2018

CHEMISTRY

CHM-201

PHYSICAL CHEMISTRY - II

Full Marks: 80

Time: 3 Hours

The figures in the margin indicate full marks for the question :

ALL QUESTIONS ARE COMPULSORY:

1. Write down the Hamiltonian operator for atomic hydrogen $\quad$ 1

2. What is compatible observable? $\quad$ 1

3. Write down the full **Schrodinger equation** (for three dimensions) $\quad$ 1

4. Prove that the operator $i \dfrac{d}{dx}$ and $\dfrac{d^2}{dx^2}$ are Hermitian $\quad$ 2+2

5. If $\hat{A}$ & $\hat{B}$ are Hermitian, show that $\widehat{AB}$ is also Hermitian if & commute $\quad$ 2

6. Write all the possible terms for configuration. Find out the ground state term. $\quad$ 2+1

7. Write down the energy expression for a linear harmonic oscillator. Draw the first five wave functions of the harmonic oscillator plotting their corresponding energies in Y-axis. $\quad$ 1+5

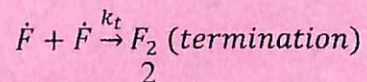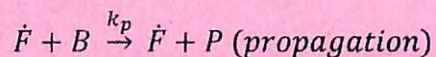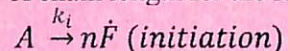8. Write down the conditions to say ψ a well-behaved wave function. $\quad$ 3

9. Match the columns $\quad$ 2

A	B	C
1. $RhCl(PPh_3)_3$	a. Aldehyde	i. Carboxylation
2. Metal Hydride	b. Monsantro Process	ii. Hydroformylation
3. $[Rh(CO)_2I_2]^-$	c. Unsymmetrical Alkene	iii. Hydrogenation
4. $HCo(CO)_4$	d. Wilkinson Catalyst	iv. Isomerization

10. Why selectivity is very much essential for a catalyst? 2
   Derive the rate expression for a catalytic hydrogenation if the hydrogen pressure is kept constant. How the Lineweaver-Burk expression helps us to calculate different kinetic data? 5+1

12. "One metal can give verities of products from a single substance simply by changing the ligands around the metal centre" Explain with examples. 4

13. "A catalyst lowers the barrier of activation of reaction". Explain with an example. 3

14. How the enzyme-catalysed reactions are different from the metal-catalysed reactions? 2

15. What are the basic assumptions, based on which the rate of a reaction is explained by CST? Discuss briefly. 3

16. Show the shift of the fraction of sufficiently energetic collisions with the increase in temperature for a particular reaction (w.r.t. activation energy). 2

17. Show that the probability factor in CST depends on entropy, S. 3

18. What caused to propose different models/mechanisms to explain the rate of a unimolecular reaction with the help of CST? 2

19. For unimolecular reaction, establish the following relation

$$k = e\frac{k_b T}{h} \exp\left(\frac{\Delta S^{\#}}{R}\right) \exp\left(\frac{-E_{Act}}{RT}\right)$$

   (Where terms have their usual significance) 7

20. Show the explosion limits and explain the causes of chain explosion with kinetics 2+5

21. Derive an expression of chain length for the following reaction 5

$$A \xrightarrow{k_i} n\dot{F} \ (initiation)$$

$$\dot{F} + B \xrightarrow{k_p} \dot{F} + P \ (propagation)$$

$$\dot{F} + \dot{F} \xrightarrow{k_t} F_2 \ (termination)$$

2

22. What are the essential conditions to generate oscillations in a chemical reaction? 3

23. How does pH influence an enzyme-catalyzed reaction? 3

24. Write a short note on enzyme inhibition. . 5

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