※ 考生請注意：本試題 ☑可 ☐不可 使用計算機

說明: **1.** 請依題序作答並標明題號，可使用一般計算機
2. 計算題需寫出計算過程，只寫答案不給分
3. $\mathbf{R = 8.314\ J\ K^{-1}\ mol^{-1} = 0.082\ atm\ L\ K^{-1}\ mol^{-1}}$, $\mathbf{h = 6.626 \times 10^{-34}\ Js}$,
4. ground state wave function of H atom: $(\pi a_o^3)^{-1/2} e^{-r/a_o}$

(一)單選題 11 題，每題 6 分，共 66 分，答錯不倒扣

(1)If a hypothetical engine extracts heat $|q_h|$ from a hot sink of temperature T_h, and releases heat $|q_c|$ to a cold sink of temperature T_c, What's the minimum value of $|q_c|$?
(A)$T_h |q_h| / T_c$　(B)$(T_h - T_c) |q_h| / T_h$　(C)$(T_h - T_c) |q_h| / T_c$　(D)$T_c |q_h| / T_h$
(E) $T_h |q_h| / (T_h + T_c)$

(2)At 35 °C, the vapor pressure of chloroform is 295.1 torr, and that of ethanol (eth) is 102.8 torr. A chloroform-ethanol solution at 35 °C with x_{eth}=0.2 has a vapor pressure of 304.2 torr and a vapor composition of y_{eth}=0.138. Calculate ΔG for the mixing of 0.2 mol of liquid ethanol and 0.8 mole of liquid chloroform at 35 °C.
(A)-1282 J　(B)-624 J　(C)-524 J　(D)-726 J　(E)-699 J

(3)At 1 atm pressure, ice melts at 273.15 K with ΔH_{fusion}= 6010 J mol^{-1} The density of ice is 920 kg m^{-3}, and the density of liquid water is 997 kg m^{-3} What pressure (in bar) is required to lower the melting temperature by 5.0°C?
(A)638　(B)726　(C)825　(D)882　(E)954

(4)For a solution of ethanol (density= 0.789 g/cm^3) and water (density= 0.998 g/cm^3) at 20 °C which has a mole fraction of ethanol of 0.2, the partial molar volume of water and ethanol is 17.9 cm^3/mol and 55.0 cm^3/mol, respectively.
What volume (in cm^3) of pure ethanol is required to make 2 liters of this solution?
(A)921　(B)826　(C)964　(D)1016　(E)1108

(5)The rotational constant of $^{12}C^{16}O_2$ is 0.39021 cm^{-1} Calculate the bond length (in pm) of the molecule ($m(^{12}C)$ = 12 u exactly, $m(^{16}O)$ = 15.9949 u).
(A)128　(B)108　(C)116　(D)135　(E)142

(6)Calculate the mean potential energy of an electron in the ground state of a hydrogen atom. ($\int_0^\infty r e^{-br} dr = b^{-2}$)
(A)$-e^2/(4\pi\varepsilon_o a_o)$　(B)$-e^2/(8\pi\varepsilon_o a_o)$　(C)$-e^2/(2\pi\varepsilon_o a_o)$　(D)$-e^2/(2\varepsilon_o a_o)$
(E)$-e^2/(\varepsilon_o a_o)$　**(背面仍有題目,請繼續作答)**

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(7)At what radius in the H atom does the radial distribution function of the ground state have 50 per cent of its maximum value?
(A)1.10a_0 (B)2.08a_0 (C)1.63a_0 (D)0.56a_0 (E)1.85a_0

(8)Consider a particle in a cubic box. What is the degeneracy of the level that has an energy $^{14}/_3$ times that of the lowest level?
(A)2 (B)3 (C)4 (D)5 (E)6

(9)Which term doesn't exist in the configuration $2p^1 3d^1$?
(A) $^3F_3$ (B) $^3D_2$ (C) $^3P_2$ (D) $^1D_2$ (E) $^1P_1$

(10)The equilibrium A $\rightleftharpoons$ B + C at 25°C is subjected to a temperature jump that slightly increases the concentrations of B and C. The measured relaxation time is 3.0 μs. The equilibrium constant for the system is 2.0×10^{-16} at 25°C, and the equilibrium concentrations of B and C at 25°C are both 2.0×10^{-4} mol dm^{-3} Calculate the rate constant (in s^{-1}) for the forward reaction.
(A)2.6×10^{-6} (B)5.4×10^{-6} (C)6.7×10^{-6} (D)1.7×10^{-7} (E)8.2×10^{-7}

(11)The gas-phase decomposition of acetic acid at 1189 K proceeds by way of two parallel reactions:
(1) $CH_3COOH \rightarrow CH_4 + CO_2$ $k_1 = 3.74\ s^{-1}$
(2) $CH_3COOH \rightarrow H_2C{=}O + H_2O$ $k_2 = 4.65\ s^{-1}$
What is the maximum percentage yield of the ketene CH_2CO obtainable at this temperature?
(A)26% (B)35% (C)41% (D)46% (E)55%

(二)計算題 4 題，共 34 分

(12)Given that $(\partial U/\partial T)_p = C_v + x$, where x is a function of α, π_T, and V, derive the mathematical expression of x. (5%)

(13)A gaseous sample consisting of 1.00 mol molecules is described by the equation of state $pV_m = RT(1 + Bp)$. Initially at 373 K, it undergoes Joule–Thomson expansion from 100 atm to 1.00 atm. Given that $C_{p,m} = {}^5/_2R$, $\mu = 0.21$ K atm^{-1}, $B = -0.525/T$ K atm^{-1} and that these are constant over the temperature range involved, calculate ΔT and ΔS for the gas. (12%)

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(14)Consider a consecutive unimolecular reaction

$$A \xrightarrow{k_a} I \xrightarrow{k_b} P$$

(a)Derive the expression of [I] and [P] in terms of $[A]_o$, k_a, k_b, and t.

(b)Plot [I] and [P] vs. time on the same plot.

(Note: The solution of $dy/dx + a\,y = g(x)$, where a is a constant,

is $e^{ax}y = \int e^{ax} g(x)\,dx + c$) (13%)

(15)The characteristic emission from K atoms when heated is purple and lies at 770 nm. On close inspection, the line is found to have two closely spaced components, one at 766.70 nm, and the other at 770.11 nm. What are the possible transitions occurred? (4%)