1M2M18018   (Pages : 2)   Reg. No:................................

Name: ....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE
Second Semester M.Sc Chemistry Degree Examination, March 2018
MCHE2B05 – Applications of Quantum Mechanics & Group Theory
(2017 Admission onwards)

Max. Time: 3 hours   Max. Weightage : 36

Section A
(Answer all questions; each question carries 1 weight)

1. Why separation of variables is not possible with Schrodinger equation of He atom?

2. The ground state energy of He atom according to perturbation method is -74.8 eV. Calculate the first ionisation potential of He atom. ($\overset{4}{E}_H$ = -13.6eV)

3. What is the difference between a primitive Gaussian and contracted Gaussian?

4. What is the difference between STO and AO

5. Which is more stable: NO or NO^+? Why?

6. What is non-crossing rule?

7. Write the sp hybrid wave functions of carbon atom and show that the linear geometry of sp hybrid orbitals is justified by them.

8. What is meant by free valence

9. What are normal modes? Represent normal modes of H_2O.

10. Show that 1 -1 i -i forms a mathematical group. Find the inverse of each element

11. Write a short note on group orbitals

12. Write the symmetry elements and determine the point groups of cis- and tras- dichloro ethylene.

(12x1=12 weightage)

Section B
(Answer any eight questions; each question carries 2 weights)

13. Apply perturbation method to He atom

14. Find the ground state energy for particle in 1D box using the trial function $e^{-\alpha r^2}$.

Given: $\hat{H} = -\frac{1}{2r^2}\frac{d}{dr}r^2\frac{d}{dr}\left(-\frac{1}{r}\right)$ and $\int_0^\infty x^n e^{-ax^2}dx = \frac{n-1}{n^2a}\left(\frac{\pi}{a}\right)^{1/2}$

15. Write the STO of Fe atom

16. What are Slater determinants? Use them to prove that an AO can accommodate only two electrons; that too with opposite spin.

17. Write the Huckel determinant of butadiene molecule. Obtain HMO coefficients and calculate π bond order.

18. Draw the MO diagram of CO and name the MO's.

19. Obtain the normalised functions of sp^2 hybridisation.

20. Write a short note on Frost - Huckel circle mnemonic device for cyclic polyenes

21. $A = \begin{bmatrix} 5 & 8 \\ 1 & 2 \end{bmatrix}$ and $B = \begin{bmatrix} 1 & 0 & 1 \\ 1 & -2 & 0 \\ 3 & 1 & -4 \end{bmatrix}$. Show that $\chi(AB) = \chi(BA) = \chi(A)\chi(B)$

22.

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$
Γ	3	0	-1	-1	2	-1

Show that $\Gamma = A_2' + E''$.

23. Predict the Raman and IR active vibrations in BF_3. Use D_{3h} character table.

24. Apply GOT to H_2O molecule and obtain the irreducible representations.

(8x2=16 weightage)

Section C
(Answer any two questions; each question carries 4 weights)

25. Explain the Hatree – Fock self consistent field method for the treatment of many electron systems

26. Compare the MO & VB methods of chemical bonding based on H_2 molecule.

27. a) List the important features of HMO treatment.

    b) Write a note on transition moment integral and its relation to spectroscopic selection rules

28. Find the conjugated π MO's of $C_3^+ H_3$ by SALC and projection operator method.

D_3h	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1	1	1	1	1	1	1		X^2+Y^2, Z^2
A_2'	1	1	-1	1	1	-1	R_Z	
E'	2	-1	0	2	-1	0	(X,Y)	(X^2-Y^2, XY)
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	Z	
E''	2	-1	0	-2	1	0		

(2 x 4 = 8 weightage

M18019   (Pages : 2) ·   Reg. No:................................

Name: ....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE
Second Semester M.Sc Chemistry Degree Examination, March 2018
MCHE2B06 – Coordination Chemistry
(2017 Admission onwards)

Time: 3 hours   Max. Weightage : 36

Section A
Answer all questions. Each carries one Weightage

Write Marcus equation and explain the terms?

Illustrate template effect with an example?

Bring out the significance of nephelauxetic series.

$[Hg(Cl)_4]^{2-}$ is thermodynamically stable and kinetically labile. What does this mean?

$[Cu(H_2O)_6]^{2+}$ and $[Cu(NH_3)_4]^{2+}$ both appear blue in solution, but $[Cu(H_2O)_6]^{2+}$ is less intense than $[Cu(NH_3)_4]^{2+}$. Why?

Show the possible stereoisomers of octahedral $[Mn(H_2O)_2(ox)_2]^{2-}$.

How the donor atom in metal-thiourea is established using IR spectroscopy?

Explain the Jahn-Teller distortion in $[Cu(H_2O)_6]^{2+}$

What are metal complex sensitizers. Give one example.

Why the magnetic moment of $[Co(H_2O)_6]Cl_2$ is higher than the spin only value?

Identify the following complexes as chiral and achiral complexes.

(a) $[Cr(ox)_3]^{3-}$; (b) cis-$[RhCl_2(NH_3)_4]^{+}$; (c) $[Ru(bipy)_3]^{4+}$; (d) $[Co(edta)]^-$.

Electronic spectra of transition metal complexes are broader than that of f-block elements. Why?

(12 x 1 = 12 weightage)

Section B
Answer any eight questions. Each carries two Weightage

Write a short note on photochemical reactions of metal complexes.

How ESR Spectroscopy can be used to distinguish between Cu(I) and Cu(II) in complexes? Explain.

Explain SN^1CB mechanism and its evidences.

Briefly explain the outer sphere electron transfer mechanism in metal complexes with examples.

17. Discuss the mechanism and synthetic applications of trans effect?

18. Draw the molecular orbital diagrams of octahedral and tetrahedral complexes?

19. Write the Irving-Williams order of stability of transition metal ions and mention the factors affecting stability of complexes?

20. What are the important merits and limitations of valence band theory?

21. How IR spectra is valuable in the study of metal carbonyls and bridged ligands?

22. Describe the kinetics of ligand substitution based on Adamson's rule?

23. Mention isomeric shift in Mossbauer spectroscopy and illustrate the Mossbauer spectra of octahedral aqua complexes of Fe^{2+} and Fe^{3+}?

24. State whether there is orbital magnetic moment contributions in the following complexes.
    i) $[Co(H_2O)_6]^{2+}$ ii) $[Co(Cl)_4]^{2-}$. Justify your answer.

$(8 \times 2 = 16$ weighta

Section C
Answer any 2 questions. Each carries 4 weightage

25. (i) The spectrum of octahedral aqua complex of chromium gives three peaks at 17000 cr

    24000 cm^{-1} and 37000 cm^{-1}. Calculate the crystal field splitting energy (Δ_0) and Nephelaux

    ratio(β).

    Given the Racah parameter (B) for free metal ion is 1310 cm^{-1}?

    (ii) Discuss the analytical applications of charge transfer spectra?

26. Explain the ligand substitution reactions in octahedral complexes.

27. Write short notes on:
    (i) Factors affecting the magnitude of crystal field splitting
    (ii) Spin-orbit coupling
    (iii) Hyperfine interactions in Mossbauer spectroscopy
    (iv) Fuoss-Eigen equation

28. Explain the determination of binary formation constants by pH-metric and spectrophotomet

    methods?

$(2 \times 4 = 8$ weight

1M2M18020 (Pages : 3) Reg. No:..........................

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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

Second Semester M.Sc Chemistry Degree Examination, March 2018

MCHE2B07 – Organic Reaction Mechanism
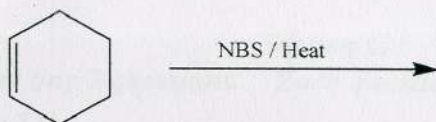
(2017 Admission onwards)

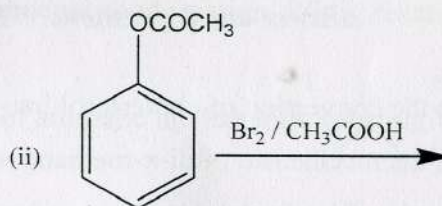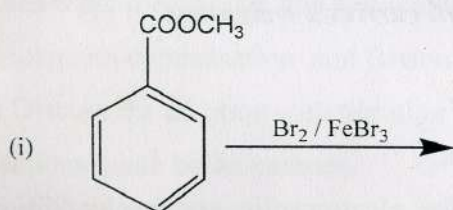Max. Time: 3 hours   Max. Weightage : 36

Section A
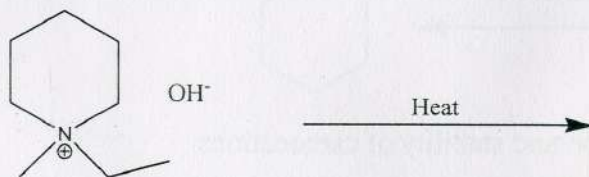
Answer all questions. Each question carries 1weightage

1. Complete the following reaction

NBS / Heat

2. What are the products obtained in the following reactions

(i) Br_2 / $FeBr_3$

(ii) Br_2 / CH_3COOH

3. Rate of S_N^2 reactions will be faster in polar aprotic solvents than in polar protic solvents. Explain why?

4. Complete the following reaction. Explain the mechanism

OH⁻   Heat

5. Methyl magnesium bromide reacts with C_4H_8O in anhydrous ether medium to form an addition product which on hydrolysis gave 3-methyl-2-butanol. Deduce the structure of C_4H_8O.

6. Explain Cope rearrangement with an example.

7. Give an example for Norrish type I cleavage.

8. Discuss the mechanism of B_{AC}^2 mechanism for the saponification .

9. What is Herzig Mayer method? What is its use?

10. Explain the mechanism of the following conversion.
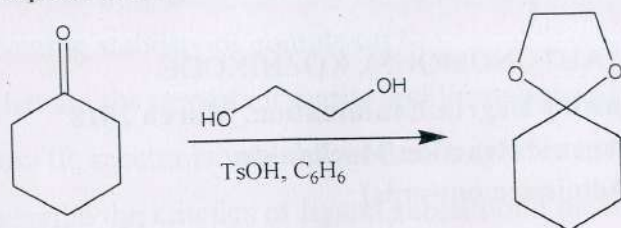
11. State and illustrate the Bredt's rule with an example.

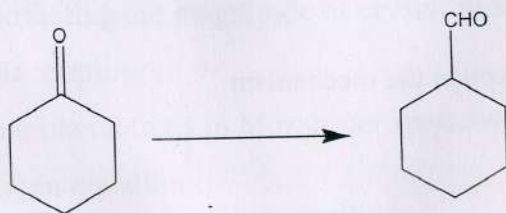12. What is the major product formed in the following reaction and explain the mechanism.
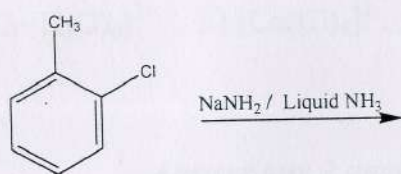

(12 x 1= 12 weightage)

Section B
Answer any 8 questions.   Each question carries 2 weightage

13. Discuss the conversion of cholesterol into testosterone.

14. Explain the mechanism of di-π-methane rearrangement.

15. Explain the Woodward Hofmann selection rules for electrocyclic and cycloaddition reactions.

16. Suggest how the following conversion can be done.

17. Write a note on generation and stability of carbocations.

18. What are the major products in the following reactions and explain the mechanism of their formation
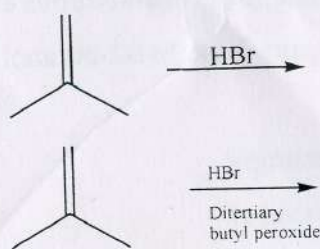
19. Explain Reformatsky reaction . Discuss the mechanism and synthetic applications.

20. Discuss the stereochemistry of Diels Alder reaction . What are the products in the following reactions and predict their optical activity.
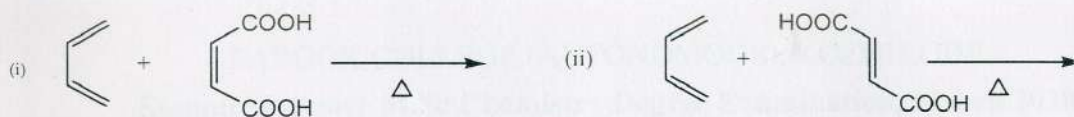
21. Explain the Jablonski diagram.

22. What are flavones and isoflavones? Outline any one method of synthesis of flavones.

23. (a) What are singlet and triplet carbenes?

    (b) What are the factors that stabilises carbanions?

24. Discuss the stereochemistry of S_N^1 and S_N^2 reactions with specific examples.

$$(8 \times 2 = 16 \text{ weightage})$$

Section C
Answer any 2 questions.   Each question carries 4 weightage

25. Explain the total synthesis of cephalosporin.

26. Discuss the mechanism and applications of Knoevenegal condensation, Wittig reaction Dieckmann condensation and Barton's reaction.

27. (i) Discuss the addition – elimination mechanism of aromatic nucleophilic substitution reactions given by haloarenes.

    (ii) Discuss the mechanism of photo-Fries rearrangement.

28. (i) Explain the mechanism of esterification of mesitoic acid.

    (ii)Discuss the chemical classification of alkaloids based on the ring structure.

    (iii)Discuss the general methods of isolation of terpenoids.

    (iv) Illustrate Oppenauer oxidation and MPV reduction with suitable examples.

$$(2 \times 4 = 8 \text{ weightage})$$

8

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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

Second Semester M.Sc Chemistry Degree Examination, March 2018

MCHE2B08 – Electrochemistry , Solid State Chemistry & Statistical Thermodynamics

(2017 Admission onwards)

Max. Time: 3 hours   Max. Weightage : 36

Section A
Answer all questions. Each carries 1 weightage

1. What is Partition function?.

2. Explain 'Ensemble'

3. Define Fermi Energy.

4. Give limitations of Einsein theory of heat capacity of solids

5. Explain potential of an electrode

6. What is distinguishing feature of a fuel cell?

7. Describe the phenomenon of polarization in cells.

8. Describe Tafel Equation.

9. Define centre of inversion.

10. What is Bravais Lattice?

11. What is Meissner Effect?

12. What do you know about paramagnetism?

(12 x 1 = 12 weightage)

Answer any 8 questions. Each question carries 2 weightage

13. Write a note on 'overpotential'

14. Describe Nerst Equation and explain the terms.

15. Explain Half Wave Potential.

16. Briefly describe decomposition potential.

17. What are a)Glide Plane and b)Screw Axis in crystals?

18. Draw stereographic projection of a crystal with C_3, σ_h and S_6

19. Write a brief note on 'colour centre'

20. Distinguish between fluorescence and phosphorescence.

21. What are the distinct features of Bose-Einsein Statistics?

22. Calculate the rotational partition function of hydrogen gas at 30^0C.

23. Write down the Sackur-Tetrode Equation and explain the terms.

24. Bring out the relationship between partition function and Gibbs Free energy.

$(8 \times 2 = 16$ weighta)

Section C
Answer any 2 questions. Each question carries 4 weightage

25. Explain superconductivity and its applications.

26. a)How would you classify solids on the basis of electrical properties .

    b)Write a short note on polarography.

27 .Discuss Bose –Einstein condensation.

28 .Briefly explain electrochemical series and its applications.

$(2 \times 4 = 8$ weighta)