

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE
Second Semester M.Sc Chemistry Degree Examination, April 2024

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) Define variation theorem. What is meant by a trial function?
- 2) Show that the BMO and ABMO of H_2^+ are orthogonal.
- 3) Give the quantum mechanical treatment of the sp hybridisation.
- 4) List the important assumptions used in the setting up of molecular mechanics methods.
- 5) What is meant by force field? Give two examples.
- 6) What is *ab-initio* method? Mention the advantages of *ab-initio* calculations.
- 7) What is a split-valence basis set? Give an example.
- 8) Give the z-matrix of NH_3 .
- 9) Explain the notations used in the basis set 6-311++G(d,p).
- 10) What is Fock operator?
- 11) Explain the concept of basis set in HF calculations.
- 12) Set up a trial function for the VBT treatment of H_2 .

Section B Short Essay

Answer 4 Questions out of 7.

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

- 13) What is meant by symmetric and antisymmetric wavefunctions? Obtain the Slater determinant for the ground state wave function of He atom.
- 14) Illustrate the variation theorem by using a suitable trial function for the ground state wavefunction of particle in a 1-D box.
- 15) Explain Born-Oppenheimer approximation and comment on the potential energy diagram of H_2 .
- 16) Using suitable examples, explain the use of Frost-Hückel circle mnemonic device for cyclic polyenes.

- 17) Write a brief note on post HF methods.
- 18) Explain the important approximation schemes used in semiempirical methods.
- 19) Write an input file for the geometry optimization of formaldehyde using Hartree-Fock method and 6-31G* basis set. Use the z-matrix of formaldehyde.

Section B Essay

Answer 2 Questions out of 4.

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

- 20) Explain the Hartree -Fock Self- Consistent Field method. Compare Slater type orbitals and Gaussian type orbitals
- 21) Discuss the time-independent perturbation method and obtain the expression for the first-order correction to energy. Apply the perturbation method to the ground state of the helium atom.
- 22) Give a detailed account of the MO treatment of H_2^+ .
- 23) Apply the HMO method to butadiene and allylic anion. Calculate the charge distribution and π -bond order of the first excited state of all the systems.

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE
Second Semester M.Sc Chemistry Degree Examination, April 2024
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 meant by macrocyclic effect?
- 2) Draw the different isomers of an octahedral complex of the type MA_3B_3 , where M is the central metal ion and A and B are unidentate ligands.
- 3) Why are low spin complexes not observed for tetrahedral coordination?
- 4) Which among $[Fe(H_2O)_6]^{+3}$ and $[Fe(CN)_6]^{3-}$ is a stronger oxidising agent. Justify .
- 5) Why $[Mn(H_2O)_6]^{+2}$ has an extremely pale pink colour?
- 6) What is spectrochemical series? Why is it called so?
- 7) Predict the magnetic moment of a compound containing Tb^{3+} ion.
- 8) How can ESR spectroscopy be used to distinguish between Cu(I) and Cu(II) complexes?
- 9) What is meant by quenching of angular momentum in coordination compounds?
- 10) Why is the aquation of reaction of $[Co(NH_3)_4Cl_2]^+$ is 10^3 faster than $[Co(NH_3)_5Cl]^{2+}$.
- 11) Give an example of photosubstitution in complexes.
- 12) What is ferrimagnetism? How does it vary with temperature?

Section B Short Essay
Answer 4 Questions out of 7.
Each question carries a weightage of 3 (4 X 3 = 12)

- 13) Explain the thermodynamic aspects of the chelate effect with suitable examples.
- 14) What is Jahn Teller effect? Give the spectral consequence of Jahn Teller effect.
- 15) Discuss the evidence which suggests that metal ligand bond is covalent in nature.

- 16) Explain spin state crossover by taking a suitable example.
- 17) Give the application of lanthanide shift reagents in NMR spectroscopy
- 18) Comment on the absorption spectra of lanthanide ions. Why are the spectra of lanthanoid complexes generally independent of the ligand type and coordination number ?
- 19) Write a note on metal complex sensitizers.

Section B Essay

Answer 2 Questions out of 4.

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

- 20) Sketch the MO diagram and explain the bonding in $[\text{Cr}(\text{NH}_3)_6]^{3+}$. Comment on its magnetic property. Discuss the merits of MOT over CFT.
- 21) What are Orgel diagrams? Discuss its applications and limitations. Why do electronic spectra of $[\text{V}(\text{H}_2\text{O})_6]^{3+}$ show only two absorption bands against three predicted for the system?
- 22) Give an account of applications of IR spectroscopy in characterization of metal complexes.
- 23) What is trans effect? Suggest the reaction pathways for preparing the different isomers of $[\text{Pt}(\text{py})\text{NH}_3\text{BrCl}]$ from $[\text{PtCl}_4]^{2-}$.

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

Second Semester M.Sc Chemistry Degree Examination, April 2024

MCH2C07 - Reaction Mechanism in Organic Chemistry

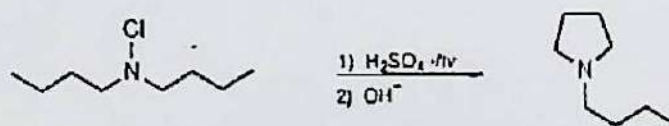
(2022 Admission onwards)

Time: 3 hours

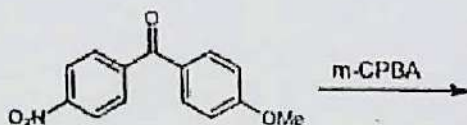
Max. Weightage : 30

Section A Short Answer**Answer 8 Questions out of 12.****Each question carries a weightage of 1 (8 X 1 = 8)**

- 1) Identify products formed when m-chlorotoluene is treated with KNH_2 in NH_3 .
- 2) Illustrate a reaction in which the following intermediates are involved.
a) Carbonium ion b) Nitrene
- 3) What is neighbouring group participation ? How does it affect the stereochemical outcome of a reaction?
- 4) Illustrate an extrusion reaction resulted in the formation of $\text{C}=\text{C}$.
- 5) Depict how can convert ethyl acetate to acetoacetic ester?
- 6) Write a short note on Ene reaction.
- 7) What is cope rearrangement?
- 8) How is *endo*-rule applied to Diels-Alder reaction.
- 9) Explain the term photosensitization and quenching.
- 10) Depict the Norrish type-I cleavage of β, γ unsaturated carbonyl compound.
- 11) Rationalize the following conversion



- 12) Identify the product and justify your answer.

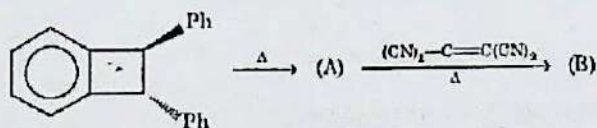
**Section B Short Essay****Answer 4 Questions out of 7.****Each question carries a weightage of 3 (4 x 3 = 12)**

- 13) Describe the effect of substrate, nucleophile and leaving group in aromatic nucleophilic substitution reaction.
- 14) Write a short note on a) Pyrolytic *syn* elimination b) Conjugate elimination and c) regiochemical outcome of saytzeff and hofmann elimination.

- 15) Discuss the generation, structure and reaction involved of the intermediate *Benzynes*.
- 16) Predict the products formed from the following reaction. Write the mechanism.



- 17) Complete the given reaction and give the mechanism of each step.



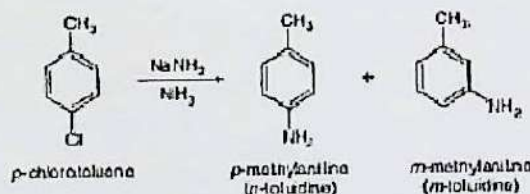
- 18) Why on thermal reaction *cis*-3,4-dimethylcyclobutene gives (2E,4Z)-2,4-hexadiene while the *trans* isomer gives the (2E,4E)-2,4-hexadiene?
- 19) Write down the catalytic cycle for Stille cross coupling reaction.

Section B Essay

Answer 2 Questions out of 4.

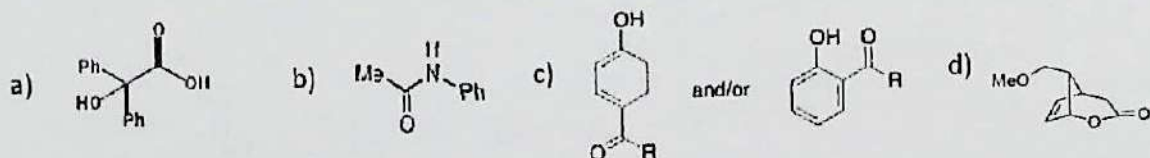
Each question carries a weightage of 5 (2 x 5 = 10)

- 20) a) Write the mechanism of the following reaction.



- b) Discuss the mechanism and stereochemical aspects of Bi-molecular Electrophilic Aliphatic Substitution.

- 21) a) Demonstrate how intra-molecular reactions such as Dieckmann and Thorpe condensation can effectively be used to prepare cyclic compounds. Illustrate with an example.
- b) What product would be formed when cyclohexanone, formaldehyde and dimethyl amine are reacted in the presence of catalytic amount of HCl. Write the mechanism of the reaction and show how the product can be used to make an enone.
- 22) a) Draw the Jablonsky diagram and discuss the major photophysical process involved in it.
- b) Write in brief (i) oxa-di- π methane rearrangement (ii) Paterno-Buchi reaction
- 23) Outline the route with tandem steps involving the rearrangements to the following compounds



FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE
Second Semester M.Sc Chemistry Degree Examination, April 2024
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 down the Nernst equation for hydrogen electrode and explain the terms.
2. What is meant by concentration polarisation? How it can be eliminated ?
3. What is meant by half wave potential? Explain its significance.
4. Write down the Tafel equation. Explain the terms
5. Explain glide plane symmetry operation and its significance.
6. Compare the properties of Laser light with normal light.
7. Explain the thermal properties of metals.
8. What is meant by a colour centre? Explain with example.
9. Define micro canonical ensemble.
10. Calculate the residual entropy of 1 mole AB type molecule.
11. Write down the significance of temperature on Boltzmann distribution
12. What is meant by Bose-Einstein condensation?

Section B Short Essay
Answer 4 Questions out of 7.
Each question carries a weightage of 3 (4 X 3 = 12)

13. Explain three theories of hydrogen over voltage.
14. Discuss the working principle, advantages and limitations of
(a) Methanol Fuel cell (b) Ni-Cd cell.
15. (a) What is the advantage of miller indices over direct lattice parameter? (b) Find
‘d’ of unit cell having an angle of reflection of crystal 28.26 deg. Using an Xray
source of wavelength 1.54 Angstrom for first order reflection.
16. Prove the non existence of fivefold degeneracy in crystals
17. Briefly explain the (a) Meisner effect and (b) superconductivity
18. What is meant by Hall Effect? how it is helpful to measure the mobility of electron.
19. Explain the classic theory of heat capacity of solids, and its failure.

Section C Essay

Answer 2 Questions out of 4.

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

20. Derive Butler-Volmer equation and explain its significance.
21. Briefly discuss the various types of imperfections in solids
22. Derive translational partition function, rotational partition function and how the temperature affects the distribution molecules in the above energy levels
23. Apply Fermi Dirac statistics for electrons in metals and explain.