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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Chemistry Degree Examination, November 2019

MCH1C04– Thermodynamics, Kinetic & Catalysis

(2019 Admission onwards)

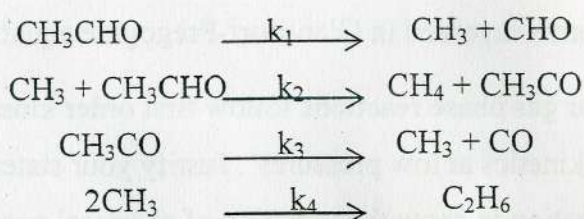Time: 3 hours   Max. Weightage : 30

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

1. Explain the terms involved in Glansdorf-Pregogine equation.

2. "Unimolecular gas phase reactions follow first order kinetics at high pressures and second order kinetics at low pressures'. Justify your statement.

3. Derive an equation to show the variation of chemical potential with pressure.

4. Using Third law of thermodynamics, show that absolute zero of temperature is un attainable.

5. Show that Freundlich adsorption isotherm is a special case of Langmuir adsorption isotherm.

6. Define Partial molar volume. How does it differ from molar volume?

7. What is meant by residual entropy? Calculate the residual entropy of H_2O molecule.

8. On raising the temperature from 27 °C to 37 °C, the rate of a reaction is doubled. Calculate the activation energy of the reaction.

9. Differentiate between attractive and repulsive surfaces by constructing its potential energy surface.

10. What is meant by excess enthalpy?

11. Explain autocatalysis with an example.

12. Write the Wynne-Jones-Eyring equation and explain its significance.

$$(8 \times 1 = 8 \text{ weightage})$$

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

13. Define phenomenological coefficient. Show that direct coefficients always dominate cross coefficients using thermo-osmosis.

14. Explain any two methods for the preparation of zeolites.

15. Explain Langmuir-Hinshelwood mechanism of the bimolecular surface reaction.

16. Explain the primary and secondary salt effects.

17. An organic decomposition reaction takes place with the following mechanism. Derive the rate-law, calculate the chain length and activation energy of the overall reaction:

$$CH_3CHO \xrightarrow{\ k_1\ } CH_3 + CHO$$
$$CH_3 + CH_3CHO \xrightarrow{\ k_2\ } CH_4 + CH_3CO$$
$$CH_3CO \xrightarrow{\ k_3\ } CH_3 + CO$$
$$2CH_3 \xrightarrow{\ k_4\ } C_2H_6$$

18. Derive Duhem-Margules equation and explain whether the equation is applicable to both ideal and non-ideal systems.

19. What is meant by surface acidity? Explain the TPD method of determination.

(4 x 3 = 12 weightage)

Section C Essay
Answer 2 Questions out of 4.
Each question carries a weightage of 5

20. Derive Michaelis-Menten equation for an enzyme catalysed reaction.

21. Derive BET equation and explain its application in calculating surface area of solids.

22. What are the drawbacks of Lindemann's theory of unimolecular reactions? How is it modified by Hinshelwood? Discuss.

23. Explain the deviations from ideal behaviour in solutions. Deduce the laws of Raoults' ebullioscopy and cryoscopy.

(2 x 5 = 10 weightage)

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Name: ....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Chemistry Degree Examination, November 2019

### MCH1C03– Structure & Reactivity of Organic Compounds

(2019 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

1. Among [18] and [10] annulenes, which one is more aromatic and why?

2. Salicylic acid is 17 times and 2,6-dihydroxy benzoic acid is 800 times stronger acid than benzoic acid. Comment on this.

3. Discuss the importance of Marcus equation.

4. Between compound I and II which would undergo solvolysis faster. Give reason?
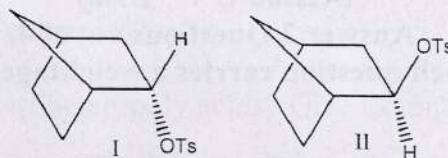
5. Draw the stable conformation of cis and trans-4-t-butylcyclohexane carboxylic acid. Which one is the stronger acid? Why?

6. Identify the isomer of 1,3-dichlorocyclohexane which gives 1,3-cyclohexadiene readily.

7. Among cis and trans isomers of 4-t-butyl cyclohexyl to sylates which will undergo E_2 reaction faster? Why?

8. Draw the structure of the isomers of benzaldehyde oxime. What happens when these compounds are treated with H^+ ions.

9. Define prochiral center. Identify prochiral hydrogens in ethanol.

10. Give an asymmetric Diels Alder reaction where chiral auxiliary have been employed.

11. What is CBS reagent. Cite an example for asymmetric reduction reaction using chiral CBS reagent?

12. Draw the structure of 3-methylhexa-2E,4Z-diene

(8 x 1 = 8 weightage)

Section B Short Essay

Answer 4 Questions out of 7.
Each question carries a weightage of 3

13. The pKa_1 of maleic acid is smaller than that of fumaric acid, whereas the pKa_2 of fumaric acid is smaller than that of maleic acid. Account for this observation.

14. Discuss the optical isomerism exhibited by isomeric 1,2, 1,3 and 1,4 dimethyl cyclohexanes.

15. 2,3-Dibromobutane has both meso and chiral diastereomers. When the meso/chiral diastereomers were boiled in acetone with KI yield different products. Which process is faster and why?

16. Discuss Curtin Hammet principle in detail.

17. Describe the substitution pattern required for allenes to be chiral. How can such chiral allenes be assigned R/S nomenclature.

18. Discuss the Cram's rule and Felkin Anh modification with suitable examples.

19. Explain asymmetric hydroboration reaction by IPC_2BH and $IPCBH_2$.

(4 x 3 = 12 weightage)

Section C   Essay
Answer 2 Questions out of 4.
Each question carries a weightage of 5

20. (a) Describe the Hammett equation and the importance of Hammett parameters σ, ρ

    (b) Discuss the aromaticity of annulenes with examples.

21. (a) Compare the rate of esterification of axial, equatorial carboxyl groups and hydrolysis of corresponding esters.

    (b) Discuss the atropisomerism in biphenyls.

22. (a) Explain the stereochemistry of aldoximes and ketoximes in detail.

    (b) Discuss the Effect of conformation on oxidation of axial and equatorial hydroxyl group to ketones by chromic acid.

23. Explain

    (a) Stereochemistry of Sharpless asymmetric epoxidation.

    (b) Diastereoselective asymmetric aldol reaction and its explanation by Zimmermann Traxler model.

(2 x 5 = 10 weightage)

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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE
First Semester M.Sc Chemistry Degree Examination, November 2019
MCH1C02–Chemistry of Elements
(2019 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

1. Explain Bronsted-Lowry concept of acids and bases

2. Calculate the styx number of $B_{10}H_{14}$.

3. Write general formula for closo, nido and arachno boranes.

4. What are borazines?

5. What are zeolites? Give examples?

6. What are different types of heteropoly acids? Give examples for each?

7. Identify the structural difference between and α-and β-P_4S_4

8. Discuss Bethe's notation of nuclear process?

9. What are super heavy elements?

10. Explain radiolysis of water?

11. Explain lithography in nanotechnology?

12. What is DLS?

                                                    (8 x 1 = 8 weightage)

Section B Short Essay
Answer 4 Questions out of 7.
Each question carries a weightage of 3

13. Illustrate the use of NH_3 as a non-aqueous solvent.

14. Give an account of classification of carbides?

15. Write briefly on metalloboranes with suitable examples?

16. Give two methods of preparation of triphosphonitrilic chloride. How does it react with NH_3 and Grignard reagent?

17. Compare magnetic and spectral properties of lanthanide and actinides.

18. Discuss the characteristics of Frost diagram using examples?

19. Explain characterisation of nano materials by using electron microscopic methods?

(4 x 3 = 12 weightage)

Section B Essay
Answer 2 Questions out of 4.
Each question carries a weightage of 5

20. Discuss reactions taking place in Liquid SO_2. What are the advantages and disadvantages of using liquid SO_2 as a non-aquous solvents?

21. What are carboranes? How is 1,2-dicarba-closo-dodecacarborane is prepared? Write a note on its isomerism? Comment on acidity of different types of hydrogen atoms present in this compounds?

22. Write a note on

    a) Neutron activation analysis

    b) Detection and measurement of radiation in nuclear chemistry

23. Explain the various methods for synthesis of nano materials?

(2 x 5 = 10 weightage)

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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Chemistry Degree Examination, November 2019

MCH1C01– Quantum Mechanics & Computational Chemistry

(2019 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

1. What is mean by conservative system? Give one example.

2. Show that two functions $\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}\right)x$ and $\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}\right)x$ of particle in one dimenional box are orthogonal.

3. Rationalise Heisenberg uncertainty principle using the operators of $\hat{P}x$ and $\hat{x}$

4. What is mean by tunnelling? Give one application of tunnelling.

5. What are polar plots? Write expression for angular function needed to plot dz^2.

6. Calculate the average value of position of electron in 1s orbital if the normalized wave function for Is orbital is $\frac{1}{\sqrt{\pi}}e^{-r}$ (in atomic units)

7. What are ladder operators? Give their significance.

8. Define Fock operator. Explain the terms.

9. What is mean by Slater determinant? Write Slater determinant for ground state Li atom

10. What are the advantages of ab initio method?

11. Explain the term electron correlation.

12. Explain pople style basis set with one example.

(8 x 1 = 8 weightage)

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

13. Define Hermition property of operators. Show that kinetic energy operator is Hermition

14. How many degenerate states are possible for a particle in a cubical box with energy $\frac{9h^2}{8ma^2}$. Explain the lifting of degeneracy in cubical box.

15. Evaluate the commutators   a) $[\hat{L}^2, \hat{L}_z]$ b) $[\hat{L}^2, \hat{L}_+]$

16. Write Rodrigues formula for Associated Laguerre polynomial and evaluate $R_{1,0}$.

17. Derive expression for first order perturbation in energy. Calculate first order perturbation in energy for a particle in a box of slanted bottom.

18. Distinguish between STO and GTO. What are the advantages of GTO?

19. Explain how we can use Molecular Mechanics model for the optimization of geometry of molecules.

<div align="right">(4 x 3 = 12 weightage)</div>

Section C (Essay)
Answer 2 Questions out of 4.
Each question carries a weightage of 5

20. Express Schrödinger equation for hydrogen atom in spherical polar coordinates. Separate in to R, Θ, and Φ equation and solve the Θ equation.

21. Apply Schrödinger wave equation for simple harmonic oscillator. Find eigen functions and eigen values.

22. State variation theorem. Give proof. Apply variation principle to ground state Helium atom.

23. a) Construct Z-matrix for H_2O and methanol

    b) What are the shortcomings of minimal basis set and explain how these shortcomings are addressed in expansion of basis sets.

<div align="right">(2 x 5 = 10 weightage)</div>