M1N17297   (Pages : 2)   Reg. No:...........................

Name: ....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2017

MCHE1B01 – Quantum Chemistry & Group Theory

(2017 Admission onwards)

Max. Time: 3 hours   Max. Weightage: 36

SECTION A

Answer *all* questions

Each question carries a weightage of 1

1. Define well behaved wave function.

2. β-carotene has maximum absorption length at 480 nm. If this transition corresponds to an n=11 to n=12 transition of an electron in a particle in a box system, what is the approximate length of β-carotene?

3. Demonstrate that for the 1-D particle in a box, $\Psi 1$ is orthogonal to $\Psi 2$.

4. Explain Zeeman effect.

5. Differentiate between a spin orbital and atomic orbital.

6. Evaluate the commutator $[\hat{P}_x, \hat{X}]$.

7. Express $\hat{L}z$ in cartesian and spherical polar co-ordinates.

8. What is radial probability distribution function?

9. Explain the degeneracy of principal quantum number.

10. Using the method of similarity transformation, deduce conjugates of C_3^1 and C_3^2 in C_{3v} point group.

11. Find out the point group of   a) H_3BO_3 b) cyclohexane (chair)

12. Generate matrices for C_6 and S_6.

(12 x 1= 12 weightage)

13. Write Rodrigues formula to obtain Lagurrea polynomial and calculate $R_{1,0}$.

14. Prove that Eigen values of hermitian operators are real and corresponding to tw

    different eigen values.

15. Write the Schrodinger equation for H atom in spherical polar coordinates and obtai

    Phi equation.

16. Evaluate a) $[\hat{L}_+, \hat{L}_z]$ and b) $[\hat{L}^2, \hat{L}_+]$.

17. Solve the Schrodinger equation for particle in a 3-D box and obtain the normalize

    eigen functions.

18. Calculate the expectation value of energy of particle on a planar rigid rotor.

19. Explain the postulate of spin by Uhlenbeck and Goudsmith and discuss spac

    quantisation of spin angular momentum.

20. Prove that 'All cyclic groups are Abelian but all Abelian groups are not cyclic'.

21. State "Great orthogonality theorem". What are the consequence of the theorem?

22. Set up the group multiplication table of C_{2h} point group.

23. What is a class? Discuss the properties of a class.

24. Explain representation of groups using C_{2v} point group.

(8 x 2= 16 weightag

SECTION C
Answer *any two* questions
Each question carries a weightage of 4

25. Apply Schrodinger equation for simple harmonic oscillator. Draw vibrational energ

    level diagram.

26. Derive C_{3v} character table Using Great Orthogonality Theorem.

27. Set up the Schrodinger equation for non-planar rigid rotor in spherical pol

    coordinates. Solve the theta part of the wave function and calculate Y_1^0.

28. Discuss the postulates of quantum mechanics. Find the eigen value and eigen functi

    of a linear momentum operator.

(2 x4 = 8 weightag

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2017

MCHE1B02 – Chemistry of Elements

(2017 Admission onwards)

x. Time: 3 hours   Max. Weightage: 36

Section A
Answer *all* questions.
Each question carries 1 weightage.

1. Name two molecules which are isoelectronic with NO_2^+ ion.

2. State electro neutrality principle. Suggest any one application.

3. Which is a better Lewis acid, BCl_3 or $B(CH_3)_3$. Explain.

4. What are 'super acids'? Give one example.

5. Brief out the allotropes of phosphorus. Which allotropic form is conducting?

6. What happens when 1, 2-dicarba-closo-dodecaborane (12) is heated?

7. What are zeolites? Mention any one synthetic application.

8. What are ultramarines? Give one example.

9. What are Pourbaux diagrams? Mention their uses.

10. The electronic spectra of most of the lanthanides are 'line like'. Why?

11. What are magic numbers?

12. Give one example for thermonuclear reactions.

(12x1=12 Weightage)

Section B
Answer any *eight* questions.
Each question carries 2 Weightage.

13. What is Walsh diagram? Discuss briefly its applications.

14. What is Bent rule of hybridization? Explain.

15. Write down Drago-Wayland equation and explain the terms. What is the importance of this equation?

16. Describe the non-aqueous chemistry of liquid SO_2.

17. What are Styx numbers? Give the structure of $B_{10}H_{14}$ and discuss the bonds present in it.

18. What is diagonal relationship? Explain with suitable examples.

19. What are silicones? How are they prepared?

20. How is S_2N_2 prepared? Depict its structure and mention one application.

21. The addition of phosphate to ammonium heptamolybdate forms a blue coloration. Discuss briefly the chemistry of this reaction.

22. What is Ellingham diagram? Discuss briefly any two applications.

23. Explain the Bethe's notation of nuclear process with example.

24. Briefly discuss the theory of nuclear fission.

<div align="right">(8x2 = 16 Weightage)</div>

Section C
Answer any *two* questions.
Each question carries 4 Weightage.

25. a) What is hydrogen bond? Discuss briefly the consequences of hydrogen bonding in molecules.

    b) How will you determine the structure of molecules by X-ray diffraction method?

26. Discuss the HSAB principle of acids and bases. What are the applications of HSAB concept?

27. a) What are super heavy elements? How are they prepared?

    b) Give the principles of neutron activation analysis.

28. Explain the various methods used for the detection and measurement of radiation.

<div align="right">(2x4=8 weightage)</div>

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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2017

MCHE1B03 – Structure & Reactivity of Organic Compounds
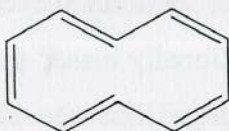
(2017 Admission onwards)

Max. Time: 3 hours   Max. Weightage: 36

Section A

(Answer all questions. Each question has 1 weightage)

1. 2-Hydroxybenzoic acid exist as a monomer whereas benzoic acid as dimer in nonpolar solvents. Why?

2. Whether the following compound is aromatic or antiaromatic? Justify your answer?

3. Explain the difference between kinetic and thermodynamic control of organic reactions?

4. What are the isotopes available for hydrogen, which can be used in mechanistic studies?

5. How can cis-4-t-butylcyclohexanol be converted to trans-4-t-butylcyclohexyl chloride?

6. Draw the most stable conformer of cis-1,3-dihydroxycyclohexane. Explain why this is more stable than the other conformations?

7. Illustrate how the HCl elimination reaction of menthyl and neomenthyl chlorides differ and why?

8. One isomer of hexachlorocyclohexane do not undergo dehydrochlorination. Draw the structure of that isomer and give reason why it is not?

9. An optically active alcohol $C_6H_{10}O$ on hydrogenation absorbs 1 mol of H_2 and becomes optically inactive. Identify the structure of alcohol?

10. Draw the structures of the following molecules.

    (a) R,R-2,3,4-trihydroxybutanal

    (b) 3-methylhexa-2E,4Z-diene.

11. Are the following molecules capable of being resolved in to optical isomers? Give reason.

    (a) Methyl-p-tolylsulfoxide   (b) N-methyl-N-ethylaniline

12. Discuss prelogs rule with suitable example?

(12x1= 12 weightage)

Section B

(Answer any 8 questions. Each question carries 2 weightage)

13. What is Huckels rule of aromaticity? Explain it on the basis of the energy levels of molecular orbitals. Comment on the structure of cyclooctatetraene.

14. 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?

15. Discuss the kinetics and stereochemistry of substitutions involving neighbouring group participation.

16. With the help of suitable example, explain the application of isotope effect in the determination of reaction mechanisms.

17. Explain the conformational aspects of substituted cyclohexanones.

18. Explain the importance of conformationally biased systems in understanding the reactivity of axial and equatorial groups. Illustrate with proper reactions and examples.

19. Draw the structure of R-2-phenylpropionaldehyde and predict the structure of the major product that would arise from it by reaction with MeMgBr and hydrolysis using crams rule.

20. The dehydrobromination of meso and racemic-1,2-dibromo-1,2-diphenylethane gives stereospecifically different products. Account this observation.

21. What are enantiotopic, homotopic and diastereotopic protons? Discuss with specific examples.

22. Discuss the optical activity in allenes. Also explain the steps involved in the assignment of R and S configurational nomenclature of allenes.

23. What is the importance of chiral pool in asymetric synthesis? Write down the chiral pool synthesis of beetle pheromone component (S)- (-) ipsenol from (S)-(-)-leucine.

24. Discuss asymmetric hydroboration with di isopinocamphenylboranes.

(8x2 = 16 weighta

Section C

(Answer any 2 questions. Each question carries 4 weightage)

(a) Discuss how Taft equation attempts to describe the polar and steric effects in organic reactions.

(b) Briefly discuss the importance of Hammett parameters.

Explain

(a) The conformational isomerism in cis and trans isomers of 1,2- 1,3 and 1,4-dimethylcyclohexanes and compare their stabilities

(b) Relative rate of esterification of cis and trans-4-t-butylcyclohexane carboxylic acids. Show which one is stronger acid?

(a) Discuss the methods by which configuration of geometrical isomers are determined.

(b) Discuss about the term conformation and intramolecular hydrogen bonding with suitable example.

What are chiral auxiliaries? What are the criteria for selection of an efficient chiral auxiliary? Discuss the importance of camphor derivatives as chiral auxilieries in Diels Alder reaction?

(2x4= 8 weightage)

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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2017

MCHE1B04 – Thermodynamic Kinetics & Catalysis

(2017 Admission onwards)

Time: 3 hours   Max. Weightage: 36

Section A

Answer all questions. Each question carries 1 Weightage.

1. Define Fugacity. What is its physical significance?

2. State and Explain third law of thermodynamics.

3. Define Force and Flux with reference to irreversible process.

4. What are coupled reactions? Explain.

5. Explain the origin of secondary salt effects.

6. Calculate the relaxation time of the following type of reversible reaction if rate constant (k) of the forward reaction is $10^8 \, s^{-1}$ and that of the backward reaction (k_{-1}) is $10^6 \, s^{-1}$.

$$A \underset{k_{-1}}{\overset{k}{\rightleftharpoons}} B$$
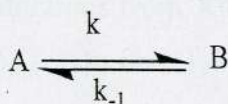
7. Distinguish between collision cross section and reaction cross section.

8. Write London equation for a triatomic molecule. Explain the terms.

9. Distinguish between general acid and specific H^+ ion catalysis.

10. Explain autocatalytic process with one example.

11. Define isosteric heat of adsorption.

12. "Unimolecular gas phase reactions follow first order kinetics at high pressure and second order kinetics at low pressure". Justify.

(12 x1 = 12 Weightage)

Section B
Answer any eight questions. Each question carries 2 Weightage.

13. Explain the variation of chemical potential with temperature and pressure.

14. Derive Duhem-Margules Equation.

15. Explain thermo-osmosis and thermo molecular pressure difference.

16. Define phenomenological coefficients. Show that direct coefficients always dominate over indirect coefficients.

17. What are the factors affecting kinetics of reaction in solution?

18. Derive expressions for kinetic chain length and activation energy of the decomposition of acetaldehyde.

19. What is mean by Potential Energy Surface? Distinguish between attractive and repulsive Potential Energy Surfaces.

20. A first order reaction has a frequency factor of 10^{15} s^{-1}. Calculate the entropy of activation at 500K.

21. Derive expression for Langmuir adsorption isotherm.

22. Discuss the analysis of solid surface using ESCA.

23. Explain Eley-Rideal mechanism for bimolecular surface reaction.

24. Derive expression for Michaelis-Menten constant in enzyme catalysis.

(8 x2 = 16 Weightage)

Section C
Answer any two questions. Each question carries 4 Weightage

25. Discuss the kinetics of H_2-O_2 reaction and explain the explosion limits.

26. Discuss oscillating chemical reactions using any two models.

27. Derive BET Adsorption isotherm.

28. a) Discuss Absolute Rate Theory and derive expression for rate constant.

    b) Show that for a rigid sphere model of a bimolecular reaction, Absolute Rate Theory agrees with Simple Collision Theory.

(2 x4 = 8 Weightage)