

編號: 55 系所: 化學系

科目: 物理化學

本試題是否可以使用計算機: 可使用, 不可使用 (請命題老師勾選)

說明: 1. 答案一律寫在答案卷上, 否則不予計分。

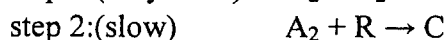
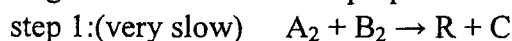
2. 請依題序作答, 並標明題號。

3. $R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$, $F = 96485 \text{ C mol}^{-1}$, $h = 6.626 \times 10^{-34} \text{ J s}$, $c = 2.998 \times 10^8 \text{ m s}^{-1}$

I. 單選題 6 題, 每題 5 分, 共 30 分 (答錯不倒扣)

(1) Which combination always results in a process being spontaneous at all temperature?

- (A) enthalpy change is negative and entropy change is negative
 (B) enthalpy change is positive and entropy change is position
 (C) enthalpy change is positive and entropy change is negative
 (D) enthalpy change is negative and entropy change is positive
 (E) none of these

(2) The following mechanism has been proposed in the reaction $2A_2 + B_2 \rightarrow 2C$ 

What is the molecularity of step 2?

- (A) unimolecular (B) bimolecular (C) trimolecular (D) quadmolecular
 (E) the molecularity cannot be determined

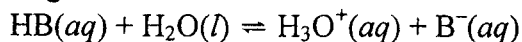
(3) A first-order reaction is 42% complete at the end of 17 minutes.

What is the value of the rate constant?

- (A) $3.2 \times 10^{-2} \text{ min}^{-1}$ (B) 20 min^{-1} (C) 31 min^{-1} (D) $5.1 \times 10^{-2} \text{ min}^{-1}$
 (E) none of these

(4) What is the probability of finding a particle in a one-dimensional box in energy level $n = 4$ between $x = L/4$ and $x = L/2$? (L is the length of the box.)

- (A) 12.5% (B) 25% (C) 33% (D) 37.5% (E) 50%

(5) The following reaction has a ΔG° value of 42.6 kJ/mol at 25°C.What is the K_a for the acid HB?

- (A) 1.63 (B) -17.2 (C) 3.41×10^{-8} (D) 42,600 (E) 14.0

(6) Calculate the following ratio for a gas at Kelvin temperatures T_1 and T_2 where $T_2 = 2T_1$.Collision frequency between O_2 molecules at T_1 : Collision frequency between O_2 molecules at T_2

- (A) 0.50 (B) 2.0 (C) 1.0 (D) 1.4 (E) 0.71

II. 簡答題 4 題, 每題 5 分, 共 20 分

(1) What are the term symbols for the first excited state of Li atom?

(2) What is the term symbol for the ground state of He_2 diatomic molecule?

(背面仍有題目, 請繼續作答)

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- (3) A reaction took 143 s for 50.0% of a particular substance to decompose. If the initial concentration is 0.060 M and the decomposition reaction follows second-order kinetics, what is the value of the rate constant?
- (4) A 1.50-mol sample of an ideal gas is allowed to expand adiabatically and reversibly to twice its original volume. In the expansion the temperature dropped from 296 K to 239 K. What is the ΔH for the gas expansion?

III. 詳細解釋下列專有名詞 4 題，每題 5 分，共 20 分

- (1) Boltzmann thermal distribution
- (2) zero-point energy
- (3) impact parameter
- (4) anharmonicity constant

IV. 計算題 3 題，每題 10 分，共 30 分（必須寫出計算過程，否則不給分）

- (1) The overall reaction and equilibrium constant value for a hydrogen-oxygen fuel cell at 298 K is
$$2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{l}) \quad K = 1.28 \times 10^{83}$$

Calculate ΔG° for the fuel cell at 298 K.
- (2) The infrared spectrum of gaseous $^1\text{H}^{35}\text{Cl}$ shows the $\nu = 0$ to $\nu = 1$ transition at 2885 cm^{-1} . Calculate the vibrational force constant for the HCl molecule.
- (3) A reflection from the [111] planes of a cubic crystal was observed at a glancing angle of 11.2° when Cu K_α X-rays of wavelength 154 pm were used. Calculate the length of the side of the unit cell?