

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE
Second Semester M.Sc Chemistry Degree Examination, April 2025
MCH2C05 - Quantum mechanics & computational chemistry
(2022 Admission onwards)

Time: 3 hours

Max. Weightage : 30

Section A Short Answer
Answer 8 Questions out of 12.

Each question carries a weightage of 1 (8 X 1 = 8)

- 1) Explain the independent particle model to solve many body problem.
- 2) What is Fock operator?
- 3) Illustrate Pauli's exclusion principle using the Slater determinant of the ground state of He atom.
- 4) Draw the MO diagram of O₂ molecule and comment on the magnetic nature.
- 5) Find the spectroscopic term symbol of H₂⁺ and He₂⁺.
- 6) Account for the orientation of two sp hybrid orbitals in opposite directions.
- 7) Explain free valence index.
- 8) Account for the anti-aromatic nature of 1,3-cyclobutadiene using Frost Hückel mnemonic device.
- 9) Define the term electron correlation.
- 10) Mention the advantages of semi-empirical methods in comparison with *ab-initio* methods.
- 11) Briefly explain the post HF methods.
- 12) Give the z-matrix of formaldehyde.

Section B Short Essay
Answer 4 Questions out of 7.

Each question carries a weightage of 3 (4 X 3 = 12)

- 13) Explain perturbation method. Calculate the total energy of particle in a one dimensional box with slanted bottom having length 0 to a.
- 14) Discuss Hartree's self-consistent field method for many electron systems.
- 15) Compare Slater type orbitals and Gaussian type orbitals.
- 16) Give the quantum mechanical treatment of sp³ hybridisation.
- 17) Give a critical comparison of MO and VB theories.

- 18) Obtain the HMOs of allylic anion. Calculate the charge distributions and bond orders.
- 19) Explain the structure of a Gaussian input file.

Section B Essay

Answer 2 Questions out of 4.

Each question carries a weightage of 5 (2 X 5 = 10)

- 20) State and prove variation theorem. Apply variation method to the ground state of the helium atom.
- 21) Briefly discuss the VB treatment of H₂ molecule. Write the singlet and triplet functions of H₂.
- 22) Give a detailed account of molecular mechanics methods. Compare MM methods with *ab-initio* methods.
- 23) Discuss the classification of basis sets and their nomenclature.

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Name:

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE
Second Semester M.Sc Chemistry Degree Examination, April 2025

MCH2C06 - Coordination Chemistry

(2022 Admission onwards)

Time: 3 hours

Max. Weightage : 30

Section A Short Answer

Answer 8 Questions out of 12.

Each question carries a weightage of 1 (8 X 1 = 8)

- 1) What is template effect?
- 2) Which among the complexes $[\text{Ni}(\text{NH}_3)_6]^{2+}$ and $[\text{Ni}(\text{en})_3]^{2+}$ will have greater overall stability constant. Justify your answer.
- 3) Why are all Cu-F bond distances not the same in CuF_2 ?
- 4) Which among $[\text{Fe}(\text{H}_2\text{O})_6]^{+3}$ and $[\text{Fe}(\text{o-Phen})_3]^{3+}$ is a stronger oxidising agent? Justify
- 5) Account for the intense yellow colour of CrO_4^{2-} .
- 6) Interelectronic repulsion is found to be weaker in complexes than in free metal ions. Why?
- 7) Derive the ground state term symbol for Tm^{3+} ion.
- 8) Why does the Mossbauer isomer shift in $[\text{Fe}(\text{CN})_5\text{L}]^n$ decrease in the order $\text{L} : \text{NH}_3 > \text{PPh}_3 > \text{CN} > \text{CO}$?
- 9) What is meant by spin orbit coupling?
- 10) Why does the aquation reaction of $[\text{Co}(\text{NH}_3)_5\text{Cl}]^{2+}$ occur slowly compared to $[\text{Co}(\text{NH}_3)_4\text{Cl}_2]^+$?
- 11) What is ferromagnetism? How does it vary with temperature?
- 12) What are delayed reactions?

Section B Short Essay

Answer 4 Questions out of 7.

Each question carries a weightage of 3 (4 X 3 = 12)

- 13) Explain the factors that affect the stability of complexes
- 14) Define CFSE. Calculate the CFSE of i) $[\text{CoCl}_4]^{2-}$ ii) $[\text{Co}(\text{NH}_3)_6]^{3+}$
- 15) How do pi donor ligands influence the magnitude of splitting parameter in pi bonded complexes?
- 16) Why does the tetrahedral complex of a metal give much more intense d-d spectra than its octahedral complex?
- 17) Explain hyperfine splitting in ESR spectrum by taking Cu(II) complex as an example.
- 18) Give the differences between 4f and 5f orbitals. Absorption spectra of Lanthanide ions are typically sharp and line like. Why?
- 19) Describe photosubstitution and photoaquation with examples.

Section B Essay

Answer 2 Questions out of 4.

Each question carries a weightage of 5 (2 X 5 = 10)

- 20) Depict MO energy level diagram for an octahedral complex involving sigma bonding. Explain its usefulness in accounting for the spectral and magnetic properties of metal complexes with the help of suitable examples.
- 21) What are Orgel diagrams? Draw and explain the Orgel diagram for d^2, d^7 octahedral and d^8 & d^3 tetrahedral metal complexes. Comment on its limitations.
- 22) Discuss the principle involved in Mossbauer spectroscopy. Explain the terms isomer shift and quadrupole splitting. How is this technique helpful in distinguishing the high spin and low spin complexes of Fe^{2+} ?
- 23) What is trans effect? Give the theories of trans effect. Design two step synthesis of cis and trans $[\text{PtCl}_2(\text{NO}_2)(\text{NH}_3)]^-$ starting from $[\text{PtCl}_4]^{2-}$

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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

Second Semester M.Sc Chemistry Degree Examination, April 2025

MCH2C07 - Reaction Mechanism in Organic Chemistry

(2022 Admission onwards)

Time: 3 hours

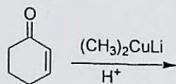
Max. Weightage : 30

Section A Short Answer

Answer 8 Questions out of 12.

Each question carries a weightage of 1 (8 x 1 = 8)

- 1) Illustrate the conversion of *p*-fluoronitrobenzene to *p*-nitroanisole.
- 2) How can the singlet and triplet nitrene are formed?
- 3) Identify the product and justify your answer



- 4) Pyrolytic elimination of 2-butyl acetate fetches three products. Why?
- 5) Illustrate the conversion of styrene to 4-phenyl-*m*-dioxane.
- 6) Describe 1,3-dipolar cycloaddition.
- 7) Discuss the regioselectivity of Diels Alder reaction by citing a suitable example.
- 8) Demonstrate the orbital interaction involved in the Cope rearrangements using FMO theory.
- 9) Explain the Lumiketone rearrangements.
- 10) Write a brief note on Paterno-Buchi reactions.
- 11) What is meant by photoenolization.
- 12) Write a name reaction that occurred at the electron deficient nitrogen.

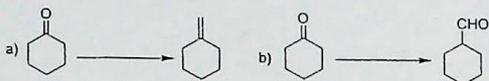
Section B Short Essay

Answer 4 Questions out of 7.

Each question carries a weightage of 3 (4 x 3 = 12)

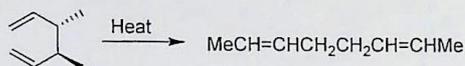
- 13) Explain the Benzyne mechanism. Predict the products obtained in the reaction of *o*-, *m*-, and *p*-chlorotoluene with NaNH₂/NH₃. Corroborate your answer.
- 14) Discuss the stereochemical aspects of reactions of enantiomers of 1,2-Dibromo-1,2-diphenylethane with sodium ethoxide.
- 15) Discuss the competitive factors affecting the S_N2 and E2 reaction during the bimolecular process by citing suitable examples.

16) How will you effect the following conversion.



17) For a [2+2] cycloaddition, thermal reaction is symmetry forbidden while photochemical reaction is symmetry allowed. Explain

18) In the following reaction, when racemic substrate is heated only one of the diastereomers of the product is formed. Identify the type of transformation and explain the term suprafacial and atarafacial.



19) Write down the catalytic cycle involved in the Suzuki coupling.

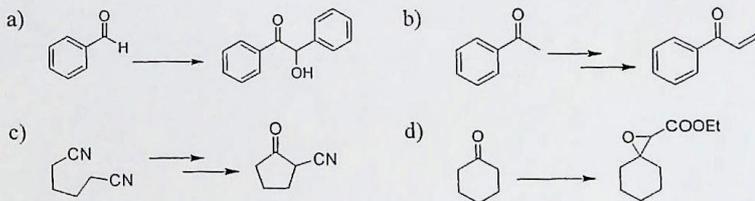
Section B Essay

Answer 2 Questions out of 4.

Each question carries a weightage of 5 (2 x 5 = 10)

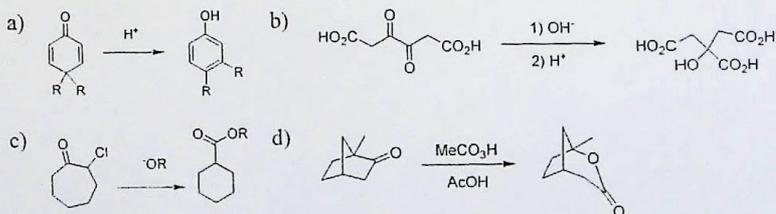
20) (a) Compare the stereochemical outcome of S_N1 and S_N2 reaction. (b) Illustrate how does the nature of the substrate influences the stereochemistry. (c) Why do vinyl and aryl halide do not undergo S_N1 and S_N2 reaction easily?

21) Identify the reagents and write the mechanism for the following transformation.



22) Briefly describe (a) Jablonski Diagram, (b) Photosensitization and Quenching, (c) Photoisomerization (d) Photooxygenation and (e) Photoreduction.

23) Outline the route with tandem steps involving to the following the rearrangements



FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

Second Semester M.Sc Chemistry Degree Examination, April 2025

MCH2C08 - Electrochemistry, Solid State Chemistry & Statistical TD

(2022 Admission onwards)

Time: 3 hours

Max. Weightage : 30

Section A Short Answer

Answer 8 Questions out of 12.

Each question carries a weightage of 1 (8 X 1 = 8)

1. Write electrode reaction in Ag/AgCl electrode. Why is it selected as a reference electrode
2. What is oxygen over voltage ?
3. Write down the Tafel equation. Explain the terms
4. Define decomposition potential.
5. What is meant by translational symmetry elements
6. Comment about the role of temperature on super conductivity.
7. Define Brillouin zone.
8. What is meant by birefringence ?
9. What does the ensemble mean and how grand canonical ensemble differs from micro canonical ensemble ?
10. Explain equipartition principle
11. Write down the expression for entropy in terms of partition function.
12. Compare the properties of Bosons and Fermions.

Section B Short Essay

Answer 4 Questions out of 7.

Each question carries a weightage of 3 (4 X 3 = 12)

13. Explain the Principle and applications of polarography.
14. Write a note on dropping mercury electrode.
15. Write a note on polymer electrolyte fuel cells.
16. Explain three different theories of hydrogen overvoltage.
17. Derive Braggs Law and its significance. Calculate the d-spacing of a simple cubic crystal having x, y, z plane intersect at a, 2b and 3c.
18. Briefly discuss (a) Meisner effect (b) Three level laser
19. Discuss Fermi statistics and how it relates to Boltzmann distribution

Section B Essay

Answer 2 Questions out of 4.

Each question carries a weightage of 5 (2 X 5 = 10)

20. Derive Debye – Huckel Limiting Law. Explain its significance and applications.
21. Briefly discuss stereographic projections.
22. Derive (a) Internal energy (b) entropy (c) Gibbs free energy in terms of partition function
23. Briefly explain the Bose-Einstein statistics.