

※ 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。

- (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 $17.42\text{ eV atom}^{-1}$.
 - (6 pts) According to Mulliken's electronegativity definition, calculate the electronegativities of these two elements.
 - (4 pts) Do you expect the molecule BF_3 to have a large molecular dipole? Explain your reasoning.
- (16 pts) Draw the Lewis structures (include the possible resonance structures, identify those with the more important contributions) of the following molecules or ion:
 - (4 pts) BF_3
 - (4 pts) N_2O where the atoms are arranged in the order N N O
 - (4 pts) NO_2 where N is in the middle
 - (4 pts) $\text{P}_3\text{O}_9^{3-}$ where three oxygen atoms and three phosphorus atoms are connected alternately to form a ring.
- (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.
 - (4 pts) $\psi_1 \propto z e^{-r/(2a_0)}$
 - (4 pts) $\psi_2 \propto y e^{-r/(2a_0)}$
 - (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.
- (10 pts) Consider the π system of cyclopropenium ion C_3H_3^+ where three carbon atoms form a ring.
 - (6 pts) Construct qualitatively the molecular orbitals. Draw the orbital energy diagram and sketch the molecular orbital wave functions.
 - (4 pts) What is the C-C bond orders of the neutral molecule C_3H_3 and the cation C_3H_3^+ respectively?
- (10 pts) HCl has the force constant $k = 475.6\text{ kg/s}^2$. The atomic mass of hydrogen and chlorine are 1.008 and 35.45 respectively.
 - (4 pts) What is the energy difference between the first vibration excited state and the vibration ground state?
 - (6 pts) Sketch qualitatively the IR absorption spectrum you expect for the HCl gas vapour.

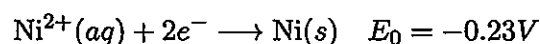
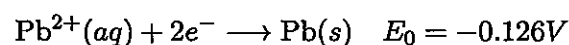
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6. (12 pts) Given the Maxwell-Boltzmann distribution of molecular speeds

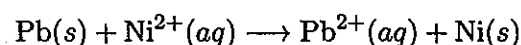
$$f(u) = 4\pi u^2 \left(\frac{m}{2\pi k_B T} \right)^{3/2} e^{-mu^2/2k_B T}$$

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) Calculate 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 $0^\circ C$.
 $H_2O_{(s)} \rightarrow H_2O_{(l)} \quad \Delta H^\circ(273K) = 16004 \text{ J mol}^{-1}$
- (a) (4 pts) What is the molar entropy change ΔS for H_2O ?
 (b) (6pts) Calculate the melting ΔG at $5^\circ C$ and $-5^\circ C$ 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) $1.0 \times 10^{-3} M$ morphine
 (b) (5 pts) $1.0 \times 10^{-6} M$ 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 $25^\circ C$



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



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