

# 淡江大學 101 學年度碩士班招生考試試題

系別：化學學系

科目：物理化學

考試日期：2月26日(星期日) 第4節

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1. (a) Propose a mechanism for the reaction  $2\text{NO}_2 + \text{F}_2 \rightarrow 2\text{NO}_2\text{F}$ . The reaction is found to be

second-order; its rate equation is  $-\frac{1}{2} \frac{d[\text{NO}_2]}{dt} = k_2 [\text{NO}_2] [\text{F}_2]$

(b) For a certain first-order reaction  $\text{A} \rightarrow \text{B} + \text{C}$ , the initial concentration of A was 0.35 M. After 30 seconds, the concentration is 0.31 M. Calculate the rate constant.

(c) Integrate the rate equation  $-\frac{dC}{dt} = kC^{1/2}$ . 15%

2. Consider the following mechanism  $\text{A} + \text{A} \xrightleftharpoons[k_{-2}]{k_2} \text{A}^* + \text{A}$  and  $\text{A}^* \xrightarrow{k_1} \text{products}$  used to

describe the decomposition of a gaseous molecule. (a) Write the differential rate equations for

$-\frac{dC_A}{dt}$  and  $\frac{dC_{A^*}}{dt}$  and assuming a steady state approximate for  $C_{A^*}$ , write  $-\frac{dC_A}{dt}$  in terms of

$C_A$  and rate constant. (b) Under what condition is this a pseudo-first-order reaction? (c) A pseudo-second-order reaction? 15%

3. For an ideal gas having  $C_p = \frac{7}{2}R$ , calculate the entropy changes of 5 mole of the gas when it is heated from room temperature (298.2 K) to 500 K (a) at constant volume and (b) at constant pressure. 10%

4. (a) Verify  $|\Psi(r,t)|^2 = |\psi(r)|^2$ , b. Describe the time-dependent and time-independent Schrödinger equation. 10%

5. Show that the frequency of the  $n = 3$  to 2 for the one particle in a 1-D box transition is 5/3 times the frequency of the 2 to 1 transition. 10%

6. Describe Frank-Condon principle! How to apply it in the electronic device and DSSC? 10%

本試題雙面印刷

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7.  $\phi_1$  and  $\phi_2$  are normalized and orthogonal to one another  $\Psi_1 = \frac{1}{\sqrt{2}}(\phi_1 + \phi_2)$  and  $\Psi_2 = \frac{1}{i\sqrt{2}}(\phi_1 - \phi_2)$ , showing that  $\Psi_1$  and  $\Psi_2$  are also normalized and orthogonal to one another. 10%
8. For each of the following processes, state which of  $\Delta U$ ,  $\Delta H$ ,  $\Delta S$ ,  $\Delta A$  and  $\Delta G$  must be zero. (a) Ice melted at  $0^\circ\text{C}$  and 1 atm. (b) A nonideal gas undergoes a Carnot cycle. (c) Hydrogen is burned in an adiabatic calorimeter of fixed volume. 10%
9. (a) Evaluate the  $\langle p_x \rangle$  for a particle in a 1-D box. (b) Please give the  $\hat{H}$  for H atom. 10%