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. 請依題序作答並標明題號，可使用一般計算機
　　　2. 選擇題為單選，答錯不倒扣
　　　3. 計算題需寫出計算過程，只寫答案不給分
　　　4. R= 8.314 J K⁻¹ mol⁻¹ = 0.082 atm L K⁻¹ mol⁻¹,

$$R= 8.314 \text{ J K}^{-1} \text{mol}^{-1} = 0.082 \text{ atm L K}^{-1}\text{mol}^{-1},$$
$$h=6.626\times10^{-34}\text{ Js, } c= 3.0\times10^{8}\text{ m/s, } \sin^2 A = [1-\cos(2A)]/2$$
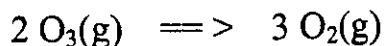
(一)選擇題 11 題，每題 6 分，共 66 分

(1)Consider $^{12}C^{16}O$ molecule as a rigid rotor with an equilibrium bond length of
112.8 pm. Calculate the wavelength of the photon emitted when the molecule
makes the rotational transition from the quantum number l =2 to 0.
(A)8.6×10^{-4} m　(B)6.2×10^{-3} m　(C)7.8×10^{-3} m　(D)1.6×10^{-4} m　(E)4.5×10^{-3} m

(2)Calculate the average linear momentum of a particle described by cos(kx).
(A)$kh/2\pi$　(B)0　(C)kh/π　(D)$2kh/\pi$　(E)$kh/4\pi$

(3)What atomic terms are possible for the electron configuration ns^1nd^1?
(A)$^3P_2, ^3P_1, ^3P_0$　(B)$^2P_{3/2}, ^2P_{1/2}$　(C)$^3D_3, ^3D_2, ^3D_1, ^1D_2$　(D)$^3P_2, ^3P_1, ^3P_0, ^1P_1$
(E)$^3D_3, ^3D_2, ^3D_1, ^1D_2, ^3P_2, ^3P_1, ^3P_0, ^1P_1$

(4)Estimate the mean ionic activity coefficient of $CaCl_2$ for a solution that is 0.01
mol/kg $CaCl_2$(aq) and 0.03 mol/kg NaF(aq).
(A)0.56　(B)0.48　(C)0.36　(D)0.62　(E)0.70

(5)Consider the reaction　　NADH(aq) + H^+(aq)　==> NAD^+(aq) + H_2(g)
at 37 °C, for which $\Delta_rG°$(at pH=0) = -21.8 kJ/mol. What's the $\Delta_rG°$ (in kJ/mol)
at pH=7?　(A)-18.2　(B)-12.5　(C)2.6　(D)9.2　(E)19.7

(6)At 25 °C, the density of a 50 % by mass ethanol-water solution is 0.914 g/cm³.
Given that the partial molar volume of water in the solution is 17.4 cm³/mol,
calculate the partial molar volume (in cm³/mol) of the ethanol.
(A)40.2　(B)32.5　(C)56.3　(D)28.3　(E)48.5

(7)The pre-exponential factor for the gas-phase decomposition of ozone
$$2 O_3(g)\quad ==> \quad 3 O_2(g)$$
at low pressure is 4.6×10^{12} L mol⁻¹ s⁻¹ and its activation energy is 10.0 kJ/mol.
What's the enthalpy of activation (in kJ/mol) at 298 K?
(A)3.28　(B)2.54　(C)6.72　(D)5.04　(E)8.65

(8)What's the entropy of activation (in $J K^{-1} mol^{-1}$) in Problem (7)?
　(A)-80.2　(B)-45.8　(C)-35.5　(D)-20.6　(E)-60.6

(9)Given that μ=0.25 K/atm and $C_{p,m}$=7R/2 for nitrogen, calculate the energy (in kJ) that must be supplied as heat to maintain constant temperature when 15.0 mol N_2 flows through a throttle in an isothermal Joule-Thomson experiment and the pressure drop is 75 atm.
　(A)4.2　(B)2.8　(C)6.5　(D)8.1　(E)9.6

(10) A sample consisting of 1.00 mol of van der Waals gas is compressed isothermally from 20.0 L to 10.0 L at 300 K.　If $C_{p,m}$= 38.4 $J K^{-1} mol^{-1}$, a= 3.60 L^2 atm/mol^2, b= 0.44 L/mol, calculate ΔU for the process.
　(A)-18.3 J　(B)-20.5 J　(C)-14.6 J　(D)-12.8 J　(E)-7.8 J

(11)What's ΔS_{sys} (in J/K) in Problem (10)?
　(A)-5.0　(B)-6.0　(C)-7.0　(D)-8.0　(E)-9.0

(二)計算題 3 題，共 34 分

(12)A particle in a one-dimensional box of length L is described by the wave function $\psi(x) = (2/L)^{1/2} \sin(n\pi x/L)$.　If n=6, calculate (a)the probability that a particle will be found between 0 and L/6, (b)the expectation value of x. (12%)

(13)Use the collision theory of gas-phase reaction to calculate the theoretical value of the second-order rate constant for the reaction $D_2(g) + Br_2(g) \rightarrow 2 DBr(g)$ at 300 K, assuming that it is elementary bimolecular. Take the collision cross-section as 0.30 nm^2, the atomic weight of Br as 80 g/mol, and the activation energy as 200 kJ/mol.　　　　　　　　　　　　　　　　(14%)

(14)Use the Maxwell relations and Euler's chain relation to express $(\partial V/\partial S)_P$ in terms of heat capacity C_p and the expansion coefficient α.　　　(8%)