

國立彰化師範大學九十六學年度碩士班招生考試試題

系所：化學系

科目：物理化學

請在答案紙上作答

共 1 頁 第 1 頁

**NOTE: You must show details of your analyses, and calculations.**

1. (16 %) The vibrational frequency of N-H bond is about  $3100 \text{ cm}^{-1}$ , what is the energy required to promote such vibration in terms of kcal/mol ? What is the zero-point vibrational energy of this motion ?
2. (30 %) Explain the following terms : (a) first law of thermodynamics, (b) second law of thermodynamics, (c) third law of thermodynamics, (d) Pauli exclusion principle, (e) expectation value, (f) eigenvalue.
3. (10 %) The Arrhenius rate constant is expressed as :  $k = Ae^{-E_a/RT}$ , given rate constants at different temperatures, describe how you can obtain the activation energy.
4. (12 %) The standard enthalpies of combustion of C(s), H<sub>2</sub>(g), and CH<sub>4</sub>(g) are -94.0, -68.3, and -212.8 kcal/mol, respectively at 298 K. Calculate the standard enthalpy of formation of CH<sub>4</sub>(g).
5. (12 %) For a particle-in-a-box (one-dimensional) system with the width of box being L, what are the expectation values for (a)  $x$  (position), and (b)  $p_x$  (momentum) operators at  $n=1$  ? Use the known wavefunctions of the system to explain "correspondence principle".
6. (20 %) Derive the rate laws for (a) first order and (b) second order reactions in which there is only one reactant, and describe how you can measure the rate constants, using the concentration versus time data of the reactant.

**Useful constants:**

Planck constant  $h = 6.626 \times 10^{-34} \text{ Js}$ ; speed of light  $c = 2.998 \times 10^{10} \text{ cm s}^{-1}$