（100）輔仁大學碩士班招生考試題目	考試日期：100年3月18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

Show all work. Indicate units for all numerical answers.

1. (20 %)

a. Please draw the basic structure of a Carnot cycle in the PV plot, and indicate the process conditions for the four steps.

b. Please derive the expression for the efficiency (ε) of the Carnot engine. Hint: Finally, you need only T_c (temperature of the cold reservoir) and T_h (temperature of the hot reservoir) for your answer.

c. For an ideal gas, derive the energy in each reversible step and prove that the entropy change over the reversible cycle is zero, $\Delta S\left(entropy\right)=\oint\frac{dq_{rev}}{T}=0$.

2. (15 %)

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^+) .

3. For hydrogen atom, $\psi_{1s}=\frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}e^{-\frac{Zr}{a_0}}$ (15 %)

a. Find the probability that the electron in the ground-state (1s) H atom is less than a distance a_0 from the nucleus ($0\le r\le a_0$).

b. Define the radial distribution function.

c. Find the maximum in the radial distribution function for the ground-state of hydrogen and plot the radial distribution function for the hydrogen atom.

(hint: $\int x^2e^{bx}dx=e^{bx}\left(\frac{x^2}{b}+\frac{2x}{b^2}+\frac{2}{b^3}\right)$)

※ 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。

Show all work. Indicate units for all numerical answers.

4. Rigid rotator: (15 %)

a. Starting from the Schrödinger equation of the rigid rotator

$$\frac{-h^2}{8\pi^2 I}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi = E\psi$$

Carry out the separation of variables to find the differential equations for **θ** and **ϕ**.

b. Show that the solution of the differential equation for **ϕ** could be expressed as

$$\Phi(\phi)=\sqrt{\frac{1}{2\pi}}\exp(im\phi)$$

5. The mechanism of destruction of stratospheric ozone: (15 %)

$$O_3 + M \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} O_2 + O + M$$

$$O_3 + O \xrightarrow{k_2} 2O_2$$

a. Please write down the differential rate equations of [O_3] and [O].

b. Please explain the concept of steady state approximation.

c. By using steady state approximation for [O], please find [O] and the rate law for the destruction of ozone. (-d[O_3]/dt)

d. Please find the rate law for the destruction of ozone (-d[O_3]/dt) at high pressure limit. (at high pressure limit, [M] would be very large.)

6. The probability that a molecule of mass ***m*** in a gas at temperature ***T*** has speed ***v*** is given by the Maxwell-Boltzmann distribution (20 %)

$$f(v)=4\pi\left(\frac{m}{2\pi kT}\right)^{3/2}v^2e^{-mv^2/2kT}$$

where k is Boltzmann's constant.

a. Find the most probable speed and the mean speed.

b. What is the ratio of the probability of finding a molecule moving with three times the average speed ?

c. How does this ratio depend on the temperature ?

(hint: $\int_0^\infty x^3\exp\left(-Bx^2\right)dx=\frac{1}{2}B^{-2}$)

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