermodynamic and kinetic stability of complexes, analyses the factors affecting stability of complexes and explains the methods of determining stability constants.	An, E	1
8.	classifies ligand substitution reactions and explains its kinetics and various mechanisms.	U, E	1
9.	analyze the chemical and physical properties of metal ions responsible for their biochemical action as well as the techniques frequently used in bioinorganic chemistry such as oxygen transport, e-transfer, communication, catalysis, transport, storage etc.	U, An	1
10.	explain the utility of metals in medicine and the underlying principles behind the same	U, Ao	1, 5
11.	explain the principles of spectroscopic methods employed in inorganic chemistry and their applications in the study of metal complexes.	An, E	1
12.	demonstrate a knowledge of fundamental aspects of the structure of the nucleus, radioactive decay, nuclear reactions, counting techniques.	R, U	1
13.	evaluate the role of nuclear chemistry to find the most suitable measures, administrative methods and industrial solutions to ensure sustainable use of the world's nuclear resources.	U, E, C	1, 4

PSO—Programme Specific Outcome

Cognitive Level:

R—Remember

An—Analyse

CO—Course Outcome

U—Understanding

E—Evaluate

Ap—Apply

C—Create

Module	Course Description	No. of Hrs	CO No.
1.0	Organometallic Compounds	18	
1.1	Nomenclature of organometallic compounds. Hapto nomenclature. 18 and 16 electron rule, isoelectronic and isolobal analogy.	2	1
1.2	Metal carbonyls, bonding in metal carbonyls. Synthesis, structure and bonding of polynuclear carbonyls with and without bridging. Carbonyl clusters-LNCC and HNCC. Ligands similar to CO: Nitrosyls, CS, CSe, and CTe Complexes (Basic idea)	2	1, 2
1.3	Fluxional molecules: $\text{Fe}(\text{CO})_5$, Cp_4Ti , $[(\eta^5\text{-Cp})\text{Fe}(\text{CO})_2(\eta^1\text{-Cp})]$, Carbonyl scrambling $[\text{Cp}_2\text{Fe}_2(\text{CO})_4]$	1	1, 3
1.4	Molecules with linear π donor ligands: Olefins, acetylenes, dienes and allyl complexes. Complexes with cyclic π donors: Cyclopentadiene, benzene complexes.	2	1, 2, 4
1.5	NMR Spectra of Organometallic compounds (Basic idea)	1	1, 3
1.6	Structure and bonding of ferrocene and dibenzenechromium complexes (MO treatment).	2	1, 4
1.7	Oxidative addition and reductive elimination, insertion (CO, SO_2 and olefin) and elimination reactions	3	1, 5
1.8	Catalysis by organometallic compounds: Terminology in catalysis- turnover number (TON), turnover frequency (TOF). Alkene hydrogenation using Wilkinson's catalyst, Hydroformylation of olefins using cobalt and rhodium catalysts, Linear to branch selectivity. Polymerization reaction by Ziegler-Natta catalyst, Monsanto acetic acid Palladium catalysed oxidation of ethylene-the Wacker process. Water gas shift reaction. Tolman Loop representation of catalytic process	5	1, 6
2.0	Coordination Chemistry-III: Reactions of Metal Complexes	18	
2.1	Energy profile of a reaction - Thermodynamic and kinetic stability, Stability of complex ions in aqueous solutions: Formation constants. Stepwise and overall formation constants. Factors affecting stability of complexes.	2	1, 7
2.2	Determination of stability constants: spectro photometric, polarographic and potentiometric methods.	3	1, 7
2.3	Stability of chelates. Thermodynamic explanation, macrocyclic effects.	1	1, 7
2.4	Classification of ligand substitution reactions-kinetics and mechanism of ligand substitution reactions in square planar complexes, trans effect theory and synthetic applications.	3	1, 8
2.5	Kinetics and mechanism of octahedral substitution- water exchange, dissociative mechanism, associative mechanism - Eigen-Wilkins mechanism, Eigen - Fuoss equation, base hydrolysis, racemisation and isomerisation reactions.	3	1, 8
2.6	Electron transfer reactions: Outer sphere mechanism- Marcus theory, inner sphere mechanism - Taube mechanism.	3	1, 8

3.0	Bioinorganic Chemistry	18	
3.1	Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium-potassium pump.	2	1, 9
3.2	Photosynthesis, porphyrin ring system, chlorophyll, PS I and PS II. Synthetic model for photosynthesis.	2	1, 9
3.3	Role of calcium in biological systems - blood coagulation, muscle contraction.	1	1, 9
3.4	Oxygen carriers and oxygen transport proteins- haemoglobin and myoglobin.	2	1, 9
35	Non-haeme iron-sulphur proteins involved in electron transfer-ferredoxin and rubredoxin.	3	1, 9
3.6	Iron storage and transport in biological systems ferritin and transferrin.	3	1, 9
3.7	Redox metalloenzymes-cytochromes, cytochrome P-450, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes- Carboxypeptidase A - structure and functions.	2	1, 9
3.8	Nitrogenases, biological nitrogen fixation. Corrin ring system- Vitamin B12 and coenzymes. Toxicity of Hg, Cd, Pb, Cr, As and chelation therapy.	2	1, 9
39	Metals in medicine - therapeutic applications of cis-platin, auranofin, transition metal radio-isotopes (example: Tc, Co and Cu etc.) and MRI contrast agents. (Mn and Fe compounds)	1	1, 10
4.0	Spectroscopic Methods in Inorganic Chemistry	18	
4.1	Infrared spectra of coordination compounds. Structural elucidation of coordination compounds containing the following molecules/ ions as ligands- NH ₃ , H ₂ O, CO, NO, OH—, SO ₄ ²⁻ , CN ⁻ , SCN ⁻ , NO ₃ ⁻ , NO ₂ ⁻ , CH ₃ COO ⁻ and X ⁻ (X=halogen). Changes in ligand vibration on coordination with metal ions.	5	1, 11
4.2	Vibrational spectra of metal carbonyls, CD and ORD spectra of metal complexes with emphasis on cobalt complexes.	3	1, 11
4.3	ESR spectra: Application to Cu(II) complexes and inorganic free radicals such as PH ₄ and [BH ₃].	3	1, 11
4.4	Nuclear Magnetic Resonance Spectroscopy: The contact and pseudocontact shifts, ¹ H NMR of biomolecules such as hemoglobin, myoglobin and ferredoxin. An overview of ³¹ P and ¹⁹ F NMR of molecules with metal nuclides, coordination chemical shift in metal complexes, ¹¹ B NMR.	4	1, 11
45	Mossbauer Spectroscopy: Application of the technique to the studies of iron and tin complexes.	3	1, 11
5.0	Nuclear Chemistry	18	
5.1	Nuclear structure, mass and charge. Nuclear moments. Binding energy. Semiempirical mass equation. Stability rules. Magic numbers.	3	1, 12

5.2	Nuclear models: Shell, Liquid drop, Fermi gas, collective and optical models.	3	1, 12
5.3	Equation of radioactive decay and growth. Half-life and average life. Radioactive equilibrium. Transient and secular equilibria.	2	1, 12
5.4	Nuclear reactions: Direct nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions. Neutron capture cross section and critical size. Radio carbon dating	3	1, 12
5.5	Nuclear fission- Nuclear cross section, Q-value, Threshold energy, Fissionable materials, Fission as a source of energy, Nuclear chain reacting systems. Principle of working of the reactors of nuclear power plants. Breeder reactor. Nuclear fusion reaction, stellar energy.	3	1, 12
5.6	Principles of counting technique such as Geiger-Muller counter, proportional, ionization and scintillation counters. Cloud chamber.	2	1, 12
5.7	Nuclear Diagnosis and Medicine: Positron Emission Tomography (PET), Proton therapy, Targeted alpha therapy	2	1, 13

References

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley and Sons, 6th edition, 1999.
2. J. E. Huheey, Inorganic Chemistry-Principles of Structure and Reactivity, Harper and Collins, 4th edition, 2011.
3. Brisdon, A.K. Inorganic Spectroscopic Methods, Oxford University Press: Oxford, 1998.
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5. Iggo, J. A. NMR Spectroscopy in Inorganic Chemistry, Oxford University Press: Oxford, 1999.
6. P. Powell, Principles of Organometallic Chemistry, Chapman and Hall, 2nd Edition, New York, 1988.
7. R. Gopalan and V. Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd.
8. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill Valley, California, 1994.
9. R. C. Mehrotra and A. Singh, Organometallic Chemistry: A Unified Approach, Wiley eastern, 1991.
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12. U.N. Dash, Nuclear Chemistry, Sultan Chand & Sons

Further Reading

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2. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, John Wiley, 3rd edition, 1978.
3. R.V. Parish, NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, Ellis Harwood, Chichester, UK 1999.
4. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, John Wiley and Sons, New York, 1967.

5. D. E. Fenton, Biocoordination Chemistry, Oxford University Press, Oxford, 1995.
6. R. W. Hay, Bioinorganic Chemistry, Ellis Horwood, Chichester, 1987.
7. H. J. Amikar, Essentials of Nuclear Chemistry, New Age International, New Delhi, 4th edition, 1995.
8. G. Friedlander and J. W. Kennady, Introduction to Radio chemistry, John Wiley and Sons New York, 1949.

APCH322: ORGANIC CHEMISTRY III

co No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	describe and explain the physical and chemical principles that underline molecular structure determination techniques such as UV-visible, IR, mass and NMR spectroscopy.	U	1
2.	apply knowledge of molecular structure determination using UV-visible, IR, mass and NMR spectroscopic techniques to identify and/or characterize chemical compounds from experimental data.	E	1
3.	calculate λ_{max} of a compound and apply IR frequency table to determine the functional groups present in the molecule, interpret mass spectrum of compound from fragmentation.	U, An	1
4.	predict likely spectral characteristics of given molecular species; solve the structures of unknown molecules using appropriate spectroscopic techniques.	An, E	1
5.	explain the basics of 2D NMR of a compound based on learned principles and solve the structure of a compound based on NMR data.	E	1
6.	identify and apply various reagents in organic synthesis	Ap, An	1
7.	explain the application of oxidizing and reducing agents in organic synthesis.	Ap, An	1

Module	Course Description	No. of Hrs	CO No.
1.0	UV-VIS, IR, and Mass Spectrometry	18	
1.1	Types of electronic transitions, absorption and intensity shift. Type of absorption bands-Woodward Fieser rules. λ_{max} calculation in dienes, α , β unsaturated ketones, and derivatives of acyl benzene. Effect of solvent on electronic spectra, applications of uv-vis spectroscopy	4	1
1.2	Principles of IR spectroscopy: Vibrational frequency of functional groups, Factors affecting vibrational frequency, coupled vibrations and ring size, +I and -I effects and hydrogen bonding, Identification of functional groups, sampling techniques	4	1
1.3	Principles of mass spectra: base peak, nitrogen rule, meta stable ion, mass spectral fragmentation patterns of long chain alkanes, alkenes, alkynes, alkyl benzene, alcohols, ethers, thiols, aldehydes, ketones, acid amides, nitro, amino and halogen compounds effect of isotope on molecular ion peak and intensity ratio. McLafferty rearrangement, Common ionization techniques in mass — EI, CI, FAB, MALDI	6	1
1.4	Spectral interpretation and structural elucidation. Solving of structural problems on the basis of numerical and spectrum-based data	4	1, 2
2.0	NMR Technique and Structural Elucidation	18	
2.1	Theory of ^1H NMR spectroscopy: Number of ^1H signals,	6	1, 2

	Chemical shifts - anisotropic effect, electronic effect, van der Waals shielding, Spin-spin coupling - coupling constant (J^2, J^3, J^4 and long-range coupling) of ortho, meta and para substituted benzene systems. Karplus equation and its applications, Chemical shift value calculation and pattern of ^1H environment in different compounds — alkenes, substituted benzenes, furan and thiophene.		
2.2	Number of ^{13}C signals, chemical shift, calculation of ^{13}C chemical shift values in acyclic systems and disubstituted benzene.	4	1, 2, 4
2.3	Number of ^1F signals in difluoro substituted ethane conformers	1	1, 2, 4
2.4	First order, and higher order spectra, NMR shift reagents, chemical exchange and double resonance	4	4
2.5	Application of NOE, DEPT, and 2D techniques — COSY, HSQC, HMQC, HMBC (basic principles only).	3	5
3.0	Selected Reagents & Reactions in Organic Synthesis — I	18	
3.1	Preparation of Grignard reagent- Application of Grignard reagent — deprotonation, addition to carbonyl groups, CO_2 addition, oxirane addition, 1,2-and 1,4 - addition to conjugated compounds. Stereo and diastereoselectivity in Grignard reaction.	3	6
3.2	Reactions of organo Li reagents — Lithiation of aromatic compounds such as benzene, alkene, alkyne, furan, thiophene and N-methylpyrrole, ortho-lithiation by preference of functional groups, halogen exchange by organo lithium. Addition reactions with ketone, carboxylic acid and amide.	4	6
3.3	Dialkyl copper lithium: preparation, reactivity to electrophiles such as epoxide, acyl halide, active aryl halides and ketones. Preference of alkyl group reactivity in Dialkyl copper lithium.	3	6
3.4	Alkynyl Cu(I) reagents Glaser coupling. Dialkyl cadmium compounds. Preparation and reaction with acylhalides.	4	6
3.5	Benzene tricarbonyl chromium-preparation and reaction with carbanions. Tebbe's reagent, Grubbs' catalyst.	4	6
4.0	Selected Reagents & Reactions in Organic Synthesis - II	18	
4.1	Application of hindered boranes such as disiamylborane, 9 BBN, Catechol borane and hexyl borane. Regio selectivity of hindered boranes, hydroboration reaction-conversion of trialkylborane to primary alcohol, tertiary alcohol, secondary alcohol, ketone and aldehyde, preparation of cis alkene from alkyne and aldehyde from terminal alkyne.	3	7
4.2	Stabilised and unstabilised sulphur ylide and their reactions to simple ketones and enones, Julia reaction, umpolung, thiazolium ion for the replacement of CN —	3	7
4.3	Phosphorous ylide — Wittig reaction- stereochemistry. Mitsunobu reaction, Inversion of alcohol, phosphorous reagents including $\text{PR}_3/\text{H}_2\text{O}$ and their applications.	3	7
4.4	Peterson reaction — acid and base catalysed elimination and their stereochemistry — Directive influence of silicon to form carbanion and for its nucleophilic attack on electrophilic carbon.	3	7

4.5	Coupling reaction — Heck, Negishi, Sonogashira — Kumada, Suzuki, Stille, Stephens — Castro.	3	7
4.6	Pauson—Khand reaction, Vollhardt Trimerization, Application of Pd(0) to vinylic epoxide ring opening by nucleophilic attack, and internal nucleophilic attack on alkene.	3	7
5.0	Selected Reagents & Reactions in Organic Synthesis - III	18	
5.1	Complex metal hydride for reduction LiAlH ₄ , NaBH ₄ . NaBH ₃ CN, DIBALH, LiBH ₄ and BH ₃ - Chemo selectivity of reduction reactions.	2	7
5.2	Electron transfer reagents application-Li/NH ₃ , Birch reduction in aromatic systems - benzene, substituted benzene, pyridine, furan, naphthalene, Clemenson reduction.	2	7
5.3	Transfer hydrogenation, Catalytic reduction and organometallics in reduction — H ₂ /Pd, H ₂ /Pt, Lindlar's catalyst, Iridium complexes and Wilkinson catalyst.	2	7
5.4	Meerwein—Ponndorf—Verley reduction, diimide reduction crowded complex metal hydride reduction, Wolf Kishner reduction, Huang-Minton modification, Mozingo method and Rosenmund reduction.	2	7
s.s	Applications of peracid - Prilezhaev reaction, Baeyer — Villiger oxidation, Sharpless asymmetric epoxidation, HIO ₄ . O ₃ , Lemieux reagent, SeO ₂ , Etard reaction, active MnO ₂ , Lead tetra acetate DDQ, PCC, CrO ₃ (H ₂ SO ₄ , DESS Martin periodinane, Tempo, OsO ₄ . alkaline KMnO ₄ and Ag ₂ CO ₃ ,	6	7
5.6	Swern reaction, Moffatt reaction, Oppenauer oxidation, Sommelet reaction, Prevost hydroxylation Woodward hydroxylation	4	7

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APCH323: PHYSICAL CHEMISTRY III

co No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	understand the theories of chemical bonding and their application with help of approximate methods predict the nature of orbitals and molecular spectra.	U,Ap,An	1
2.	compare MO and VBT.	An	1
3.	understand the properties of gases and liquids and the nature of the intermolecular forces in them.	U, Ap, An	1
4.	describe the principle behind the determination of surface tension and coefficient of viscosity.	U	1
5.	describe and explain the physical and chemical principles that underlie molecular structure determination techniques like NMR, ESR, Mossbauer, and photoelectron spectroscopy.	U, Ap, An	1
6.	judge the degrees of freedom of systems and understand theories of irreversible thermodynamic systems.	U, Ap, An, E	1
7.	understand the quantum mechanical and non-quantum mechanical methods in computational chemistry, potential energy surface and basis functions.	U, An	1
8.	write the Z-matrix of simple molecules.	U, Ap	1
9.	acquire skill in solving numerical problems.	Ap	1

Module	Course Description	No. of Hrs	CO No.
1.0	Approximation Methods and Chemical Bonding	18	
1.1	Need for Approximation methods in quantum mechanics: Method of Variation-variation theorem. Linear variation functions. Secular equations and secular determinants. Application of variation theorem using a trial function [e.g., $x(a-x)$] for particle in a 1D-box.	2	1
1.2	Method of Perturbation-successive correction to an unperturbed problem. Detailed treatment of first order non-degenerate case only. Application of perturbation theory to a particle in 1D-box with slanted bottom.	3	1
1.3	MO theory- The Born-Oppenheimer approximation -MO Theory-LCAO MO method applied to H_2 and H_2^+	2	1
1.4	MO diagram of homo nuclear diatomic molecules Li_2 , Be_2 , B_2 , C_2 , O_2 and F_2 and hetero nuclear diatomic molecules LiH , CO , NO and HF . Bond order and its relation to stretching frequencies in CO , CO^+ , NO and NO^+ (qualitative idea only)	2	1
1.5	Representation of MOs based on symmetry properties, MO configuration of homonuclear diatomic molecules, Spectroscopic term symbols for homonuclear diatomic molecules, selection rules for molecular spectra-allowed and forbidden transitions.	1	1
1.6	Valence bond theory - VB treatment of hydrogen molecule only.	2	1
1.7	Comparison of MO and VB theories.	1	2
1.8	Quantum mechanical treatment of sp , sp^2 and sp^3 hybridisation.	2	1

1.9	HMO theory of conjugated systems. Overlap and Hamiltonian integrals, Bond order and charge density calculations. Application of HMO method to ethylene, butadiene, allyl, and benzene systems, Development of Huckel theory of aromaticity.	3	1, 9
2.0	Gaseous and Liquid State	18	
2.1	Maxwell's distribution of molecular velocities, influence of temperature, types of molecular velocities- derivation of molecular velocities from Maxwell's equation.	4	3, 9
2.2	Transport phenomena in gases - viscosity of gases, Chapman equation, determination of viscosity of gases, calculation of mean free path.	3	4, 9
2.3	Thermal conductivity, diffusion	1	3
2.4	Degrees of freedom of gaseous molecules - Translational, Rotational and vibrational.	1	3
2.5	Equation of state of real gases- van der Waal's equation, other equation of states - Virial equation, second virial coefficient and determination of diameter of a molecule.	3	3, 9
2.6	Inter molecular forces - Dipole-dipole interaction, induced dipole-dipole, induced dipole-induced dipole interactions.	2	3
2.7	Liquid state: Liquid vapour equilibria, vapour pressure- methods of measuring vapour pressure - barometric method and dynamic method - equation of state for liquids, structure of liquids-short range order.	2	3
2.8	X-ray diffraction of liquids. Vacancy model for a liquid, radial distribution function.	1	3
2.9	Surface tension - determination of surface tension by drop weight method and drop number method. Viscosity - determination of coefficient of viscosity by Ostwald viscometer.	1	4, 9
3.0	Spectroscopy II	18	
3.1	Resonance spectroscopy: Nuclear Magnetic resonance Spectroscopy, Nuclear spin. Precessional frequency, Gyromagnetic ratio, Interaction between nuclear spin and applied magnetic field.	2	5
3.2	Proton NMR. Population of energy levels.	1	5
3.3	Nuclear resonance. Relaxation methods T1 and T2. Introduction to MRI. Contrast agents in MRI. Spin-spin coupling. Fine structure.	2	5
3.4	FT-NMR Spectroscopy: Instrumentation - experimental aspects magnets, radio frequency transmitter, NMR probe and computer. Radio frequency pulses effect of pulses, rotating frame reference, FID, FT technique - data acquisition and storage, signal averaging. Pulse sequences- pulse width, spins and magnetization vector. Solid state NMR, magic angle spinning.	4	5, 9
3.5	ESR spectroscopy: Electron spin. Interaction with magnetic field. Kramer's rule. McConnell equation, The g-factor. Fine structure and hyperfine structure-selection rules Analytical applications of ESR, Determination of reaction rates and mechanisms by ESR, Structural determination by ESR.	5	5, 9

	Elementary idea of double resonance (ENDOR and ELDOR).		
3.6	Mossbauer spectroscopy: Basic principles. Doppler effect, chemical shift, recording of spectrum, application. Quadrupole effect, Effect of magnetic field.	4	5
4.0	Irreversible Thermodynamics and Phase equilibria	18	
4.1	Simple examples of irreversible processes.	1	6
4.2	General theory of non-equilibrium processes. Concept of local equilibrium. The phenomenological relations. Onsager reciprocal relations. Principle of minimum entropy production.	2	6
4.3	Generalized equation for entropy production, Entropy production from heat flow, matter flow and current flow.	3	6, 9
4.4	Application of irreversible thermodynamics to diffusion. Thermal diffusion, thermo osmosis and thermo-molecular pressure difference.	3	6
4.5	Electro-kinetic effects, the Glansdorf-Pregogine equation. Far from equilibrium region.	3	6
4.6	Three component systems: Graphical representation. Three component liquid systems with one pair of partially miscible liquids. Influence of temperature. Systems with two pairs and three pairs of partially miscible liquids.	3	6
4.7	Solid- liquid system: Two salts and water systems-no chemical combination, double salt formation, one salt forms hydrate, double salt forms hydrate, Isothermal evaporation. Thermodynamics of solid-liquid and solid- vapour equilibrium	3	6
5.0	Computational Chemistry	18	
5.1	Introduction to computational chemistry: As a tool and its scope. Potential energy surface-stationary point, saddle point or transition state, local and global minima. Basis functions-Slater type orbitals (STO) and Gaussian type orbitals (GTO).	3	7
5.2	Basis sets: minimal, split valence, polarized and diffuse basis sets, contracted basis sets, Pople's style basis sets and their nomenclature.	2	7
5.3	Quantum mechanical computational methods — <i>Ab initio</i> methods: Introduction to SCF, Slater determinants, Hartree-Fock Self-Consistent Field (HF-SCF) method, RHF, ROHF and URHF (no need of calculation). Wave functions for open shell state, Roothan concept, Electron correlation and introduction to post-HF methods.	3	7
5.4	Semi empirical methods: Huckel and extended Huckel methods. Strengths and weaknesses. PPP, ZDO, NDDO, INDO, MNDO (AM1, PM3) and CNDO approach. (Mentioning only).	2	7
5.5	Density functional theory methods (DFT)-Hohenberg-Kohn theorems, Exchange correlational functional Kohn-Sham orbitals.	2	7
5.6	Non-quantum mechanical computational methods - Molecular mechanics: Force fields - bond stretching, angle	2	7

	bending, torsional terms, non-bonded interactions, electrostatic interactions and the corresponding mathematical expressions. Commonly used forcefields - AMBER and CHARMM.		
5.7	Construction of Z-matrix for simple molecules. H ₂ O, H ₂ O ₂ , H ₂ CO, CH ₃ CHO, NH ₃ and CO ₂ .	2	8
5.8	Structure drawing and energy calculation (geometry optimization) using free software Arguslab, Tinker, NAMD, DL-POLY	2	7

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- 4.R.S. Drago, Physical Methods in Chemistry, Saunders College,2nd Edn., 1992.
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APCH4PIV: INORGANIC CHEMISTRY PRACTICALS II

Total 125 h

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	interpret data from an experiment, including the construction of appropriate graphs and the evaluation of errors.	U, An	3, 7, 8
2.	estimate a simple mixture of ions (involving quantitative separation) by volumetric and gravimetric methods.	An	7, 8
3.	perform COD, BOD, DO, TDS analysis.	Ap, An	4, 7, 8
4.	predict likely spectral characteristics of given metal complexes solve the structures of unknown metal complexes using appropriate spectroscopic techniques and magnetic measurements	Ap, An	6, 8
5.	analyse the XRD of simple substances.	An	8
6.	interpret TG and DTA curves.	An	8
7.	Synthesise and characterise inorganic nanomaterials	An	8

Module	Course Description	No. of Hrs	CO No.
1.	Estimation of simple mixture of ions (involving quantitative separation) by volumetric and gravimetric methods. a) Iron (gravimetric) and Chromium (volumetric) b) Iron (gravimetric) and Zinc (volumetric) c) Copper (volumetric) and Nickel (gravimetric) d) Iron and Copper e) Copper and Nickel	40	1, 2
2.	Environmental Analysis — COD, BOD, DO, TDS	15	1, 3
3.	Spectral Interpretation of metal complexes using IR, UV-vis. spectral data. Supplementary information like metal estimation, CHN analysis, conductivity measurements and magnetic measurements to be provided to the students. Assessment is based on arriving at the structure of the complex and assignment of IR spectral bands.	25	4
4.	Analysis of XRD of simple substances.	15	5
5.	Interpretation of TG and DTA curves.	25	6
6.	Synthesis and characterisation of Inorganic nano materials a. Nanocrystalline hydroxyapatite b. Nano Iron oxide particles	5	7

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2. Willard Merrit and Dean, Instrumental Methods of Analysis, 7th edition, 1986.
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4. B. A. Skoog and D. M. West, Principles of Instrumental Analysis, Saunders College, 4th edition, 1991.

5. R. S. Drago, Physical Methods in Inorganic Chemistry, Van Nostrand, 1992.
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APCH4PV: ORGANIC CHEMISTRY PRACTICALS II

Total 125 h

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	interpret data from an experiment, including the construction of appropriate graphs and the evaluation of errors.	U, An	3, 7, 8
2.	predict likely spectral characteristics of given molecular species; solve the structures of unknown molecules using appropriate spectroscopic techniques	Ap, An	6, 7, 8
3.	develop paper chromatogram of a compound and determine its purity	C	7, 8
4.	estimate quantitatively the Aniline, Phenol, glucose, Ascorbic acid and Aspirin in a sample	Ap	7, 8
5.	estimate colorimetrically paracetamol, protein and ascorbic acid	Ap	7, 8
6.	use green chemical principles in the synthesis	Ap	4, 7, 8

Module	Course Description	No. of Hrs	CO No.
A.	Volumetric estimation of 1) Aniline 2) Phenol 3) Glucose 4) Ascorbic acid 5) Aspirin	25	4
B.	Colorimetric estimation 6) paracetamol with potassium ferricyanide 7) protein by biuret method 8) Ascorbic acid by folin-phenol reagent or phosphotungstic acid methods	25	5
C.	Spectral identification 9) UV, IR, ¹ H NMR, ¹³ C NMR, EI mass spectral identification of Organic compounds from a library of organic compounds (Each students have to record the spectral analysis of a minimum of 40 compounds)	40	1, 2
D.	Separations of mixtures by Paper Chromatography 10) Identification of amino acids	10	3
E.	Single stage preparation of organic compounds by green chemistry	25	4
	11) Preparation of p-bromoacetanilide using CAN.		
	12) Radical coupling — 1,1-Bis-2-naphthol.		
	13) Synthesis of dihydropyrimidinone.		

	14) Synthesis of dibenzalacetone - with lithium hydroxide.		
	15) Photoreduction of benzophenone to benzopinacol (not for end semester evaluation).		
The board of examiners have to choose the combination of a volumetric estimation, a colorimetric estimation, a green synthesis OR paper chromatography and spectral analysis.			

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6. J. B. Cohen, Practical organic chemistry, Forgotten Books, 2015.
7. P. F. Shalz, Journal of Chemical Education 1996, 173: 267.
8. Monograph on green laboratory experiments, DST, Govt. of India, pp 1-79.
9. For spectral data of organic compounds, see: http://sdb.sriodb.aist.go.jp/sdb/cgi-bin/direct_frame_top.cgi

APCH4PM: PHYSICAL CHEMISTRY PRACTICALS II

Total 125 h

CO NO.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	interpret data from an experiment, including the construction of appropriate graphs and the evaluation of errors.	U, E	3, 7, 8
2.	determine the strength of strong/weak acids by conductometric titrations	Ap	7, 8
3.	verify Onsager equation and Kohlraush's law conductometrically.	An, E	7, 8
4.	determine the activity and activity coefficient of electrolyte.	Ap, An	7, 8
5.	determine the concentration of a solution potentiometrically or pH metrically.	Ap, An	7, 8
6.	employ spectrophotometry in determining unknown concentration.	Ap, An	7, 8
7.	Determine the specific rotation of a substance using polarimeter	Ap, An	7, 8
8.	Determine the half-wave potential of different ions using polarography	Ap, An	7, 8
9.	determine the concentration of a liquid mixture using a refractometer.	Ap, An	7, 8
10.	determine the unknown concentration of a given KI solution.	Ap, An	7, 8

11	determine the solubility and heat of solution of ammonium oxalate, succinic acid etc.	Ap, An	7, 8
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Module	Course Description	No. of Hrs	CO No.
1.	Conductometry a) Determination of strength of strong and weak acids in a mixture b) Determination of strength of a weak acid. c) Precipitation titration ($\text{BaCl}_2 \times \text{K}_2\text{SO}_4$) d) Titration of dibasic acid ($\text{H}_2\text{C}_2\text{O}_4/\text{H}_2\text{SO}_4$). e) Verification of Onsager equation. f) Verification Kohlraush's law. g) Determination of activity and activity coefficient of electrolyte.	20	1, 2, 3, 4
2.	Potentiometry a) Determination of emf of Daniel cell and temperature dependence of emf of a cell. b) Titrations involving redox reactions — Fe^{2+} vs KMnO_4 , $\text{K}_2\text{Cr}_2\text{O}_7$, $(\text{NH}_4)_2\text{Ce}(\text{SO}_4)_2$ and KI vs KMnO_4 c) Determination of the emf of various ZnSO_4 solutions and hence the concentration of unknown ZnSO_4 solution. d) Determination of activity and activity constant of electrolytes. e) Determination of thermodynamic constants of reactions.	20	1,5
3.	pH metric titrations Titrations involving a) Strong acid against strong base b) Weak acid against strong base c) Mixture of strong and weak acid against strong base d) Dibasic acid against strong base	15	1, 5
4.	Spectrophotometry a) Verification of Beer-Lambert's law. b) Absorption spectra of conjugated dyes (malachite green, methylene blue). c) Determination of concentration of potassium dichromate & potassium permanganate in a mixture. d) To study the complex formation between Fe^{3+} and salicylic acid. e) Determination of pKa of an indicator.	15	1, 6
5.	Polarimetry a) Measurement specific rotation of glucose. b) Determination of specific rotation of sucrose c) Determination of unknown concentration of glucose solution and rate constant of its hydrolysis in presence of HCl	15	1, 7

6.	Polarography a) Determination of half wave potential ($E_{1/2}$) of various ions and identification of the nature of the species. b) Determination of the concentration of a given reducible ion (Cd^{2+})	10	1, 8
7.	Refractometry a) Determination of molar refraction of pure liquids b) Determination of concentration of KCl solution/glycerol solution c) Determination of solubility of KCl in water. d) Determination of molar refraction of solid KCl e) Study the stoichiometry of potassium iodide-mercuric iodide complex. f) Determination of concentration of KI solution.	15	1, 9,10
8.	Solubility and Heat of solution Determination of solubility and molar heat of solution of a substance (e.g., ammonium oxalate, succinic acid) from solubility data - analytical method and graphical method	15	1,11

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Model Question Papers

General instruction to question paper setters

- There will be a 15 main questions in each question paper divided into 3 sections — A, B and C
- Each of the sections A, B and C will have 5 questions each, 1 from each module.
- Each question in Section A will have 3 sub questions (a), (b) and (c), of which the candidate has to answer any two (2 marks each).
- Each question in Section B will have 2 sub questions (a) and (b), of which the candidate has to answer any one (5 marks each).
- Candidate should answer any three out of the five questions in Section C (10 marks each).
- Section A carries a total of 20 marks, Section B carries 25 marks, and Section 3 carries 30 marks.
- The maximum marks will be 75 and the duration of the exam will be 3 hrs.

Third Semester M.Sc. Degree Examination - Model question paper
APCH321: INORGANIC CHEMISTRY - III
(2025 admission Onwards)

Time: 3 Hrs

Max. Marks: 75

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) Explain the haptic nomenclature of organometallics with a suitable example
(b) Represent the structures of $\text{Fe}(\text{CO})_5$, $\text{Fe}_2(\text{CO})_9$ and $\text{Fe}_3(\text{CO})_{12}$.
(c) What is the Wilkinson's catalyst? What is its use?
2. (a) Write down the Marcus equations.
(b) What is macrocyclic effect?
(c) Discuss the Taube mechanism.
3. (a) What are the functions of biological membranes?
(b) What is the difference between photosynthesis I and photosynthesis II?
(c) Explain briefly the coordination environment of the metal ion in Vitamin B12.
4. (a) Using IR spectroscopy how will you distinguish between NH_3 and H_2O ligands of a metal complex?
(b) Distinguish between contact shifts and pseudocontact shifts in NMR.
(c) How many signals are obtained in the ^{19}F nmr spectra of the following
(i) SF_6 (ii) SF_4 (iii) XeOF_4 . Give reasons for your answer
5. (a) What are magic numbers? What are their specialties?
(b) Distinguish between transient and secular equilibria
(c) Summarise the liquid drop model of the nucleus.

[2 x 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) With a suitable example, describe the oxidative addition reaction
(b) Explain Wacker process.
7. (a) Describe the dissociative mechanism in metal complexes
(b) Using $[\text{PtCl}_4]^{2-}$ as the starting material, how can the cis and trans isomers of $[\text{PtCl}_2(\text{NH}_3)(\text{PPh}_3)]$ and $[\text{PtCl}_2(\text{NO}_2)(\text{NH}_3)]$ be prepared
8. (a) Briefly explain the mechanism of ion transport across membranes
(b) Explain the iron storage and transport in biological systems.
9. (a) Explain the use of ORD spectra in studying metal complex formation
(b) Discuss the utility of Mossbauer spectroscopy in the study of complexes of iron.
10. (a) Discuss the principle of working of the reactors of nuclear power plants.
(b) What is meant by radioactive equilibrium? The ratio between atoms of two radioactive elements A & B at equilibrium was found to be $3.1 \times 10^4 : 1$. If the half life period of A is 2×10^{10} years what is the half life of B.

[5 x 5 = 25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. Construct the MO diagram Ferrocene and explain the bonding using MOT.
12. Explain the kinetics and mechanism of ligand substitution reactions in square planar complexes.
13. Discuss in detail the function of PS-I and PS-II in photosynthetic activity.
14. Explain the use of various NMR techniques in inorganic chemistry.
15. Explain the various nuclear models.

[10 × 3 = 30]

Third Semester M.Sc. Degree Examination — Model question paper
APCH322: ORGANIC CHEMISTRY — III
 (2025 admission Onwards)

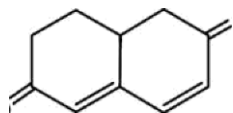
Time: 3 Hrs

Max. Marks: 75

SECTION A

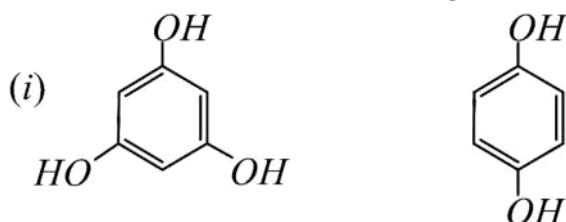
Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) What will be the Q_{max} for the following?



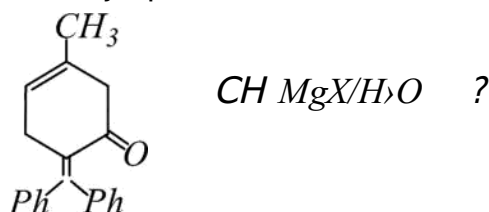
- (b) What will be the IR vibrational frequency of "CO" group in the following compound?
 (i) Benzylacetate (ii) Vinylacetate
 (c) What will be the base peak for 2-pentanone?

2. (a) What will be the number of ^{13}C signals in

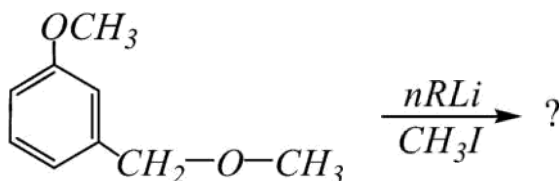


- (b) Give two examples for NMR shift reagent?
 (c) What is Nuclear Overhauser Effect?

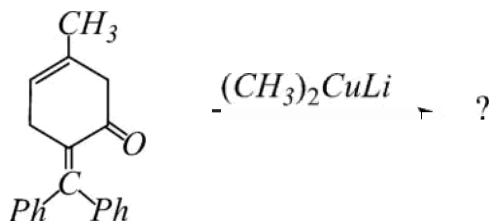
3. (a) The major product formed in the following reaction is



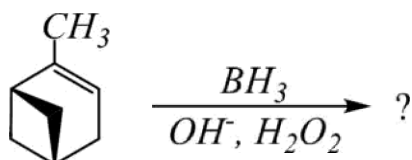
- (b) The major product formed in the following reaction is



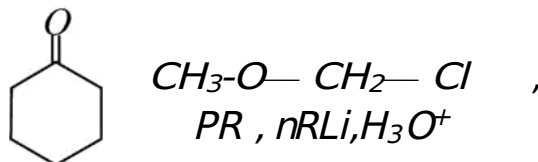
- (c) The major product formed in the following reaction is



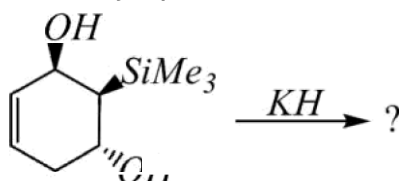
4. (a) The major product formed in the following reaction is



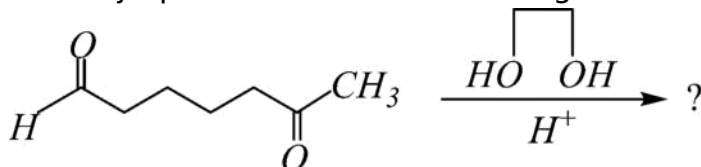
- (b) The major product formed in the following reaction is



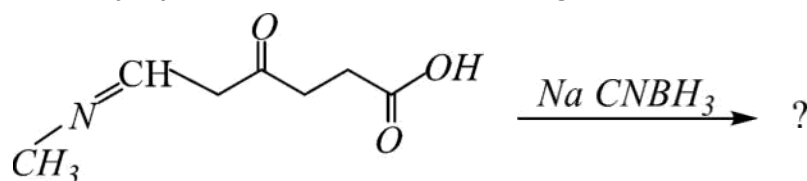
- (c) The major product formed in the following reaction is



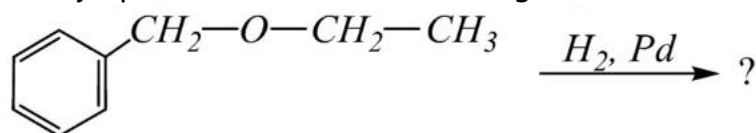
5. (a) The major product formed in the following reaction is



- (b) The major product formed in the following reaction is



- (c) The major product formed in the following reaction is

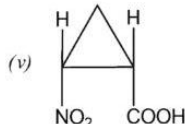
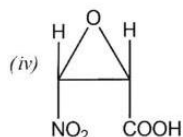
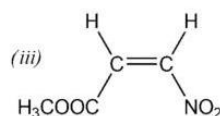
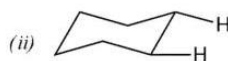
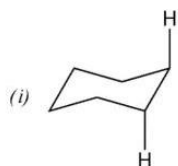


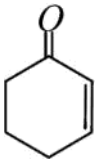
[2 × 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) What will be the 'J' values of vicinal hydrogen in the following compounds?



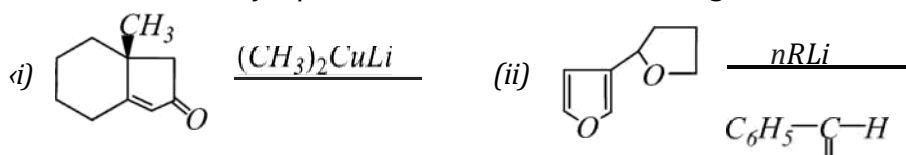
- (b) Write down the fragmentation pattern for 2-hexene?
7. (a) What are the basic principles of COSY?
 (b) Write the ^{13}C NMR values of the following compound?
- 
8. (a) Write a note on the application of $n\text{RLi}$?
 (b) Write a note on the preparation and application of Tebb's reagent?
9. (a) Write a note on the application of hindered boranes?
 (b) Write a note on the Sonogashira coupling reaction?
10. (a) Write a note on the reduction of aromatic rings by $\text{Li}/\text{C}_2\text{H}_5\text{OF}/\text{NH}_3$
 (b) Write a note on Bayer villager oxidation?

[5 x 5 = 25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. (a) Write a note on the Karplus equation and outline its application?
 (b) Write down the fragmentation pattern for n-propyl phenyl ketone including McLafferty rearrangement?
12. Write down the applications of NOE and DEPT?
13. (a) Write down the application of benzene tricarbonyl chromium?
 (b) Write down the major product involved in the following reaction?



14. (a) Write a note on Julia reaction?
 (b) Write a note on Suzuki coupling reaction?
15. (a) Write down the mechanism for Prevost hydroxylation?
 (b) Write down the application of Iridium complexes as a reducing agent?

[10 x 3 = 30]

Third Semester M.Sc. Degree Examination - Model question paper
APCH323: PHYSICAL CHEMISTRY — III
(2025 admission Onwards)

Time: 3 Hrs

Max. Marks: 75

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) State variation theorem
(b) What is overlap integral? Give its significance.
(c) Derive the term symbol of hydrogen molecule in the ground state.
2. (a) Predict and justify the condition at which a real gas obeys the following equation of state $PV = RT + Pb$.
(b) The van der Waals constant a for two gases are 4.17 and 0.024 dm³atm mol⁻² respectively. Explain which is easily liquefiable and why?
(c) At what pressure does the mean free path of argon gas at 25°C become comparable to the diameter of the atoms themselves? Given $a = 0.36$ nm²
3. (a) The shift in frequency shown by a proton from TMS is 180 Hz, when measured on a 100 MHz instrument. Calculate the chemical shift in ppm.
(b) Calculate the ESR frequency of an unpaired electron in a magnetic field 0.33 Tesla. Given for free electron $g=2$, $\hbar = 9.273 \cdot 10^{-27}$ J/T.
(c) What is meant by contrast agents in MRI?
4. (a) Apply phenomenological equation in thermal diffusion.
(b) What is the principle of minimum entropy production?
(c) What are the conditions under which linear relations are valid to understand irreversible processes?
5. (a) What is a minimal basis set?
(b) Construct the z-matrix of CO₂ molecule.
(c) Differentiate STO and GTO.

[2 x 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) Calculate the first order correction to the energy levels for a one-dimensional box with a slanted bottom whose potential energy varies as v_x/a where a is the length of the box.
(b) Apply HMO theory to 1, 3-butadiene molecule and discuss the molecular orbitals and their corresponding energy levels.
7. (a) Briefly explain the various intermolecular forces acting in gases.
(b) Discuss the barometric method of measurement of vapour pressure.
8. (a) What is ENDOR spectroscopy? How it is different from ELDOR spectroscopy?
(b) Discuss the application of Mossbauer spectroscopy.
9. (a) Derive expressions for entropy production in the case of system contains both the matter flow and current flow.

- (b) Describe the phase diagram of two salts and water system with double salt formation?
10. (a) Illustrate the Density functional theory method.
 (b) What is potential energy surface? Explain its significance.

[5 x 5 = 25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. (a) Discuss the quantum mechanical treatment of sp^2 hybridization.
 (b) Sketch the MO diagram of NO molecule and calculate bond order
 (c) Comment on the variation in stretching frequency of NO when it is changed to NO^+ .
12. Explain the various methods for the determination of surface tension of a liquid.
13. (a) Explain the principle and applications of solid-state NMR spectroscopy.
 (b) What is meant by hyperfine splitting in ESR spectra? Give the selection rule for hyperfine transitions?
 (c) Briefly explain the analytical applications of ESR spectroscopy.
14. (a) Draw the phase diagram of a three-component liquid system with three pairs of partially miscible liquids. Explain.
 (b) How would you understand (i) thermoosmosis and (ii) thermal diffusion from irreversible thermodynamics? [5+5]
15. (a) Write briefly on ab-initio methods used in computational chemistry? What are the merits and demerits of the method?
 (b) Explain the terms i) force field ii) contracted Gaussians. [7+3]

[10 x 3 = 30]

SEMESTER - IV

APCH421: CHEMISTRY OF ADVANCED MATERIALS AND RESEARCH METHODOLOGY

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	understand dimensions, synthesis, physicochemical properties of nanomaterials and its applications.	U, Ap, An	1
2.	understand and apply characterization tools for analysing nano structures.	U, Ap, An	1
3.	outline and recognize the types of polymerization, kinetics and mechanisms.	U, Ap, An	1
4.	understand the stereochemical aspects and methods for the determination of molecular weights of polymers.	U, Ap, An	1
5.	discuss the synthesis and applications of selected classes of speciality polymers.	U, Ap, An	1, 5
6.	distinguish the types and important applications of smart materials.	U, Ap, An	1, 5
7.	identify and discuss the basic concepts and problems involved in chemical research.	U, Ap,	1

PSO—Programme Specific Outcome

CO—Course Outcome

Cognitive Level:

R—Remember

U—Understanding

Ap—Apply

An—Analyse

E—Evaluate

C—Create

Module	Course Description	No. of Hrs	CO No.
1.0	Introduction to Nanomaterials and Nanotechnology	18	
1.1	Nanomaterials: 0D, 1D, 2D and 3D nanomaterials fundamental physicochemical principles - size dependence of the properties of nanomaterials - quantum confinement Nanocomposites.	3	1
1.2	Synthesis of nanomaterials: Sol-Gel, colloidal precipitation, co-precipitation, hydrothermal, vapour deposition, and sonochemical method.	3	1
1.3	Carbon nanostructures and clusters: Graphenes, carbon nanotubes and fullerenes (C ₆₀) - Synthesis, properties and applications.	4	1
1.4	Metal nanoparticles: Synthesis and properties (optical, electronic, magnetic), surface plasmon resonance.	3	1
1.5	Evolving interfaces of nanotechnology: Nanobiotechnology, nanoelectronics, nano sensors, nano-biosensors, nano tweezers, elementary ideas about nano catalysts, nano photocatalysts, nanofiltration.	3	1
1.6	Nanomedicines-nanoparticles for medical imaging and targeting cancer cells and nano encapsulation for drugdelivery to tumours. Nanotoxicology.	2	1
2.0	Characterization Tools in Nanotechnology	18	
2.1	Electron microscopies: Scanning electron microscopy (SEM), Transmission Electron Microscopy (TEM), High	4	2

	Resolution Transmission Electron Microscopy (HR-TEM).		
2.2	Probe microscopies: Atomic Force Microscopy (AFM), Scanning tunnelling microscopy (STM), Scanning tunnelling electron microscopy (STEM).	4	2
2.3	X-ray methods: X-ray diffraction (XRD), X-ray Photoelectron spectroscopy (XPS), Energy Dispersive X-ray Spectroscopy (EDAX), X-ray Fluorescence (XRF)	4	2
2.4	Laser scattering method: Dynamic light scattering (DLS)	1	2
2.5	Spectroscopic techniques: IR spectroscopy for surface functionalization of nanoparticles, UV-visible - Diffused reflectance spectroscopy, photoluminescence, Raman spectroscopy. (Basic understanding of each technique with special emphasis on characterization at nano scale).	5	2
3.0	Polymerization processes and Speciality Polymers	18	
3.1	Methods of polymerization - bulk, solution, melt, suspension and emulsion techniques. Step growth polymerization - Linear Vs Cyclic polymerization. Free radical addition polymerization - kinetics and mechanism. Chain transfer. Cationic and anionic polymerization: Kinetics and mechanism	4	3
3.2	Polymer stereochemistry: Configuration and conformation. Tacticity. Chiral polymers. Polymer characterization-Methods for determining molecular weights – static and dynamic light scattering, viscometry, and GPC	4	4
3.3	Crystalline and amorphous states-glassy and rubbery States. Glass transition temperature and crystalline melting of polymers. Degree of crystallinity - X-ray diffraction. Thermal analysis of polymers using DSC	3	4
3.4	Synthesis and Applications of Industrial Polymers-carbon chain and hetero chain polymers. Polymeric reagents, catalysts, and substrates. Conducting polymers: Synthesis & applications of polyacetylenes, polyanilines & polypyrroles	4	5
3.5	Basic concepts about polymer based LEDs and lithium polymer batteries. Main chain and side chain liquid crystalline polymers. Phase morphology	3	5
4.0	Smart materials	18	
4.1	Piezoelectric, magnetostrictive, halochromic, chromogenic, electrochromic, thermochromic, magnetocaloric and thermoelectric materials.	4	6
4.2	Chemistry behind photochromism in spiropyrans, spirooxazines, diarylethenes, azobenzenes, quinones. Examples for photochromic coordination compounds.	4	6
4.3	Shape-memory polymers, pH-sensitive polymers, Temperature-responsive polymers, dielectric elastomers.	3	6
4.4	Self-healing polymers and concept of mechanophores. Photo responsive and photorefractive polymers.	3	6
4.5	Introduction to ferrofluids, concept of pseudo elasticity.	3	5
5.0	Research Methodology in Chemistry	18	
5.1	Definition of research, objectives and motivations in research, scientific methods, role of theory, significance of research.	3	7

5.2	Types of research: historical, fundamental, analytical, conceptual, qualitative, quantitative, applied, clinical or diagnostic and experimental research.	2	7
5.3	Research approaches, research method vs. research methodology, research process, criteria and qualities of good research. Importance of research quality management, accountability in research.	3	7
5.4	Scientific writing: research proposal, research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.	3	7
5.5	Chemical literature: primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Reference management softwares: Mendeley, Endnote, Zotero	3	7
5.6	Literature databases: Web of Science, ScienceDirect, SciFinder, Scopus. Chemical abstract.	2	7
5.7	Important scientific and chemistry journals. Peer-reviewed journals, journal impact factor, citation index	2	7

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6. Lead J., and Smith, E., Environmental and Human Health Impacts of Nanotechnology, John Wiley & Sons. 2009.

APCH422a: ADVANCED INORGANIC CHEMISTRY

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	explain the schemes for σ and π bonding with examples.	U	1
2.	explain MO and Ligand field theory with the support of group theory and construct the MO diagram of octahedral complexes.	U, C	1
3.	apply character tables to find out the Infrared and Raman active modes for C_{2v} , C_{3v} and D_{4h} .	Ap, An	1
4.	assimilate the concepts of molecular recognition, self-assembly, dynamic combinatorial chemistry and supramolecular chirality, and be aware of the most important work in the field.	U	1
5.	understand the nature of bonding in metal atom clusters and distinguish Low nuclearity and High nuclearity carbonyl clusters.	U, An	1
6.	perform the electron counting schemes in cluster compounds.	Ap, An	1
7.	differentiate the different types of cluster molecules and understand their utility in catalysis.	An	1
8.	understand and explain the role of metal ions in biological systems and give examples for the use of metals in medicine.	U, An	1
9.	differentiate the defects arising due to deficiency and excess presence of metal ions in the body.	An	1
10.	explain the acid base concept in non aqueous media and identify the reactions taking place in selected non aqueous solvents.	An	1

Module	Course Description	No. of Hrs	CO No.
1.0	Applications of Group Theory	18	
1.1	Hybrid orbitals and molecular orbitals for simple molecules. Transformation properties of atomic orbitals. Hybridisation schemes for s and p bonding with examples	3	1
1.2	MO theory for AB_n type molecules. Molecular orbitals for regular octahedral, tetrahedral and metals and sandwich compounds.	3	2
1.3	Ligand field theory: Splitting of d orbitals in different environments using group theoretical considerations.	3	2
1.4	Construction of energy level diagrams. Correlation diagram. Method of descending symmetry. Tanabe-Sugano diagrams. Selection rules for electronic spectra.	3	2
1.5	Molecular orbitals in octahedral complexes. Formation of symmetry adapted group orbitals of ligands. MO diagram.	3	2
1.6	Symmetry and selection rules: Symmetry properties of common orbitals. Application of character tables to infrared and Raman spectroscopy. Infrared and Raman active modes for C_{2v} , C_{3v} and D_{4h} .	3	3

2.0	Supramolecular Chemistry	18	
2.1	Concepts and language. Molecular recognition: Molecular receptors for different types of molecules, design and synthesis of coreceptors and multiple recognition.	4	4
2.2	Strong, weak and very weak Hydrogen bonds. Utilisation of H-bonds to create supramolecular structures. Use of H bonds in crystal engineering and molecular recognition.	4	4
2.3	Supramolecular reactivity and catalysis. Transport processes and carrier design.	3	4
2.4	Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching device.	4	4
25	Examples of self-assembly in supramolecular chemistry.	3	4
3.0	Metal-Metal bonds and Metal Clusters	18	
3.1	Metal—Metal bonds and metal atom clusters. Conditions favourable for formation of M—M bonds, Compounds with M—M multiple bonds.	4	5
3.2	Dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding: systems with and without quadrupole bond.	3	5
3.3	Tri, Tetra and hexa nuclear clusters, Isoelectronic and isolobal relationships, Low nuclearity and High nuclearity carbonyl clusters (LNCCs and HNCCs),	3	5
3.4	Hetero atoms in metal atom clusters, electron counting schemes for HNCCs — Capping Rule.	3	6
3.5	Cubane Clusters, Chalcogenide Clusters, Zintl Anions and Cations.	4	7
3.6	Molecular Clusters in catalysis	1	7
4.0	Selected Topics in Bioinorganic Chemistry	18	
4.1	Copper on biochemical systems. Oxidase activity, superoxide dismutase activity. Electron transport in biology.	4	8
4.2	Structure and function of copper proteins in electron transport process. Oxygen transport copper proteins. Hemocyanin-copper transport, copper enzymes-Azurin, plastocyanin.	4	8
4.3	Inorganic medicinal chemistry. Metals in medicine. Metal deficiency and diseases. Toxic effects of metals. Effect of deficiency and excess of essential metal ions.	3	9
4.4	Toxicity due to non-essential elements and speciation. Detoxification mechanism.	3	8
4.5	Role of lithium and aluminium in biological systems. Chelation therapy and chemotherapy.	2	9
4.6	Anticancer drugs and vanadium based diabetics drugs.	2	9
5.0	Acids, Bases and Non-aqueous Solvents	18	
5.1	Acid base concept in non aqueous media-HSAB concept, solvent effects, linear free energy relationship — mechanism and methods of determination, super acids	4	10
5.2	Reactions in non-aqueous solvents. Ammonia-solutions of metals in liquid ammonia.	3	10
5.3	Protic solvents: anhydrous sulfuric acid, hydrogen halides.	3	10
5.4	Aprotic solvents: non-polar solvents, non-ionizable polar	8	10

	solvents, polar solvents undergoing autoionization, liquid halogens, interhalogen compounds, oxyhalides, dinitrogen tetroxide, sulphur dioxide.		
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References

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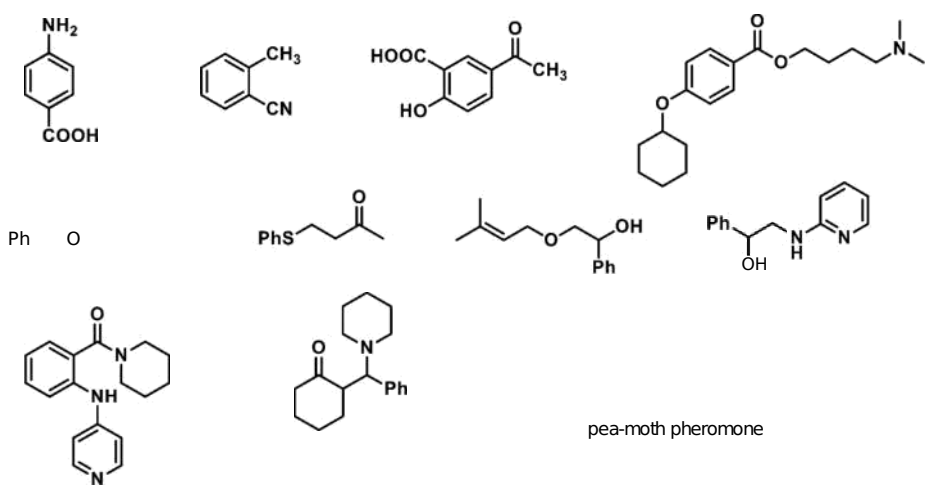
Further Reading

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4. Structural Methods in Molecular Inorganic Chemistry. D.W.H. Rankin, N.W. Mitzel, C.A. Morrison John Wiley & Sons, Ltd, 2013
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APCH422b: ADVANCED ORGANIC CHEMISTRY

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	explain the total synthesis of some steroids and structural elucidation of cholesterol.	Ap, An	1
2.	explain the structural elucidation of some terpenes and alkaloids by various methods	Ap, An	1
3.	explain the structure of proteins	Ap	1
4.	explain the basic principles of molecular recognition and supra molecular chemistry and to apply them.	U, An	1, 5
5.	describe the importance of drug designing and the chemistry of some important drugs.	U, Ap	1, 5
6.	identify, analyse and evaluate synthetic routes to target molecules using retrosynthesis	U, An, Ap	1, 5, 8
7.	understand the 12 principles of Green Chemistry.	R, U	4
8.	identify greener solvents and recycling of these including catalysts.	U, Ap	1, 4
9.	apply the principles for Green Chemistry in order to make a life cycle assessment for a chemical product	Ap, An	1, 5
10.	explain how green chemistry principles can be used to advance UN Sustainable Development Goals	U, Ap	1, 5

Module	Course Description	No. of Hrs	CO No.
1.0	Natural Products and Biomolecules	18	
1.1	Synthesis of testosterone, androsterone, progesterone (from cholesterol), synthesis of quercetin and estrone, Structural elucidation of cholesterol, colour reactions of steroids, Oral contraceptives	6	1
1.2	Structural elucidation of menthol, abietic acid and β – carotene	3	2
1.3	Degradation of alkaloids — Hoffman exhaustive methylation and limitation — Emde's degradation — von Braun's method. Total synthesis of morphine. Application of Ergot alkaloids	4	2
1.4	Denaturation of protein. Peptide bond formation methods — SPPS — Merrifield resin.	1	3
1.5	Biosynthesis of steroids and terpenes from acetyl CoA	1	2
2.0	Molecular Recognition and Supramolecular Chemistry	18	
2.1	Introduction to supra molecular chemistry — The concepts of molecular recognition, forces involved in molecular recognition — Hydrogen bonding, ionic bonding, π stacking van der Waals and hydrophobic interaction.	4	4
2.2	Receptors — Guanidine group, expanded sapphyrins, organometallic receptors [Cobaltocenium (1) with amide functionally], β -cryptand, molecular clefts with tweezers Kemp's triacid, cyclodextrins, and calixarenes.	4	4
2.3	Molecular self-assembly — supramolecular devices -	4	4
2.4	Importance of molecular recognition in DNA and protein structure,	4	4

	their function and protein biosynthesis - transcription and translation— basic aspects only.		
2.5	Supramolecular systems like organic zeolites, clathrate hydrates of gases, Helicates, liquid crystals — elementary ideas only.	2	4
3.0	Medicinal Chemistry	18	
3.1	Concept of 'LEAD' with examples. Factors governing drug-design. Rational approach to drug design. Drug-design: The method of variation. Drug-design and development. Molecular hybridisation - rigidity and flexibility versus drug design.	5	5
3.2	Pro drugs - classification - carrier linked, mutual, Bio processor. Pro drugs of functional moieties. Enzyme inhibition and classification.	5	5
3.3	Different classes of drugs with examples newer drugs, prostaglandin, Anticonvulsant drugs, hormone Antagonists, Antithyroid drugs, antimicro bacterial drugs, cardiac steroids, Heparin, cromakalim and drugs to compact AIDS.	4	5
3.4	Synthesis of paracetamol, phenobarbital diazepam, sulphamethoxazole, benzylpenicillin, chloramphenicol.	4	5
4	Retrosynthetic Analysis	18	
4.1	Retrosynthetic disconnections: The basis for retrosynthetic analysis and terminologies, Concepts of synthons reagents, synthetic equivalents (formyl/acyl anion, enolate, homo enolate, etc.) functional group interconversion	3	6
4.2	One group and two group carbon-heteroatom disconnection: chemo selectivity and umpolung concept	3	6
4.3	Protecting groups: Selective protection and deprotection of various functional groups and its application in total synthesis. Alcohol protecting agents — tetra hydropyranyl, silyl t-butyl trichloro ethyl. Carbonyl protecting agents — ethylene glycol, ethane 1,2 dithiol and propane 1,3-dithiol. Amino protecting agent — tertiary butoxy carbonyl chloride and benzyloxy carbonyl chloride, FMoc.	4	6
4.4	Synthetic routes based on retrosynthetic analysis —  benzyl penicillin and longifolene	8 (4+4)	6

5.0	Green Chemistry	18	
5.1	Twelve principles of green chemistry organic synthesis in Benign Green solvents — water, supercritical carbon dioxide, ionic liquids, olyethylen glycol, and fluoruous solvents.	5	7
5.2	Organic synthesis using green reagents — oxygen, ozone, hydrogen peroxide dioxiranes, peroxy acids, Dimethyl carbonate, poly supported reagents — PNBS, Polymeric organo tin dihydride reagents, polystyrene anhydride and polymeric sulfonazide.	5	8, 9, 10
5.3	Synthesis using scavenger resins, catalysis, biocatalysis, Green processes — microwave synthesis — Two principal mechanism for interaction with matter - The microwave effect with examples - single mode and multimode microwave effect with examples — single mode and multimode microwave cavities.	6	8, 9, 10
5.4	Biodegradable polymers	2	10

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2. N. R. Krishnaswamy, Chemistry of Natural Products a unified approach, Universities Press, 1999
3. O. P. Agarwal, Natural products Vol 1 and 2, Goel publishing, 2010.
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6. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reaction, Ane Books, 2006.
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14. A. L. Lehninger, D. L. Nelson, M. M. Cox, Lehninger, Principles of Biochemistry, 5th Edn., W.H. Freeman, 2008.
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APCH422c: ADVANCE PHYSICAL CHEMISTRY

cO No.	Expected Course Outcomes Upon completion of this course, the students will be able to	Cognitive Level	PSO Ho.
1.	apply the group theory in the identification of IR and Raman active normal modes in molecules coming under various point groups such as C_{2v} , C_{3v} , C_{4v} , T_d and O_h .	Ap	1
2.	apply group theory in solving spectroscopic problems.	Ap	1
3.	solve the problems in Exactly solvable systems like Simple Harmonic Oscillator, rigid rotor and the Hydrogen atom.	Ap, An	1
4.	explain the approximation methods used in quantum mechanics	U	1
5.	illustrate trial wave functions for calculation of H atom and particle in a 1D-box as examples.	U, Ap	1
6.	set up secular determinants	C	1
7.	explain the variation in the state of a system with time	U, An	1
8.	apply computational methods as potential tools for practicing chemistry	An	1
9.	construction of Z-matrices of simple molecules H_2 , H_2O , H_2O_z , H_2CO , CH_3CHO , CH_4 , C_2H_4 and with dummy atom, CO_2 , NH_3 , C_6H_6 .	C	1
10.	explain the commonly using force fields (MM3, MMFF, AMBER and CHARMM) and Softwares.	Ap	1
11.	Compare Molecular Mechanics, <i>Ab-initio</i> method, Semi-empirical method and DFT method of computations.	E	1

Module	Course Description	No. of Hrs	CO No.
1.0	Applications of Group Theory	18	
1.1	Spectroscopic applications: Transition moment integral transition moment operator. Vanishing matrix element. Symmetry selection rule for IR, Raman and electronic spectra. Dipole and polarizability transition moment operator.	3	1, 2
1.2	Identification of IR and Raman active normal modes in molecules coming under various point groups such as C_{2v} , C_{3v} , C_{4v} and C_{2h}	3	1, 2
1.3	Mutual exclusion and complementarity principle of IR and Raman spectra and their use in the identification of molecular structures	3	1, 2
1.4	Probability of overtone and combination bands. Identification of allowed and forbidden electronic transitions in carbonyl groups. Vibronic transitions.	3	1
1.5	Application to MO theory: Symmetry adapted LCAO-MO theory of π (pi)-bonded hydrocarbons	3	1
1.6	Projection operator and its use in the construction of wave functions of n — molecular orbitals of cyclopropenyl cation. secular equations and use of symmetry for simplifying the calculations of energy and wave functions of ethylene, butadiene and benzene	3	1

2.	Exactly Solvable Systems	18	
2.1	Simple Harmonic Oscillator: Wave equation for 1D harmonic oscillator. Complete solution and their properties. 3D-Harmonic oscillator. Potential energy in three dimension and Schrodinger wave equation in Cartesian coordinate. Separation of variables and solution of the equation for energy and wave function. Degeneracy.	3	3
2.2	Rigid rotor: Schrodinger equation in polar Coordinate. Angular momentum operator for rigid rotor. Separation of variables and complete solution for 0 and g equations.	3	3
2.3	Legendre polynomials and associated Legendre functions. Normalization of associated Legendre functions and evolution of the values of orbital angular momentum quantum number. Recursion relations. Rigid rotor wave function and energy.	3	3
2.4	The Hydrogen atom: Schrodinger wave equation in polar coordinate. Separation of variables and complete solution of the radial part. The associated Laguerre polynomial. Normalization. The evolution of the value of the principal quantum number.	3	3
2.5	The spherical harmonics and the radial part of the wave function. The total wave function of H atom. The wave functions of Hydrogen like atomic orbitals and explanations for the shapes of various orbitals.	3	3
2.6	Angular momentum, angular momentum operators (L_x , L_y , L , and L^2) and their commutation properties. Spherical harmonics as eigen functions of angular momentum operator L and L^2 . Ladder operator method for angular momentum. Space quantisation.	3	3
3.0	Approximation Methods — I	18	
3.1	Schrodinger wave equation for He atom and anharmonic oscillator and difficulty to get the exacts solution.	3	4
3.2	The Variation method: Variation theorem. The variation integral and its properties. Variational parameters. Trial wave functions.	3	4
3.3	Illustration of trial wave functions for calculation of H atom and particle in a 1D-box as examples.	3	5
3.4	Trial functions as linear combination of orthonormal functions, linear combinations of functions containing variational parameters as trial functions.	3	5
3.5	Setting up of secular determinants. Variation methods of normal state of He.	3	6
3.6	The SCF method, SCF and variation method. Strength and limitation of the method.	3	6
4.0	Approximation Methods — II	18	
4.1	The perturbation method. The generalized perturbation method. The idea of successive correction to unperturbed systems.	3	4
4.2	First order perturbation. Correction of wave function	3	4

	and energy. Theory of non - degenerate level perturbation. The normal Helium atom.		
4.3	The first order perturbation of the degenerate level. The hydrogen atom.	3	4
4.4	Second order perturbation theory. Correction for wave function and energy. Stark effect.	3	4
4.5	Time dependent wave equation: Variation in the state of a system with time. Emission and absorption of radiation.	3	7
4.6	The Einsteins transition probability and its calculation. Selection rules and intensity of spectrum for harmonic oscillator, rigid rotor and hydrogen atom.	3	4
5.0	Computational Methods	18	
5.1	Computational methods as potential tools for practicing chemistry. Potential energy surface, saddle point, local minima and global minima. Geometry optimisation. Exchange and overlap integrals. Difficulty in evaluating them with H-like wave functions. Slater Type functions (STO), approximation of STO with Gaussian type functions. Contracted Gaussians.	3	8
5.2	Basis sets: minimal basis set, split valance basis set, polarised basis set and diffused basis set. Model chemistry and notations. Geometry input - in terms of Cartesian coordinates and internal coordinates. Z-matrix, construction of Z-matrices of simple molecules H ₂ , H ₂ O, H ₂ , H ₂ CO, CH ₃ CHO, CH ₄ . C ₂ H ₂ and with dummy atom, CO ₂ , NH ₃ , C ₆ H ₆ .	3	9
5.3	Molecular mechanics method: Force fields, potential energy expressions for bond stretching, bending, torsion, non-bonded interactions, electrostatic interaction and H-bonding. Setting up of force field expressions. Method of parameterisation. Use of molecular mechanics. Brief introduction to commonly using force fields (MM3, MMFF, AMBER and CHARMM) and Softwares.	3	10
5.4	Ab-initio method: Hartree-Fock Self Consistent Field method. Slater determinant. Post Hartree-Fock methods —Configuration Interaction (CI) and Moller Plesset (MP) methods.	3	11
5.5	Semi empirical method: Basic principle of the method. Its variants, ZDO, CNDO and INDO.	3	11
5.6	Density Functional method: Functional. Hohenberg-Kohn theorems. Kohn-Sham orbitals. Basic idea of Local Density (LD) approximation, Generalised Gradient approximation and hybrid (BLYP, B3LYP) methods. Comparative study of Molecular Mechanics, Ab-initio method, Semi-empirical method and DFT method of computations.	3	11

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8. D. A. McQuarrie, J. D. Simon, Physical Chemistry - A Molecular Approach, Viva Publishers
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APCH423: Dissertation

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	demonstrate an advanced theoretical and technical knowledge of chemistry as a creative endeavour; analyse, interpret and critically evaluate scientific information.	Ap, An	1
2.	present information, articulate arguments and conclusions, in a variety of modes, to audiences in their field of research.	E, C	5, 8
3.	as part of a team or individually, design, conduct, analyse and interpret results of an experiment, and effectively communicate these in written reports and other formats.	Ap, An	3, 7
4.	develop an understanding of the requirements to undertake independent research in a chemistry field.	U	6, 9
5.	demonstrate an understanding of the relationship between scientific research and the progress of new knowledge in a global scenario.	An	5, 6, 9

APCH424: Comprehensive Viva Voce and Visit to R & D Centre

CO No.	Expected Course Outcomes <i>Upon completion of this course, the students will be able to</i>	Cognitive Level	PSO No.
1.	Understand the relevance of independent supervised research in a chemistry field and the need of well-developed judgement, adaptability and accountability as a practitioner or learner	U, An	2, 9

Model Question Papers

General/ Instruction to question paper sellers

- There will be a 15 main questions in each question paper divided into 3 sections — A, B and C.
- Each of the sections A, B and C will have 5 questions each, 1 from each module.
- Each question in Section A will have 3 sub questions (a), (b) and (c), of which the candidate has to answer any two (2 marks each).
- Each question in Section B will have 2 sub questions (a) and (b), of which the candidate has to answer any one (5 marks each).
- Candidate should answer any three out of the five questions in Section C (10 marks each).
- Section A carries a total of 20 marks, Section B carries 25 marks, and Section 3 carries 30 marks.
- The maximum marks will be 75 and the duration of the exam will be 3 hrs.

**APCH421: CHEMISTRY OF ADVANCED MATERIALS AND
RESEARCH METHODOLOGY**

(2025 admission Onwards)

Time: 3 Hrs

Max. Marks: 75

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) What is meant by quantum confinement?
(b) Explain the synthesis of metal nanoparticles with an example.
(c) Write a short note on nano toxicology?
2. (a) What is EDAX?
(b) How XPS is used in nano technology?
(c) How diffused reflectance spectroscopy is used in characterisation of nanoparticles?
3. (a) What do you mean by chain transfer in polymerization process?
(b) Mention two advantages and two disadvantages of solution polymerization over bulk polymerization.
(c) Explain briefly "auto acceleration" in radical polymerization? Why does it happen?
4. (a) What are conducting polymers?
(b) Name any two polymeric reagents.
(c) Which are the polymers used in optical lithography?
5. (a) What are halochromic materials?
(b) Write a note on pH-sensitive polymers.
(c) What are piezo electric materials?

[2 x 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) Explain the relation between size and properties of nano-materials.
(b) Explain the CVD method used in the preparation of nanoparticles.
7. (a) Explain the use of powder XRD in determination of particle size of nanomaterials.
(b) How is electron microscopy used as characterisation techniques?
8. (a) What are chain transfer agents? Describe their effect on rate expression and molecular weight obtained in the presence of chain transfer agent.
(b) Unlike radical polymerisation both cationic and anionic polymerization show a marked dependence on the type of solvent used. Discuss on this.
9. (a) Discuss the structure and working principle of lithium polymer batteries.
(b) Explain in detail the synthesis of polythiophenes.
10. (a) Explain the chemistry behind photochromism in spirooxazines and quinones.
(b) Write short note on synthesis and application of ferrofluids.

[5 x 5 = 25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. Explain application and role of metal nano particles in catalysis with examples.
12. Discuss the applications of DLS and IR spectroscopy in the analysis of nanomaterials.
13. Elaborate any two methods to determine the molecular weight of polymers.
14. Explain the application of polymers in drug delivery and in catalysis.
15. Describe with proper examples:
(a) magnetostrictive materials (b) thermoelectric materials
(c) self-healing polymers (d) dielectric elastomers.

[10 3 = 30]

Fourth Semester M.Sc. Degree Examination - Model question paper
APCH422a: ADVANCED INORGANIC CHEMISTRY
(2025 admission Onwards)

Time: 3 Hrs

Max. Marks: 75

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) What is the point group of NO_3^- ? How does its symmetry change when complexed as unidentate ligand?
(b) Give the splitting of d-orbitals in a square pyramidal geometry?
(c) Demonstrate that C_3 and C_3^2 belong to the same class in C_3 point group.
2. (a) What is meant by macrocyclic effect?
(b) Give any two examples of self-assembly in supramolecular chemistry.
(c) What are the three basic functions of supramolecular species?
3. (a) What are anionic clusters? Give examples
(b) Explain Wade's rules to calculate the number of framework electrons in clusters.
(c) Clusters of $\text{Co}(\text{CO})_{12}$ and $\text{Co}_3\text{FeH}(\text{CO})_9$ are isolobal to each other. Explain
4. (a) What is cisplatin? What is its importance?
(b) What is the role of Lithium in biological systems?
(c) Write any two diseases caused by the deficiency of copper in the body.
5. (a) Give examples of room-temperature molten salts that could be used as non-aqueous solvents?
(b) What is meant by levelling effect of solvent?
(c) Which species would act as a base in (1) BrF_2 and (2) liquid SO_2 . Why?

[2 x 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) Give the salient features of Tanabe-Sugano diagram taking d ion as an example.
(b) Discuss the application of group theory in arriving at the selection rules for the electronic spectrum of metal complexes.
7. (a) Explain the importance of supramolecular chemistry in the field of catalysis
(b) What are the advantages and applications of supramolecular chemistry in Nanotechnology?
8. (a) Explain the concept of Chevrel phases.
(b) What are LNCC's? Give eg: Discuss their structures.
9. (a) The toxicity of metals have been variously correlated with their (1) electronegativity, (2) insolubility of sulphides and (3) stability of chelates. Discuss.
(b) What are dismutation reactions? Give eg: What type of metal is in superoxide dismutase?

10. (a) What are the advantages and disadvantages of using protic solvents as non-aqueous solvents?
 (b) Write a note on the reactions in liquid HF.

[5 x 5 = 25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. Deduce the normal modes of trans-N₂F₂ molecule and predict the IR and Raman activity of the modes. Given the character table for C_{2h}.

C ₂	E	C ₂	i	σ _h	
A _g	1	1	1	1	R, x ² , y ² , z ² , xy
B _g	1	-1	1	-1	Ry, Ry XZ, yz
A _u	1	1	-1	-1	z
B _u	1	-1	-1	1	x, y

12. Discuss with suitable examples the different types of interaction in supramolecular compounds.
13. Discuss and draw the structure and bonding of (Re₂Xe)²⁺.
14. Explain the structure and functions of hemocyanin and plastocyanin
15. Write a detailed account of the reactions in the following non-aqueous solvents:
 (1) NH₃ and (2) N₂

[10 x 3 = 30]

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) Write any two colour reaction for vitamin D?
(b) Mention any two application of Ergot alkaloids?
(c) Give the structure of cholesterol. How will you determine its carbon skeleton through Hoffmann degradation?
2. (a) What are cyclodextrins? Give one example?
(b) Explain the term π -stacking?
(c) What are liquid crystals?
3. (a) Write any two drugs to combat "AIDS"?
(b) Give the structure of chloramphenicol and benzyl penicillin?
(c) What are the factors governing drug design?
4. (a) What are synthons?
(b) What is umpolung?
(c) Write any two amino protecting agents?
5. (a) Give two examples for dimethyl carbonate as a green reagent in organic synthesis?
(b) Give two advantage of scavenger resins?
(c) What are the types of phase transfer catalyst?

[2 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) Write note on synthesis of testosterone?
(b) Write note on structural elucidation of menthol?
7. (a) Write note on π -stacking and hydrogen bonding interaction in supramolecular chemistry?
(b) Write note on organometallic receptors?
8. (a) Name the steps involved in drug design?
(b) Give the synthesis route for diazepam and sulphamethoxazole.
9. (a) Describe various protecting agent for alcohols?
(b) Write a synthetic route for benzyl penicillin based on retro synthetic analysis?
10. (a) Explain briefly some organic reaction involving microwave synthesis?
(b) Explain briefly some organic reaction involving phase transfer catalyst?

(5 x 5 = 25)

SECTION C

Answer any three questions. Each question carries 10 marks

11. (a) Write down the steps involved in the total synthesis of testosterone from cholesterol?
(b) Write down the steps involved in the total synthesis of estrone?

12. Write a note on the molecular receptors such as Kemp's triacid, cyclodextrins and calixarenes?
13. (a) Write a note on drug design and development?
(b) Give one example each for AIDS drug, hormone Antagonists, newer drugs and antibiotic.
14. Write a note on solid supported reagents for green chemical reactions with suitable examples.
15. Write the synthetic routes for longifolene based on retro synthetic analysis.
[10 3 = 30]

Fourth Semester M.Sc. Degree Examination - Model question paper
APCH422c: ADVANCED PHYSICAL CHEMISTRY
 (2025 admission Onwards)

Time: 3 Hrs

Max. Marks: 75

SECTION A

Answer two among (a), (b) and (c) from each. Each sub question carries 2 marks

1. (a) Define projection operator.
 (b) Explain vanishing and non-vanishing integral with one example each.
 (c) Discuss the mutual exclusion principle using group theory.
2. (a) Explain space quantization.
 (b) Express the angular momentum operators in terms of spherical coordinates.
 (c) Write the three Legendre polynomials when $m=0$ and $l=1, 2, 3$.
3. (a) Write one trial function to solve Helium by variation method. Justify the result.
 (b) Briefly discuss SCF method.
 (c) State and explain variation theorem.
4. (a) State and explain selection rules for vibrational transitions in simple harmonic oscillator.
 (b) The potential energy term for an harmonic oscillator is $\frac{1}{2}kx^2 + bx^3$ Predict the correction term according to first order perturbation method. Justify the result.
 (c) What is Stark effect?
5. (a) What is the meaning of the notation 3-21G**?
 (b) What is parametrisation? How does it simplify ab initio calculations?
 (c) Write the z-matrix of Ammonia molecule.

[2 x 10 = 20]

SECTION B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6. (a) HCHO belongs to C_{2v} point group. Using group theory, find out the lowest energy electronic transition.
 (b) Find the IR and Raman active vibrations of NH_3 ? C_{3v} character table given.

C_{3v}	E	$2C_3$	$3C_2$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (xz, yz)$

7. (a) Write Schrodinger wave equation for a rigid rotor. Transform it into the Legendre equation.
 (b) Solve the time independent Schrödinger wave equation for a 3D-harmonic oscillator whose potential energy is

$$V_{(x,y,z)} = \frac{1}{2}(k_1x^2 + k_1y^2 + k_1z^2)$$

8. (a) Estimate the ground state energy of normal Helium atom using variation method.
(b) What are the strength and limitations of variation method?
9. (a) Show that the first order Stark effect on the ground state of hydrogen atom is zero.
(b) Find the ground state energy of a particle in one dimensional box with slanted bottom using first order perturbation method.
10. (a) Explain DFT method of computational chemistry.
(b) Discuss the need of Post Hartree-Fock method.

[5 5 = 25]

SECTION C

Answer any three questions. Each question carries 10 marks

11. Find energy of R molecular orbitals of benzene using HMO method. Use C6 character table.
12. Apply Schrodinger wave equation for simple harmonic oscillator. Find eigen function and eigen values.
13. What is linear variation method? Illustrate using one example.
14. Briefly discuss time dependent perturbation theory.
15. Discuss the various computational methods based on wave function. Make a critical comparison.

[10 • 3 = 30]