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1M2A23020 (Pages : 2) Reg. No:.....

Name: .....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

Second Semester M.Sc Chemistry Degree Examination, April 2023

MCH2C05 - Quantum Mechanics and 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 by applying it to Helium atom.
2) Explain the Fock's modification to the Hartree's SCF method.
3) What does a basis function represent? Write the general forms of STO and GTO.
4) Illustrate Pauli's exclusion principle using the Slater determinant of the helium atom.
5) Explain Born-Oppenheimer approximation.
6) Write the Hückel determinant for benzene.
7) Obtain the normalised functions of sp hybridisation.
8) What is meant by free valence?
9) Explain the term electron correlation.
10) Compare the advantages and disadvantages of semi-empirical and ab-initio methods.
11) Briefly explain the basic idea of two post HF methods.
12) Give the general structure of Gaussian input file.

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

13) Apply time independent perturbation method to particle in a 1D-box with slanted bottom and calculate the total energy.
14) Briefly explain the Hartree's SCF method for many electron atoms.
15) What is meant by symmetric and antisymmetric wave functions? Obtain the Slater determinant for the excited state of He atom.
16) Draw the MO diagram of HF and name the MO

17) Write the Hückel determinant of 1,3-butadiene molecule. Obtain HMO coefficients and calculate π bond order.

18) Write a short note on Frost - Hückel circle mnemonic device for cyclic polyenes.

19) Construct 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) Define variation theorem. Prove the theorem and illustrate it using any suitable trial function.

21) Give a brief account of the VB treatment of H_2 molecule. Show that VBT holds the concept of electron pair bond between two atoms.

22) Give a detailed account of molecular mechanics and semi-empirical methods.

23) Explain the classification of basis sets with suitable examples.

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1M2A23021 (Pages : 2) Reg. No:.....

Name: .....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

Second Semester M.Sc Chemistry Degree Examination, April 2023

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) Draw all the possible geometrical isomers for the complex $[Cr(en)_2(CN)_2]^+$.
2) Mention the types of hybridisation and shapes of a) $Cr(CO)_6$ and b) $V(CO)_6$
3) Explain EAN rule.
4) Write the order of increasing energies of different d orbitals in square-planar geometry.
5) Write a short note on quenching of orbital angular momentum.
6) Write ground state term symbol of Ce^{3+} and Pr^{3+}
7) Write on absorption spectra of lanthanides and actinides?
8) Write on magnetic properties of actinides.
9) Low spin and high spin complexes can be distinguished by Mossbauer spectra. Explain this statement.
10) In the IR spectrum of the polymeric complex $Na_2[Co(CN)_5]_x$ two CN stretching frequencies occur.Explain
11) Explain an experimental method to distinguish between isomers of $[PtClBr(PR_3)_2]$
12) How does the racemization of tris chelate complexes take place?

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

13) Explain Adamson's rule of photo substitution of chromium complexes.
14) State and explain the Jhan Teller Theorem. What are its consequences?
15) Illustrate photolysis of water.

16) Arrange the following in increasing order of energy and justify your answer
^4F, ^2P, ^3G, ^6H, ^3I.

17) Describe the magnetic properties of lanthanides

18) Compare the complex formation ability of transition and inner transition elements

19) What is base hydrolysis? Discuss the possible mechanisms?

Section B Essay

Answer 2 Questions out of 4.

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

20) Discuss the spectrophotometric method for the determination of stability constant of complexes?

21) a) LMCT transitions in tetraoxoanions such as MnO_4^- *and* CrO_4^- are prominent explain?

b) Calculate the effective magnetic moment of $[Ni(H_2O)_6]\ 2^+$ using following data
i)$\lambda = -350cm^{-1}$ ii)$10Dq = 8500cm^{-1}$

22) Explain relevant points in epr spectra with respect to its application to Cu(II) complexes

23) How does the ligand field affect the choice between SN1 and SN2 paths in the substitution reactions of octahedra complexes? Also, explain how is this choice influenced by the basicity and pi bonding capacity of a non reacting ligand?

1M2A23022 (Pages : 3) Reg. No:.....

Name: .....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

Second Semester M.Sc Chemistry Degree Examination, April 2023

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) Explain how the branching at α-carbon of the substrate affects the rate of S_E2 (front) reaction.

2) How can the nitrene, Ph-N: and Ph-CO-N: be formed as intermediates. Write the examples of the subsequent reaction.

3) Solvolysis by acetate of 2-phenyl ethanol is found to be much faster than that of n-propanol. Account for the observation.

4) Give two examples for extrusion reaction.

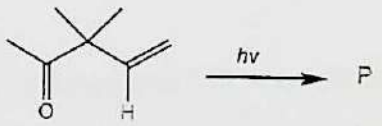
5) Write the mechanistic aspects of BAc2 Ester hydrolysis.

6) Derive Woodward Hoffmann rule for [1, 3] sigmatropic shifts.

7) Identify the photoproduct and write the scheme of reaction that would arise by irradiating cyclohex-2-en-1-one.

8) Fetch the product that obtained when 3-methyl-hexa-1,5-diene were heated at high temperature. Explain.

9) Identify the product of the reaction and write the mechanism.



10) Explain the term photoreduction.

11) Illustrate the photoreactions of Benzene.

12) Give two examples of reactions involving palladium catalyst for the formation of carbon – carbon bond formation.

Section B: Short Essay

Answer 4 Questions out of 7.

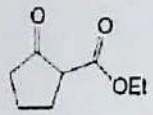
Each question carries a weightage of 3 (4 x 3 = 12)

13) Discuss the 'ion pair mechanism' in Nucleophilic Substitution reaction and comment on its stereochemical outcome by citing a suitable example.

14) Write a brief note on mechanical and stereochemical aspects of E1 elimination.

15) Discuss the major factors that affect the stability and reactivities of carbocation intermediate.

16) How would you employ a base catalyzed reaction for the preparation of the following cyclic compound and write the mechanism of the reaction.



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

18) Write the mechanism of a) Claison rearrangement b) Ene reaction.

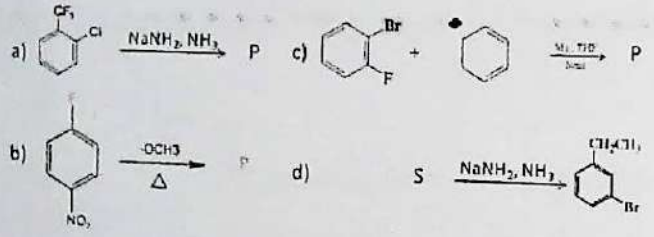
19) Write the catalytic cycle involved for Suzuki reaction.

Section B: Essay

Answer 2 Questions out of 4.

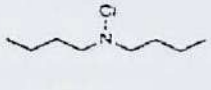
Each question carries a weightage of 5 (2 X 5 = 10)

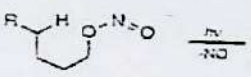
20) Complete the following reaction and outline the mechanism of the reaction

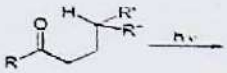


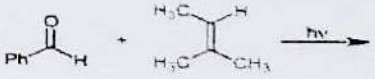
21) Write the mechanism of the following reaction. a) Darzen, b) Reformatsky, c) Knoevenagel, and d) Wittig.

22) What product would you expect from the following reaction and outline the mechanism

a) 

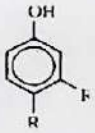
b) 

c) 

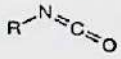
d) 

23) Outline the route involving the rearrangements to the following compounds

a) 

b) 

c) 

d) 

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1M2A23023 (Pages : 2) Reg. No:.....

Name: .....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

Second Semester M.Sc Chemistry Degree Examination, April 2023

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) Define half wave potential. Mention its significance.
3) Write down the Tafel equation. Explain the terms
4) Explain concentration polarization
5) Illustrate glide plane symmetry operation
6) Explain the characteristics of piezoelectric crystals.
7) Draw the stereographic projection of monoclinic systems $2, \bar{2}, 2/m$
8) Explain the lasing action of a three stage laser.
9) Explain thermodynamic probability.
10) Write down the equation for vibration partition function and define the terms.
11) Write down the temperature independent equation for entropy and discuss its significance.
12) Explain Dulong – Petits law of heat capacity of solids.

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

13) Explain any two theories of hydrogen over voltage.
14) Derive Butler-Volmer equation and mention its significance
15) Write a note on dropping mercury electrode. Mentions its advantages.
16) Briefly explain the Cooper pair theory of super conductivity
17) What is meant by Hall Effect? How it can be used to measure the mobility of charge carriers ?
18) Explain Einstein's theory of heat capacity of solids. Mention its drawbacks.
19) Prove the non existence of fivefold degeneracy in crystals

Section C

Essay Answer 2 Questions out of 4.
Each question carries a weightage of 5 (2 X 5 = 10)

20) Derive Debye Huckel Limiting Law. Discuss its significance

21) a) Derive Braggs Law. Mention its significance.

b) Discuss line and plane defects.

22) Derive translational partition function, rotational partition function and its temperature effects.

23) Derive Bose-Einstein statistics and explain how it relates to Boltzman distribution.