（101）輔仁大學碩士班招生考試題目	考試日期：101 年 3 月 9 日第 3 節
	本試題共 2 頁（本頁為第 1 頁）

科目：物理化學　　系所組：化學系碩士班甲組

1. (20%) An ideal gas at 27°C expands isothermally and reversibly from 10 to 1 bar against a pressure that is gradually reduced. For this process, please calculate (i) the transfer heat *q* per mole, the work done on a system *w* per mole and (ii) each of the thermodynamics quantities ΔU, ΔH, ΔG, ΔA, and ΔS.

2. (20%) There is considerable interest in hydrogen adsorption on carbon nanotubes and porous carbons as a method of storage for transport and related energy applications. The hydrogen adsorption isotherms are markedly dependent on temperature and isobars were measured to provide data on the amounts adsorbed as a function of temperature. The hydrogen amount adsorptions on sample carbon G212 at 100kPa are 9.15mmolg^{-1} at 77K and 4.75 mmolg^{-1} at 114K, respectively. Calculate the isosteric enthalpy of adsorption of adsorption at zero surface coverage.

3. (20%) To get a sense of the effect of cellular conditions on the ability of ATP to drive biochemical processes, compare the standard Gibbs energy of hydrolysis of ATP to ADP with the reaction Gibbs energy in an environment at 37°C in which pH = 7.0 and the ATP, ADP, and P_i^- concentrations are all 1.0 μmol dm^{-3}. (Hint: the biological standard free energy ΔG of -31 $Jmol^{-1}K^{-1}$ for ATP → ADP+ P_i^- +H^+).

4. (20 %) It's well known that raising the temperature increases the reaction rate. Quantitatively the relationship between the rate a reaction proceeds and its temperature is determined by the Arrhenius Equation k = A exp(-E_a/RT) , where k is the rate coefficient, R is the gas constant, T the absolute temperature, E_a the activation energy and A the frequency factor. For the reaction $2N_2O_4$ (g) + O_2(g) →$2N_2O_5$(g), rate constants were measured at two temperatures:

T/K	298.15	318.15
k/ s^{-1}	4.69 x 10^{-5}	6.29 x 10^{-4}

(a) Find the value of the activation energy E_a.
(b) Find the value of the frequency factor A.
(c) Calculate the rate constant at 338.15 K.
(d) Sketch a plot of ln(k) versus (1/T). Indicate on your graph ln A and the relation of the slope to the activation energy E_a.

※ 注意：1. 考生須在「彌封答案卷」上作答。
2. 本試題紙空白部分可當稿紙使用。
3. 考生於作答時可否使用計算機、法典、字典或其他資料或工具，以簡章之規定為準。

5. (20 %) For the ground state of a particle in a 1D box, evaluate the mean values $\langle x \rangle$ and $\langle p \rangle$ and the mean-square value $\langle x^2 \rangle$ and $\langle p^2 \rangle$ of the position and the linear momentum, respectively. Form the root-mean-square deviations $\Delta x \equiv (\langle x^2 \rangle - \langle x \rangle^2)^{1/2}$ and $\Delta p \equiv (\langle p^2 \rangle - \langle p \rangle^2)^{1/2}$, investigate the consistency of the outcome with the uncertainty principle that $\Delta x \, \Delta p \geq \hbar/2$.

Useful Information:

Speed of light	c	2.9979×10^{8} ms^{-1}
Boltzman constant	k_B	1.38065×10^{-23} JK^{-1}
Avogadro constant	N_A	6.02214×10^{23} mol^{-1}
Planck constant	h	6.62608×10^{-34} Js
Gas constant	R	8.314 JK^{-1}mol^{-1}