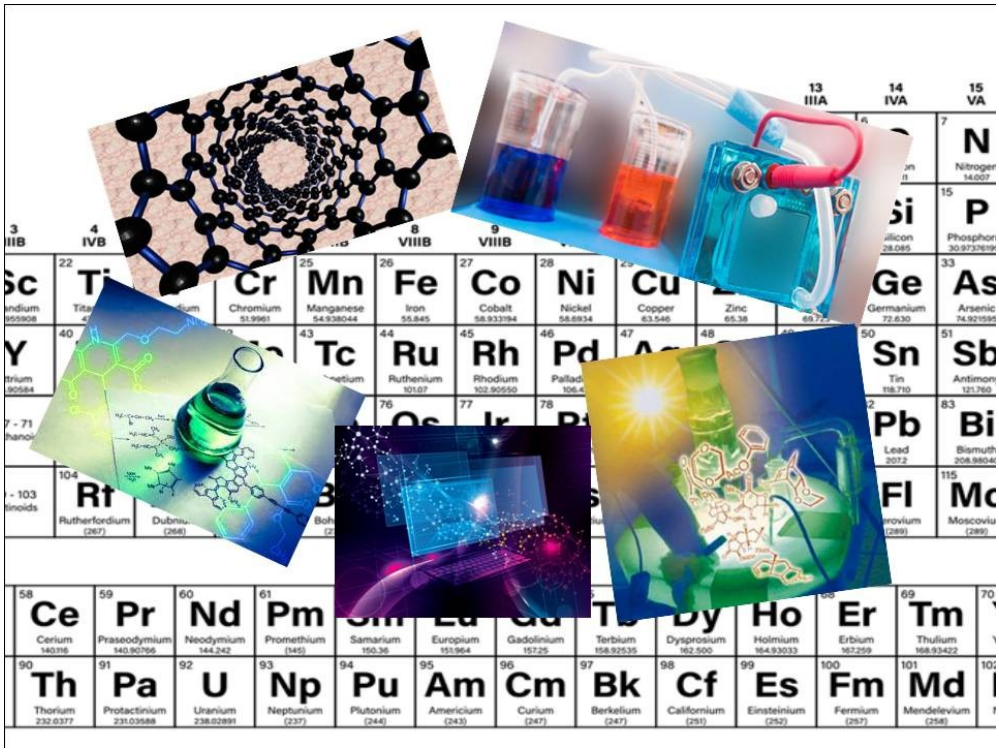
# Learning Outcomes-based Curriculum Framework (LOCF) for Post-graduate Programme



## M.Sc. Programme in Chemistry

(Syllabus effective from 2020 Admission onwards)

**UNIVERSITY OF KERALA**

Department of Chemistry

**2020**

## PREAMBLE

The role of higher education is vital in securing the gainful employment and providing further access to higher education comparable to the best available in the world-class institutions elsewhere. The improvement in the quality of higher education, therefore, deserves to be given tom-most priority to enable the young generation of students to acquire skill, training and knowledge to enhance their thinking, comprehension and application abilities and prepare them to compete, succeed and excel globally. Sustained initiatives are required to reform the present higher education system for improving and upgrading the academic resources and learning environments by raising the quality of teaching and standards of achievements in learning outcomes across all undergraduate programs in science, humanities, commerce and professional streams of higher education.

One of the significant reforms in the undergraduate education is to introduce the Learning Outcomes-based Curriculum Framework (LOCF) which makes it student-centric, interactive and outcome-oriented with well-defined aims, objectives and goals to achieve. The University Grants Commission (UGC) took the initiative of implementing the LOCF in the Colleges and the Universities of the country. Accordingly, the University of Kerala has decided to implement the LOCF in all its departments under the auspices of Internal Quality Assurance Cell (IQAC). A series of teacher training workshops were organised by IQAC and the office of the Credit and Semester System (CSS), and the departments have revised the syllabus accordingly, through workshops and in consultation with academic experts in the field.

## GRADUATE ATTRIBUTES (GAs)

The Graduate Attributes (GAs) reflect particular qualities and abilities of an individual learner including knowledge, application of knowledge, professional and life skills, attitudes and human values that are required to be acquired by the graduates of University of Kerala. The graduate attributes include capabilities to strengthen one's professional abilities for widening current knowledge and industry-ready skills, undertaking future studies for global and local application, performing creatively and professionally, in a chosen career and ultimately playing a constructive role as a socially responsible global citizen. The Graduate Attributes define the characteristics of learners and describe a set of competencies that are beyond the study of a particular area and programme.

**The GAs of University of Kerala**

- Continue life-long learning as an autonomous learner
- Continuously strive for excellence in education
- Apply and nurture critical and creative thinking
- Promote sustainable development practices
- Promote co-operation over competition
- Balance rights with responsibilities
- Understand and respect diversity & difference
- Not be prejudiced by gender, age, caste, religion, or nationality.
- Use education as a tool for emancipation and empowerment of humanity

## BRIEF HISTORY OF THE DEPARTMENT

The origin of the Department of Chemistry may be traced to the establishment of the University of Travancore, 1937. It currently offers M.Sc., M.Phil. and Ph.D. programmes and is one of the active teaching and research departments in the state. The M.Sc. programme was named as M.Sc. Analytical Chemistry when it started in the year 1960, and later converted to M.Sc. in Chemistry in 1997. The faculty members, past and present, and the alumni have made valuable contribution to the teaching and research in chemistry. Theirprestigious recognitions include the Vice Chairmanship of UGC, Directorship of NAAC, Vice-Chancellorships at M. G. and IGNO Universities, Humboldt Foundation Fellowships, DAAD Fellowship, Fogarty NIH Travel Award and Bhatnagar Award.

# UNIVERSITY OF KERALA

## DEPARTMENT OF CHEMISTRY

## Syllabus for M.Sc. Chemistry

| Programme Specific Outcomes (PSO) for M.Sc. Chemistry | |
|---|---|
| **PSO 1** | Develop asolid understanding on the fundamental principles and major concepts in the core disciplines of chemistry with the ability to analyze at an advanced level |
| **PSO 2** | Generate an understanding on the importance of application of Chemisry in academic, industrial, environmental and social context. |
| **PSO 3** | Provide an intellectual training to develop a rational and rigorous scientific approach in synthesizing information and concepts. |
| **PSO 4** | Develop skills to handle modern analytical and spectroscopic instruments. |
| **PSO 5** | Equip the students to perform standard laboratory procedures, monitor by observation and measurement events or changes and record data. |
| **PSO 6** | Develop research and analytical skills in basic research with the ability to undertake research in multidisciplinary teams. |
| **PSO 7** | Provide a detailed training in written and verbal communication of scientific information and ideas |
| **PSO 8** | Develop ability to work independently or as part of a team in a research setting to adapt to wide range of available career option in the future. |

**PSO=Program Specific Outcome**

**R=Remember**
**Un=Understanding**
**Ap=Apply**
**An=Analyse**
**E=Evaluate**
**C=Create**
**FK=Factual Knowledge**
**CK=Conceptual Knowledge**
**PK=Procedural Knowledge**
**MK=Metacognitive Knowledge**

## Programme Structure of M.Sc. Chemistry

| Semester | Course Code | Name of the course | Core Courses (CC) | Discipline-Specific Elective (DSE) | Generic Course (GC) | Skill Enhancement Elective (SEE) | Credits |
|---|---|---|---|---|---|---|---|
| I | **Core Courses (CC)** | | | | | | |
| | CHE-CC-511 | Inorganic Chemistry I | + | | | | 3 |
| | CHE-CC-512 | Organic Chemistry I | + | | | | 3 |
| | CHE-CC-513 | Physical Chemistry I | + | | | | 3 |
| | CHE-CC-514 | Inorganic Chemistry Lab I | + | | | | 3 |
| | CHE-CC-515 | Organic Chemistry Lab I | + | | | | 3 |
| | CHE-CC-516 | Physical Chemistry Lab I | + | | | | 3 |
| II | CHE-CC-521 | Inorganic Chemistry II | + | | | | 3 |
| | CHE-CC-522 | Organic Chemistry II | + | | | | 3 |
| | CHE-CC-523 | Physical Chemistry II | + | | | | 3 |
| | CHE-CC-524 | Inorganic Chemistry Lab II | + | | | | 3 |
| | CHE-CC-525 | Organic Chemistry Lab II | + | | | | 3 |
| | CHE-CC-526 | Physical Chemistry Lab II | + | | | | 3 |
| | **Discipline-Specific Elective (DE)** | | | | | | |
| | CHE-DE-527 | Advanced Inorganic Chemistry | | + | | | 2 |
| | CHE-DE-528 | Advanced Organic Chemistry | | + | | | 2 |
| | CHE-DE-529 | Advanced Physical Chemistry | | + | | | 2 |
| III | **Core Courses (CC)** | | | | | | |
| | CHE-CC-531 | Inorganic Chemistry III | + | | | | 3 |
| | CHE-CC-532 | Organic Chemistry III | + | | | | 3 |
| | CHE-CC-533 | Physical Chemistry III | + | | | | 3 |
| | CHE-CC-534 | Inorganic Chemistry Lab III | + | | | | 2 |
| | CHE-CC-535 | Organic Chemistry Lab III | + | | | | 2 |
| | CHE-CC-536 | Physical Chemistry Lab III | + | | | | 2 |
| | **Discipline-Specific Elective (DE)** | | | | | | |
| | CHE-DE-537 | Electronic Structure Theory and Applications | | + | | | 4 |
| | CHE-DE-538 | Photophysical Processes and Applications | | + | | | 4 |
| | CHE-DE-539 | New Methods in Organic Synthesis | | + | | | 4 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | CHE-DE-540 | Introduction to Chemical Biology and Anti-Cancer Research | | + | | | 4 |
| **IV** | **Core Courses (CC)** | | | | | | |
| | CHE-CC-541 | Comprehensive Viva | + | | | | 2 |
| | CHE-CC-542 | Dissertation | + | | | | 11 |
| | **Discipline-Specific Elective (DE)** | | | | | | |
| | CHE-DE-543 | Applied Chemistry | | + | | | 4 |
| | CHE-DE-544 | Analytical and Instrumental Methods | | + | | | 4 |
| **Any Sem** | **Generic Course (GC)** | | | | | | |
| | CHE-GC-501 | Analytical and Environmental Chemistry | | | + | | 2 |

## FIRST SEMESTER

| | | |
|---|---|---|
| 1. | Semester | **1** |

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

| **MOD. No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | **Introduction to Coordination Chemistry**: Types of ligands and complexes. Coordination number and geometry: Classification of complexes based on coordination numbers and possible geometries. Isomerism: Structural, geometrical and optical isomerism. Stability of complex ions in aqueous solution: Formation constants. Stepwise and overall formation constants. Factors affecting stability of complexes. Determination of stability constants. Irving William order of stability, Chelate and macrocyclic effects. | **CO1** |
| II | **Theories of Structure and Bonding in Metal Complexes**: Valence bond theory and its limitations. Ligand field theory: Splitting of d orbitals in different ligand fields such as octahedral, tetragonal, square planar, tetrahedral, trigonalbipyramidal and square pyramidal fields. Jahn Teller effect. LFSE and its calculation. Thermodynamic effects of LFSE. Factors affecting the splitting parameter. Spectrochemical series. Molecular orbital theory based on group theoretical approach and bonding in metal complexes. MO diagrams of complexes with and without π bonds. Effect of π bond on the stability of the complex. Sigma and pi bonding ligands such as CO, NO, CN-, R3P, and Ar3P. Nephelauxetic series. | **CO1** |
| III | **Bioinorganic Chemistry**: Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na+ and K+. Photosynthesis-chlorophyll a, PS I and PS II. Z-scheme of photosynthesis. Role of manganese complex in oxygen evolution. Coordination compounds in medicine- Anticancer drugs: Platinum complexes-cisplatin. Various types of interaction of metal complexes with nucleic acids. | **CO2** |
| IV | **Oxygen carriers and oxygen transport proteins**-Hemoglobins, myoglobins and hemocyanin, hemerythrins and hemevanadins, Iron-Sulphur proteins. Nature of heme-dioxygen binding. cooperativity in hemoglobin. Iron storage and transport in biological systems-ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. NonredoxmetalloenzymesCarboxypeptidaseA and Carbonic anhydrase – structure, function and mechanism of action. Nitrogen Fixation nitrogenase, vitamin B12 and the vitamin B12 coenzymes. | **CO2** |
| V | **Acid-Base Chemistry and Chemistry in Non-aqueous Solvents**: Relative strength of acids, Pauling rules, Lux-Flood concept, Lewis concept, Measurement of acid base strength systematics of Lewis acid-base interactions steric and solvation effects acid – base anomalies , Pearson's | **CO3** |

| | | |
|---|---|---|
| | HSAB concept, acid- base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness. Chemistry in non-aqueous solvents, reactions in NH3, liquid SO2, solvent character, reactions in SO2, acetic acid, solvent character, reactions in CH3COOH and some other solvents. Molten salts as non-aqueous solvents, solvent properties, room temperature molten salts, unreactivity of molten salts, solutions of metals. | |
| VI | **Chemistry of noble gases and halogens**: Early chemistry, Xenon fluorides and oxofluorides; Synthesis, properties, structure and bonding. Xenon compounds with bonds to other elements. Chemistry of Krypton and Radon. Chemistry of halogens: Halogens in positive oxidation states. Interhalogen compounds, pseudohalogens and polyhalide ions including polyiodide anions. | **CO4** |

**References:**


1. Banerjea, D. "Coordination Chemistry", 3rd Edn., Asian books, 2009.
2. Cotton, F. A. and Wilkinson, G., "Advanced Inorganic Chemistry", 6th Edn, Wiley Interscience, New York, 1999.
3. Huheey, J. E. Keiter, E. A. and Keiter, R. L. "Inorganic Chemistry - Principles of Structure and Reactivity", 4th Edn, HarperCollins, New York., 1993.
4. Kettle, S. F. A. "Physical Inorganic Chemistry: A Coordination Chemistry approach", Oxford University press, 2000.
5. Lippard, S. J. and Berg, J. M. "Principles of Bioinorganic Chemistry", University Science Books, 1994.
6. Atkins, P. W. and Shriver, D. F. "Inorganic Chemistry", 5th Edn, OUP, 2009.
7. Bertini, I, Gray, H. B., Lippard, S. J. and Valentine, J. S., "Bioinorganic Chemistry", University science books, 1994.
8. Cowan, J. A. "Inorganic Biochemistry - An Introduction", 2nd Edn.,Wiley-VCH, 1997.
9. Figgis, B. N and Hitchman, M. A. "Ligand Field Theory and its Applications," Wiley-India, 2010.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10. Holleman, A. F. and Wiberg, E. "Inorganic Chemistry", Academic press, 2001.
11. Lee, J. D. "Concise Inorganic Chemistry," 4th Edn., Wiley-India, 2008.
12. Purcell, K.F and Kotz, J. C. "Inorganic Chemistry", Holt-Saunders, 2010.
13. Reddy, B. E. Douglas, D. H. McDanial and .Alexander, J. J "Concepts and Models of Inorganic Chemistry", 3rd Edn, John Wiley, 2001.
14. Reddy, K. H. "Bioinorganic Chemistry", New Age international, 2003


**Model Question Paper**

## FIRST SEMESTER M.Sc. DEGREE EXAMINATION Month Year

## Branch: CHEMISTRY

### CHE-CC-511: INORGANIC CHEMISTRY I

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

### SECTION-A

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

1. What is meant by step-wise formation constant of a complex? In the formation of the complex $[ML_4]$ show that $\beta_4 = K_1.K_2.K_3.K_4$.
2. Give a note on Irving William order of stability.
3. Which ligand makes higher $\Delta_0$ value; $H_2O$ or $OH^-$ ? Justify your answer.
4. Which one exhibits higher nephelauxetic effect; $NH_3$ or $CN^-$ ? Substantiate your answer.
5. Give a short note on ionophores.
6. Trans-platin has no anticancer activity, though Cis-platin is a promising anticancer drug. Why ?
7. Distinguish between ferrintin and transferrin.
8. Discuss the role of P cluster in Nitrogenase.
9. Indicate the conjugate acids of the following : i) $NH_3$ ii) $NH2^-$ iii) $H_2O$ iv) HI
10. 'Liquid ammonia is called a levelling solvent.' Justify the statement.
11. Why are the O-F bonds in $O_2F_2$ longer than $OF_2$ whereas the O-O bond in $O_2F_2$ is short compared with that in $H_2O_2$ ?
12. Draw the structure of $XeF_2$, $XeF_4$ and $XeF_6$.

### SECTION-B

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

13. Draw the structure of Cis and trans – dichloro-bis(ethylene diamine)Cobalt(III) ion. Which isomer is optically active ? Justify your answer.
14. Chelate effect is an entropy effect. Justify the statement.
15. Discuss about the various factors affecting the magnitude of splitting parameter ($\Delta$) in complexes.
16. What is valinomycin ? How can you explain that valinomycin binds $K^+$ more tightly than $Na^+$ ?
17. Discuss the structural features and function of Catalase.
18. Give a brief note on Iron-Sulphur proteins.
19. With suitable examples, explain the utility of molten salts as solvent in reactions.
20. Give the structure of $IF_5$. How does $IF_5$ reacts with $XeF_2$ and $XeF_4$ ? Liquid $IF_5$ conduct electricity. What is the reason behind it ?

### SECTION-C

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

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

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

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

23. Illustrate the z-scheme of photosynthesis.

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

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

| | | |
|---|---|---|
| 1. | Semester | **1** |
| 2. | Course Title | **ORGANIC CHEMISTRY I** |
| 3. | Course Code | **CHE-CC-512** |
| 4. | Credits | **3** |

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

| MODULE No | COURSE CONTENT | CO No. |
|---|---|---|
| I | Structural Organic Chemistry - Aromaticity, Hückel's rule, criteria for aromaticity, annulenes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions, anti- and homo- aromatic systems, Fullerenes, Carbon nanotubes and graphenes, Physical organic chemistry - kinetic and thermodynamic control of reactions, Hammond's postulate, kinetic isotope effects with examples, linear free energy relationships, Hammett and Taft equations, Curtin-Hammett principle, Catalysis by acids and bases with examples like acetal, cyanohydrin, ester formations and hydrolysis reactions, Acidity and Basicity of organic compounds, pKa values, kinetic and thermodynamic acidity. Hard and soft acids and bases - HSAB principle and its applications. | 1 |
| II | Stereochemistry of Organic Molecules - Conformational analysis of alkanes and cycloalkanes, Effect of conformation on reactivity of cyclohexane and decalin derivatives. Anomeric effect, Sawhorse and Newmann projections, Geometrical isomers, E-Z nomenclature, Molecular symmetry and chirality, chiral centres – enantiomers and diastereomers, CIP rules. R and S, threo, erythro nomenclatures, non-carbon chiral centres, Axial and Planar chirality, Atropisomerism, Helicity, stereochemical descriptors for chiral axis and planes, Prostereoisomerism, topicity, Stereoselective and stereospecific reactions, regioselective and regiospecific reactions, calculation of enantiomeric excess and specific rotation, Chiral separation methods, Chiral shift reagents, non-carbon chirality. | 2, 3 |
| III | Reactions of sp3 Carbons - Stereochemical and mechanistic aspects of SN reactions, Effect of solvent, leaving group and substrate structure, Neighbouring group participation, Non-classical carbocations and ion pairs in SN reactions, Ambident nucleophiles and substrates, SN′ and SNi reactions, Isotopic and salt effects, Formation and ring opening of epoxides in cyclohexyl systems (Fürst Plattner rule). Elimination reactions leading to C=C bond formation. E1, E2 and E1CB mechanisms, Hoffman and Saytzeff modes of elimination, Effect of leaving group and substrate structure, Pyrolytic eliminations – Chugaev and Cope eliminations, Cis eliminations. Substitution vs elimination. | 3 |
| IV | Reactions of sp2 Carbon and Aromatic Systems - Electrophilic addition to C=C - Mechanistic and stereochemical aspects of bromine addition, halolactonization, hydrogenations, hydroborations, epoxidation including Sharpless asymmetric epoxidation, hydroxylations including Woodward-Prevost hydroxylations, oxy-mercuration and de-mercuration and singlet carbene addition. Stereochemistry of | 4 |

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

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- Smith, M. B. and March, J. "March’s Advanced Organic Chemistry", 6$^{th}$Edn, Wiley. 2007.
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- PS Kalsi “Stereochemistry and Mechanism Through Solved Problems” New Age International, 2001
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- McMurry, “Organic Chemistry”, Thomson Brooks/Cole, 1999.


**Model Question Paper**

## FIRST SEMESTER M.Sc. DEGREE EXAMINATION 2020

# Branch: CHEMISTRY

## CHE-CC-512 : ORGANIC CHEMISTRY I

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

### SECTION-A

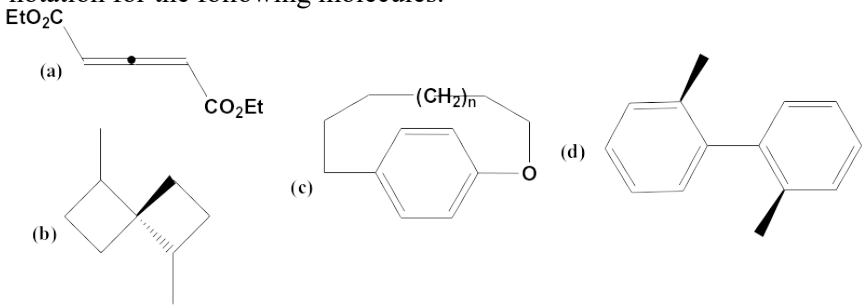
Answer **any 10** questions. **Each** question carries **2** marks

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

### SECTION-B

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

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

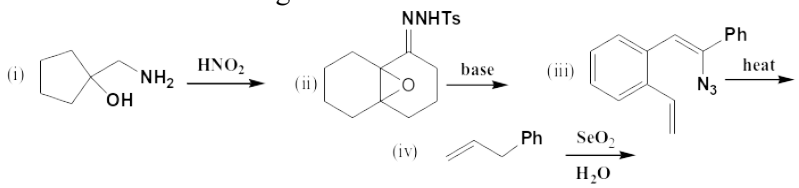



34. 2(R)-Hydroxy, 3(S) bromo butane when treated with a small amount of base yields compound **A**. Identify the structure of compound A and show the correct stereochemistry, reaction scheme and mechanism.
35. In each pair of similar substitution reactions below write the structures of the products of each; indicating which reaction is likely to have the faster rate and why.

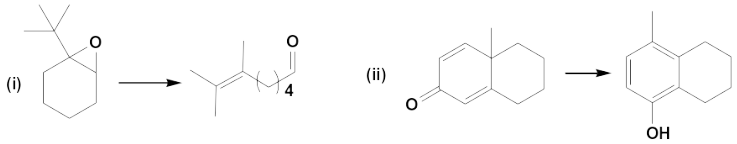
    i) Phenylmethyl chloride (benzyl chloride) or 2-phenylethyl chloride with silver acetate in methanol ii) Sodium cyanide in acetone with 1-methyl-1-idomethyl-cyclopentane or 2-cycopentylethyl iodide iii) 2-phenyl-2-propanol or 3-phenyl-2,4-dimethyl-3-pentanol on warming

in concentrated HBr iv) Sodium salt of methyl malonate and ethyl iodide in methanol or in acetonitrile ($CH_3CN$)

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




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




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

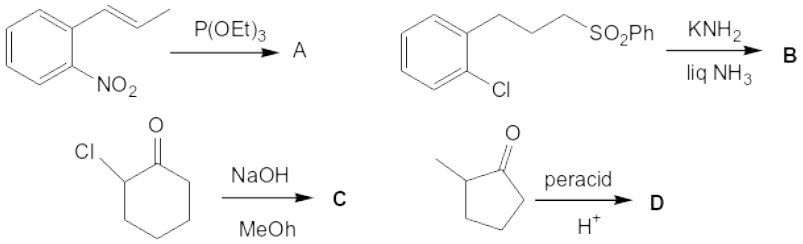
## SECTION-C

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

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

22. i) In the following reactions, decide whether it is likely to proceed by $S_N1$ or $S_N2$ mechanisms. Predict the products including the stereochemistry
    a) S-1-Pheny1-1-bromobutane + NaCN in dimethylformamide
    b) S-1-Pheny1-1-bromobutane + AgOAc in ethanol
    ii) Give 2 mechanisms for nucleophilic aromatic substitutions providing suitable examples. (4+4)

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




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

| | | |
|---|---|---|
| 1. | Semester | **1** |
| 2. | Course Title | **PHYSICAL CHEMISTRY I** |
| 3. | Course Code | **CHE-CC-513** |

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

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Historic evolution of quantum mechanics: The wave nature of sub-atomic particles. The uncertainty principle and its consequences. The postulates of quantum mechanics. Wave functions, well-behavedness, Orthogonality theorem. Orthonormality. Concept of operators: Laplacian, Hamiltonian, linear and Hermitian operators. Angular momentum operators and their properties. Operator algebra, Commutators, Eigen function and eigen values. Expectation value. Time dependent and independent Schrodinger equation. Separation of variables. | 1,2 |
| II | Exactly solvable problems: Solutions of Schrodinger wave equations for:<br>1. A free particle in 1D. Particle in 1D box of infinite and finite potential wells. Tunnelling. Particle in 3D box. Zero point energy and significance. Applications in conjugated dyes.<br>2. 1D- Harmonic oscillator. Hermite equation and Hermite polynomials. Recurrence formula. 3D- harmonic oscillator. Oscillator model and Molecular vibrations. Selection rule for vibrational transitions. | 3 |
| III | Schrodinger equation in polar coordinates and exactly solvable problems: Solutions of Schrodinger wave equations for<br>1. Rigid rotator. Particle on a ring. Separation of variables. Real and Imaginary Wave functions.<br>2. Non-planar rigid rotator. Legendre and Associated Legende equations and polynomials. Rodrigue's formula. Spherical Harmonics. Polar Diagrams. Salient features. Space quantization.<br>Hydrogen atom. Laguerre and Associated Laguerre equations and corresponding polynomials. Space quantization. Zeeman effect, Uhlenbeck and Goudsmith postulate of spin, Stern Gerlach experiment. Orbitals and Spin orbitals. Radial probability distribution function and graphs. Selection rules for spectral transitions. | 3 |
| IV | Symmetry and character tables: Symmetry elements and symmetry operations. Point groups. Multiplication of operations. Conditions for a set of elements to form a group. Group multiplication table. Similarity transformation and classification of symmetry operations. Matrix representation of point group. Reducible and irreducible representations. Character of a matrix. Orthogonality theorem. Rules derived from | 4,5 |

| | | |
|---|---|---|
| | orthogonality theorem (proof not required). Setting up of the character tables of simple groups - $C_{2v}$, $C_{2h}$, $C_{3v}$ and $C_{4v}$ on the basis of the rules. Reduction of reducible representations to irreducible representations. Molecular dissymmetry and optical activity. Applications of character tables to spectroscopy. Transition moment operators, vanishing integrals, determination of number of active IR and Raman lines. Application of character table to orbitals. Construction of hybrid orbitals. Construction of Symmetry adapted LCAO | |
| V | Types of surfaces. Measurements of surface pressure and surface potential. Surfactants and micelles. The gas-solid interface. Types of adsorption. Heat of adsorption. Adsorption isotherms. Gibbs adsorption equation and its verification. Langmuir isotherm. Multilayer adsorption. Freundlich isotherm. BET isotherm. Solid-liquid interface. Influence of surface tension on adsorption. Measurements of surface area of solids.Harkin-Jure method. Entropy and point B methods. Use of Langmuir isotherm and BET method. Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism | 6 |
| VI | Colloids- zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium. Emulsions: macro- and micro-emulsions; aging and stabilization of emulsions; Phase behaviour of microemulsions. Surface Enhanced Raman Scattering, Surfaces for SERS studies, Chemical enhancement mechanism, Surface selection rules, Applications of SERS. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces. | 7,8 |

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- McQuarrie, D. A., "Quantum Chemistry", 2ndEdition,University Science Books, 2008.
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- GreggS. J., “The Surface Chemistry of Solids”, 2nd Edition, Chapman Hall, 1961.
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- Somorjai, A., “Introduction to Surface Chemistry and Catalysis”, 2nd Edition, Wiley-Interscience, 2010.


**Model Question Paper**

## FIRST SEMESTER M.Sc. DEGREE EXAMINATION, Month Year
## Branch: CHEMISTRY

## CHE-C513: PHYSICAL CHEMISTRY-I

Times: 3 Hours Max. Marks: 60

### SECTION- A

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

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

### SECTION- B

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

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

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

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| E" | 2 | -1 | 0 | -2 | 1 | 0 | $(R_x,R_y)$ | (xz,yz) |

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

| **P/torr** | 30 | 40 |
|---|---|---|
| **T(K)** | 200 | 240 |

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

**SECTION C**

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

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

| $C_2v$ | E | $C_2z$ | $\sigma_v(xy)$ | $\sigma_v(yz)$ | | | |
|---|---|---|---|---|---|---|---|
| A1 | 1 | 1 | 1 | 1 | z | $x^2,y^2,z^2$ | |
| A2 | 1 | 1 | -1 | -1 | Rz | xy | |
| B1 | 1 | -1 | 1 | -1 | x,Ry | xz | |
| B2 | 1 | -1 | -1 | 1 | y,Rx | yz | (4+4) |

22. a) Write down the Schrodinger equation for H-atom in spherical polar coordinates and separate the variables.
    b) What is the probability of finding the electron within radius of $a_0$ from the nucleus (Given ground state wave function of H-atom is $(1/\pi a_0^3)^{1/2}e^{-r/a0}$) (4+4)

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

24. a) Calculate the expectation values of Px and $Px^2$ for a particle in 1-dimensional box. Rationalize the results.

b) The 1s orbital of H-atom is given by the expression $1s= (1/\pi a_0^3)^{1/2}e^{-r/a_0}$), where $a_0$ is the Bohr radius. Show that the most probable radius at which the electron will be found in the 1s orbital is $a_0$. (4+4)

| 1. | Semester | **1** |
|---|---|---|
| 2. | Course Title | **Inorganic Chemistry Lab I** |
| 3. | Course Code | **CHE-CC-514** |

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

**References:**


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


| | | | | | |
|---|---|---|---|---|---|
| 1. | Semester | **1** | | | |
| 2. | Course Title | **ORGANIC CHEMISTRY LAB I** | | | |
| 3. | Course Code | **CHE-CC-515** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO** | | **TL** | **KL** | **PSO** |

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

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

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


| | | |
|---|---|---|
| 1. | Semester | **1** |
| 2. | Course Title | **PHYSICAL CHEMISTRY LAB I** |
| 3. | Course Code | **CHE-CC-516** |
| 4. | Credits | **3** |

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

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Distribution law: Partition of iodine, ammonia and aniline between water and organic solvents. Association of benzoic acid. Equilibrium constants of Tri-iodide and copper-ammonium complexes. Enthalpy change for tri-iodide formation. | 1,6 |
| II | Refractometry: Refractive index and molar refraction of liquids. Atomic refractions. Composition of solid solutes. Molecular and ionic radii from molar refraction. Study of the complex $K_2[HgI_4]$. | 2,6 |
| III | Chemical kinetics: Acid hydrolysis of esters. Comparison of strengths of acids. Saponification of esters. Persulphate-iodide second order reaction. Activation energy. Arrhenius parameters. Primary salt effect. | 3,6 |
| IV | Thermochemistry: Determination of water equivalent. Heat of neutralization and heat of ionization. Integral and differential heats of solution. Thermometric titrations. Determination of concentrations of strong acids. | 4,6 |
| V | Polarimetry: Inversion of cane sugar. Velocity constants for different acid strengths. Comparison of strengths of two acids. | 5,6 |
| VI | Adsorption: Verification of Langmuir and Freundlich isotherms for solute adsorption on solids. Estimation of surface area. First order kinetics. Computation of adsorption thermodynamics. Exothermic and endothermic reactions. | 6 |

**References:**


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


## SECOND SEMESTER

| 1. | Semester | **2** |
|---|---|---|
| 2. | Course Title | **INORGANIC CHEMISTRY II** |

| | | | | | |
|---|---|---|---|---|---|
| 3. | Course Code | **CHE-CC-521** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO:** *On completion of the course, students should be able to:* | | **TL** | **KL** | **PSO No.** |
| | *1. Describe and compare the electronic, spectral and magnetic properties of metal complexes* | | 2-Un, 4-An, 5-E | FK, CK | PSO1, PSO3 |
| | *2. Execute their fundamental knowledge in co-ordination chemistry to understand and evaluate properties of various metal complexes* | | 3-Ap, 4-An, 5-E | FK, CK | PSO1, PSO3 |
| | *3. Classify and distinguish the stability and reactivity of metal complexes* | | 4-An, 5-E | FK, CK | PSO1, PSO2 |
| | *1. Explain and demonstrate the coordination chemistry of lanthanides and actinides* | | 4-An, 5-E | FK CK | PSO1, PSO2 |
| | *2. Describe, demonstrate and compare the fundamental concepts of organometallic chemistry* | | 2-Un, 4-An, 5-E | FK CK | PSO1, PSO2 |
| | *3. Explain and examine the reactions of various organometallic complexes* | | 3-Ap, 4-An 5-E | FK, CK | PSO1, PSO2 PSO3 |
| | *7. Evaluate the applications of organometallic complexes in various domains* | | 4-An, 5-E | FK, CK | PSO2,PSO3 |
| **MOD No** | **COURSE CONTENT** | | | | **CO No.** |
| I | **Electronic Spectra of complexes**-Term symbols of dn system. Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for dn and d10-n ions in octahedral and tetrahedral fields (qualitative approach), d-d transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling. Orgel diagrams. Tanabe Sugano diagrams. Effects of Jahn Teller distortion and spin orbit coupling on spectra. Charge transfer spectra. luminescence spectra. | | | | **CO1, CO2** |
| II | **Magnetic properties of metal complexes**: Types of magnetism shown by complexes- paramagnetic and diamagnetic complexes, molar susceptibility, Magnetic susceptibility measurements. Gouy method. Spin only value. Orbital contribution to magnetic moment. Temperature dependence of magnetism-Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Ferromagnetism and antiferromagnetism in complexes. Anomalous magnetic moments. Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments. | | | | **CO1, CO2** |
| III | **Reactions of Metal Complexes**: Kinetics and mechanism of reactions involving complexes in solution. Inert and labile complexes. Kinetics and mechanism of nucleophilic substitution (Ligand displacement) reactions in square planar complexes. trans effect-theory and applications. Kinetics and mechanism of octahedral substitution, Dissociative and associative mechanisms, Ligand field effects on reaction rate. Influence of acid and base on reaction rate. Racemization and isomerization. Redox reactions in complexes: Electron transfer and electron exchange reactions. Theories of Electron transfer reactions-outer sphere mechanism-Marcus theory, inner sphere mechanism, electron transfer in metalloproteins. | | | | **CO3** |
| IV | **Coordination Chemistry of Lanthanides and Actinides**: General characteristics of lanthanides-Electronic configuration, Term symbols for lanthanide ions, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents. General | | | | **CO4** |

| | | |
|---|---|---|
| | characteristics of actinides-difference between 4f and 5f orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties. | |
| V | **Organometallic Compounds**-Synthesis, Structure and Bonding: Compounds with transition metal to carbon bonds, classification of ligands, eighteen electron rule. Organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding. Complexes with cyclic pi donors-metallocenes and cyclic arene complexes structure and bonding. Carbene and carbyne complexes. Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. | **CO5** |
| VI | **Reactions of Organometallic Compounds**: Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands. Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions. Catalysis by organometallic compounds: Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst. Reactions of carbon monoxide and hydrogen-the water gas shift reaction, the Fischer-Tropsch reaction (synthesis of gasoline). Hydroformylation of olefins using cobalt or rhodium catalyst. Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $Co_2(CO)_8$ catalyst in adipic ester synthesis. Palladium catalysed oxidation of ethylene-the Wacker process. | **CO6, CO7** |

**References:**


1. Banerjea, D. “Coordination Chemistry”, 3rd Edn., Asian books, 2009.
2. Cotton, F. A. and Wilkinson, G. “Advanced Inorganic Chemistry”, 6th Edn, Wiley
3. Cotton, S. “Lanthanide and Actinide Chemistry”, John Wiley & Sons, 2007.
4. Dutta, R. L and Syamal, A. “Elements of Magnetochemistry”, 2nd Edn., East West press, 1993.
5. Huheey, J. E. Keiter, E. A. and Keiter, R. L. “Inorganic Chemistry - Principles of Structure and Reactivity”, 4th Edn, HarperCollins, New York., 1993.
6. Kettle, S. F. A. "Physical Inorganic Chemistry: A Coordination Chemistry approach", Oxford University press, 2000.
7. Mehrotra, R. C. and Singh, A. “Organometallic Chemistry: A Unified Approach”, New age international, 2007.
8. Purcell, K. F. Kotz, J. C. ‘Inorganic Chemistry”, Holt-Saunders, 2010.
9. Sathyanarayana, D. N. “Electronic Absorption Spectroscopy and Related Techniques”, Universities press, 2001.
10. Miessler, G. L., Fischer, P. J and Tarr, D. A “ Inorganic Chemistry” 5$^{th}$edn. Pearson, 2014.


**Additional references**


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


**Model Question Paper**

## SECOND SEMESTER M.Sc. DEGREE EXAMINATION Month Year

## Branch: CHEMISTRY

### CHE-CC-521: INORGANIC CHEMISTRY II

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

### SECTION-A

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

1. $[Ti\ Cl_6]^{3-}$ and $[Ti\ (CN)_6]^{3-}$ gives $\lambda_{max}$ at 13,000 $cm^{-1}$ and 22,300 $cm^{-1}$ in their respective electronic spectra. Justify the statement.
2. The term symbols for $d^3$ and $d^4$ configuration is $^4F$. Explain.
3. Predict the geometries and magnetic moments of $[Ni\ Cl_4]^{2-}$ and $[Ni\ (CN)_4]^{2-}$ on the basis of valence bond theory.
4. Calculate the magnetic moment for $[Co\ Cl_4]^{2-}$ taking into account the fact that there is angular momentum contribution to the magnetic moment. ($\Delta = 3100\ cm^{-1}$).
5. Which isomer of $[Pt\ (NH_3)_2\ Cl_2]$ is formed when $[Pt\ (NH_3)_4]^{2+}$ is reacted with 2 moles of HCl? Why?
6. 'The inert complexes are not necessarily thermodynamically stable'. Justify this statement with an example.
7. Lanthanides ions give rise to very sharp bands in their electronic spectra. Why?
8. Yttrium is concentrated along with lanthanides; why?
9. Draw the structures of the following 18 electron compounds and mention the hapticity of organic ligands:
   i) $[Mn\ (CO)_4\ (C_3H_5)]$ ii) $[Fe\ (CO)_2\ Cp\ (CH_3)]$
10. The IR stretching frequency of CO in metal carbonyls is lower than that for free CO molecule. Why?
11. What are oxidative addition and reductive elimination reactions, as applied to organometallic chemistry?
12. Write a catalytic cycle for the synthesis of acetic acid from methanol.

### SECTION-B

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

13. Discuss the spectral consequence of Jahn- Teller distortion in transition metal complexes.
14. The electronic spectrum of $[Co\ (NH_3)_6]^{3+}$ has a weak band in the red – and two medium intensity bands in the visible to near UV region. Assign these transitions using Orgel diagram.
15. What is spin-only magnetic moment? How it is useful in the structural elucidation of transition metal complexes?
16. Illustrate the mechanism of inner-sphere electron transfer reactions using a specific example.

17. What is trans effect? What is its theoretical basis?
18. Discuss the bonding in metal nitrosyls.
19. ) Exemplify and briefly discuss the structure and bonding in cyclic arene complexes.
20. Draw and discuss the catalytic cycle for hydroformylation of alkenes using rhodium complex as catalyst.

## SECTION-C

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

21. Write briefly on Tanabe-Sugano diagrams with special reference to their construction and advantages in the interpretation of electronic spectra.
22. i) Discuss briefly about the temperature dependence on magnetism.
    ii) What is meant by aquation reaction? Using suitable examples, explain the mechanism of aquation reactions of octahedral complexes.

(4 + 4)

23. Compare lanthanide and actinide complexes based on their oxidation state, electronic spectra and magnetic properties.

24. i) Discuss the general methods of preparation of metal carbonyls.

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

(4 + 4)

| | | | | | |
|---|---|---|---|---|---|
| 1. | Semester | **2** | | | |
| 2. | Course Title | **ORGANIC CHEMISTRY II** | | | |
| 3. | Course Code | **CHE-CC-522** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO** | | **TL** | **KL** | **PSO** |

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

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Radicals in Organic Synthesis - Structure, stability and generation of free radicals, Baldwin's rules of ring closure, Inter and intramolecular additions of radicals to alkenes and alkynes, Radical chain reactions, Introduction to polymers and free-radical polymerizations, Named reactions – Pinacol, acyloin, McMurry, Hoffmann-Lofler-Freytag and Barton reactions, Use of NBS and tributyl tin hydrides, Ullmann coupling. | 1, 4 |
| II | Organic Photochemistry - Primary photoprocesses. Jablonski diagram, Photoreactions of C=O systems, enes, eneones, dienes and arenes. Photoisomerisations, Norrish type I and II reactions. Patterno-Buchi and Barton reactions. Di-π-methane and aromatic photo rearrangements. Photochemical remote functionalisation and hydrogen abstraction reactions. Introduction to PET, chemi and bioluminescent reactions. Chemistry of singlet oxygen. Photochemistry in nature. Photosynthesis. Introduction to organic applied photochemistry and femtochemistry, photochromism and thermochromism. | 3, 4 |
| III | Concerted Reactions - Symmetry properties of MOs. Principle of conservation of orbital symmetry. Pericyclic reactions - theory, mechanism and stereocourse of electrocyclic reactions, cycloaddition reactions and sigmatropic rearrangements, 1,3-dipolar cycloadditions, ene reactions, chelotropic reactions, Sommelet-Hauser, Cope, Claisen and Mislow-Evans rearrangements, thermal eliminations. Woodward-Hoffmann selection rules, secondary orbital interactions in [4+2] cycloadditons, factors affecting rates of cycloaddition reactions. | 2, 4 |
| IV | NMR Spectroscopy - Magnetic nuclei with emphasis on 1H and 13C, shielding, de-shielding and chemical shifts, factors affecting chemical shifts - Field and anisotropic factors, relaxation processes, chemical and magnetic non-equivalence, 1H and 13C NMR scales, Spin-spin splitting – AX, AX2, AX3, A2X3, AB, ABC and AMX type coupling, Coupling constants.. Pascals triangle, first order and non-first order spectra, Karplus curve, Quadrapule broadening, virtual and long-range coupling, Shift reagents and their role, Decoupling and double | 5, 6 |

| | | |
|---|---|---|
| | resonance, Off-resonance decoupling, NOE.<br>Introduction to 2D NMR. Correlation, NOE and quantum correlation spectroscopy techniques like COSY, HETCOR, HMQC, HMBC, NOESY and EXCY. Application of DEPT technique, Problems on spectral interpretation. | |
| V | UV-Vis and IR Techniques - UV-VIS spectra of enes, eneones, arenes and conjugated systems. Woodward-Fieser rules, Solvent effect on absorption spectra. Chiroptical properties – introduction to CD and ORD, Cotton effect, octant rule, axial haloketone rule. Characteristic IR bands of functional groups. Factors affecting the IR stretching frequency – vibrational coupling, hydrogen bonding, electronic, inductive and field effects, Identification of functional groups and other structural features by IR. | 5 |
| VI | MS in organic structure analysis. EI, CI, SIMS, FAB, ES and MALDI ion production methods. Characteristic EIMS fragmentation modes and MS rearrangements including McLafferty rearrangement, Spectral interpretation, structure identification and solving of structural problems using numerical and spectral data. | 5, 6 |

**REFERENCES**


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


**ADDITIONAL REFERENCES**


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


**Model Question Paper**

## SECOND SEMESTER M.Sc. DEGREE EXAMINATION 2020

## Branch: CHEMISTRY

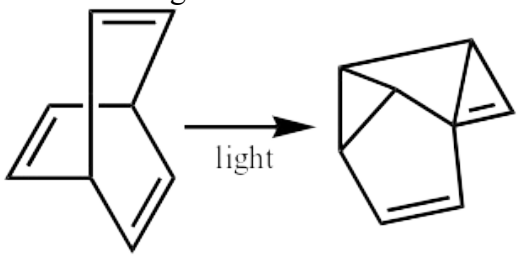
### CHE-CC-522: ORGANIC CHEMISTRY II

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

**SECTION-A**

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

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

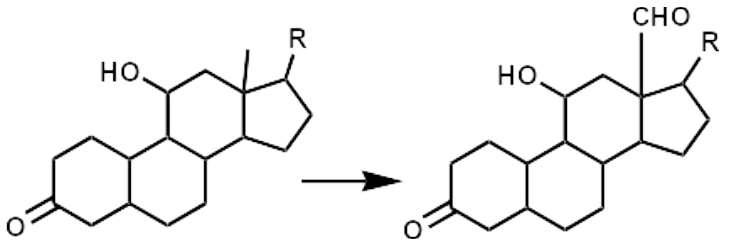



25. Predict the products formed when the following molecules are irradiated (i) (2Z, 4E)-hexadiene and (ii) (2Z, 4Z, 6E)-octatriene.
26. Depict the cycloaddition of tropone with butadiene.
27. Illustrate the product formed when benzyne undergoes cycloaddition to i) anthracene and ii) furan.
28. How many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

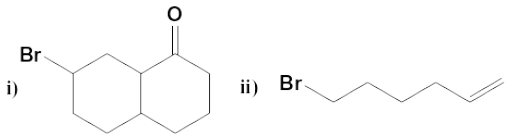
**SECTION-B**

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

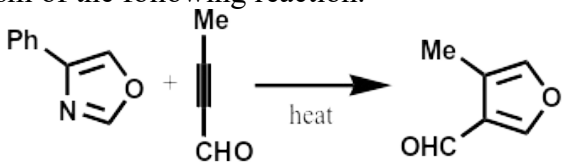
33. How can the following conversion be effected? Give the reagents and mechanism.




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




35. Explain the mechanism of the following reaction.



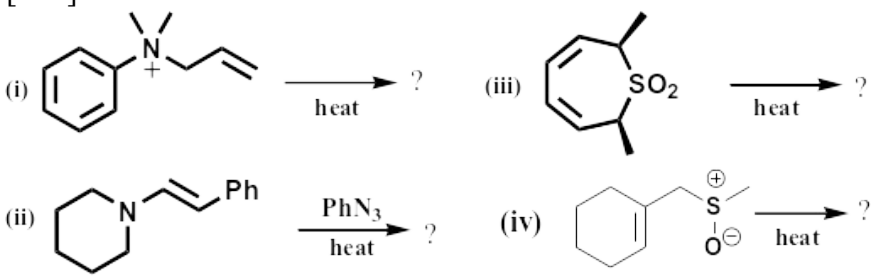

36. Based on the FMO theory predict and explain the product formation when (2E, 4Z, 6E)-octatriene electrocyclizes a) thermally and b) photochemically
37. A compound with molecular formula $C_4H_6O_2$ shows an IR band at 1770 $cm^{-1}$. The $^{13}$CNMR peaks are at 178, 68, 28 and 22 ppm. The compound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

**SECTION-C**

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

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

[4+4]




22. a) How can *cis*-2-butene be differentiated from *trans*-2-butene using i) IR spectroscopy and ii) NMR spectroscopy?

b) Depict and explain the $^{1}H$-$^{1}H$ COSY spectrum of *iso*-butyl acetate [4+4]

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

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

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

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

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

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

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Many electron atoms- Approximations. Independent particle model. Variational method. Theorem and proof. Variational treatment of hydrogen and helium atom. Secular determinant. Perturbation method – 1st and 2nd order perturbation to energy and wave function. Application to particle in 1-D box of increasing potential, Helium atom. self-consistent field method. Pauli's exclusion principle. Symmetry and antisymmetry wave functions. Slater determinants. Vector atom model. Spin orbit coupling. Spectroscopic Term symbols and spectral lines. | 1,2 |
| II | Molecular problems. Born-Oppenheimer approximation. Molecular Orbital Theory. MO theory of hydrogen molecule ion. Valence Bond theory ($H_2$). MO theory of $H_2$ and other homonuclear diatomic molecules. Molecular orbital diagrams, Bond order and stability. MO theory of simple heterogeneous diatomic molecules like HF, LiH, CO and NO. Defects in simple MO and VB theories.Semi empirical MO treatment of planar conjugated molecules. HuckelMO theory and calculation of energy and MO of ethylene, butadiene and allylic anion and cyclic systems – cyclobutadiene and benezene. Calculation of charge distribution, bond order and free valency. | 2,3 |
| III | Ab initio methods. Hartree equations and Hartree-Fock equations for molecular problems. Roothaan modification. Hartree Fock Roothan equations.Basis sets andBasis functions. Slater type orbital (STO) and Gaussian type orbital (GTO). Contracted and primitive. Basis sets and classification. Minimal, multiple zeta, split-valence, polarized and diffused. Pople style basis sets. Electron correlation and relativistic effects, Configuration interaction. Z-matrtix. | 4 |
| IV | Spectra of diatomic molecules: Microwave spectroscopy. Rotation of diatomic molecules. Rotational spectrum. Intensity of spectral lines. Calculation of internuclear distance. Nonrigid rotors and centrifugal distortion. Introduction to instrumentation. Infrared spectroscopy: Rotational spectra of polyatomic molecules. Linear and symmetric top molecules. Vibrational spectra of harmonic and anharmonic diatomic molecules. Fundamental and overtones. Determination of force constants. Vibrational rotational couplings. Different branches of spectrum. Symmetry of vibrational-rotation spectrum. | 5,6 |

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

**References:**


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


**ADDITIONAL REFERENCES**


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


**Model Question Paper**

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

Times: 3 Hours Max. Marks: 60

SECTION- A

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

1. Write down the perturbation term in the Hamiltonian of Helium atom.
2. Write down the Slater determinant of Li atom.
3. What is Born-Oppenheimer approximation? Why is it important?

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

## SECTION- B

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

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

## SECTION- C

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

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

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

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

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

| | | | | | |
|---|---|---|---|---|---|
| 1. | Semester | **2** | | | |
| 2. | Course Title | **Inorganic Chemistry Lab II** | | | |
| 3. | Course Code | **CHE-CC-524** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO:** On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | ***1.*** *Perform colorimetric experiments for the quantitative determination of various metals* | | 3-Ap<br>4-An | CK, PK | PSO5<br>PSO6 |
| | ***2.*** *Perform simple inorganic synthesis and conduct characterization techniques such as IR, UV-Vis absorption and NMR spectroscopy* | | 3-Ap<br>4-An | PK, MK | PSO4<br>PSO5<br>PSO6 |
| | ***3.*** *Discuss coordination chemistry of Ni complexes* | | 2-Un<br>4-An | CK | PSO1<br>PSO2 |
| **MOD. No** | **COURSE CONTENT** | | | **CO No.** | |
| I | Colorimetric estimation of Iron after plotting calibration graph. | | | **CO1** | |
| II | Quantitative estimation of Chromium by colorimetry. | | | **CO1** | |
| III | Quantitative estimation of Manganese by colorimetry. | | | **CO1** | |
| IV | Colorimetric estimations of Ti, W and Cu., after plotting calibration graph. | | | **CO1** | |
| V | Synthesis and Characterization of Ni(II) Complexes<br>a. The preparation of $[Ni(en)_3]Cl_2\ 2H_2O$<br>b. The preparation of $[Ni(NH_3)_6]Cl_2$<br>c. The preparation of $[Ni(en)_2]Cl_2 . 2H_2O$ | | | **CO2, CO3** | |
| VI | Synthesis and characterization of tetraphenylporphyrin and its Zn(II) complex | | | **CO2** | |

**References:**


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

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

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

**REFERENCES**


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

| | | |
|---|---|---|
| 1. | Semester | **2** |
| 2. | Course Title | **PHYSICAL CHEMISTRY LAB II** |
| 3. | Course Code | **CHE-CC-526** |
| 4. | Credits | **3** |

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

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

**References:**


- Daniels,F. and Mathews,J. H. "Experimental Physical Chemistry", McGraw Hill, 1970.
- Finlay, A. and Kitchener,J. A. "Practical Physical Chemistry", Longman, 1977.
- James,A. M. "Practical Physical Chemistry", Longman, 1981.
- Shoemaker, D. P. and Garland,C. W. "Experiments in Physical Chemistry", McGraw Hill, 1998.

- Willard,H. H. Merritt , L. L. and Dean,J. A. "Instrumental Methods of Analysis" 7th Edition, CBS Publishers, 2004..
- Viswanathan, B.; Raghavan, P. S. "*Practical Physical Chemistry*," Viva Books, 2004.
- YadavJ. B., "Advanced Practical Chemistry", Krishna Prakashan Media, 2015.


| | | |
|---|---|---|
| 1. | Semester | **2** |
| 2. | Course Title | **ADVANCED INORGANIC CHEMISTRY** |
| 3. | Course Code | **CHE-DE-527** |
| 4. | Credits | **2** |

| 5. | **CO** On completion of the course, students should be able to: | **TL** | **KL** | **PSO No.** |
|---|---|---|---|---|
| | 1. summarize and describe concepts and practices in nuclear /radiation chemistry | 1-R; 2-U | FK, CK | 01, 02 |
| | 2. Compare and explain various special techniques for the synthesis of inorganic compounds | 5-E; 2-U | FK, CK | 01, 02 |
| | 3. Analyze various inorganic chemistry reactions for the synthesis of metal complexes | 4-An; 5-E | CK | 02, 03 |
| | 4. Rationalize the use of spectroscopic techniques IR and NMR for the characterization of inorganic complexes | 4-An; 2-U | CK | 01, 02 |
| | 5. Apply their knowledge in spectroscopic methods to elucidate the structure of inorganic complexes | 3-Ap; 4-An | CK, MK | 02, 03 |
| | 6. solve problems regarding the structure of various metal complexes using ESR and Mössbauer spectroscopy | 3-Ap; 4-An | CK | 02, 03 |
| | 7. Appreciate the photocatalytic ability of metal complexes in solar energy conversion | 2-Un;5-E | CK | 01, 02, 03 |
| | 8. Explain and analyze the chemistry and applications of industrial inorganic materials | 2-Un; 4-An | FK, CK | 01, 02 |

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Nuclear and radiation chemistry: Fission products and fission yield. Neutron capture cross section and critical size. Nuclear fusion reactions and their applications. Neutron activation analysis, Chemical effects of nuclear transformations. Positron annihilation and autoradiography. Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109. Radiation safety precaution, nuclear waste disposal. Radiation chemistry of water and aqueous solutions. Measurement of radiation doses | 1 |
| II | Inorganic synthesis: Special techniques such as chemical vacuum line, plasmas, photochemical apparatus and electrolysis. Synthesis of transition metal complexes involving the following methods: Electron transfer reaction, substitution reaction, reactions of coordinated ligands, aldol condensation, imine bromination hydrolysis, substituent exchange reaction, template effect and macrocyclic ligands. Complexes with interlocking ring ligands. Formation of supramolecular species. | 2, 3 |

| | | |
|---|---|---|
| III | Inorganic Spectroscopic Methods:Studies of simple inorganic compounds and metal complexes using IR, Raman and NMRSpectroscopy- Metal ligand vibrations, bonding modes of acetate, nitrate, sulphate and perchlorate and metal atoms. Application of IR spectroscopy for the identification of these bonding modes. Far IR spectra. Vibrational spectra of metal carbonyls. Application of NMR spectroscopy for the structural investigation of diamagnetic metal complexes from chemical shift and spin-spin coupling. | 4, 5 |
| IV | ESR and Mössbauer spectroscopy of coordination compounds: ESR spectra of metal complexes- hyperfine splitting, g values, zero field splitting and Kramers degeneracy. Application of ESR spectroscopy in the structural investigation of copper(II) and manganese(II) complexes. Mössbauer spectroscopy- Mössbauer effect, hyperfine interactions, isomer shift, electric quadrupole and magnetic hyperfine interactions. Application of Mössbauer spectroscopy in the structural study of iron and tin complexes. | 6 |
| V | Inorganic photochemistry: Photochemical laws and kinetics. Photophysical processes. Excited states, ligand field states, charge-transfer states. Fluorescence and phosphorescence. Photochemical reactions-substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes. Applications-synthesis and catalysis, chemical actinometry and photochromism. Metal complex sensitizers-electron relay, semiconductor supported metal oxide systems, solar energy conversions; water photolysis and $CO_2$ reduction. Chlorophyll and light reaction in photosynthesis. | 7 |
| VI | Chemistry of Materials:Glasses, ceramics, composites, nanomaterials-preparative procedures. Sol-gel synthesis, glassy state-glass formers and glass modifiers, ceramic structures, mechanical properties, clay products, refractories- characterizations, properties and applications. Ultramarines, zeolites and Metal organic frameworks (MOF); Synthesis structure and applications. | 8 |

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- Goshal,S. N. "Nuclear Physics", S. Chand and Company, 2006.
- Adamson, W and Fleischauer, P.D. "Concepts of Inorganic Photochemistry", Wiley, 1975.
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- Drago, R. S. "Physical Methods in Chemistry", Saunders College, 1992.
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- Roundhill, D. M. "Photochemistry and Photophysics of Metal Complexes", Plenum press, 1994.
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- Jain, P. C abd Jain, M. "Engineering Chemistry", 12th Edn., Dhanpat Rai Pub., 2006.
- MacGillyvray, L. R and Lukehart, C. M. "Metal Organic framework materials", Wiley, 2014
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**Model Question Paper**

## SECOND SEMESTER M.Sc. DEGREE EXAMINATION Month Year

## Branch: CHEMISTRY

### CHE-CC-527:ADVANCED INORGANIC CHEMISTRY

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

### SECTION-A

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

1. What is nuclear fission energy ?
2. Define neutron capture cross section.
3. Describe a scheme for the synthesis of hexaamminecobalt(III) from cobalt(ii) chloride in aqueous medium.
4. What are cryptates and cryptands ?
5. Suggest an experimental method to distinguish between terminal and bridging binding modes of CO ligands in transition metal carbonyl complexes.
6. How can you use NMR spectroscopic technique to identify fluxional behaviour in transition metal complexes?
7. What is Kramers degeneracy ?
8. Explain how the anisotropy in g value can be used to provide information about the electronic ground state of transition metal ion complexes.
9. What is photochromism ?
10. How do you explain the intense purple colour of KMnO4 ?
11. Explain the structure of sodalite.
12. What is meant by glass modifier ?

### SECTION-B

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

13. Phosphorus-32 has a half-life of 14.3 days. What fraction ofa sample of phosphorus-32 would remain after 5.5 days ?

14. Discuss different classes of substitution reactions in inorganic chemistry.
15. Explain the effect of macrocyclic ligands in stabilizing transition metal complexes.
16. Illustrate the use of IR spectroscopy in distinguishing the hapticity of cyclopentadienyl ligand in transition metal complexes.
17. How do you distinguish high and low spin iron complexes using Mössbauer spectroscopy ?
18. Explain Jablonski diagram with a neat sketch.
19. Explain photochemical redox reaction using Cr(III) complexes as an example.
20. Explain the difference between the composite and blend with suitable examples.

## SECTION-C

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

21. Discuss the chemical vacuum line and plasma technique used in inorganic synthesis.
22. i) Write a note on neutron activation analysis.
    ii) Illustrate mutual exclusion principle with suitable transition metal complexes as examples.
    (4 + 4)
23. Discuss the importance of metal complexes in solar energy conversion.
24. i) How do you use ESR spectroscopy in structural determination of manganese(II) complexes ?

ii) Write a short note on the synthesis, structure and applications of metal organic frameworks.

(4 + 4)

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|---|---|---|---|---|---|
| 1. | Semester | **2** | | | |
| 2. | Course Title | **ADVANCED ORGANIC CHEMISTRY** | | | |
| 3. | Course Code | **CHE-DE-528** | | | |
| 4. | Credits | **2** | | | |
| 5. | **CO**<br>On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | 1. Get an overview of supramolecular assemblies and their importance | | I-R, 2-Un | FK, CK | I, II |
| | 2. Comprehend the green chemistry principles and how they are being implemented | | 2-Un, 3-Ap, 4-An | FK, CK | II, III |
| | 3. Get an introduction to medicinal chemistry and drug action | | 1-R, 2-Un, | FK | I, II |
| | 4. Understand polymerization mechanisms and processes | | 2-Un, 3-Ap | FK | I, II |
| | 5. Analyze and estimate functional groups present in oils, milk, starch etc. | | 4-An 5-E | FK, CK | III, VI |

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Supramolecular Chemistry - Noncovalent interactions: Molecular and chiral recognition, Host-Guest chemistry and inclusion complexes: crown ethers, cryptands, calixarenes, cyclophanes and cyclodextrins, Self-Assembly and Self-Organization, Molecular Aggregates: lipid membranes, nanotubes, micelles and liquid crystals, Fullerene based supramolecular systems, Dendrimers, Molecular devices: molecular switches and wires, Molecular recognition in biological systems like DNA and proteins. | 1 |
| II | Chemistry of Biomolecules - DNA replication, Codon and anticodon recognition. Protein biosynthesis, transcription and translation, Genetic code, DNA sequencing. DNA profiling and the Polymerase Chain Reaction (PCR). | 1 |
| III | Green Chemistry - Background, origin and principles of green chemistry. Atom economy and other metrics of greenness. Examples of green processes. Solid supports, Supercritical carbon dioxide, Microwave and sonochemical synthesis. Synthesis using solventless or alternate media conditions: fluorous and ionic liquid media. | 2 |
| IV | Medicinal Chemistry and the Chemistry of the Cell - Introduction to drug discovery and design, drug administration, Drug action – pharmacokinetic and pharmacodynamic phases, receptor proteins, drug | 3 |

| | | |
|---|---|---|
| | receptor interaction, drug action, drug selectivity, drug metabolism, Classification of drugs, Anti-anginal drugs, antihypertensive agents, antimalarial drugs, aminoquinolines, Antibiotics and analgesics with examples. Drug stability, Penicillins, tetracyclins and cephalosporins. Drugs for cancer, AIDS and diabetes, Composition and structural features of lipids. | |
| V | Polymer Chemistry - Classes of polymers. Types and mechanisms of polymerization reactions (free-radical, cationic and anionic). Methods of molecular mass and size distribution determination. GPC and Light scattering techniques, Polymer structure and property characterisation. Synthesis of stereoregular polymers. Polymerization techniques. Bulk, Solution, melt, suspension, emulsion and dispersion techniques, Group Transfer, metathesis and ring opening polymerization. Copolymerization. Polymers as supports, reagents and catalysts, Biodegradable polymers, conducting polymers. | 4 |
| VI | Quantitative analysis of organic functional groups - Analysis of oils and fats. Principle of the analysis of milk and starch based food materials. Organic trace analysis using spectrophotometry and fluorimetry. | 5 |

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- Lehn, J. M. "Supramolecular Chemistry – Concepts and Perspectives", VCH, 1995
- Anastas, P. T. and Warner, J. C. "Green Chemistry: Theory and Practice," OUP.
- Ahluwalia, V. K and Chopra, M. "Medicinal Chemistry", Ane Books, 2008.
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- Gunzler, H. and Williams, A. Handbook of Analytical Techniques, Vol. 1&2, Wiley VCH


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- VK Ahluwalia "Green Chemistry – Environmentally Benign Reactions", Paperback 2012
- VR Gowarikar "Polymer Science" , New Age International, 2015
- Wilson and Gisvolds."Text book of Organic, Medicinal and Pharmaceutical Chemistry", J. B. Lippincott Williams and Wilkins, 2011
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- Holmes, D. J. and Peck, H. "Analytical Biochemistry", 3rd Edn, Longman, 1998


**Model Question Paper**

## SECOND SEMESTER M.Sc. DEGREE EXAMINATION 2020

## Branch: CHEMISTRY

**CHE-DE-528ADVANCED ORGANIC CHEMISTRY**

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

**SECTION-A**

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

1. Suggest a synthesis method for 18-crown-6 and explain one application.
2. How can calixarenes and porphyrins form supramolecular systems?
3. Give the structures of RNA and DNA
4. What is PCR? Explain the important points.
5. Give any two examples for sonochemical synthesis.
6. What are ionic liquids? Illustrate an example of its synthesis and application.
7. What are prodrugs? Give an example.
8. What are the factors affecting the degree of drug absorption?
9. Explain the light scattering method for molecular weight determination of polymers.
10. Give two examples each of i) biodegradable polymer and ii) conducting polymer
11. How can the iodine content in a organic compound be analyzed?
12. What are POP's? Give examples.

## SECTION-B

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

13. Illustrate the self-assembly of i) barbituric acid and 2,4,6-triamino pyrimidine and ii) bipyridine in presence of Cu(I).
14. How are liquid crystals classified? Give examples.
15. Explain the primary structure determination of a protein.
16. Provide examples of reactions taking place in i) MW conditions and ii) in solid supports
17. Explain the SFE and SFC techniques.
18. What is meant by ADME of a drug? Explain.
19. Explain bulk and emulsion polymerization techniques.
20. How is the lactose content in milk determined?

## SECTION-C

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

21 a) What are the essential features that a molecule should possess to act as a molecular wire? Give example.
   b) Luminescent cryptates of Eu(III) can be used to construct photonic devices. Explain.

22. a) Discuss the principles of green chemistry
   b) Discuss any two green chemistry experiments which can be done in a lab.

23. a) Explain group transfer and ring opening polymerization techniques.
   b) What are stereoregular polymers and how are they synthesized?

24 a) Explain protein biosynthesis.
   b) How can the amount of detergent in a water sample be analyzed and how can it be removed?

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|---|---|---|---|---|---|
| 1. | Semester | **2** | | | |
| 2. | Course Title | **ADVANCED PHYSICAL CHEMISTRY** | | | |
| 3. | Course Code | **CHE-DE-529** | | | |
| 4. | Credits | **2** | | | |
| 6. | **CO**<br>On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | 1. Explain industrially important metal complex catalyzed reactions | | 3-Ap | CK,PK | II, III |
| | 2. Understand the basics of ultrafast reactions | | 2-un | FK | I, II |
| | 3. Understand various corrosion methods and determine ways to control them. | | 2-Un; 5-Ev | FK,CK | I, II, III |
| | 4. Explain and differentiate various energy storage cells | | 3-Ap; 4-An | FK,CK | II, III, VI |
| | 5. Understand the concepts and theories of photochemical and photophysical process of energy transfer and its applications | | 2-Un; 3-Ap | FK | II, III, VI |
| | 6. Understand the basics of computational chemistry for quantum chemical calculations | | 2Un | CK,PK | II,III, VI |

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Surface area and porosity measurement. Preparation of catalysts, Precursor compound, Preactivation and activation process. Basic steps of phase transfer catalyzed reactions, transfer and intrinsic rates of catalysis.<br>Metal complex catalyzed reactions. Hydrogenation. Wacker oxidation. Monsanto acetic acid synthesis. Hydroformylation. Thermal and photochemical Water Gas Shift reactions. Olefin metathesis. Fischer-Tropsch reaction. Mobil process for the conversion of methanol to gasoline hydrocarbons. Ultrafast reaction dynamics. Introduction. Ultrafast lasers. Supersonic beams - pump-probe spectroscopy. Applications. | 1,2 |
| II | Corrosion and its Control:Nernst Theory, Standard Electrode Potential, Galvanic Series, Concentration cell, Types of corrosion: Uniform and Galvanic, Erosion, Crevice, Pitting, Exfoliation and Selective leaching, Inter-angular Stress, Waterline, Soil, Microbiological. Theories of corrosion: Acid, Direct Chemical attack, Electrochemical, Corrosion reactions, Factors affecting corrosion, Protective measures against corrosion, Sacrificial anode, and impressed current cathode protection. | 3 |
| III | Protective Coatings:Paints: Constituents, functions & mechanism of drying. Varnishes and Lacquers; surface preparation for metallic coatings, electroplating (gold) and electrode less plating (Nickel), anodizing, phosphate coating, powder coating & antifouling coating. Laser assisted surface engineering, Micro-Arc oxidation, Electro-spark coating. | 3 |

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|---|---|---|
| IV | Electrochemical storage cells: Charging and discharging, storage density, energy density. Different types of batteries: (i) Lead Acid (ii) Nickel-Cadmium, (iii) Zinc manganese dioxide. Modern batteries: (i) Zinc-Air (ii) Nickel-Metal Hydride, (iii) Lithium battery. Fuel cells; thermodynamic efficiency, electromotive force of fuel cells: Low temperature fuel cells: Hydrogen–oxygen fuel cells– alkaline and polymeric membrane types. Basics of Microbial fuel cells: construction, electrodes used, electron transfer mechanism. | 4 |
| V | Advanced Photochemistry:Energy transfer- theories of energy transfer, Photosensitization of organic and inorganic molecules – Singlet oxygen – methods of singlet oxygen generation and detection – chemistry of singlet oxygen – photodynamic therapy of cancer. Photoinduced electron transfer (PET) - concepts and theories. Photochemistry and Photophysics of semiconductors – semiconductor photocatalysis and applications. Artificial solar energy harvesting- photochemical splitting of water, dye sensitized solar cells. | 5 |
| VI | Computational Chemistry:Empirical, Semi empirical and ab initio methods. Hartree-Fock SCF methods. Basis functions- STO and GTO, primitive and contracted functions. Basis sets. Minimal, split-valence, polarized and diffused, Effective core potential (ECP). Pople style basis sets and examples. Calculating the number of basis functions for a molecular calculation. Molecular properties. Mulliken charges. Dipole moments. Geometry. Molecular orbitals-occupied and virtual. Overlap and overlap population. Specification of molecular geometry in Cartesian coordinates and internal coordinates. Z-matrix of molecules $H_2O$, $NH_3$, $CH_4$, eclipsed and staggered ethane. Dummy atoms and ghost atoms. | 6 |

**References:**


- Appleby, A. S. J. and Foulkes, F. K., Fuel cell Hand Book, Von Nostrand Reinhold, 1989.
- Banerjee, S.N., "An Introduction to Corrosion Science and Corrosion Inhibition", OxonianPress P. Ltd., New Delhi, 1985.
- Bruce G Gates, "Catalytic Chemistry", John Wiley & Sons, Inc. USA, 1992
- Cramer, C. J., "Essentials of Computational Chemistry- Theories and Models", 2nd Edition, Wiley, 2004.
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- Jensen, F., "Introduction to Computational Chemistry", 3rd Edition, Wiley, 2017.
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- Photoinduced Electron Transfer by Marye Anne Fox and ChanonM., Part A, B. C and D, Elsevier Science Publishing Company, 1988.
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**Model Question Paper**

## SECOND SEMESTER M.Sc. DEGREE EXAMINATION, Month Year
## Branch: CHEMISTRY
## CHE-DE-529: ADVANCED PHYSICAL CHEMISTRY

Times: 3 Hours Max. Marks: 60

SECTION- A

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

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

## SECTION- B

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

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

## SECTION- C

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

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

22. a) Explain the term corrosion? Describe the different theories to explain. How can you prevent a metal from corrosion?
    b) What are paints? What are their constituents and uses? (4+4)

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

24. a) Write the z-matrix of ammonia and staggered ethane

b) What are the basic approximations in HF theory? Explain, how the energy in HF limit differ from exact energy? (3+5)

## THIRD SEMESTER

| | | | | | |
|---|---|---|---|---|---|
| 1. | Semester | **3** | | | |
| 2. | Course Title | **INORGANIC CHEMISTRY III** | | | |
| 3. | Course Code | **CHE-CC-531** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO:** *On completion of the course, students should be able to:* | | **TL** | **KL** | **PSO No.** |
| | *1. Describe the fundamentals of solid state chemistry and X-ray diffraction* | | 2-Un, 4-An | FK | PSO1, PSO3 |
| | *1. Explain and compare solid properties based various binding forces and imperfections in solids* | | 2-Un, 4-An | FK, CK | PSO1, PSO3 |
| | *2. Describe and apply the basics of electrical and magnetic properties of solids* | | 2-Un, 3-Ap, 4-An | FK, CK | PSO1, PSO3 |
| | *3. Examine and correlate the solid state properties with real life materials* | | 2-Un, 3-AP | FK, CK | PSO1, PSO2 |
| | *4. Get an insight about the chemistry of open and closed structure compounds of important non-metallic elements* | | 2-Un, 4-An | FK | PSO1, PSO3 |
| | *5. Describe and examine the structure and properties of various metallic clusters* | | 2-Un, 4-An | FK, CK | PSO1, PSO3 |
| **MOD No** | **COURSE CONTENT** | | | | **CO No.** |
| I | **Introduction to Solid State**: Crystal systems and lattice types. Bravais lattices. Crystal symmetry. Point groups and space groups. Miller indices. Reciprocal lattice concept. Close packed structures: BCC, FCC and HCP. Voids. Coordination number. X Ray diffraction by crystals: Functions of crystals. Transmission and reflection grating. Braggs equation. Diffraction methods. Powder, rotating crystal, oscillation and Weisenberg methods. Indexing and determination of lattice type and unit cell dimensions of cubic crystals. Structure factor. Crystal defects: Point, line and plane defects. | | | | **CO1** |
| II | **Solid State Theories and Properties**: Binding forces in solids: Ionic bonding and potential energy field. Lattice energy. Born theory and Born Haber cycle. Molecular, ionic, covalent, metallic and hydrogen bonded crystals. Free electron theory and band theory of solids. Conductors, insulators and semiconductors. Mobility of charge carriers. Hall effect. Electrons and holes. Imperfections and nonstoichiometry (oxides and sulphides). Techniques of introducing imperfections in solids.Electrical properties of solids: Conductivity of pure metals. Superconductivity. Photoconductivity. Photovoltaic effect. Dielectric properties. Piezoelectricity and ferroelectricity. Magnetic properties | | | | **CO2,CO3,CO4** |

| | | |
|---|---|---|
| | of solids: Diamagnetism, paramagnetism, ferromagnetism, ferrimagnetism and antiferromagnetism. Lasers and their applications. | |
| III | **Inorganic nanomaterials and applications:** Popular and scientific perspective of nanotechnology; Fabrication of nanomaterials-top-down and bottom-up methods; Different types of nanostructures- 0D, 1D and 2D materials-nanoparticles, nanorods, nanocombs, nanotubes, nanowires and quantum dots, semiconductor nanoparticles; Carbon based nanomaterials and applications-Fullerene, graphene, carbon nanotubes and diamondoidnanomaterials; Nonocomposites- natural, organic polymer, metal and ceramic nanocomposite; Nanomaterials in various applications-Magnetic nanoparticle for information storage applications, Light-emitting devices based on direct band gap semiconductor nanoparticles. Nanomaterials for energy applications-fuel cell, photovoltaic and rechargeable batteries. Nanometerials in biomedical applications. | **CO5** |
| IV | **Structures of Sulphur, Nitrogen, Phosphorus and Silicone Compounds**: Sulphur Nitrogen compounds: Tetrasulphurtetranitride, disulphurdinitride and polythiazyl. $S_xN_y$ compounds. S-N cations and anions. Other S-N compounds. Sulphur phosphorus compounds: Molecular sulphides such as $P_4S_3$, $P_4S_7$, $P_4S_9$ and $P_4S_{10}$. Phosphorus-nitrogen compounds: Phosphazines. Cyclo and linear phosphazines. Other P-N compounds. Silanes, silicon halides, silicates; Classification and structure, silicones. | **CO6** |
| V | **Structure of Boron Compounds**: Boron hydrides: Reactions of diborane, and its structure and bonding. Polyhedral boranes: Preparation, properties, structure and bonding. The topological approach to boron hydride structure. Styx numbers. Wade's rules. Carboranes: Closo, nido and arachnocarboranes. Metalloboranes and metallocarboranes. Organoboron compounds and hydroboration. Boron-nitrogen compounds: Borazine, substituted borazines and boron nitride. | **CO6** |
| VI | **Other Metal clusters**: Factors favouring metal-metal bonds, Dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)_2$-trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons. Polyatomic zintl anion and cations. Infinite metal chains. Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W. | **CO7** |

**References:**


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


**Additional references**


13. Emeleus, H. J. Sharpe, A. G. "Modern Aspects of Inorganic Chemistry", 4th Edn., ELBS, 1973.
14. Holleman, A. F. and Wiberg, E. "Inorganic Chemistry", Academic press, 2001.
15. Kittel, C. "Introduction to Solid State Physics", Wiley.

16. Lee, J. D. "Concise Inorganic Chemistry," 4th Edn., Wiley-India, 2008.
17. Purcell, K.FandKotz, J. C. "Inorganic Chemistry," Holt-Saunders, 2010.

**Model Question Paper**

## THIRD SEMESTER M.Sc. DEGREE EXAMINATION Month Year

## Branch: CHEMISTRY

### CHE-CC-531: INORGANIC CHEMISTRY III

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

### SECTION-A

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

1. Explain the basis for classification of lattices into 7 crystal systems and 14 Bravais lattices.
2. Calculate the number of atom in a unit cell of BCC and FCC crystal structure.
3. Discuss the defect structure in non-stoichiometric sulphides.
4. What are the similarities and differences between ferrimagnetism and antiferromagnetism ?
5. What is meant by a 2D nanomaterial ? Give example.
6. Explain with example 'quantum confinement'.
7. Discuss the structure of $S_4N_4$.
8. Describe the structure of $P_4S_9$ and $P_4S_{10}$.
9. Find styx numbers for$B_6H_{10}$.
10. Even though borazine is isoelectronic with benzene, borazine is far more reactive than benzene. Why ?
11. Predict the number of metal-metal bonds in $Co_2(CO)_8$.
12. Establish the isolobal analogy between $CH_3$ and $Mn(CO)_5$.

### SECTION-B

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

13. Differentiate between FCC and HCP close packed structures.
14. What are intrinsic and extrinsic semiconductors ?

15. What is superconductivity and critical transition temperature ?
16. Explain with example 'bottom-up' approach of nanomaerial synthesis.
17. Discuss the bonding and aromaticity in cyclic phosphazenes.
18. Differentiate closo and nido carboranes with examples.
19. Compare the stability of o- and p- Dicarbadodecarborane.
20. Discuss the different types of bonding modes of carbonyl ligands in LNCCs.

## SECTION-C

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

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

ii) Discuss the bonding in $[Re_2Cl_8]^{2-}$ .

(4 + 4)

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

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Construction of Carbocyclic and Heterocyclic Rings - Importance of heterocyclic compounds, Structure and aromaticity of heterocycles, Trivial and Systematic Hantzsch Widman Nomenclature of heterocyclic compounds, Different methods of ring synthesis, Three and four membered heterocycles, Named reactions for synthesis of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline including Paal-Knorr, Feist-Benary, Fischer indole, Hantzsch, Skraup, Pictet-Spengler and Bischler-Napieralski methods, Electrophilic and nucleophilic substitutions of 5-membered, 6-membered, indole, quinoline and isoquinoline rings, Heterocycles with more than one heteroatom – synthesis and reactivity. Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Olefin metathesis. | 1 |
| II | Organic Synthetic Strategies - Introduction to retrosynthetic analysis. Linear and convergent synthesis, Synthons, functional group interconversions (FGI), Role of protecting groups in organic synthesis, Enolate and enamine alkylation reactions including Stork-enamine | 1, 2 |

| | | |
|---|---|---|
| | reaction, Dipole inversion - Umpolung. Organometallic reagents like Grignard, alkyl lithium and Gilman Reagents and their utility, Organocuprates, DABCO and Baylis-Hilman reaction, Role of palladium in organic synthesis, Heck, Sonogashira, Suzuki, Stille and Negishi coupling reactions. Glaser coupling, Tebbe olefination, Sakurai reaction, Brook rearrangement, Mitsunobu reaction, PPh3-CBr4 reagent | |
| III | Reagents for oxidation - Oxidations using manganese and chromium reagents, PCC, PDC Collins and Jones reagents, Etard reaction, Use of SeO2, MnO2, Ag2CO3 and lead tetraacetate, DMSO based reagents - Swern oxidation, Oppenauer oxidation. Oxidation of alkenes - OsO4, RuO4, HIO4, ozone and peracids. Sharpless asymmetric epoxidation, Woodward and Prevost hydroxylations, Dehydrogenation to aromatic compounds. Baeyer-Villiger oxidation, Dakin reaction. | 3 |
| IV | Reagents for reduction - Catalytic hydrogenation and stereochemistry. Hydrogenation catalysts and their selectivity. Adam's catalyst, Rosenmund reduction, Lindlar catalyst, Wilkinson's catalyst, Homogeneous hydrogenations. Fe, Zn, Na and Li reductions. Dissolving metal reductions – Clemmenson reduction, metal-alcohol reductions, Birch reduction, Hydride transfer reductions – MPV reduction, Reduction using NaBH4, LAH, LAH-AlCl3, DIBAL-H and NaCNBH3, selectrides. Reductions using borane reagents, hydroboration, Luche reduction, Wolff Kishner and diimide reductions.. | 3 |
| V | Natural Products Chemistry - Classification, Isolation, identification, typical examples and structures of secondary metabolites - Alkaloids, Terpenoids, Steroids, Prostaglandins, Coumarins and flavones. Degradation methods for structural elucidation – Hoffmann and Emde methods, examples of alkaloids, Total synthesis of reserpine, Classification of terpenes, Cationic rearrangements and formation of cyclic terpenes, Structural elucidation of santonin, Structure and importance of quercetin; β-carotene and ascorbic acid. Synthesis of Vitamin C from glucose, Biosynthesis of fatty acids and polyketides by acetate pathway, monoterpenes by mevalonic acid pathway and alkaloids by shikimic acid pathway, biosynthesis of higher terpenes and steroids. Structure of cholesterol and other important steroids, Barbier Wielander degradation and Blanc rule | 4, 5 |
| VI | Chemistry of nucleic acids and proteins - Amino acids, proteins and peptides: Structures and synthesis of amino acids – Strecker synthesis, Azlactone synthesis and enantioselective synthesis. Reactions of amino acids due to the NH2 group, COOH group and its reaction with ninhydrin, Structure of proteins, Introduction to enzyme and co-enzymes, structure and relevance of NAD, chymotrypsin, pyridoxal and thiamine, Peptide bond formation methods, amino and carboxy protection in SPPS. ADP and ATP. Automated polypeptide and oligonucleotide synthesis. Structure of polysaccharides including starch, cellulose, glycogen and chitin. | 6 |

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


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- Warren, S. “Organic Synthesis: The Disconnection Approach”, John Wiley, 2004.
- Hanson, J. R “Organic Synthetic Methods” RSC , 2002.
- Norman, R. O. C. and Coxon, A. "Modern Synthetic Reactions", Chapman Hall, 1993
- Mackie, R. K., Smith, D. M. and Aitken, R. A. “Guidebook to Organic Synthesis”, 3 Edn, Longman.1990
- Krishnaswamy, N. K. “The Chemistry of Natural Products,” Universities Press 2010
- Mann, J. “Chemical Aspects of Biosynthesis”, Oxford primer 20, OUP.1994
- Simmonds, R. J. "Chemistry of Biomolecules", RSC. 1992
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**Model Question Paper**

## THIRD SEMESTER M.Sc. DEGREE EXAMINATION 2020

## Branch: CHEMISTRY

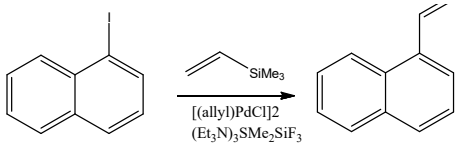
### CHE-CC-532 : ORGANIC CHEMISTRY III

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

### SECTION-A

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

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



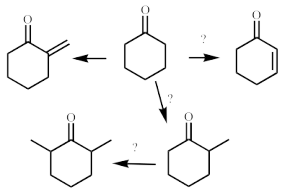

4. Illustrate the retrosynthetic analysis for paracetamol.
5. How do you convert 2-butyne to (i) *cis*-2-butene and (ii) *trans*-2-butene
6. What product is formed when trans-2-butene is treated with iodine and silver acetate under anhydrous conditions?
7. An aldehyde can be coupled with ethyl acrylate in presence of DMAP. Illustrate the reaction with mechanism.

**8.** What reagents are used for conversion of i) ethyl cinnamate to cinnamyl alcohol and ii) ethyl benzoate to benzaldehyde?
9. Suggest and illustrate a method to convert bromo benzene to biphenyl.
10. How are fatty acids biosynthesized in living cells?
11. Illustrate formation of shikimic acid in cells.
12. Depict the Strecker synthesis of aminoacids.

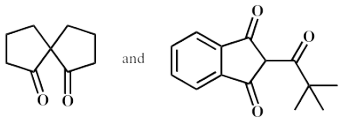
## SECTION-B

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

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



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

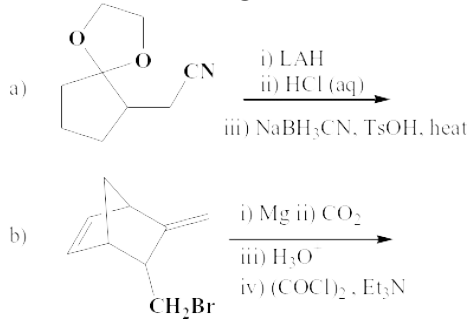



17. Illustrate biosynthesis of monoterpene.
18. Explain the secondary and tertiary structure of proteins.
19. Explain Barbier Wielander degradation and Blanc rule
20. Predict the product formed when isoquinoline is treated with lithium in liquid ammonia.

## SECTION-C

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

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



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

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

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | First and second laws of thermodynamics. Thermodynamic criteria for equilibrium and spontaneity. The Clausius inequality, Maxwell relations. The third law of thermodynamics. Need for the third law. Nernst heat theorem. Apparent exceptions to third law. Applications of third law. Thermodynamics of irreversible processes: Simple examples of irreversible processes. General theory of nonequilibrium processes. Entropy production. The phenomenological relations. Onsager reciprocal relations. Application to the theory of diffusion, thermal diffusion, thermoosmosis and thermomolecular pressure difference. Electrokinetic effects. The Glansdorf-Pregogine equation. | 1 |
| II | Statistical thermodynamics: Mechanical description of molecular systems. Thermodynamic property and entropy. Microstates. Canonical and grand canonical ensembles. Equation of state for ideal quantum gases. Maxwell-Boltzman distribution. The partition functions. Partition function for free linear motion, for free motion in a shared space, for linear harmonic vibration. Complex partition functions and partition functions for particles in different force fields. Langevins partition function and its use for the determination of dipole moments. Electrostatic energies. Molecular partition | 2 |

| | | |
|---|---|---|
| | functions. Translational, rotational, vibrational and electronic partition functions. Total partition functions. Partition functions and thermodynamic properties. Heat capacity of gases. Equipartition principle and quantum theory of heat capacity. | |
| III | Quantum statistics: Bose-Einstein statistics. Examples of particles. Theory of paramagnetism. Bose-Einstein condensation. Liquid helium. Super cooled liquid. Fermi-Dirac statistics. Thermionic emission. Relations between Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac statistics. Heat capacity of solids. The vibrational properties of solids. Einstein theory of heat capacity. The spectrum of normal modes. The Debye theory. The electronic specific heat. Structure of liquids, X-ray diffraction studies, Short range order, radial distribution function, configurational partition function for liquids. Theories of liquids state. Free space and van der Waals theories. Lennard-Jones theory of melting. Specific heats and communal entropy of liquids. | 3 |
| IV | Order and molecularity of reactions. Time dependency of order. Complex reactions: Reversible, consecutive, concurrent and branching reactions. Free radical and chain reactions. Steady state treatment. Reactions like $H_2$-$Cl_2$ and $H_2$-$Br_2$. Decomposition of ethane, acetaldehyde and $N_2O_5$. Rice-Herzfeld mechanism. Unimolecular reaction. Lindemann treatment. Semenoff-Hinshelword mechanism of chain reactions and explosion. Kinetics of fast reactions: Relaxation method. Relaxation spectrometry. Flow method, Stopped-flow technique. Shock method. Pulse method. Flash photolysis. Factors influencing reaction rates in solution. Salt effects. Curtin-Hammett equation, kinetic isotope effect.<br>Theories of reaction rates. Arrhenius equation, Collision theory, potential energy surfaces and reaction coordinate, TransitionState theory, comparative study of the theories. Kinetics of reactions in solution. Diffusion controlled reactions. Ionic reactions and effect of ionic strength, Effect of solvents, effects of pressure on velocity of gas reactions. | 4,5 |
| V | Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Acid-base catalysis. Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanisms, acidity function. Enzyme catalysis. Michaelis-Menton equation, effect of pH and temperature on enzyme catalysis. Mechanism of heterogeneous catalysis-Unimolecular and Bimolecular surface reactions. Langmuir-Hinshelwood mechanism.<br>Introduction to photochemistry: Laws of photochemistry. Quantum yield. Radiative and non-radiative transitions. Fluorescence and phosphorescence. Intensity and concentration. Fluorescence indicators. Quenching of fluorescence. Chemiluminescence. Explosion reaction. Kinetics of photochemical reaction of $H_2$and $Cl_2$, and $H_2$and $Br_2$. | 6 |
| VI | Ionic activity. Ion-solvent interaction. Strong electrolytes. Ion transport. Debye-Huckel theory of strong electrolytes, Debye-Huckel limiting law. Mean ionic activity coefficient. Debye-Huckel- Onsagar equation and its derivation. Debye-Falkenhagen effect. Wein effect.<br>Types of electrodes. Electrochemical cells. Liquid junction potential and its determination. Evaluation of thermodynamic properties and activities. Electrical double layer, and its various models. Electrode-electrolyte interface. Electrokinetic phenomena. Current-potential curves. Over potential and its theories. Butler-Volmer equation. Tafel and Nernst equations. Corrosion and methods for prevention. Porbaux diagram and Evans diagram. Introduction to polarography, cyclic voltammetry. Theory and working of Fuel Cells. | 7 |

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- Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3rd edition, 2006, Springer.
- Houston, P. A., "Chemical Kinetics and Reaction Dynamics", Dover, 2006.

- Panchenkov, G. M. and Labadev, V.P., "Chemical Kinetics and Catalysis", MIR Publishing.
- Laidler, K. J. "Chemical Kinetics" 3rd Edition, Prentice Hall, 1987.
- Moore, J. W. and Pearson, R. G. "Kinetics and Mechanism", 3rdedition, 1981, John Wiley and Sons.
- Bokris, J. O. M.; Reddy, A. K. N., "Modern Electrochemistry", Wiley-Interscience, 1972.
- Glasstone, S., "Introduction to Electrochemistry", East West Press Pvt Ltd. 1965.

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- Berry, R. S.; Rice, S. A. and Ross, J. "Physical Chemistry", Oxford University Press, Oxford, 2000.
- Sears, F. W., "Introduction to Thermodynamics, Kinetic Theory of Gases and Statistical mechanics", 2nd Edition, Addison Wesley, 1972.


**Model Question Paper**

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

Times: 3 Hours Max. Marks: 60

SECTION- A

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

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

## SECTION- B

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

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

## SECTION- C

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

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

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

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

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

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

(4+4)

| | | | | | |
|---|---|---|---|---|---|
| 1. | Semester | **3** | | | |
| 2. | Course Title | **Inorganic Chemistry Lab III** | | | |
| 3. | Course Code | **CHE-CC-534** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO:** On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | ***1.*** *Implement the analytical techniques learned earlier to the real cases* | | 3-AP<br>5-E | CK,<br>PK<br>MK | PSO4,<br>PSO5<br>PSO6 |
| | ***2.*** *Describe and execute ion-exchange separation technique* | | 2-Un<br>4-An | CK,<br>PK<br>MK | PSO4,<br>PSO5<br>PSO6 |
| | ***3.*** *Execute inorganic synthesis of model coordination complexes* | | 4-An<br>5-E | PK | PSO5<br>PSO6 |
| | ***4.*** *Interpret and compare the electronic properties of complexes based on the given experimental results* | | 3-Ap<br>4-An<br>5-E | PK,<br>MK | PSO3<br>PSO4<br>PSO5 |
| | ***5.*** *Describe and operate analytical and spectroscopic tools to characterize and analyse various inorganic complexes* | | 3-AP<br>4-An<br>5-E | PK,<br>MK | PSO4<br>PSO5<br>PSO6 |
| **MOD. No** | **COURSE CONTENT** | | | | **CO No.** |
| I | Analysis of some typical ores: Carbonate ore, sulfate ore, ilmenite and monazite. | | | | **CO1** |
| II | Analysis of fertilizers: Estimation of nitrogen in ammonium compounds. NPK estimations in synthetic fertilizers | | | | **CO1** |
| III | Ion exchange separation of binary mixtures: Zn & Mg and Co & Ni. | | | | **CO2** |
| IV | Synthesis of [Ti(urea)6]I3: An air stable d1 Complex. Compare the electronic property with $[Ti(H_2O)_6]^{3+}$ | | | | **CO3, CO4, CO5** |
| V | Preparation of various transition metal complexes | | | | **CO3** |
| VI | Characterizations of prepared metal complexes by UV-VIS, IR, magnetic susceptibility and electrical conductivity | | | | **CO4, CO5** |

**References:**


1. Drago, R. S. "Physical Methods in Inorganic Chemistry", Affiliated East West.

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


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|---|---|---|---|---|---|
| 1. | Semester | **3** | | | |
| 2. | Course Title | **ORGANIC CHEMISTRY LAB III** | | | |
| 3. | Course Code | **CHE-CC-535** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO**<br>On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | 1. To estimate the various functional groups present in organic molecules | | 3-Ap, 4-An | CK, PK | II, III, V |
| | 2. To apply volumetry for organic analysis | | 3-Ap | FK, PK | V |
| | 3. To apply UV-Vis spectrophotometry to analyze certain functional groups | | 3-Ap, | CK, PK | III, IV |

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

**REFERENCES**


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

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|---|---|---|---|---|---|
| 1. | Semester | **3** | | | |
| 2. | Course Title | **PHYSICAL CHEMISTRY LAB III** | | | |
| 3. | Course Code | **CHE-CC-536** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO**<br>On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | 1. Use conductometer to perform conductometric titrations, and to measure equivalent conductance | | 2-Un; 3-Ap | CK,PK | IV; V; VI |
| | 2. Perform potentiometric titrations | | 3-Ap | CK,PK | IV; V; VI |
| | 3. Perform polarographic estimations | | 3-Ap; 5-Ev | CK,PK | IV; V;VI |
| | 4. Perform flame photometry or Karl-Fischertitrator estimations | | 3-Ap;5-Ev | CK,PK | V; VI |
| | 5. Create a program in C++ or calculate simple properties of molecules employingsemiempirical MOT program. | | 3-Ap; 6-Cr | PK,MK | V;VI |
| | 6. Understand the basic principles of lab techniques adopted in physical<br>Laboratories,monitor, record and present data in a scientific form | | 2-Un | FK | V, VII, VIII |

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Conductance: Verification of Onsagar equation. Solubility of sparingly soluble substances. Oswald's dilution law. Basicity of acids. Dissociation constants of acids and bases. Conductometric titrations involving acid-base and precipitation reactions. Equivalent conductance of solutions of strong electrolytes and weak electrolytes. | 1,6 |
| II | Potentiometry: Single electrode potentials of hydrogen and glass electrodes. Quinhydrone electrode. Potentiometric titrations involving acid-base, redox and precipitation reactions. pH of buffer solutions. Solubility of AgCl. Determination of dissociation constant. | 2,6 |
| III | Polarography: Polarographic estimation of cadmium, zinc and lead. Composition of mixtures. | 3,6 |
| IV | Flame photometry: Estimation of $Na^+$, $K^+$, $Li^+$, $Ca^{2+}$ and $Mg^{2+}$. Composition of the mixtures. | 4,6 |

| | | |
|---|---|---|
| V | Karl-Fischer titrator: Estimation of water contents in pharmaceuticals, oils, fats and paints. | 4,6 |
| VI | Computers in Chemistry: Writing, compiling, and executing a computer program in C++, for any four chemical problems given: Determination of molecular weight of an organic compound, Determination of decay constant, half life and average life of a radioactive element, Calculating the normality/molarity/ molality of a given solution, Calculating the pH of a solution.<br>**OR**<br>Calculate the equilibrium geometry, geometrical parameters and energy of molecules: water, methane, ethane, acetone, and acetaldehyde using **MOPAC** semi empirical program. | 5,6 |

**References:**


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


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

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Molecular dynamics: Brief description of computational methods: *abinitio*, semi empirical, and empirical methods. Molecular mechanics. Potential energy functions. Force fields. Geometry minimization, Molecular dynamics. Periodic boundary conditions, Propagation of Newton's equation using Verlet, Velocity verlet and Leap-Frog algorithm. | 1 |
| II | *Ab initio* Methods: Approximations. HartreeFock method. Self consistent field. Slater determinants. Roothan approximation. Restricted HartreeFock (RHF), Restricted open HF (ROHF), and Unrestricted HF (UHF) methods. Semi empirical treatments: Extended Hückel theory. Introduction to CNDO, INDO, NDDO. Applications. Computing the matrix elements. | 2 |

| | | |
|---|---|---|
| | Slater's rules for matrix elements. Convergence. Optimization. | |
| III | Basis sets andBasis functions. Slater type orbital (STO) and Gaussian type orbital (GTO). Contracted and primitive. Basis sets. Minimal, multiple zeta, split-valence, polarized and diffused. Pople style basis sets, designation of basis set size –Dunnings correlation consistent basis sets Relativistic effects - Effective core potential, ECP. | 3 |
| IV | Post HF methods-Exchange and Correlation energy. Static and dynamic electron correlation, Avoided crossings and configuration mixing. Configuration Interaction (CI). Couple cluster, Multi-Configuration and Complete active space SCF (MCSCF, and CASSCF), Moller-Plesset Perturbation methods ($MP_n$). Pros and Cons of these methods. | 4 |
| V | Density Functional Theory: Development of density function theory (DFT). Density matrices. Thomas-Fermi model. Hohenberg-Kohn existence and variational theorems. Chemical potential. Kohn-Sham self consistent field method. Exchange correlation functionals. Local density approximation (LDA), density Gradient corrections (GGA). Hybrid and meta–GGA functionals. Advantages and applications of DFT. | 5 |
| VI | Specifying the molecule in Cartesian and internal coordinates: Writing the Z-matrix of $H_2O$, $CH_4$, ethane, Cyclopentadiene, and benzene with suitable point group. Dummy atoms and Ghost atoms. Influence of point group in computations. Illustration by taking $H_2O$, and $NH_3$. Computing the quantities- structure, potential energy surface, and chemical properties such as Mulliken and natural charges. Dipole moments.SCF orbital energies. Koopmann's theorem and Brillouin theorem. | 6,7 |

**References:**


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


## Model Question Paper

**FOURTH SEMESTER M.Sc. DEGREE EXAMINATION, MONTHYEAR**
**Branch: CHEMISTRY**
**CHE-DE-537 ELECTRONIC STRUCTURE THEORY AND APPLICATIONS**

Times: 3 Hours Max. Marks: 60

SECTION- A

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

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

10. Differentiate between LDA and GGA.
11. What type of computation will be performed to verify if the molecule is indeed a minimum on the potential energy surface.
12. Differentiate dummy and ghost atoms.

SECTION- B

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

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

SECTION- C

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

21. a) Explain 'Force Fields'
    b) What are Pople style basis sets? Briefly explain the classification and its relevance. (4+4)

22. Explain and differentiate with examples the various approximations employed under density functional theory methods.
23. Explain in detail the various steps involved in HF methods. Also, differentiate RHF and UHF methods.
24. Explain Kohn-Sham theorem and applications

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

| | | | | |
|---|---|---|---|---|
| | systems and compare it to those in natural photosynthetic systems | E | MK | 03 |
| **MODULE No** | **COURSE CONTENT** | | | **CO No.** |
| I | Photophysical Properties of the Electronically Excited Molecules:Basic principles of photochemistry: Absorption of radiation-Beer Lambert's law. Electronic transitions. Frank Condon principle. Jablonski diagrams. Nonradiative transitions. Internal conversion and inter system crossing. Radiative transitions: Fluorescence emission, triplet states and phosphorescence. Absorption complexes. Charge transfer absorption. Excimers. Exciplexes. Delayed fluorescence. Chemiluminescence. | | | 1, 2 |
| II | Bimolecular Processes: Fluorescence quenching. Collisional quenching. Stern-Volmer equation. Static quenching Photoinduced electron transfer (PET): Concepts and theories, electron donors and acceptors, quantum yield, efficiencies and lifetimes, intermolecular, intramolecular and supramolecular PET. Fluorescence resonance energy transfer (FRET): Trivial or radiative mechanism; Forster and Dexter type energy transfer. Energy transfer versus electron transfer. Applications of electron transfer and energy transfer. | | | 3 |
| III | Techniques and Instrumentation:Light sources, filters and monochromators: Incandescent lamps and arc lamps, optical filters, spectrographs and monochromators. Lasers as excitation sources: General principles, Two, three and four level lasers, Solid state lasers (Ruby and Nd/YAG) and gas lasers. Luminescence measurements: Steady-state fluorescence spectroscopy. Luminescence quantum yield measurements, Time-resolved fluorescence spectroscopy, single photon counting, Detection and kinetics of reactive intermediates, Transient absorption spectroscopy: Nanosecond laser flash photolysis and Picosecond laser flash photolysis. | | | 4 |
| IV | Application of fluorescence in chemical sensing: Various approaches of fluorescence sensing, Fluorescent pH indicators, Fluorescent molecular sensors based on ion or molecular recognition: Recognition units and topology, recognition based on photoinduced electron transfer(PET), photoinduced charge transfer (PCT), Excimer formation and disappearance and Forster resonance energy transfer (FRET). Fluorescent sensors for Metal ions (based on all above mentioned recognition mechanisms), Fluorescent sensors for anions and neutral molecules. | | | 5 |
| V | Novel Fluorophores:Semiconductor Nanoparticles: Spectral properties of quantum dots, Labeling cells with quantum dots, Quatum dots and Resonance Energy Transfer (RET), Lanthanides: RET with lanthanides, Lanthanide nanoparticles, Near-infrared emitting lanthanides, Long-lifetime metal–ligand complexes: Introduction to metal–ligand probes, Spectral properties of MLC probes, Metal-ligand complex sensors, Aggregation induced emissive (AIE) fluorophores: Mechanism of AIE and applications. | | | 6,7 |
| VI | Solar Energy Conversion:Natural photosynthetic system: Light dependant reactions, photosynthetic reaction centre, Z-scheme of photosynthesis. Artificial photosynthesis, conversion of solar energy to chemical and other forms of energies. Solar water splitting. Photocatalytic hydrogen production, Photocatalytic carbon dioxide reduction. Photovoltaic cells: Polymer solar cells and dye sensitized solar cells. Photo-biochemical energy production. | | | 8,9 |

**REFERENCES**


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

**ADDITIONAL REFERENCES**


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


**Model Question Paper**

## THIRD SEMESTER M.Sc. DEGREE EXAMINATION Month Year

## Branch: CHEMISTRY

## CHE-DE-538: PHOTOPHYSICAL PROCESSES AND APPLICATIONS

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

### SECTION-A

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

1. State and Explain Frank Condon principle.
2. Guanosine has a maximum absorbance of 275 nm. $\varepsilon_{275}$ = 8400 $M^{-1}$ $cm^{-1}$ and the path length is 1 cm. Using a spectrophotometer, you find that the absorbance at 275 nm is 0.70. What is the concentration of guanosine?
3. What is Stern-Volmer equation? How it is useful in distinguishing static and dynamic quenching?
4. Explain the concept of donor and acceptor in photoinduced electron transfer (PET) with suitable examples.
5. Which are the light sources used in the UV-Vis absorption spectrophotomerter?
6. Experimentally how can you characterise the triplet state of an organic chromophore?
7. What is a fluorescent pH indicator? Explain with an example.
8. Exemplify the concept of excimer based fluorescence sensor.

9. Luminescence lifetimes of metal-ligand complexes are usually high compared to that of pure organic fluorophores. Why?
10. How luminescence originates in quatum dots?
11. What is the function of redox couple in dye sensitized solar cell?
12. Write a note on photocatalytic carbon dioxide reduction.

## SECTION-B

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

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

## SECTION-C

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

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

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

(4 + 4)

| 1. | Semester | **3** | | |
|---|---|---|---|---|
| 2. | Course Title | **NEW METHODS IN ORGANIC SYNTHESIS** | | |
| 3. | Course Code | **CHE-DE-539** | | |
| 4. | Credits | **3** | | |
| 5. | **CO**<br>On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | 1. Use retrosynthetic method for the logical dissection of complex organic molecules and devise synthetic methods | | 3-Ap, 4-An, 6-C | CK | II, III, VI |
| | 2. Use various reagents and organic reactions in organic synthesis | | 3-Ap | FK, CK | III, VI |
| | 3. Gain expertise in asymmetric synthesis and catalysis | | 3-Ap | FK, CK | VI |

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | The Disconnection Approach - Designing a synthesis, FGI, Synthons, order of events, choosing a disconnection, synthesis of aromatic compounds, chemoselectivity in synthesis – one group C-X disconnections – alcohols, ethers, sulphides, alkyl halides, two group C-X disconnections, 1,1- and 1,2- C-C disconnections, one group C-C disconnections, enolate chemistry, two-group disconnections, 1,1-, 1,2-, 1,3-, 1,4- and 1,5- difunctionalized compounds. | 1 |
| II | Retrosynthesis in Action - Advanced strategies, retrosynthesis in industry, stereoselectivity and regioselectivity in synthesis, using alkenes, alkynes and nitro compounds in synthesis, reconnections, | 1 |

| | | |
|---|---|---|
| | retrosynthetic analysis and synthesis – practice problems | |
| III | Heterocyclic Ring Synthesis - Three, four, five and six membered ring synthesis and retrosynthesis, aromatic heterocycles, aromatic heterocycles with two heteroatoms, rearrangements in synthesis, electrophilic substitution reactions, named reactions in heterocyclic synthesis. | 2 |
| IV | Modern Organic Synthesis - Nef reaction, Kulinkovich reaction, Ritter reaction, Seyferth-Gilbert homologation, Tishchenko reaction, Fritsch-Buttenberg-Wiechell rearrangement, Corey-Fuchs reaction, Noyori reaction. Brook rearrangement. Tebbeolefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Suzuki-Miyaura, Negishi-Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Wohl-Ziegler reaction. Introduction to MCR, Ugi and Passerini reactions, Click reactions, olefin metathesis. | 2 |
| V | Asymmetric Synthesis - Organocatalysis, Prolines and NHCs – synthesis and reactivity, Transition metal mediated reactions in organic synthesis, Olefin metathesis, Grubbs catalysts, Enantiomers and diastereomers. resolution methods, Stereospecific and stereoselective synthesis, Asymmetric Synthesis - Principles, General strategies, Chiral Pool strategy, Chiral Auxiliaries, Asymmetric Diels Alder Reaction, Chiral Reagents – Binol Derivatives of LiAlH4, Chiral Catalysts – CBS Catalyst. | 3 |
| VI | Reagents – Use of DDQ, iodobenzenediacetate, CAN, manganese acetate, FeCl3, NMO, Dess Martin periodinane, SmI2, N-heterocyclic carbenes, Na tetracarbonyl ferrate, benzenetricarbonyl chromium: TEMED, TEMPO, TMS, CBr4 + Ph3P | 2 |

**REFERENCES**


- Warren,S. “Organic Synthesis – The Disconnection Approach”, John Wiley and Sons, 2004
- P. S. Kalsi “Organic Synthesis through Disconnection Approach” MEDTEC, 2014
- Gilchrist, T. L. “Heterocyclic Chemistry.” Pearson, Third Edn., 2005.
- Norman, R. O. C. “Principles of Organic Synthesis”, Chapman and Hall, 2nd Edition, 1995.
- Clayden, J., Geeves, N and Warren, S. “Organic Chemistry”, OUP.


**ADDITIONAL REFERENCES**


- Joule J. A and Mills K. “Heterocyclic Chemistry”, 4th Edition, UK, Blackwell Science, 2000.
- Taber, D “Organic Synthesis – State of the Art 2003-2005”.


**Model Question Paper**

## THIRD SEMESTER M.Sc. DEGREE EXAMINATION 2020

## Branch: CHEMISTRY

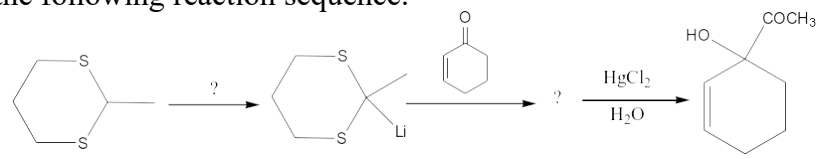
**CHE-DE-539NEW METHODS IN ORGANIC SYNTHESIS**

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

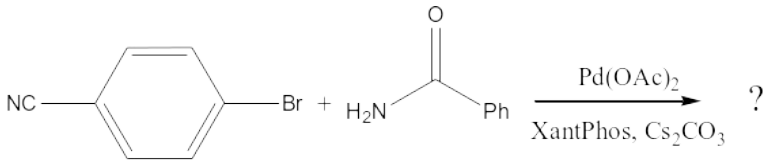
**SECTION-A**

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

1. Suggest synthetic equivalents for a) $PhCH_2^-$ and b) $PhCH_2^+$
2. 1-Butyne can be converted to butanal by using hydroboration oxidation. Illustrate.
3. Reaction of 4-hydroxy aniline with acetyl chloride is used for the synthesis of an analgesic. Identify the compound and depict the synthetic scheme.
4. How is *m*-nitro toluene synthesized from toluene?
5. Complete the following reaction sequence.




6. How is thiophene converted to thiophene-2-carbaldehyde?
7. How are azetidines and azetidine-2-ones synthesized?
8. Suggest a method to convert benzophenone to diphenyl acetylene and illustrate the mechanism.
9. Predict the product

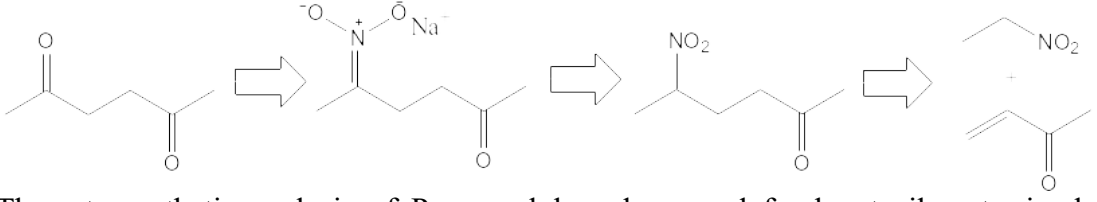



10. Give an example each for Grubbs 1st and 2nd generation catalysts.
11. How are BINOL derivatives of $LiAlH_4$ synthesized? Give one application.
12. What is the product formed when benzene tricarbonyl chromium complex is treated with BuLi followed by TMSCl? Illustrate.

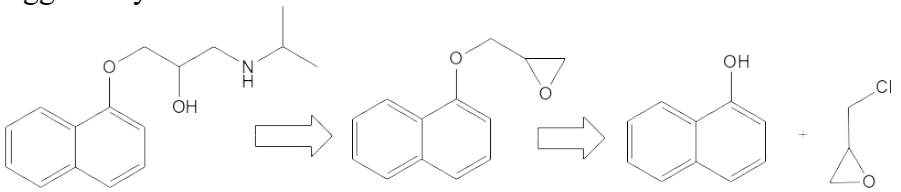
**SECTION-B**

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

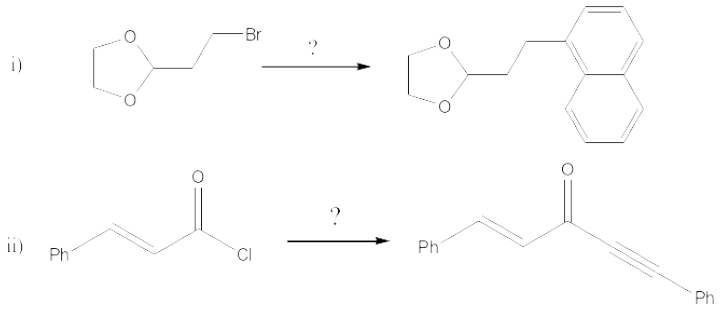
13. Retrosynthesis of a 1,4-diketone is shown below. Complete it and suggest the synthesis.



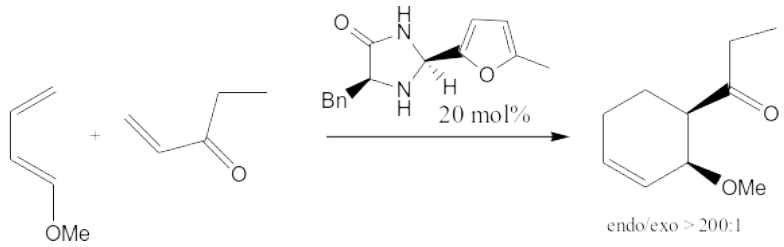

14. The retrosynthetic analysis of Propranolol, a drug used for heart ailments, is shown below. Suggest a synthetic route.



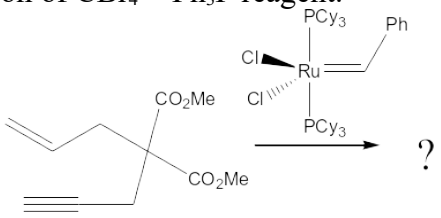

15. Explain Hantzsch pyridine synthesis.
16. How are the following conversions done?




17. Give an example each for ROM and RCM.
18. Explain this reaction



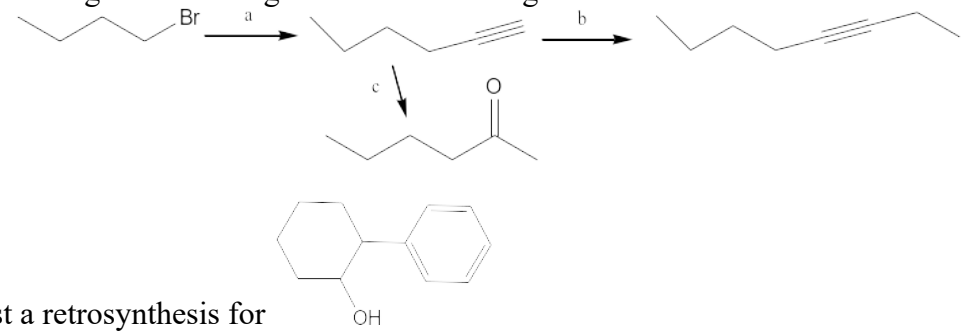

19. Depict one application of $CBr_4$ + $Ph_3P$ reagent.
20. Predict the product.




## SECTION-C

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

21 What reagents can bring about the following conversions




22. Suggest a retrosynthesis for
23. i) Describe the reactivity of $SmI_2$, CAN and $Mn(OAc)_3$ providing examples. (3x3)
    ii) What is DDQ? What is it used for?
    iii) Explain the structure and importance of TEMPO
24. Depict the schemes with reagents and illustrate the mechanisms of Perkin, Stobbe, Dieckmann and Knoevenagel reactions.

| | | | | | |
|---|---|---|---|---|---|
| 1. | Semester | **3** | | | |
| 2. | Course Title | **Introduction to Chemical Biology and Anti-Cancer Research** | | | |
| 3. | Course Code | **CHE-DE-540** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO:** On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | *1. Describe the basic structural difference between prokaryotic and eukaryotic cells* | | 1-R, 2-Un | FK | PSO2 |
| | *2. Describe the structure and chemical composition of nucleic acids, protein, carbohydrates and lipids.* | | 2-Un, 3-Ap | FK | PSO2 |
| | *3. Describe and evaluate the chemical aspects of biological process and cell anatomy* | | 2-Un, 3-AP 5-E | FK, CK | PSO2, PSO3 |
| | *4. Describe in interlink between the nucleic acid sequence and protein synthesis to control various functions in cells* | | 2-Un, 3-Ap | FK, CK | PSO2, PSO3 |
| | *5. Correlate the evolutionary history with cellular and molecular biology* | | 2-Un, 3-Ap, 5-E | FK, CK | PSO2 PSO3 |
| | *6. Explain and correlate the genetic information with cancer growth and new therapeutic techniques in anti- cancer researchworking protocols.* | | 2-Un, 4-An, 5-E | FK, CK PK | PSO2 PSO3 |
| | *7. Describe about some fundamental aspects biochemical assays* | | 2-Un, 3-Ap | FK,PK | PSO2 PSO4 |
| **MOD** | **COURSE CONTENT** | | | **CO No.** | |
| I | **The beginning of life, the cell**: Cells, the structural and functional units of all living organisms; Three distinct domains of life; Eukaryotic and prokaryotic cell | | | **CO1 CO3** | |

| | | |
|---|---|---|
| | structure; Structural hierarchy in the molecular organization of cells; Cell Cycle and Cell-Growth Control; Macromolecules in cell constitution; Stereospecific interaction between biomolecules; Basics of energy production in cell; Genetic foundations in cell; Prebiotic chemistry and biological evolution; Molecular anatomy and evolutionary relationships. | **CO5** |
| II | **Nucleic acids: structure and biological relevance**:Deoxyribose nucleoside and nucleotide; Phosphodiester and glycosidic bond; Double helix structure of DNA; DNA super coiling; DNA topologies; Significance of DNA G-quadruplex; DNA-replication, repair and recombination; Reversible denaturation and annealing (renaturation) of DNA; DNA stability and damage; Chemical synthesis of DNA; Amplification of a DNA segment by the polymerase chain reaction (PCR).DNA sequencing by the Sanger method; Nucleotides as a carrier of chemical energy in cells; Adenine nucleotides as a components of enzyme cofactors; Gene and chromosomes; Ribose nucleic acid (RNA); secondary structures of RNA; Different types of RNAs and their biological role in cell; DNA-Dependent Synthesis of RNA; RNA Processing; Transcription and translation; RNA-Dependent Synthesis of RNA and DNA. | **CO2**<br>**CO4** |
| III | **Proteins, carbohydrates and lipids**: Amino acids; classifications of amino acids; acid-base properties of amino acids; peptides and polypeptides; structure of protein; Chemical synthesis of peptides; Ramachandran plot; secondary structure of protein; Protein tertiary and quaternary structures; Structural diversity and functional diversity in globular proteins; Stable folding patterns in proteins; Protein denaturation and folding; Enzymes and the working principle; Primary structure of carbohydrate; monosaccharides and disaccharides; Fischer projection and Haworth perspective formulas; Polysaccharides; Structural and functional roles of polysaccharides; Lipids;Sphingolipids; Storage lipids; Polyunsaturated fatty acids; Structural lipids in membrane; Lipids as signals, cofactors, and Pigments | **CO2**<br>**CO4** |
| IV | **Membrane transport, biosignaling, bioenergetics and metabolism:**The composition and architecture of membranes;membrane proteins; Transbilayer movement of lipids; Receptor-mediated endocytosis, caveoline mediated transport; Solute transport across membrane; Glucose transport; Ion transport; ATP driven transport; Ion channels; General features of signal transduction; G protein–coupled receptors and second messengers; GPCRs in vision, olfaction, and gustation; Receptor Tyrosine Kinases; Biochemical reactions in biological energy transduction; Free energy change associated with ATP, acetyl-coenzyme A, and phosphoenolpyruvate (PEP); ATP as the energy source for cell functions; Biological Oxidation-Reduction Reactions; Types of coenzymes and proteins serve as electron carriers; Glycolysis-the two phase of glycolysis; Feeder pathways for glycolysis; Fates of pyruvate under anaerobic conditions: Fermentation; Gluconeogenesis. | **CO4** |
| V | **Strategies in cancer therapeutics and imaging:**Oncogenes, Tumor suppressor genes, and programmed cell death-apoptosis; Cancer metabolism; Multidrug resistance; Personalized medicine; Cancer therapeutic and imaging techniques-Metal complexes as anti-cancer drugs; photodynamic therapy (PDT), Photothermal therapy (PTT), Immunotherapy and gene therapy; Positron Emission tomography (PET), ImmunoPET, Magnetic resonance imaging (MRI) in cancer imaging; Nanomaterial for therapy and theranostics; Protein inhibition; heat shock protein (HSP) inhibition; Synergistic cancer therapy; Mitochondria targeting therapies. | **CO6** |
| VI | **Biochemical tools and working protocols:**Cell culture protocol; Cell proliferation assays; Fluorescence and confocal microscopy; Fluorescence life time imaging (FLIM); DNA cloning and recombinant DNA technology; Bacterial and yeast artificial chromosomes; reverse transcriptase PCR (RT-PCR); quantitative PCR (q-PCR); Polypeptide sequencing; Purification, Detection, and Characterization of | **CO7** |

| | | |
|---|---|---|
| | Proteins; Ion exchange chromatography; SDS Gel electrophoresis; Investigating proteins with mass spectrometry; Fusion proteins and immunofluorescence proteins for localization of proteins in cells; Protein-protein interaction studies; Tandem affinity purification (TAP) tags; DNA microarrays to investigate RNA expression patterns and other Information; CRISPR/Cas systems; Human genome sequencing-applications. | |

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- Functional Nanomaterials for Phototherapies of Cancer, L. Cheng, C. Wang, L. Feng, K. Yang and Z. Liu, Chem. Rev. 2014, 114, 10869−10939.
- Metal Drugs and the Anticancer Immune Response, B.Englinger, C.Pirker,P.Heffeter, A.Terenzi,C. R. Kowol, B. K. Keppler and W. Berger, Chem. Rev. 2019, 119, 1519−1624


**Model Question Paper**

# THIRD SEMESTER M.Sc. DEGREE EXAMINATION 2020

## Branch: CHEMISTRY

### CHE-DE-540: Introduction to Chemical Biology and Anti-Cancer Research

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

**SECTION-A**

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

1. Mention four points to differentiate eukaryotic and prokaryotic cells.
2. Silicon is in the same group of the periodic table as carbon and, like carbon, can form up to four single bonds. In that case, what is the possibility of replacing silicon with carbon in biomolecules? Justify your answer.
3. What is prosthetic group in a protein? Explain with example.
4. How a phosphodiester linkage is formed in a DNA and how it is important in determining the structural features?

5. Compare the stability of DNA and RNA in alkaline condition. Justify your answer.
6. Differentiate Watson-crick and Hoogsteen hydrogen bonding with example.
7. How PCR and RT-PCR differs?
8. What is recombinant DNA?
9. What is apoptosis?
10. What is a plasmid?
11. Describe the advantages of FLIM over normal fluorescence microscopy.
12. Write a short note on DNA G4 structure and its biological relevance.

## SECTION-B

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

13. Write a note on abiotic origin of biomolecules.
14. Sketch in detail the mutual dependence of DNA and protein.
15. Explain the difference between ion exchange, size exclusion and affinity chromatography for protein purification.
16. Plot the reaction sequence in Edman degradation method of peptide sequencing.
17. If you want to make a double stranded DNA with the oligomer 5'-ACCTGGTCACATTGG-3', how you will execute the synthesis? Explain in detail.
18. What is the chemical background of MTT assay?
19. Sketch the conformational difference in the polysaccharides cellulose and amylose.
20. In samples of DNA isolated from two unidentified species of bacteria, X and Y, adenine makes up32% and 17%, respectively, of the total bases. What relative proportions of adenine, guanine,thymine, and cytosine would you expect to find in the two DNA samples? One of these species was isolated from a hot spring (64 °C). Which species is most likely thethermophilic bacterium, and why?

## SECTION-C

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

21. Explain in detail the PCR procedure of DNA amplification. (8)

22. (i) What is HSP90 and how HSP90 inhibitors can act as an anti-cancer drug? (4)
    (ii)What are the major components in PDT and how the therapeutic effect is generated? (4)

23. (i) Explain Ramachandran plot and how this helps to test the quality of a predicted 3D structure of a protein. (5)
    (ii) Explain the effect of pH on the conformation of α-helical secondary structures of poly(Glu) and poly(Lys). (3)
24. Explain the role of G protein–coupled receptors (GPCRs) in vision, olfaction, and gustation. (8)

## FOURTH SEMESTER

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|---|---|---|---|---|---|
| 1. | Semester | **4** | | | |
| 2. | Course Title | **COMPREHENSIVE VIVA** | | | |
| 3. | Course Code | **CHE-CC-541** | | | |
| 4. | Credits | **2** | | | |
| 5. | **CO**<br>With this, the student should be able to | | **TL** | **KL** | **PSO No.** |
| | 1. Do a comprehensive revision of the topics studied so far in the programme | | 4-An,5-E | CK | III, VII, VIII |
| | 2. Get trained to attend an interview-mode examination | | 4-An, 5-E | MK | III, VII,VIII |
| | **COURSE CONTENT** | | | | **CO No.** |
| Comprehensive viva will include various topics of the core courses studied in the first three semesters | | | | | |

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|---|---|---|---|---|---|
| 1. | Semester | **4** | | | |
| 2. | Course Title | **DISSERTATION** | | | |
| 3. | Course Code | **CHE-CC- 542** | | | |
| 4. | Credits | **14** | | | |
| 5. | **CO**<br>On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | 1. Conduct a literature survey | | 3-Ap, 5-E | PK | VI, VII,VIII |
| | 2. Design and execute small reaction schemes | | 5-E, 6-C | PK, MK | VI,VII,VIII |
| | 3. Independently write scientific reports | | 6-C | CK,PK | VII, VIII |
| | 4. Communicate through various forms of presentation | | 3-Ap | CK | VIII |

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|---|---|---|---|---|---|
| 1. | Semester | **4** | | | |
| 2. | Course Title | **APPLIED CHEMISTRY** | | | |
| 3. | Course Code | **CHE-DE-543** | | | |
| 4. | Credits | **3** | | | |
| 5. | **CO**<br>On completion of the course, students should be able to: | | **TL** | **KL** | **PSO No.** |
| | 1. Understand various chemical industry processes | | 1-R, 2-Un, | FK, CK | I, II |
| | 2. To appreciate the role of chemistry in day-to-day human life | | 2-Un, 3-Ap 4-An | FK, CK | I, II, III |
| | 3. To apply chemistry principles in industry and chemical engineering | | 3-Ap, 5-E | CK, PK | I, III |

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Petroleum, Fuels &Combustion, Lubricants - Petroleum:Petroleum, cracking, Synthetic petrol, Refining of gasoline, Reforming, Chemical structure of fuel and knocking. Octane Rating of fuels, Cetane Rating, Diesel engine fuel, Kerosene, LPG as a fuel.<br>Fuels &Combustion:Classification, Calorific value, Types, Determination by Bomb calorimeter, Dulong's Formula, Analysis of Coal, Proximate and Ultimate analysis, Fuel gas analysis, Significance, Numericals, Carbonization of Coal, Manufacture of metallurgical coke by Otto Hoffman's by product oven, Combustion calculations.<br>Lubricants:Functions of lubricant, Mechanism of lubrication, Fluid or Hydrodynamic Lubrication, Thin film or Boundary lubrication & Extreme pressure lubrication. Lubricants for Extreme ambient conditions and for special applications. Properties of lubricants and tests. | 1, 3 |
| II | Corrosion and Protective Coatings - Corrosion and its Control:Nernst Theory, Standard Electrode Potential, Galvanic Series, Concentration cell, Types of corrosion: Uniform and Galvanic, Erosion, Crevice, Pitting, Exfoliation and Selective leaching, Inter-angular Stress, Waterline, Soil, Microbiological. Theories of corrosion: Acid, Direct Chemical attack, Electrochemical, Corrosion reactions, Factors affecting corrosion, Protective measures against corrosion, Sacrificial anode, and impressed current cathode protection.<br>Protective Coatings:Paints: Constituents, functions & mechanism of drying. Varnishes and Lacquers; surface preparation for metallic coatings, electroplating (gold) and electroless plating (Nickel), anodizing, phosphate coating, powder coating & antifouling coating. | 1, 2, 3 |

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|---|---|---|
| III | Applied Inorganic Chemistry - Introduction to chemical industry: Flow sheet preparation. Principles of process selection and operation selection. Basic raw materials and routes to major inorganic products. Flow sheets and engineering aspects of the manufacture of sulfuric acid, ammonia, urea, glass.Refractories:Definition, Classification with examples; Criteria of a good refractory material; Causes for the failure of a Refractory Material. Flow sheet and engineering aspect of the manufacture of Refractories. | 1,3 |
| IV | Portland Cement:Manufacture of cement, Dry and Wet process, Flow sheet and engineering aspect of the manufacture of Portland cement, Important process parameters for manufacturing a good cement clinker. Characteristics of the constitutional compounds of cement.Additives for cement, Properties, General composition, testing of cement, Chemical & physical requirement. | 1, 3 |
| V | Applied Organic Chemistry - Raw materials and routes to major organic products. Flow sheets and engineering aspects of the manufacture of important products such as nitrobenzene, vinyl chloride, soaps, detergents and hydrogenation of oils.<br>Pharmaceuticals: manufacturing process of aspirin, vitamin A and paracetamol.<br>Pesticides: manufacture of BHC, DDT, Carbaryl and Malathion. Manufacture of dyes.<br>Cosmetics: Talcum Powder, Tooth pastes, Shampoos, Nail Polish, Perfumes, soaps, and detergents - General formulations and preparation - possible hazards of cosmetics use.<br>Adulterants: Adulterants in milk, ghee, oil, coffee powder, tea, asafoetida, chilli powder, pulses and turmeric powder - identification. Color chemicals used in food-soft drinks and its health hazards. | 1,3 |
| VI | Polymer Chemistry - Polymers: Types of Polymerization. Thermoplastics & thermosetting polymers. Preparation, properties and applications of the Polyethylene, Teflon, PVC, Nylon, Phenol formaldehyde & Urea Formaldehyde. Silicone resins, silicone fluids, silicone greases. Polyurethanes, foamed or cellular plastics.Elastomers: Natural rubber, Vulcanization of rubber & Synthetic rubber. | 1,2,3 |

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**Model Question Paper**

## FOURTH SEMESTER M.Sc. DEGREE EXAMINATION 2020

## Branch: CHEMISTRY

### CHE-DE-543: APPLIED CHEMISTRY

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

**SECTION-A**

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

1. Differentiate between octane number and cetane number.
2. A furnace is heated by combusting a gaseous fuel of composition 29% CO, 9% $CO_2$, 16% $H_2$ and 46% $N_2$ with dry air. The Orsat analysis of products of combustion (POC) is 15% $CO_2$, 7% $O_2$ and 78% $N_2$. Calculate the volume of products of combustion (POC) at STP and at 1000 deg C.
3. What are the various types of corrosion?
4. Differentiate between electroplating and electroless plating.
5. What are the criteria for a good refractory material?
6. What are the common additives added in cements?
7. Depict the flowsheet for manufacture of sulphuric acid.
8. Differentiate between soaps and detergents chemically.
9. How is BHC and DDT manufactured?
10. What are the chief adulterants in milk and how are they determined?
11. How is Teflon manufactured? What are its applications?
12. Discuss monomers for polyurethane synthesis.

**SECTION-B**

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

13. Discuss the process of rubber vulcanization and its importance.
14. How is paracetamol and Vitamin A synthesized in lab?
15. Differentiate between thermoplastics and thermosetting plastics giving applications for both.
16. Discuss the dry and wet processes for cement manufacture.
17. Explain the factors causing corrosion and prevention strategies.
18. How is glass manufactured industrially? Explain using a flow chart.
19. What is meant by hydrodynamic lubrication? Give examples.
20. A natural gas analysing 85% $CH_4$, 5% $C_2H_6$ and 10% $N_2$ with air such that percentoxygen in POC remains at 2% on dry basis. Assume complete combustion, calculate (a) analysis of POC (dry basis), and (b) % excess air.

**SECTION-C**

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

21. Depict a diagram for the bomb calorimeter. Explain its principle, working and application.
22. Estimate the redox potential of a natural water that is in equilibrium with the atmosphere at pH 7 and 298 K. What fraction of a dilute solution $Fe^{2+}$ will be in its oxidized form $Fe^{3+}$ in such a water?The relevant E°s are1.23V for $O_2(g) + 4H^+ + 4e \longrightarrow 2H_2O$ and0.77V for the $Fe^{3+}/Fe^{2+}$ couple.
23. Why is hydrogenation of oil important? Explain the process, give example and application.
24. Discuss the synthesis of nylon, phenol-formaldehyde, urea-formaldehyde and silicone resin.

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|---|---|---|---|---|
| | Semester | **4** | | |
| | Course Title | **ANALYTICAL AND INSTRUMENTAL METHODS** | | |
| | Course Code | **CHE-DE- 544** | | |
| | Credits | **3** | | |
| | **CO:** On completion of the course, students should be able to: | **TL** | **KL** | **PSO No.** |
| | ***1**. Describe and implement the fundamentals of data analysis and analytical procedures involved in environmental quality control* | 2-Un, 3-Ap | FK<br>PK | PSO1<br>PSO2<br>PSO4 |
| | ***2**. Describe and classify principles and theory behind various chromatographic techniques.* | 2-Un | FK<br>CK<br>PK | PSO1<br>PSO4 |
| | ***3**. Explain and demonstrate the theory, principle and instrumentation of various analytical and spectroscopic instruments* | 2-Un, 3-AP | CK<br>PK | PSO1<br>PSO4 |
| | ***4.** Explain the basic principles and instrumentation of radiation analysis methods* | 2-Un | FK<br>CK | PSO1<br>PSO2<br>PSO4 |
| | ***5.** Explain and compare the principle, instrumentation and application of thermal, electro and surface analysis techniques* | 2-Un, 4-An | FK<br>CK<br>PK | PSO1<br>PSO4 |
| **MOD. No** | **COURSE CONTENT** | | | **CO No.** |
| I | **Data Analysis and Procedures Involved in Environmental Analysis:** Accuracy and precision. Evaluation of analytical data, The mean and median. Standard deviation, variance and coefficient of variation. Classification of errors. Minimization of errors. Significant figures and computations. Statistical methods in analysis. Students T test, Rejection of suspected value, Q test. Analytical procedures involved in the environmental monitoring of water quality- BOD, COD, DO, nitrite and nitrate, iron, fluoride, soil moisture, salinity, soil colloids, cation and anion exchange capacity. Air pollution monitoring: Control measures for air pollutants. sampling and collection of air pollutants-SO2, NO2, NH3, O3, and SPM. Principle of the analysis of milk and starch based food materials, Analysis of drugs, oils and fats. | | | **CO1** |
| II | **Chromatographic Methods**: Principles, instrumentation and applications of column chromatography, paper chromatography, thin layer chromatography, ion-exchange chromatography, Gas chromatography and HPLC. Detectors, Hyphenated techniques, Capillary Electrophoresis, Introduction to Chiral Chromatography, Molecular Exclusion Chromatography, Affinity Chromatography. Introduction to Method development and analysis of samples using the above techniques. | | | **CO2** |
| III | **Introduction to Instrumental Methods**: Electrical and nonelectrical data domains- | | | **CO3** |

| | | |
|---|---|---|
| | transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods precision, sensitivity, selectivity, and detection limits. Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio– hardware and software methods. Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals. | |
| IV | **Radiation Analysis Methods**: Measurement of radioactivity. Detection counters. Ionization chamber, Cloud chamber, Bubble chamber, Proportional counter, Geiger counter, Scintillation counters, Neutron activation analysis. Isotope dilution methods. Introduction to Positron emission Tomography, Working of nuclear reactors. | **CO3, CO4** |
| V | **Thermal, Electro and Surface Analysis Methods**: Principles, instrumentation and applications of thermogravimetry (TG), derivative thermogravimetry (DTG), differential thermal analysis (DTA) and differential scanning calorimetry (DSC). Analysis of samples using the above instruments- Principles, instrumentation and applications of Electrogravimetry, Coulometry, Polarography, Amperometry, Cyclic voltametry, Potentiometry and Conductometry. Analysis of samples using the above instruments. Introduction to SEM, TEM, AFM and other surface characterization techniques. | **CO3, CO5** |
| VI | **Fundamentals of Spectrochemical Methods:** Spectrophotometers - Sources of Light , Lamp and lasers, Monochromators, Detectors- PMT, Photodiode array, Charge coupled device, Infrared Detectors, Optical Sensors, Dealing with noise-Signal Averaging, Types of Noises, Fourier transformation in infrared Spectroscopy and NMR, Michelson interferometer, Instrumentation of UV-Vis, IR, Fluorescence Spectrometer Atomic Spectrometry- Atomization, Flames, furnaces and plasmas, Temperature Effects on Atomic spectroscopy, Inductively coupled Plasmas, Hollow Cathode Lamp, Interferences, Isobaric Interference Back ground Correction techniques, Mass Spectrometry, Ionization Methods Types of Mass Spectrometer, Quadrupole Spectrometer, Time of Flight, Orbitrap, Ion Mobility Mass Spectrometer Chromatography Mass Spectrometry Hyphenated methods, Introduction to ICPMS, XPS. | **CO3** |

**References:**


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16. Kolasinski, K.W. Surface Science: Foundations of Catalysis and Nanoscience, 2nd Edn., Wiley, 2009.
17. Mermet, J. Otto, M. Kellner, M. R. Analytical chemistry, Wiley-VCH, 2004.

18. Wilson, C. L. Wilson, D. W. Comprehensive Analytical Chemistry, Elsevier, 1982.

**Model Question Paper**

## FOURTH SEMESTER M.Sc. DEGREE EXAMINATION 2020

## Branch: CHEMISTRY

### CHE-DE-544: ANALYTICAL ANDINSTRUMENTAL METHODS

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

**SECTION-A**

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

1. Write down significant figures of i)0.0009 Kg ii) 9.50 mm iii) 85000 iv) 4.5600 X $10^4$
2. Plot a titration curve for the titration between a strong acid *vs* strong base. Which indicator can be used for this titration?
3. Explain a method to separate polymers according to their size.
4. How can two stereoisomers of a compound be separated?
5. Enumerate the methods to improve S/N ratio while handling instruments.
6. Why are FETs also known as unipolar transistors?
7. What is the principle of neutron activation analysis?
8. How does positron emission tomography work?
9. Depict a cyclic voltammogram and explain completely.
10. What is meant by fourier transformation in IR or NMR?
11. Explain MALDI and FAB mass techniques.
12. Differentiate between DSC and DTA.

**SECTION-B**

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

13. What is meant by distribution of random errors? Explain
14. Discuss the principle and application of any one electrokinetic separation method.
15. What technique is used to determine polydispersity indices?
16. What are hyphenated techniques? Give the principle of any two.
17. What are the techniques to measure radioactivity?
18. Explain the difference between SEM and TEM.
19. What are the different types of optical sensors and what are their applications?
20. What are the temperature effects on atomic spectroscopy in general?

**SECTION-C**

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

21. Explain various ways to minimize the errors encountered during an analysis.
22. Explain the various thermoanalytical techniques that can be used to study the thermal properties of a material.
23. Explain the working of nuclear fission and fusion reactors.

24. Compare the techniques EDX, XPS, AAS and ICPMS.

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

| **MODULE No** | **COURSE CONTENT** | **CO No.** |
|---|---|---|
| I | Data Analysis - Accuracy and precision. Evaluation of analytical data, The mean and median. Standard deviation, variance and coefficient of variation. Classification of errors. Minimization of errors. Significant figures and computations. Statistical methods in analysis. Students T test, Rejection of suspected value, Q test. | 1 |
| II | Volumetric Analysis and Precipitation Methods - Classification of reactions in volumetry (titrimetry). Acid-base equilibria in water. Buffers. Titration curves. Theories of indicators. Theory of complexometric titrations and applications, Solubility product. Common ion effect. Super saturation and precipitate formation. Precipitation from homogeneous solutions. The purity of precipitate. Co-precipitation and post precipitation. Contamination of precipitates. Washing of precipitate. Ignition of precipitate. Organic reagents used in gravimetry | 1, 2 |
| III | Chromatographic Methods**:** Principles, instrumentation and applications of column chromatography, paper chromatography, thinlayer chromatography, ion-exchange chromatography, Gas chromatography and HPLC. Detectors, Hyphenated techniques, Introduction to Chiral Chromatography, Molecular Exclusion Chromatography, Introduction to Method development and Analysis of samples using the above techniques. | 3 |

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|---|---|---|
| IV | Introduction to Environmental Chemistry - Components of Environment. Earth's atmosphere, Stratosphere chemistry, Ozone formation and depletion, Protection of ozone layer, Chlorofluorocarbons, Chemistry of photochemical smog, Acid rain, Atmospheric production of nitric acid, sulphuric acid, Rain, snow and fog chemistry, Aerosols, Adverse effects of acid rain, Green house effect. Impact of greenhouse effect on global climate. | 4 |
| V | Air and Water Pollution - Air pollution incidents. Control measures for air pollution. Water pollution, Incidents of water pollution in India – examples – causes, effects and remedial measures, Case studies, Humic material, Metal complexes of ligands of anthropogenic origin, Soaps and detergents. Eutrophication. | 5 |
| VI | Solid Waste Management - Heavy metals. Industrial waste water treatment: Solid wastes from mining and metal production, Organic wastes, Mixed urban wastes, Solid waste management, Pollutants in soil. Radioactive pollutants. Pollutants from industries and agriculture. Chemical toxicology. Biochemical effects of pesticides and heavy metals. | 6 |

**References**


- Bailey, R. A. Clark, H. M. Perris, J. P. Krause, S. and Strong, R. L. "Chemistry of the Environment",Academic.
- De, A. K. "Environmental Chemistry",Wiley Eastern.
- Manjooran,K. B. "Modern Engineering Chemistry", Kannatheri Publications, Kochi.
- Skoog,D. A. West, D. M. and Holler,F. J. "Fundamentals of Analytical Chemistry", Saunders
- Sodhi,G. S. "Fundamental Concepts of Environmental Chemistry", Narosa.
- van Loon, G. W. "Environmental Chemistry", OUP.
- Vogel, I. "A Textbook of Quantitative Inorganic Analysis", Longman.
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**Model Question Paper**

## FIRST SEMESTER M.Sc. DEGREE EXAMINATION 2020

## Branch: CHEMISTRY

### CHE-GC-501: ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

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

**SECTION-A**

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

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

**SECTION-B**

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

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

**SECTION-C**

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

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