說明：1.請依序作答並標明題號。

2.計算題必須寫出計算過程，只寫答案不給分。

3.R＝8.314　$JK^{-1}mol^{-1}$

4.考生可使用一般計算機。

1) (a) The fundamental vibrational wavenumber for stretching of a C-H bond is 3000 $cm^{-1}$. Predict the vibrational wavenumber as the H is replaced by D. (b) The rate of breaking a C-D bond is lower than of a C-H bond. Why ? (15%)

2) Derive the integrated rate law for a second order reaction A + B ------>P ([A]=$[A]_o$ and [B]=$[B]_o$ at t=0, k = rate constant). (10%)

3) Write down the rotational energy terms for a linear molecule and the partition function for the rotor. (10%)

4) Draw the unit cell for face-centered cubic lattice. (5%)

5) Derive the Langmuir adsorption isotherm. (The dynamic equilibrium is A(g) + M(surface) $\rightleftharpoons$ AM(surface) with rate constant $k_a$ for adsorption and $k_d$ for desorption, $\theta$ for surface coverage, and p for pressure.) (10%)

6) Suppose two electrons in an atom occupy an orbital $\psi$, then in the orbital approximation the overall wavefunction is $\psi(1)\psi(2)$. Write the total wavefunction, the wavefunction including spin, that is allowed by Pauli principle. (10%)

7) Using potential energy curves to explain Dissociation and Predissociation for a chemical bond. (15%)

8) Explain in detail the principle of a four-level laser. (10%)

9) (a) State the third-law of thermodynamics
(b) Calculate the change in entropy that occurs when a sample containing 1.0 mole water is heated from 50°C in liquid state to 100°C in vapor state. The molar heat capacity for $H_2O(l)$ is 75.3 $JK^{-1}mol^{-1}$ and the enthalpy of vaporization of water is 40.7 $kJmol^{-1}$ at 100°C. (15%)