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Reg. No:.....

Name: .....

FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2018

MCHE1B01 – Basic Concepts in Quantum Chemistry & Group Theory

(2016 Admission onwards)

Max. Time: 3 hours

Max. Weightage: 36

**SECTION A**

**Answer all questions**

**Each question carries a Weightage of 1**

1. Explain the Born interpretation of the wave function.
2. Determine the average value of the position of an electron at the lowest energy level in a particle-in-a-box.
3. Determine the uncertainty in position for an electron travelling at  $2 \times 10^6$  m/s with an uncertainty in velocity of 1% of the true value.
4. Examine if  $e^{ikx}$  is an eigen function of momentum operator  $\hat{P}_x$ .
5. Define well behaved wave function.
6. Evaluate the commutator  $[\hat{L}_+, \hat{L}_z]$ .
7. What are Hermitian operators?
8. What are spin orbitals? Write the general form of spin orbitals.
9. Based on the plot of vibrational wave function at  $v = 0$ , explain quantum mechanical tunnelling.
10. Define cyclic groups and abelian groups.
11. Give the point group of i)  $\text{PCl}_3$ , ii) ethylene, iii) allene, iv)  $\text{NH}_3$ .
12. What is meant by reducible representations and irreducible representations of point groups?

(12 x 1 = 12 Weightage)

**SECTION B**

**Answer any eight questions**

**Each question carries a Weightage of 2**

13. Explain space quantisation of orbital and spin angular momentum.
14. Briefly discuss the postulates of quantum mechanics.
15. Distinguish between radial density plots and radial distribution plots.
16. For a particle on a ring, how are the rotational quantum numbers generated?
17. Apply Schrodinger equation for particle in a 1-D box. Obtain the normalized wave function.



18. What are spherical harmonics? Calculate  $Y_0^0$  and  $Y_1^0$ .
19. Show that  $\hat{L}^2$  and Hamiltonian operator of a rigid rotator have the same set of eigen functions.
20. Show that in associated Legendre polynomial,  $|m|$  cannot have values greater than  $l$ .
21. Write the matrix representation for inversion operation and proper rotation.
22. Show that symmetry elements of  $C_{2v}$  point group forms a mathematical group.
23. Set up the group multiplication table for  $C_{3v}$  point group.
24. What is reduction formula? Find out the irreducible representation of  $C_{3v}$  point group using the character table

$C_{3v}$	E	$2C_3$	$3\sigma_v$
$A_1$	1	1	1
$A_2$	1	1	-1
E	2	-1	0

(8 x 2 = 16 Weightage)

### SECTION C

Answer any two questions  
Each question carries a Weightage of 4

25. Discuss the quantum mechanical treatment of simple harmonic oscillation and calculate  $\Psi_0(x)$ .
26. Using Great Orthogonality Theorem derive the  $C_{4v}$  character table.
27. 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.
28. Solve Schrodinger equation for particle on a ring. Calculate the expectation value of energy and angular momentum.

(2 x 4 = 8 Weightage)



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FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE

First Semester M.Sc Degree Examination, November 2018

**MCHE1B02 – Chemistry of Elements**

(2018 Admission onwards)

Max. Time: 3 hours

Max. Weightage: 36

**Section A**

**Answer all questions.**

**Each question carries 1 Weightage.**

1. What are hypervalent molecules? Give two examples.
2. What are Van der Waals forces? Suggest any four Van der Waals forces existing between molecules.
3. Explain Usanovich concept of acids and bases.
4. Would you expect  $\text{HNO}_3$  and  $\text{SbF}_5$  to behave as an acid or base in liquid HF? Explain giving equations.
5. Which has higher electron affinity, C or N? Why?
6. How is diborane converted to borazine?
7. What are molecular sieves?
8. What is polythiazil? How it is prepared?
9. What are the hydrolysis products of uranyl ion in aqueous solutions?
10. What is Latimer diagram? Give any two applications.
11. What is radiation dosimetry?
12. Give one example for thermonuclear reactions.

(12x1=12 Weightage)

**Section B**

**Answer any eight questions.**

**Each question carries 2 Weightage.**

13. Explain electroneutrality principle with suitable examples.
14. Explain briefly the principle for the construction of Walsh diagram. What is the information obtained from these diagrams?
15. State HSAB principle. Give any two applications of HSAB principle.
16. How will you determine the enthalpies of acid-base reactions?
17. State and explain Wade's rule.



18. Explain the structure and bonding in  $B_2H_6$ .
19. What are silicones? How are they synthesised? Give any two uses.
20. State VSEPR theory. Discuss the applications of VSEPR theory with suitable examples.
21. What are super heavy elements? How are they prepared?
22. What is diagonal relationship? Explain with suitable examples.
23. Briefly explain the principles of neutron activation analysis.
24. Discuss the working principle of GM counter.

(8x2 = 16 Weightage)

### Section C

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

25. What is Ellingham diagram? Discuss applications.
26. Discuss the important chemical reactions that can occur in liquid sulphur dioxide. Mention the important advantages of liquid sulphur dioxide as a solvent.
27. Discuss the synthesis, structure and bonding in Phosphorous-Nitrogen and Phosphorous-Sulphur compounds.
28. Write notes on
  - a) Radiolysis of water
  - b) Nuclear models

(2x4=8 Weightage)



FAROOK COLLEGE (AUTONOMOUS), KOZHIKODE  
First Semester M.Sc Degree Examination, November 2018  
MCHE1B04 – Thermodynamic, Kinetics & Catalysis  
(2016 Admission onwards)

Max. Time: 3 hours

Max. Weightage: 36

**Section A****(Answer all questions. Each question has 1 Weightage)**

1. Derive Gibbs-Duhem equation.
2. Derive an equation to show the variation of chemical potential with temperature.
3. Explain the principle of micro reversibility and Onsager reciprocal relations.
4. Differentiate between diffusion controlled and activation controlled reactions.
5. Explain the influence of pressure and solvation on the reaction rate in solution.
6. "Unimolecular gas phase reactions follow first order kinetics at high pressures and second order kinetics at low pressures". Justify your statement.
7. Show that Freundlich adsorption isotherm is a special case of Langmuir adsorption isotherm.
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. Explain the principle of ESCA technique.
10. Explain the terms involved in London equation for the activation energy calculation.
11. Distinguish between coupled and non-coupled reactions.
12. What is the effect of pH and temperature on enzyme catalysis?

**(12 × 1 = 12 Weightage)****Section B****(Answer any 8 questions. Each question carries 2 Weightage)**

13. Explain any two methods for the determination of partial molar quantities.
14. What is meant by excess functions? Explain the expressions for excess functions for free energy, entropy, enthalpy and volume.
15.  $C_v$  for uranium metal is  $3.04 \text{ JK}^{-1}\text{mol}^{-1}$  at 20 K. Calculate the absolute entropy of the metal in  $\text{JK}^{-1}\text{mol}^{-1}$  at 20K.
16. Explain molecular beam and flash photolysis methods employed to monitor the progress of fast reactions.



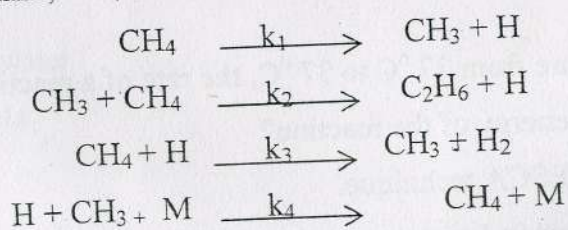
17. Show that absolute rate theory agrees with simple collision theory for atom combination reactions.
18. Differentiate between primary and secondary salt effects.
19. Derive Gibbs'-Duhem- Margules equation.
20. Explain the concept of attractive and repulsive surfaces by constructing its potential energy surface.
21. Explain the effect of temperature and pressure on explosion limits in  $H_2-O_2$  reaction.
22. The adsorption of a gas is described by Langmuir adsorption isotherm with  $K_a = 0.85 \text{ kPa}^{-1}$ . Find the pressure at which the surface coverage is (a) 15% , (b) 95%.
23. Explain general acid and specific acid catalysis with suitable examples.
24. Derive the Eyring equation?

(8 × 2 = 16 Weightage)

### Section C

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

25. (i) Deduce the laws of Raoult's ebullioscopy and cryoscopy.  
 (ii) An aqueous solution of a non-volatile solute boils at  $100.17^\circ\text{C}$ . At what temperature would it freeze? (For water,  $K_b = 0.52 \text{ K kg mol}^{-1}$  and  $K_f = 1.86 \text{ K kg mol}^{-1}$ ).
26. (i) Discuss briefly the Rice-Herzfeld mechanism of organic decomposition reaction.  
 (ii) The following Rice-Herzfeld mechanism has been proposed for the gas phase pyrolysis of methane,  $\text{CH}_4$



Assuming steady state approximation for  $[\text{H}]$  and  $[\text{CH}_3]$ , derive the rate-law for the formation of  $\text{C}_2\text{H}_6$ .

27. (i) Explain the BET theory of adsorption.  
 (ii) Discuss the use of Langmuir and BET isotherms for surface area determination.
28. Explain the Michaelis and Menten theory of the mechanism of enzyme catalysis?

(2 × 4 = 8 Weightage)