※ 注意：請於試卷上「非選擇題作答區」標明大題及小題題號，並依序作答。

1. (10 pts) Element boron has the electron affinity 27kJ mol^{-1} and the first ionization energy 8.30 eV $atom^{-1}$; the element fluorine has the electron affinity 328kJ mol^{-1} and the first ionization energy 17.42 eV $atom^{-1}$.
   (a) (6 pts) According to Mulliken's electronegativity definition, calculate the electronegativities of these two elements.
   (b) (4 pts) Do you expect the molecule BF_3 to have a large molecular dipole? Explain your reasoning.
2. (16 pts) Draw the Lewis structures (include the possible resonance structures, identify those with the more important contributions) of the following molecules or ion:
   (a) (4 pts) BF_3
   (b) (4 pts) N_2O where the atoms are arranged in the order N N O
   (c) (4 pts) NO_2 where N is in the middle
   (d) (4 pts) $P_3O_9^{3-}$ where three oxygen atoms and three phosphorus atoms are connected alternately to form a ring.
3. (12 pts) Given the following atomic wave functions of the hydrogen atom, identify their quantum numbers (n, l, m *etc.*) to name the atomic orbitals. Use suitable plots to describe the electron density of these atomic orbitals.
   (a) (4 pts) $\psi_1 \propto z\, e^{-r/(2a_0)}$
   (b) (4 pts) $\psi_2 \propto y\, e^{-r/(2a_0)}$
   (c) (4 pts) $\psi_3 \propto (2z^2 - x^2 - y^2)e^{-r/(3a_0)}$

   where $r = \sqrt{x^2 + y^2 + z^2}$, a_0 is the Bohr radius.
4. (10 pts) Consider the π system of cyclopropenium ion $C_3H_3^+$ where three carbon atoms form a ring.
   (a) (6 pts) Construct qualitatively the molecular orbitals. Draw the orbital energy diagram and sketch the molecular orbital wave functions.
   (b) (4 pts) What is the C-C bond orders of the neutral molecule C_3H_3 and the cation $C_3H_3^+$ respectively?
5. (10 pts) HCl has the force constant $k = 475.6$ kg/s^2. The atomic mass of hydrogen and chlorine are 1.008 and 35.45 respectively.
   (a) (4 pts) What is the energy difference between the first vibration excited state and the vibration ground state?
   (b) (6 pts) Sketch qualitatively the IR absorption spectrum you expect for the HCl gas vapour.

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6. (12 pts) Given the Maxwell-Boltzmann distribution of molecular speeds

$$f(u) = 4\pi u^2 \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-mu^2/2k_B T}$$

where u is the molecular speed, m the mass of the molecule, k_B the Boltzmann constant, T the temperature.

   (a) (5 pts) Calculate the most probable molecular speed

   (b) (7 pts) Calcuate the root-mean-square velocity. Is it larger than the most probable speed? (Hint: $\int_{-\infty}^{\infty} dx \exp(-x^2) = \sqrt{\pi}$)

7. (10 pts) One mole of H_2O melt from ice to water with ΔH at 0°C.

   $H_2O_{(s)} \longrightarrow H_2O_{(l)}$　　$\Delta H°(273K)$= 16004 J mol^{-1}

   (a) (4 pts) What is the molar entropy change ΔS for H_2O?

   (b) (6pts) Calculate the melting ΔG at 5°C and -5°C from the (metastable) solid to (metastable) liquid. Which melting process can happen spontaneously? (Hint: You can neglect the specific heat difference of ice and the liquid water.)

8. (10 pts) A weak base morphine has $K_b = 8 \times 10^{-7}$. Calculate the pH for the aqueous solutions which contain

   (a) (5 pts) 1.0×10^{-3}M morphine

   (b) (5 pts) 1.0×10^{-6}M morphine.

9. (10 pts) A solution contains both solid Pb and solid Ni, and $NiSO_4$(aq)/$PbSO_4$(aq). Given the standard reduction potential data at 25°C

$$Pb^{2+}(aq) + 2e^- \longrightarrow Pb(s) \quad E_0 = -0.126V$$

$$Ni^{2+}(aq) + 2e^- \longrightarrow Ni(s) \quad E_0 = -0.23V$$

   Calculate the maximal $[Pb^{2+}]/[Ni^{2+}]$ ratio at which the following reaction is spontaneous at 25°C:

$$Pb(s) + Ni^{2+}(aq) \longrightarrow Pb^{2+}(aq) + Ni(s)$$

$R = 8.314$J $mol^{-1}K^{-1}$, $F = 96485$C mol^{-1}, $k_B = 1.38 \times 10^{-23}$J K^{-1}, $h = 6.626 \times 10^{-34}$ J s, 1eV=1.602×10^{-19}J, $N_A = 6.02 \times 10^{23} mol^{-1}$, $c = 3.00 \times 10^8$ m s^{-1}

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