

說明：1. 請標明題號並依序作答。

2. 計算題必須寫出計算過程，只寫答案不給分。可使用一般計算機。

3.  $R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$ ,  $h = 6.626 \times 10^{-34} \text{ J s}$ ,  $c = 2.998 \times 10^8 \text{ m s}^{-1}$

1. Draw all normal modes of  $\text{H}_2\text{O}$  and rank the mode frequencies of  $\text{H}_2\text{O}$  in increasing order. (10%)
2. Determine the ratio of (a) the mean speeds, (b) the mean kinetic energies of  $\text{H}_2(\text{g})$  and  $\text{O}_2(\text{g})$  at 300 K. (5%, 5%)
3. The communication frequency of cell phones is around 900 MHz or 1800 MHz. Can the electromagnetic radiation of communication be absorbed by the most air molecules  $\text{N}_2$  and  $\text{O}_2$ ? Explain your answer. (10%)
4. For the first-order reaction  $\text{A} \rightarrow 3\text{B} + \text{C}$ , when  $[\text{A}]_0 = 0.015 \text{ mol L}^{-1}$ , the concentration of B increases to  $0.018 \text{ mol L}^{-1}$  in 3.0 min. (a) What is the rate constant for the reaction? (b) How much more time would be needed for the concentration of B to increase to  $0.030 \text{ mol L}^{-1}$ ? (5%, 5%)
5. (a) What is spin-orbit coupling? (b) The first two sodium D lines are 589.158 nm and 589.755 nm in vacuum which are due to  $3p$  to  $3s$  transitions. Derive the spin-orbit coupling constant for the  $3p$  state levels of sodium. (4%, 8%)  
(hint:  $E = hcA\{j(j+1) - l(l+1) - s(s+1)\}/2$  A: spin-orbit coupling constant)
6. (a) Why are so many exothermic reactions spontaneous?  
(b) Using the relationship  $\ln(K) = -\frac{\Delta H^\circ}{RT} + \frac{\Delta S^\circ}{R}$  show that for a system at equilibrium the equilibrium will shift to the right for an endothermic process when the temperature is increased. (4%, 8%)
7. (a) What is photoelectron? (b) Explain in detail of the "X-ray photoelectron spectroscopy". (4%, 8%)
8. The enthalpy of vaporization of chloroform is  $29.4 \text{ kJ mol}^{-1}$  at its normal boiling point of 335 K. Calculate (a) the entropy of vaporization of chloroform at this temperature and (b) the entropy change of the surroundings. (6%, 6%)
9. Explain (a) dispersion interaction (b) Lennard-Jones potential (c) impact parameter (12%)