

國立嘉義大學九十六學年度
應用化學系碩士班招生考試(甲組)試題

科目：綜合化學 II

I. Physical Chemistry (50 points)

- (a) What are the three quantum numbers of $3p_z$ orbital? (b) Can you give the magnetic quantum number of $2p_x$ orbital? (c) Why? (6 points)
- The electron configuration of Be in the excited state is $1s^2 2s^1 2p^1$. (a) Show the term symbols correspond to the electron configuration (b) What is the term symbol for ground state? (c) What are the spin wave functions of the ground states? (d) What are the spatial wave functions of the ground states? (8 points)
- For NH_3 at 300 K, (a) what value of $C_{p,m}$ is predicted by the equipartition principle? (In the unit of R) (b) Would NH_3 actually have this value of $C_{p,m}$ at 300 K (In the unit of R) (c) Under what condition(s) would NH_3 have the equipartition –principle value of $C_{p,m}$? (6 points)
- Assume that a molecule has only three energy levels, whose energies and degeneracy are $\varepsilon_1/k = 0, g_1=1; \varepsilon_2/k = 100\text{K}, g_2=3; \varepsilon_3/k = 300\text{K}, g_3=5$.
(a) Calculate partition function z at 0 K. (b) Calculate partition function z at 100 K. (c) Calculate partition function z at $T \rightarrow \infty$. (d) What is the most populated level at 100 K. (8 points)
- The Gibbs equation for dG is $dG = -SdT + VdP$. Use the Euler reciprocity relation to derive one of the Maxwell relations. (2 points)
- If the $J=1$ to 2 rotational transition for diatomic molecule occurs at $\lambda = 2\text{ cm}$, find λ for the $J=6$ to 7 transition of this molecule. (2 points)
- An overall reaction is third order. What is the unit for the rate constant? (2 points)
- For $\text{H}^{35}\text{Cl}, \text{H}^{37}\text{Cl}, \text{D}^{35}\text{Cl}$ and D^{37}Cl , which one has the largest rotational partition function? (2 points)
- (a) What is Raman scattering? (b) What is Stokes lines and anti-Stokes lines? (4 points)
- (a) What is the selection rule of vibration-rotation spectra of H^{35}Cl ? (b) What is **R branch**? (c) What is **P branch**? (d) Please simply draw the **vibration-rotation spectra** of H^{35}Cl and assign the peaks. (Assume that at room temperature) (e) Point out the **band origin** in the spectra that you drew. (10 points)

II. Analytical chemistry (50 points)

- The concentration of Ca^{2+} in a serum sample is determined using a Ca ion-selective electrode (Ca-ISE) and one-point standard addition. A 10.00-mL sample is transferred to a 100-mL volumetric flask and diluted to volume. A 50.00-mL aliquot of diluted sample solution is placed in a beaker with the Ca-ISE and a reference electrode, and the potential is measured as -0.1090V. After a 2.00-mL of $1.50 \times 10^{-3}\text{ M}$ Ca^{2+} solution is added, the measured potential is -0.0872V. What is the ppm concentration of Ca^{2+} in the original serum sample? (Ca: 40.08) (8 points)
- (a) What is the order in which the following compounds: benzoic acid, benzene, phenol, and p-hydroxybenzoic acid, would be eluted from a C18 column by using acetonitrile/ H_2O as eluent? (3 points)
(b) Explain the order considering the stationary phase and the mobile phase. (5 points)
- Electromagnetic radiation is divided into different regions based on the type of atomic or molecular transition. State the molecular transition and give an example of spectroscopic technique according to the following regions of electromagnetic radiation: X-ray, UV/Vis, infrared, microwave and radio wave. (10 points)
- How to prepare 500. mL buffer solution (total acetate = 0.100 M) at pH 4.90 by using sodium acetate (Formula weight = 82.03) and glacial acetic acid (17.5 M, $\text{pK}_a=4.76$)? (8 points)
- Write charge balance and mass balance equations for the mixed solution of 0.100 M Na_2CO_3 and 0.200 M Na_2HPO_4 . (8 points)
- The following calibration data were obtained by an instrumental method for the determination of species X in aqueous solutions.

conc. X, ppb	No. replications	mean signal	standard deviation
0.00	25	0.028	0.0072
2.00	5	0.170	0.0088
6.00	5	0.415	0.0090
10.00	5	0.688	0.0085
15.00	5	1.022	0.0084

- (a) Calculate the calibration sensitivity? (5 points)

(hint: $y = mx + b$, wherein $m = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}$, $b = \frac{\sum y_i - m \sum x_i}{n}$)

- (b) Calculate the detection limit for the method? (3 points)