

八十四學年度 生命科學 所 甲 組碩士班研究生入學考試

科目 物理化學 科號 0904 共 5 頁第 1 頁 *請在試卷【答案卷】內作答

(60%) Part 1. Only one answer is correct for each following question. 3 points will be given for a correct answer, 3 points will be deducted for an incorrect answer and no point for no answer.

() 1. What is the quantum mechanical operator for the kinetic energy? (1)

$-(\hbar^2/m)\frac{\partial^2}{\partial q^2}$ (2) $-i\hbar\frac{\partial}{\partial q}$ (3) $-i(\hbar^2/m)\frac{\partial^2}{\partial q^2}$ (4) $-\frac{\hbar}{i}\frac{\partial}{\partial q}$

() 2. What are the energy levels for a rigid diatomic rotor? (1) $(J+1/2)\frac{\hbar^2}{2I}$

(2) $J(J+1/2)\frac{\hbar^2}{2I}$ (3) $J(J+1)\frac{\hbar^2}{2I}$ (4) $(J+1)(J+2)\frac{\hbar^2}{2I}$ (I is the moment of

inertia)

() 3. If $\langle m|\Omega|n\rangle \equiv \int \psi_m^* \Omega \psi_n dt$, what is the most general definition of

hermiticity? (1) $\langle m|\Omega|n\rangle = \langle n|\Omega|m\rangle^*$ (2) $\langle m|\Omega|n\rangle = \langle n|\Omega|m\rangle$ (3) $\langle m|\Omega|n\rangle = \langle m|\Omega|n\rangle^*$ (4)

$\langle m|\Omega|n\rangle = -\langle n|\Omega|m\rangle$

() 4. Is the operator id/dx Hermitian? (1) yes (2) no.

() 5. What is the usual length for a hydrogen bond? (1) 1.0 Å (2) 1.20 Å (3)

2.0 Å (4) 3.5 Å.

() 6. What are the energy levels for a harmonic oscillator? (1) $n\hbar\omega$ (2) $n\hbar\omega$

(3) $(n+1/2)\hbar\omega$ (4) $(n+1/2)\hbar\omega$

() 7. How many normal modes of vibration for H₂O? (1) 3 (2) 4 (3) 5 (4) 6

() 8. What is the degeneracy of a rotational level J for a spherical top

molecules (1) $2J+1$ (2) $(2J+1)^2$ (3) $2J(2J+1)$ (4) $(2J+1)(2J-1)$

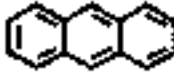
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- () 9. The pK_a value of H_2O is around 15. What is the sign of the corresponding free energy ΔG^0 ? (1) $\Delta G^0 > 0$ (2) $\Delta G^0 < 0$ (3) $\Delta G^0 = 0$.
- () 10. Which of the following relationships between temperature T and the velocity v is true? (1) $\langle v \rangle \propto T$ (2) $\langle v^2 \rangle \propto T$ (3) $\langle v \rangle \propto T^2$
- () 11. The rate constant in Transition State Theory is written as $A \exp(-\Delta G^* / kT)$, where ΔG^* is the activation free energy, k_B the Boltzmann constant and T temperature - what is the value of the frequency factor A at $300^\circ K$? (1) $6 \times 10^6 \text{ s}^{-1}$ (2) $6 \times 10^8 \text{ s}^{-1}$ (3) $6 \times 10^{10} \text{ s}^{-1}$ (4) $6 \times 10^{12} \text{ s}^{-1}$
- () 12. For the molecule CO , which of the formulae describes the charge distribution properly? (1) $C^{-\delta}O^{-\delta}$ (2) $C^{+\delta}O^{-\delta}$.
- () 13. What is quantum mechanical operator for position q if the operator for the momentum p is taken to be multiplication by p ? (1) $i\hbar(d/dp)$ (2) $-i\hbar(d/dp)$ (3) $\frac{i}{\hbar}(d/dp)$ (4) $-\frac{i}{\hbar}(d/dp)$
- () 14. When liquid water is vaporized at $100^\circ C$ and 1 atm, which of the following quantities is zero. (1) ΔE (2) ΔH (3) ΔG (4) ΔA
- () 15. For an irreversible cycle, $\oint \frac{dq}{T}$ is always (1) > 0 (2) $= 0$ (3) < 0 .
- () 16. For an ideal gas, which of the following is not true? (1) $PV = nRT$ (2) $(\partial H / \partial V)_T \neq 0$ (3) $(\partial C_V / \partial V)_T = 0$.
- () 17. What is the point group for C_2H_6 (in the eclipsed conformation)?
 (1) D_{3d} (2) D_{3h} (3) D_{3d} (4) D_{2h}

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- () 18. What is the point group for anthracene ? (1) $C_{\infty v}$ (2) C_{2h}
 (3) C_{2v} (4) D_{2h} .
- () 19. What is the force between the particles in an ideal gas? (1) none (2) only attraction (3) only repulsion (4) both attraction and repulsion.
- () 20. What is the value of RT at room temperature? (R is the gas constant and T the temperature) (1) 0.2 cal/mol (2) 0.6 kcal/mol (3) 2.4 kcal/mol (4) 4.8 kcal/mol.

Part 2 . (40%) Answer the following questions and show your calculation.

$$R = 8.314 \times 10^7 \text{ erg deg}^{-1} \text{ mol}^{-1} = 1.987 \text{ cal deg}^{-1} \text{ mol}^{-1} = 8.314 \text{ JK}^{-1} \text{ mol}^{-1}$$

$$h = 6.626 \times 10^{-34} \text{ J s}$$

- (10) 1. What will be the free energy of forming 1 mol of H_2O at $1000^\circ K$ if
 (a) 10 atm of O_2 and 10 atm of H_2 are reacted to give 0.01 atm of H_2O ;
 (b) 0.01 atm of O_2 and 0.01 atm of H_2 are reacted to give 10 atm of H_2O ?
 Is the reaction favored relative to standard conditions in each case?
 For part (b), $H_2O(g)$ could be introduced with the reactants to give a high enough product partial pressure.

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(20) 2. The stoichiometric equation for a reaction is



The initial rate of formation of C is measured with the following results:

initial concentration of A (M)	initial concentration of B (M)	initial rate (Ms ⁻¹)
1	1	10 ⁻³
2	1	4×10 ⁻³
1	2	10 ⁻³

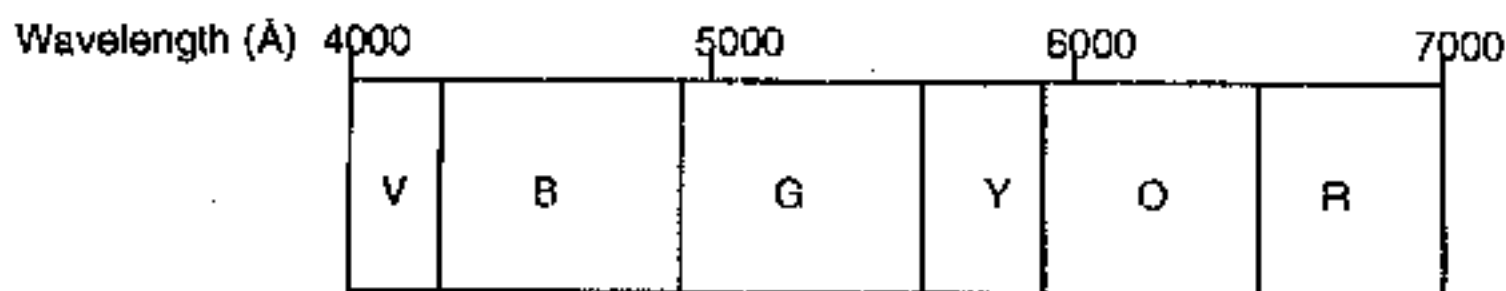
- What is the order of the reaction with respect to A?
- What is the order of the reaction with respect to B?
- Use your conclusions in part (a) and (b) to write a differential equation for the appearance of C.
- What is the rate constant k for the reaction? Do not omit the units of k.
- Give a possible mechanism for the reaction and discuss in words, or give equations to show, how the mechanism is consistent with the experiment.

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(10) 3. Use the figure to decide what color flame would one expect to see if a potassium compound such as potassium chloride is heated in a Bunsen burner flame, given that potassium containing materials emit light of frequency $7.41 \times 10^{14} \text{ sec}^{-1}$.



V-Violet B-Blue G-Green Y-Yellow O-Orange R-Red