系所組：化學系應用化學碩士班

日期節次：101 年 3 月 17 日第 3 節 13:00~14:30

科目：物理化學

1. (a) One mole of an ideal gas at 300 K is reversibly and isothermally compressed from 25.0 L to 10.0 L. Suppose the surrounding is also at 300 K, calculate ΔS and $\Delta S_{surrounding}$. (10 points)
   (b) Under the same condition of Problem 1(a) except the compression is now done by a constant external pressure 2.49×10^5 Pa, is the process spontaneous or non-spontaneous? Why? (10 points)

2. A prolate molecule like CH_3I has moment of inertia $I_a < I_b = I_c$, show that its rotational energy can be expressed by $E_{JK}(cm^{-1}) = BJ(J+1) + K^2(A-B)$, where J and K are quantum numbers, A and B are rotational constants. (10 points)

3. Draw the π orbitals of benzene and fill in the π electrons. (10 points)

4. Derive the equilibrium constant of reaction $CaCO_{3(s)} \rightleftarrows CaO_{(s)} + CO_{2(g)}$ in terms of substance activities. (10 points)

5. Suppose an enzyme catalyzed reaction has mechanism $E + S \overset{k_1}{\rightarrow} ES$, $ES \overset{k_{-1}}{\rightarrow} E + S$, $ES \overset{k_2}{\rightarrow} E + P$. Here E, S, ES and P stand for the enzyme, substrate, intermediate, and product, respectively. If the initial concentration of E is $[E]_0$, derive the rate law by the steady-state approximation. (10 points)

6. (a) SO_2 is a C_{2v} molecule and the p_x orbitals are defined as perpendicular to this exam paper. Now with the p_x orbitals of S, O_A, and O_B atoms as the basis (p_S, p_A, p_B), derive the matrix representation of the C_2 axis with respect to this basis. (10 points)
   (b) If we have a new basis (p_S, p_1, p_2), where $p_1=p_A+p_B$ and $p_2=p_A-p_B$, derive the matrix representation of the C_2 axis with respect to this new basis. (10 points)

7. Term explanations: (5 points for each)
   (a) The third law of thermodynamics.
   (b) Arrhenius preexponential factor.
   (c) The uncertainty principle.
   (d) Normalized wave functions.