

科目：綜合化學(II)
 考試時間：100 分鐘

系所：應用化學系
 本科原始成績：100 分

是否使用計算機：是

Physical Chemistry

一、選擇題 (每題兩分)

1. Which of the following is not one of the Maxwell relation ?

- a) $\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V$ b) $\left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P$
 c) $-\left(\frac{\partial T}{\partial S}\right)_P = \left(\frac{\partial V}{\partial T}\right)_P$ d) $\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V$

2. Which of the following is incorrect ?

- a) the first law of thermodynamics explains the relation between internal energy and work
 b) the third law of thermodynamics defines free energy
 c) the second law of thermodynamics defines the entropy of the universe
 d) none of the above

3. When describing the free energy of mixing of a solution, what fraction should we use ?

- a) mole fraction
 b) volume fraction
 c) mass fraction
 d) pressure fraction

4. The work done by expanding an ideal gas from initial state (*i*) to final state (*f*) isothermally at temperature *T* is

- a) $-nRT \ln \frac{V_i}{V_f}$ b) $nRT \ln \frac{V_i}{V_f}$
 c) $nC_V \Delta T$ d) $nRT \ln \frac{V_f}{V_i}$

5. For a particle in one dimensional box with length *a*, which of the following is incorrect ?

- a) The ground state wavefunction is $\sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$
 b) The ground state energy is $\frac{h^2}{8ma^2}$

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c) The ground state energy is $\frac{\hbar^2}{8ma^2}$

d) The wave functions form an orthonormal set

6. Which of the following is correct?

a) $[\hat{L}_x, \hat{L}_y] = [\hat{L}_y, \hat{L}_x]$

b) $[\hat{x}, \hat{p}_x] = [\hat{p}_x, \hat{x}]$

c) $[\hat{L}_z, \hat{L}^2] = [\hat{L}^2, \hat{L}_z]$

d) $[\hat{L}_x, \hat{L}_y] = \hat{L}_z$

7. The term symbol for an ns^1np^1 electron configuration are 3P_2 , 3P_1 , 3P_0 , and 1P_1 . According to Hund's rule, which of the term symbol corresponds to the ground state?

a) 3P_2

b) 3P_1

c) 3P_0

d) 1P_1 .

8. The canonical partition function Q for indistinguishable particles has the particle partition function q can be written as

a) $Q = q^N / N!$

b) $Q = q^N / N$

c) $Q = q^N$

d) none of the above

9. For Infrared absorption spectrum of a diatomic molecule; which of the following statement is true ?

a) Equally spaced peaks observed due to equally spaced rotational energy levels

b) Greater the bond length results larger spacing between the peaks

c) The spacing between peaks is approximately equal to $2B$ (B : rotational constant)

d) None of the above

10. Which of the following thermodynamic function has absolute zero value ?

a) Enthalpy

b) Entropy

c) Gibbs Free Energy

d) Helmholtz Free Energy

二、計算題 (每題六分，請清楚標示答案否則不予計分)

11. The $^{12}\text{C}^{16}\text{O}$ molecule has an equilibrium bond distance of 112.8 pm and the fundamental vibrational frequency is 2169.814 cm^{-1} , calculate

a) the reduced mass in kg

b) the moment of inertia in kg m^2

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- c) the wavelength of the photon emitted when the molecule makes the transition from $J = 1$ to $J = 0$ in meter
 d) the force constant in Newton/meter

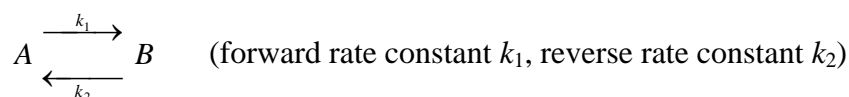
12. Consider a gas whose equation of state over a certain temperature range can be represented by $PV = RT + aT^2$ for 1 mole of gas, where a is a constant. Using the second law, we can

show that $\left(\frac{\partial U}{\partial V}\right)_T = \frac{aT^2}{V}$. When the gas is expanded isothermally and reversibly from V_1 to

V_2 . a) Derive an expression for the work associated with this process. b) Obtain an expression giving the change in the internal energy for this process. c) Obtain an expression giving q for this process.

13. At 1:3 mixture of nitrogen and hydrogen was processed over a catalyst at 450°C . It was found that 2.04% by volume of ammonia was formed when the total pressure was maintained at 10.13 bar. Calculate the value of equilibrium constant (K) for $3/2 \text{H}_2(\text{g}) + 1/2 \text{N}_2(\text{g}) \rightleftharpoons \text{NH}_3(\text{g})$ at this temperature.

14. Set up the rate expression for the following mechanism



If the concentration of B is small compared with concentrations of A, C, and D, then Steady State approximation can be used to derive the rate law. Show that this reaction may follow the first order equation at high pressure and the second order equation at low pressure.

15. A quantum mechanical system has two energy levels ϵ_1 and ϵ_2 . Derive equations for the probability P_1 that the system will be in state 1 and the probability P_2 that the system will be in state 2. What are the probabilities at $T/k_B = 0$ and ∞ ? What are the values of P_1 and P_2 at $\Delta\epsilon = k_B T$? (k_B is Boltzmann Constant)

Analytical Chemistry

16. (每子題 2 分) Explain the difference between

a、 qualitative analysis and quantitative analysis

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- b、 weak electrolyte and strong electrolyte
- c、 direct titration and back titration
- d、 normal-phase chromatography and reversed-phase chromatography
- e、 faradaic current and charging current

17. (5 分) What is the pH of 1 M NaOH (aq)?
18. (5 分) A solution is mixed with 20.0 mL of 0.20 M formic acid (HCOOH) and 20.0 mL of 0.20 M sodium formate (HCOONa). The pH of the solution is 3.74. What is the pK_a of the solution? Explain.
19. (10 分) Why the sensitivity of fluorescence is better than UV/Vis?
20. (10 分) List the names of universal detector for GC and the names of solute property detector for HPLC.
21. (10 分) Why the commonly used ionization sources of GC/MS are EI and CI but not ESI or other ionization techniques?