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1N16018 (Pages :2) Reg. No:.....

Name: .....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2016

CH1C01 – Quantum Chemistry & group theory

(2016 Admission onwards)

ıx. Time: 3 hours Max. Weightage: 36

Section A

(Answer all questions, Each question carries a weightage of 1)

Evaluate the expression for the following operators

a) $(x \frac{d}{dx})^2$ b) $(\frac{d}{dx} x)^2$

Show that $[A^2 B] = A [A B] + [A B] A$

Show that the wave function of a particle in a 1-D box is not an eigenfunction of the momentum operator.

Prove that $< A^2 > = (< A >)^2$ where A is the K.E operator for particle in a 1-D box.

Write Rodrigus formula

Differentiate between a spin orbital and an atomic orbital.

Write down the expression for $\hat{L}_z$ in the Cartesian co-ordinates and spherical polar co-ordinates.

Normalize the wave function $e^{im\varphi}$ over the interval $0 \leq \varphi \geq 2\pi$

Find out the point group of a) Ethane (staggered) b) $CH_2=C=C=C=CH_2$ c) Ferrocene (staggered) d) cyclohexane (chair form)

10 By using the 3×3 matrix for C_n and C_n^{-1} prove $C_n \times C_n^{-1} = E$ (identity operation)

11 Explain why conjugate symmetry elements are included in the same class.

12 Explain the different rules of selecting a principle axis of a molecule.

(12 x 1 = 12)

Section B

(Answer any eight questions. Each question carries a weightage of 2)

13 Find out the expression for energy of a two particle rigid rotar using the spherical harmonics wave function.

14 Prove that for two non- interacting particles the total energy is the sum of the two individual energies and the total wave function is the product of two individual wave functions.

15 Write the operator postulate of quantum mechanics. Show that Heisenberg's Uncertainty principle is one of the consequences of the operator postulate of quantum mechanics.

16 The radial part of the 2S orbital wave function is $1/\sqrt{32\pi}$ (2-r) $e^{-r/2}$. Plot the wave function. Find out the value of r corresponding to maxima and minima. Also find out the number of nodes.

17 Prove that the operators $\hat{L}^2$ and $\hat{L}_z$ commute with each other using their expressions in spherical polar co-ordinates.

18 Using the spherical harmonics functions for l=1and m = -1, 0,+1 prove that

$$\sum_{m=-1}^{+1} |Y_l^m(\theta\phi)|^2 = \text{constant}$$

19 Find the most probable position of the ground sate of a particle in a three dimensional box of length a, breadth b, and height c.

20 Show that the four symmetry operations of the C_{2h} point groups forms a mathematical group under multiplication.

21 Using Great Orthogonality theorem prove that the sum of the squares of the characters in any irreducible representation is equal to the order of the group.

22 Using the C_{3v} given below find out E × E and reduce it.

	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

23 Prove by taking suitable example that "All cyclic groups are Abelian but all abelien groups are not cycylic

24 Generate 3 × 3 matrix for all the operations of the C_{2v} point group. Using this result prove that C_2 is its own inverse

(8 x 2 = 16)

Section C

(Answer any two questions. Each question carries a weightage of 4)

25 Apply Schrodinger wave equation for one dimensional harmonic oscillator. Find out the eigenfunctions and eigenvalues.

26 Set up the Schrodinger equation for Hydrogen atom and solve the radial part of the equation to find out the wave function. Also get the expression for the energy.

27 Derive the C_{2v} character table including the IR's for the rotations, translations and the binary products of translational components (x,y,z).

28 a) Define Hermitian operator. Test for the hermiticity of momentum operator in x direction.

b) Prove that, If A and B are two hermitian operators the product AB is hermitian if and only if A and B commute with each other.

(2 x 4 = 8)

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3M1N16019 (Pages : 1) Reg. No:.....

Name: .....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2016

CH1C02 – Chemistry of Elements

(2016 Admission onwards)

Max. Time: 3 hours Max. Weightage: 36

Section A
Answer all questions
Each question carries 1 weightage.

1. What are heteropoly anions? Give examples
2. What is the styx number of B_5H_9 and B_4H_{10}?
3. Explain Symbiosis with an example.
4. What are Super acids? Give two examples.
5. Discuss Wade's Rule for classifying boranes
6. What are isoelectronic molecules? Illustrate with examples.
7. What are Zeolites? Give any two applications.
8. What are allotropes? Give the structure of allotropes of phosphorous.
9. Discuss the structure of diborane.
10. What do you mean by lanthanide contraction? What are its consequences?
11. Briefly explain compound nucleus theory.
12. What is Magic Number? How is it affecting the stability of a nucleus?

(12 × 1 = 12 weightage)

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

13. Discuss the bonding in closoPolyhedral borane anions.
14. Discuss the different types of borides based on their structure with examples.
15. Illustrate the solvent system concept of acids and bases.
16. Discuss the preparation and properties ofcyclophospazenes
17. Explain the different types of reactions of boranes.
18. Explain why Borazine is called inorganic benzene. Give its reactions.
19. Discuss the structure and bonding of S_4N_4.
20. Discuss the applications of the HSAB Principle.
21. Explain hydrogen bond and its consequences.
22. Explain Nuclear activation analysis.
23. What are photonuclear and thermonuclear reactions?
24. Discuss radiolysis of water

(8 × 2 =16 weightage)

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

25. Discuss the principle and operation of Geiger-Mullerand Scintillation counters
26. Discuss liquid ammonia as non-aqueous solvent.
27. Discuss the synthesis, structure and applications of silicones.
28. What are super heavy elements? Discuss their methods of preparation.

(2 × 4 =8 weightage)

1M1N16020 (Pages : 2) Reg. No:.....

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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2016

CH1C03 – Structure & Reactivity of Organic Compounds

(2016 Admission onwards)

Max. Time: 3 hours Max. Weightage: 36

Section A

(Answer all questions. Each question has 1 weightage)

State Hammond postulate.

Identify the most stable conformation of chlorohydrins.

Among menthyl chloride and neomenthyl chloride, which would readily undergo HCl elimination? Why?

Write a brief note on stereochemistry of aldoximes.

State whether Cyclooctatetraene is aromatic or not? Why?

What is froast diagram?

What is ring flip?

Write Felkin-ahn model with an example.

What is homotopic hydrogen atoms? Give example.

0. What is bond angle strain?

1. Discuss the use of L-brucine in resolution.

2. What is racemisation?

(1 x 12 = 12)

Section B

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

3. Discuss the stability of benzylic cations and radicals.

4. Explain the aromaticity of fused ring systems.

5. Explain neighbouring group participation.

6. Discuss the effect of semipinacolic deamination of cis and trans-2-aminocyclohexanols.

7. Predict the different products formed by the dehydration of cis and trans 2-phenylcyclohexanol.

18. Discuss the conformations of alkene dihalides and glycols.

19. Discuss chirality due to folding of helical structures?

20. Write a note on Cahn- Ingold-Prelog rules applied to chiral biphenyls.

21. Discuss chiral pool synthesis of(-)ipsenol from S-(-)-leucine.

22. Explain with appropriate example the use of chiral auxiliaries in asymmetric synthesis.

23. Explain (a) prochiral centre (b) linear free energy relationships.

24. Explain (a) Bredt's rule (b) Pyrolytic elimination of esters with an example.

(8 x 2 = 16)

Section C

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

25. Explain

(a)aromaticity of annulenes (b)homo aromaticity.

26. Write brief note on

(a) Taft equation and its application]

(b) Marcus equation

(c) Isotopic labelling experiment.

27. Discuss

(a)asymmetric reduction using BINAL-H

(b) asymmetric hydroboration using $(IPC)_2BH$ and $IPCBH_2$.

28. Describe

(a) conformations of disubstituted cyclohexane

(b)3^0-butyl cyclohexane

(4 x 2 = 8)

12 ✓

1N16021 (Pages : 2) Reg. No:.....

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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2016

CH1C04 – Thermodynamic Kinetics & Catalysis

(2016 Admission onwards)

ax. Time: 3 hours Max. Weightage: 36

]Section A

(Answer all questions. Each question has 1 weightage)

State and explain Nernst heat theorem.

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

What is meant by residual entropy? Calculate the residual entropy of NO molecule.

Show that $\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P$

Define mean ionic activity coefficient and explain its significance.

"Unimolecular gas phase reaction catalyzed by solid surfaces follow first order kinetics at low pressures and zero order kinetics at high pressures'. Justify your statement.

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

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

Explain the principle of Scanning Electron Microscopy technique.

0. Explain the terms involved in London equation for the activation energy calculation.

1. Distinguish between coupled and non-coupled reactions.

2. What is pressure jump method in relaxation methods?

(12 × 1 = 12 weightage)

Section B

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

13. Explain the Lotka-Volterra and Brusselator mechanism in oscillating chemical reactions.
14. Define phenomenological coefficient. Show that direct coefficients always dominate cross coefficients using thermo-osmosis.
15. Derive an expression for the net branching factor and explain how it influences a branching chain reaction.
16. Explain crossed molecular beam methods employed to monitor the progress of fast reactions.
17. Explain Langmuir-Hinshelwood mechanism of the bimolecular surface reaction.
18. Differentiate between primary and secondary salt effects.
19. Explain the statistical distribution of energy for particle with many degrees of freedom.
20. Explain the concept of attractive and repulsive surfaces by constructing its potential energy surface.
21. 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

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

22. Show that for the rigid sphere model of bimolecular reactions absolute rate theory agrees with simple collision theory.
23. Illustrate the Eley-Rideal mechanism using the reaction $2CO + O_2 \rightarrow 2CO_2$.
24. Derive the Eyring equation?

(8 × 2 = 16 weightage)

Section C

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

25. Using irreversible thermodynamics account for thermal diffusion and thermal osmosis.
26. What are the drawbacks of Lindemann's theory of unimolecular reactions? How is it modified by Hinshelwood? Discuss.
27. Derive BET equation and explain its application in calculating surface area of solids.
28. Explain the Michaelis and Menten theory of the mechanism of enzyme catalysis?

(2 x 4 = 8 weightage