FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2021

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 are conservative and non-conservative systems? Give examples.

2. Calculate the normalization constants for the given functions in the interval x = -a to x = +a

    (i) $\psi_1(x) = N_1(a^2-x^2)$

    (ii) $\psi_2(x) = N_2x(a^2-x^2)$

3. Explain the Born interpretation of wave function.

4. Based on the plot of vibrational wave funtion at v = 0, explain quantum mechanical tunnelling.

5. Express $\hat{L}x$, $\hat{L}y$ and $\hat{L}z$ in cartesian and spherical polar co-ordinates.

6. Write a note on the postulate of spin by Uhlenbeck and Goudsmith.

7. Illustrate perturbation method by application to particle in 1D- box with slanted bottom.

8. Illustrate Pauli's antisymmetry principle using the Slater determinant for the ground state of He atom.

9. Explain the term force field. Give two examples.

10. What is meant by electron correlation?

11. Write the Schrodinger equation for H atom and separate Φ equation.

12. What is meant by self –consistent field method?

(**8 x 1 = 8 weightage**)

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

13. Set up Schrodinger equation and solve it for particle in a 1-D box with one finite potential wall.

14. Evaluate the Hermite polynomial $H_1(x)$ and obtain the normalized vibrational wave function $\Psi_1(x)$.

15. Evaluate the commutators (i) $[L_x, L_y]$, and (ii) $[L_+, L_z]$.

16. Explain Zeeman effect. How does it originate?

17. What is meant by perturbation method? Obtain the expression to calculate first order correction to energy.

18. Give an account of Slater type orbitals and Gaussian type orbitals.

19. Explain the basic concepts of ab initio and semi empirical methods with suitable examples

(4 x 3 = 12 weightage)

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

20. (a) Discuss the postulates of Quantum Mechanics.

    (b) Prove that eigen function of a Hermitian operator corresponding to different eigen values are orthogonal.

21. Explain variation theorem with proof. Apply variation method to He atom in the ground state.

22. Write the Schrodinger equation for Hydrogen atom in spherical polar coordinates. Separate the variables and solve the radial part of the wave function. Also get the expression for energy.

23. (a) Explain the classification of basis sets.

    (b) Write Gaussian input file for the geometry optimization of water at HF/6-31G(d,p) level of theory (Use z-matrix of H_2O).

(2 x 5 = 10 weightage)

1M1N21024

(Pages : 2)

Reg. No:..........................

Name: ....

Time: 3 hours

Max. Weightage : 30

Section A Short Answer
Answer any 8 questions
Each question carries a weightage of 1

1. What are Super acids? Give one example.

2. Give one example for photo nuclear reactions.

3. What is Nanolithography?

4. What are interstitial Carbides? Give example.

5. Which allotropic form of phosphorous is an insulator?

6. Compare and contrast the chemistry of borazine with benzene derivatives.

7. Polythiazyl behaves as a one dimensional metal. Explain

8. What are the different types of heteropolyacids? Give example for each.

9. What are Pourbaix diagrams?

10. Explain Usanovich concept of acids and bases.

11. Compare the magnetic and spectral properties of lanthanides and actinides.

12. What are zeolites?

(8 x 1 = 8 weightage)

Section B Short Essay
Answer any four questions
Each question carries a weightage of 3

13. Discuss the characteristics of Latimer diagram using an example.

14. Explain any three methods for the synthesis of nanomaterials?

15. Give an account of preparation, properties and structure of $(PNCl_2)_3$.

16. What is meant by 'styx' numbers? Explain with two examples.

17. Write a note on different types of silicates.

18. Explain the diagonal relationship of first and second group of elements.

19. Write a note on graphenes.

(4 x 3 = 12 weightage)

Section C Essay
Answer any two questions
Each question carries a weightage of 5

20. (a) Explain any one method used for the characterisation of nanomaterials.

    (b) Write a note on Dynamic light scattering (DLS) technique.

21. Discuss the synthesis, structure and bonding of S-N compounds.

22. (a) Discuss the Liquid drop model of nucleus.

    (b) Give a note on neutron activation analysis.

23. Discuss reactions taking place in liquid SO_2. What are the advantages and disadvantages of using liquid SO_2 as non-aqueous solvents?

(2 x 5 = 10 weightage)

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2021

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. How will you account the stability of ninhydrin molecule which is having a carbon bearing two OH groups.

2. Why resonance stabilization energy of phenanthrene (92 Kcal/mole) is higher than anthracene (84 Kcal/mole). Give suitable explanation for this difference.

3. The Hammet acidity function of conc H_2SO_4 is (-)12. What are the informations that you can obtain from this value.

4. Discuss the importance of Bell Evans Polanyi principle.

5. Draw the most stable conformers of the following molecules and explain the reason for their stability (a) 1,2-dibromo cyclohexane (b) 1,3-dihydroxy cyclohexane.

6. Which one of the two compounds, trans-1-chloro-4-methyl cyclohexane or cis-1-t-butyl-4-fluoro cyclohexane would be more likely undergo conformational transformations. Explain why?

7. Among the stable conformers of cis and trans-4-t-butyl cyclohexanols which will react faster with (a) CrO_3/Pyridine (b)Acetic anhydride/pyridine

8. Whether cis-1-chloro-2-methyl cyclohexane is optically active or inactive. Give suitable reasonfor your finding.

9. Draw the structures of R and S isomers of 6,2'-diiodo biphenyl-2-carboxylic acid.

10. What will be the product formed when S-2-bromo butane is reacted with aqueous KOH. Write the stereochemical structure of the product and assign its configuration.

11.
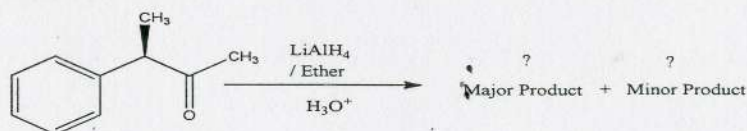
Write the stereo selectivity of above reaction using Felkin-Ahn model.

12. Discuss the importance of CBS reagent in asymmetric reduction reaction citing a suitable example.

(8 x 1 = 8 weightage)

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

13. (a) Discuss the structure and bonding in electron donor-acceptor complexes and explain why these compounds are highly coloured. (2 weightage)

    (b) Discuss the criteria for aromaticity and antiaromaticity with suitable Illustrations. (1 weightage)

14. (a) Differentiate kinetically and thermodynamically controlled reactions with the help of hydrobromination reaction of 1,3-Butadiene. (2 weightage)

    (b) Discuss Neighbouring group participation with the participation of carboxylate ion and hydroxyl group. (1 weightage)

15. (a) Discuss the different factors affecting the conformational stability of molecules citing different examples. (1 weightage)

    (b) Explain conformational preferences of 2-bromo cyclohexanone and cis&trans isomers of 2,6-dibromocyclohexanones. (2 weightage)

16. (a) Compare the rate of esterification in menthol, neoisomenthol, neomenthol and isomenthol with suitable explanation. (2 weightage)

    (b) Discuss the stereochemistry of decalins. (1 weightage)

17. (a) Explain the condition for rotation restriction and optical activity in biphenyls using different examples. (2 weightage)

    (b) Illustrate stereomutation of geometrical isomers taking a specific example. (1 weightage)

18. (a) Describe the substitution pattern required for allenes to be chiral. How can such chiralallenebe assigned for R/S nomenclature (2 weightage)

    (b) Hexahelicene and transcyclooctene, both are optically active despite the fact that they do not possess chiral carbons. Why? (1 weightage)

19. (a) Explain the importance of chiral auxiliaries in asymmetricα alkylation of enolates. (1 weightage)

    (b) Discuss the stereochemistry of Sharpless asymmetric epoxidation. (2 weightage)

(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 with the importance of Hammett parameters σ, ρ in understanding reaction mechanisms. Explain why Hammett equation is a lenear free energy relationship.   (3 weightage)

(b) Discuss the effect of inter and intramolecular hydrogen bonding on boiling point, acidity, basicity using appropriate examples.   (2 weightage)

21. (a) What are conformationally biased systems? Illustrate with examples that, how these systems are useful in understanding the reactivity of axial and equatorial groups.   (3 weightage)

(b) Discuss the conformational aspects of semipinacolic deamination of erythro and threo1,2-diphenyl-1-(p-chlorophenyl)-2-aminoethanol.   (2 weightage)

22. (a) Explain three different resolution methods by which resolution of racemates can be achieved efficiently.   (3 weightage)

(b) Explain the chirality due to folding of helical structures with example.(2 weightage)

23. Explain (a) Chiral pool synthesis of beetle pheromone component S(-)ipsenol from S(-)leucine.   (2 weightage)

(b)Diastereoselective asymmetric aldol reaction and its explanation by Zimmermann Traxler model.   (3 weightage)

(2 x 5 = 10 weightage)

1M1N21026   (Pages : 2)   Reg. No:.........................

Name: ....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2021

MCH1C04– Thermodynamics, Kinetics & 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. What is the significance of third law of thermodynamics?

2. Explain the term entropy production with examples.

3. What is meant by phenomenological relations?

4. State and explain steady state approximation.

5. Explain the term 'explosion limits' in branching chain reactions.

6. Distinguish between diffusion controlled and activation controlled reactions.

7. What is meant by partial molar property?

8. Explain the term 'reaction coordinate'.

9. Spontaneous adsorption is always exothermic. Justify your answer.

10. What is Michaeli's menton constant? Write its significance.

11. Define isosteric heat of adsorption.

12. Write a note on residual entropy.

(8 x 1 = 8 weightage)

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

13. Define excess thermodynamic function. Describe one method to determine excess Gibbs free energy.

14. Derive Duhem-Margules equation and mention its application.

15. Write a note on sol-gel method for the preparation of catalysts.

16. Write BET adsorption isotherm. Show that it is appropriate to Langmuir adsorption isotherm under limiting cases.

17. How would you determine surface acidity using TPD method?

18. Write the principle of crossed molecular beams.

19. What are the assumptions of Absolute reaction rate theory?

(4 x 3 = 12 weightage)

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

20. How will you study the kinetics of fast reactions?

21. Define Electro kinetic phenomena. How would you rationalize electro-kinetic properties using irreversible thermodynamics?

22. (a) Using one of the models, discuss oscillating chemical reactions.

    (b) Discuss the surface area determination using BET method.

23. Comment on Langmuir Hinshelwood mechanism and Eley Reidel mechanism for bimolecular reactions.

(2 x 5 = 10 weightage)