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 $\Delta S$ 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 $2.49 \times 10^5$ 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 $\pi$ orbitals of benzene and fill in the $\pi$ 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 $E + S \xrightarrow{k_1} ES$, $ES \xrightarrow{k_{-1}} E + S$, $ES \xrightarrow{k_2} E + P$. 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.