

國立臺北科技大學 101 學年度碩士班招生考試

系所組別：3712 有機高分子研究所甲組

第二節 物理化學 試題 (選考)

第一頁 共二頁

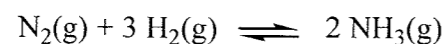
注意事項：

1. 本試題共九題，配分共 100 分。
2. 請標明大題、子題編號作答，不必抄題。
3. 全部答案均須在答案卷之答案欄內作答，否則不予計分。

<< 請寫出計算或推導過程 >>

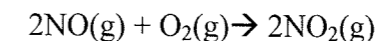
<< 常用物理常數請參考最後一頁 >>

1. Calculate the final temperature and the change in internal energy when 500 J of energy is transferred as heat to 0.9 mol $O_2(g)$ at 298 K and 1.00 atm at (1) constant volume; (2) constant pressure. Treat the gas as ideal. (16 分)
2. Allow 1.00 mol of idea gas molecules expand from 8.00 L to 20.00 L at 292 K. Please calculate the ΔS in the isothermal reversible expansion process. (4 分)
3. The standard reaction enthalpy for the hydrogenation of propene is -124 KJ/mol.
 $CH_2=CHCH_3(g) + H_2(g) \rightarrow CH_3CH_2CH_3(g)$
 The standard reaction enthalpy for the combustion of propane is -2220 KJ/mol.
 $CH_3CH_2CH_3(g) + 5 O_2(g) \rightarrow 3 CO_2(g) + 4 H_2O(l)$
 Given standard enthalpy of $H_2(g) + \frac{1}{2} O_2(g) \rightarrow H_2O(l) \Delta H^0 = -286$ KJ/mol
 Calculate the standard enthalpy of combustion of propene. (5 分)
4. Calculate the equilibrium constant for the ammonia synthesis reaction at 298 K. (10 分)



$$\Delta G_f^0(NH_3, g) = -16.45 \text{ KJ/mol}$$

5. NO and O_2 are two important molecules in our life. The chemical reaction of these two molecules is given as following,

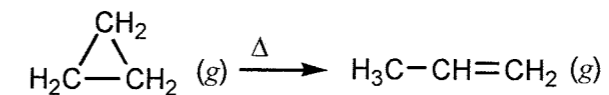


Given some experimental data as following,

Experiment	Initial concentration (mol/L)		Initial Rate (mol NO) $L^{-1}s^{-1}$
	NO	O_2	
1	0.012	0.020	0.102
2	0.024	0.020	0.408
3	0.024	0.040	0.816

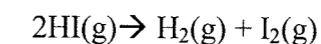
Please write the rate law for the consumption of NO and determine the value of rate constant k . (10 分)

6. Cyclopropane is the smallest cyclic hydrocarbon. Because its 60° bond angles allow poor orbital overlap, its bonds are weak. As a result, it is thermally unstable and rearranges to propene at $1000^\circ C$ via the following first-order reaction



The rate constant is $9.2s^{-1}$, (1) What is the half-life of the reaction? (2) How long does it take for the concentration of cyclopropane to reach one-quarter of the initial value? (10 分)

7. The decomposition of hydrogen iodide,



has rate constants of $9.51 \cdot 10^{-9} \text{ L/mol} \cdot \text{s}$ at 500 K, and $1.10 \cdot 10^{-5} \text{ L/mol} \cdot \text{s}$ at 600 K. Please find the activation energy $E_a = ?$ (10 分)

8. (1) Given a particle moving in a one dimensional box with an infinite potential well as following, please solve the Schrödinger equation to obtain the energy levels and its corresponding state function. (10 分)

$$V(x) = 0 \text{ if } 0 \leq x \leq l$$

$$V(x) = \infty \text{ if } x > l \text{ or } x < 0$$

(2) Please calculate expectation value of $\langle x \rangle$ and $\langle p_x \rangle$. (10 分)

(3) Based on the uncertainty principle, $\Delta x \Delta p_x \geq h/4\pi$, please calculate the lowest energy of particle in a box case as in (1). (5 分)

注意：背面尚有試題

9. Evaluate the following commutator results (10 分)

$$(1) [\hat{x}, \hat{H}] = ? \quad (2) [\hat{L}^2, \hat{L}_x] = ?$$

Physical constants:

Gas Constant : $R = 0.0821 \text{ atm L/mol-K} = 8.314 \text{ J/mol-K}$

Avogadro constant $N_A = 6.022 \times 10^{23} / \text{mol}$

Atomic Properties

Electron charge : $e = 1.602 \times 10^{-19} \text{ C}$; Electron rest mass : $m_e = 9.109 \times 10^{-31} \text{ kg}$

Neutron rest mass : $m_n = 1.675 \times 10^{-27} \text{ kg}$; Proton rest mass : $m_p = 1.673 \times 10^{-27} \text{ kg}$

Fundamental Constants

Planck's constant : $h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s}$; Boltzmann's constant : $k = 1.381 \times 10^{-23} \text{ J/K}$

Speed of light in a vacuum : $c = 2.998 \times 10^8 \text{ m/s}$

Unit equalities:

Energy

$1 \text{ J} = 1 \text{ kg m}^2 / \text{s}^2 = 1 \text{ C V}$; $1 \text{ cal} = 4.184 \text{ J}$; $1 \text{ L-atm} = 101.3 \text{ J}$

Pressure

$1 \text{ atm} = 1.01325 \times 10^5 \text{ Pa}$; $1 \text{ Bar} = 1 \times 10^5 \text{ Pa}$