

1. (5 points) Write the ground-state electron configurations of (a) C, (b) Na, (c) Fe, (d) Cu, and (e) Cu^{2+} . 5

(15 points) When we solve Schrodinger equation of the hydrogenic atoms (containing one electrons and one nucleus), we can get the wavefunctions (atomic orbitals) of an electron in the atoms, which are represented by principal quantum number (n), orbital angular quantum number (l), and magnetic quantum number (m_l). The energy levels of the wavefunctions are given by $E = -RZ^2/n^2$ (Z is the atomic number and R is a constant.).

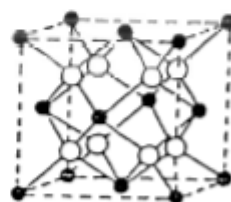
(a) Determine the n , l , and m_l values of the following atomic orbitals. **1s, 2s, 2p, 3d, 4s.** 5

(b) If the electron of the ground-state hydrogen atom is first excited to $n=2$ level by an external light, can we determine the orbital in which the excited electron should be placed? Say **yes** or **no**. If the answer is **yes**, write the orbital. If the answer is **no**, write the reasoning. 2

(c) How about for Li^{2+} ? (The same question as (b).)

(d) For B atom, the 2s orbital has lower energy than the 2p orbital. Explain the reason. 5

3. (15 points) The following figure shows a unit cell structure of an ionic solid structure.



(a) What is the name of the structure? 3

(b) In the figure, black dots represent the sites of cations and the open circles represent the sites of anions. What kind of packing array do the cations lie in? What kind of hole do the anion occupy in the cation array? 3

(c) What are the coordination numbers of the cation and the anion? 3

(d) What is stoichiometric formula? 3

Give one example which adopt the above structure? 3

(25 points) The total potential energy of a solid is given by

$$V = \frac{N_A e^2}{4\pi\epsilon_0} \left(\frac{z_A z_B}{d} \right) A + N_A C \exp\left(-\frac{d}{d^*}\right)$$

as a function of the separation (d) between the nearest cation and anion.

Here, N_A , e , ϵ_0 , z_A , z_B , A , C , and d^* are the Avogadro number ($N_A = 6.022 \times 10^{23}/\text{mol}$), the electron charge ($e = 1.602 \times 10^{-19} \text{ C}$), the vacuum permittivity ($4\pi\epsilon_0 = 1.113 \times 10^{-10} \text{ C}^2/\text{Jm}$), the cation charge number, the anion charge number, the Madelung constant, a constant, and $0.345 \text{ \AA}$, respectively.

(a) Derive the equation for the minimum potential energy. (Born-Mayer Equation) 5

(b) The ionic solid structure of AgCl is **Rock-Salt**. The Madelung constant for the Rock-Salt structure is 1.748. When the separation between Ag^+ and Cl^- is $2.514 \text{ \AA}$, calculate the minimum potential energy of AgCl solid? (Unit should be kJ/mol.) 5

(c) Calculate the lattice enthalpy of AgCl (s) using a Born-Harber cycle and the following data. 10

Formation of AgCl (s) $H = -127 \text{ kJ/mol}$

Sublimation of Ag (s) $H = 285 \text{ kJ/mol}$

Ionization of Ag (g) $H = 731 \text{ kJ/mol}$

Dissociation of Cl_2 (g) $H = 244 \text{ kJ/mol}$

Electron gain by Cl (g) $H = -355 \text{ kJ/mol}$

Compare the results of (b) and (c) to discuss the ionic properties of AgCl . 5

5. (10 points) (a) Draw the Lewis structures of the following molecules or ions. CH_4 , ICl_2^- , BeCl_2 , NH_3 , SF_6 . 5
(b) Predict the structures of the molecules or ions of (a) by using VSEPR theory. Draw the structures and Write the names of the structures (both including and excluding the lone pairs). 5

(15 points) O_2 molecule has the following characteristics 1. A double bond holds two O nuclei. 2. Each O atom has two lone pairs. 3. O_2 molecule is paramagnetic. Explain these characters as the following order.

Draw the Lewis structure of O_2 molecule. 3

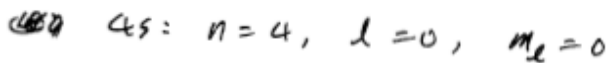
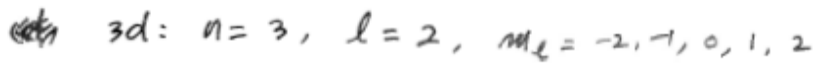
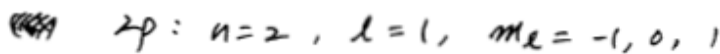
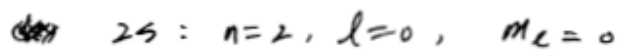
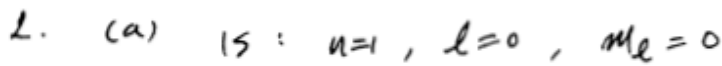
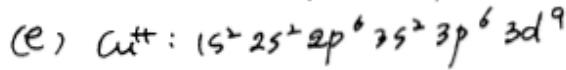
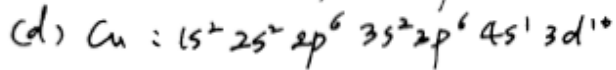
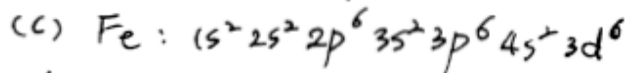
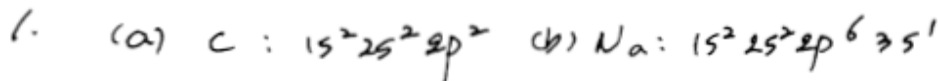
(b) The double bond is comprised of one σ -bond and one π -bond. Explain these with sp^2 -hybrid and p-orbital of O atoms. 3

(c) Draw the energy levels of the molecular orbitals. Represent the ground-state electron configuration with arrows on the energy level diagram. Show the bond order of two and the paramagnetic properties of O_2 molecule using the electron configuration. 6

(d) In the process of $\text{O}_2 \rightarrow \text{O}_2^+ + e^-$, is the bond length increasing or decreasing? Give your reasoning. 3

7. (5 points) What are the formal charges and the oxidation numbers of O atoms and N atom in NO_3^- ?

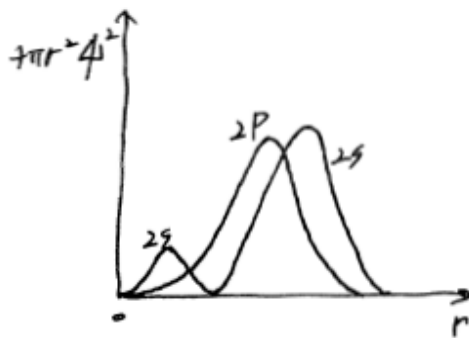
8. (Bonus! 10 points) Give your comments about the inorganic chemistry I lecture. (Anything about the lecture. Things were good, bad, and ugly. Thing should be improved, changed, and added.)



(b) no. 2s and 2p orbitals are degenerated.

(c) no. " "

(d) Radial distribution functions for 2s and 2p.



As in the figure, 2s orbital can penetrate closer to the nucleus than 2p orbital. When electrons are placed in 2s orbital, 2p orbitals feel the effective nuclear charge, which is less than the original nuclear charge, due to the shielding effect of 2s orbital. From the equation

$E = -\frac{R_H Z^2}{n^2}$, we can predict $E_{2s} < E_{2p}$.

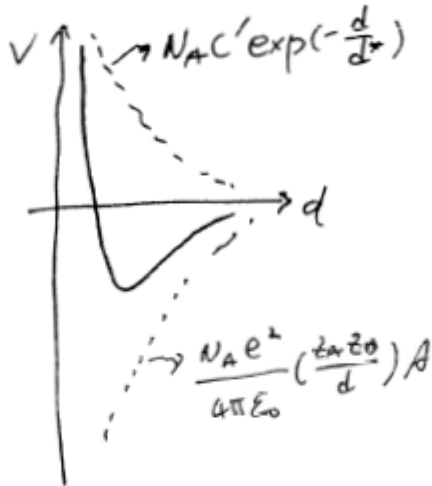
nuclear charge

3. (a) fluorite (b) cation: fcc, anion: tetrahedral holes

(c) cation: 8, anion: 4 (d) AB_2 (A: cation, B: anion)

(e) CaF_2 , BaCl_2 , NiSi_2 , ...

4. (a)



$$V = \frac{N_A e^2}{4\pi\epsilon_0} \left(\frac{z_A z_B}{d} \right) A + N_A C' \exp\left(-\frac{d}{d^*}\right)$$

at minimum

$$\frac{dV}{dd} = 0$$

$$\frac{dV}{dd} = \frac{N_A e^2}{4\pi\epsilon_0} \left(\frac{z_A z_B}{-d^2} \right) A$$

$$- \frac{1}{d^*} N_A C' \exp\left(-\frac{d}{d^*}\right)$$

$$= 0$$

$$\therefore N_A C' \exp\left(-\frac{d}{d^*}\right) = \frac{N_A e^2}{4\pi\epsilon_0} \left(\frac{z_A z_B}{-d^2} \right) A \frac{d}{d^*}$$

$$\therefore U_{\min} = \frac{N_A e^2}{4\pi\epsilon_0} \left(\frac{z_A z_B}{d} \right) A - \frac{N_A e^2}{4\pi\epsilon_0} \frac{z_A z_B}{d^2} \cdot d^*$$

$$= \frac{N_A e^2}{4\pi\epsilon_0} \frac{z_A z_B}{d} \left(1 - \frac{d^*}{d} \right) A \quad \text{: Born-Mayer Equation}$$

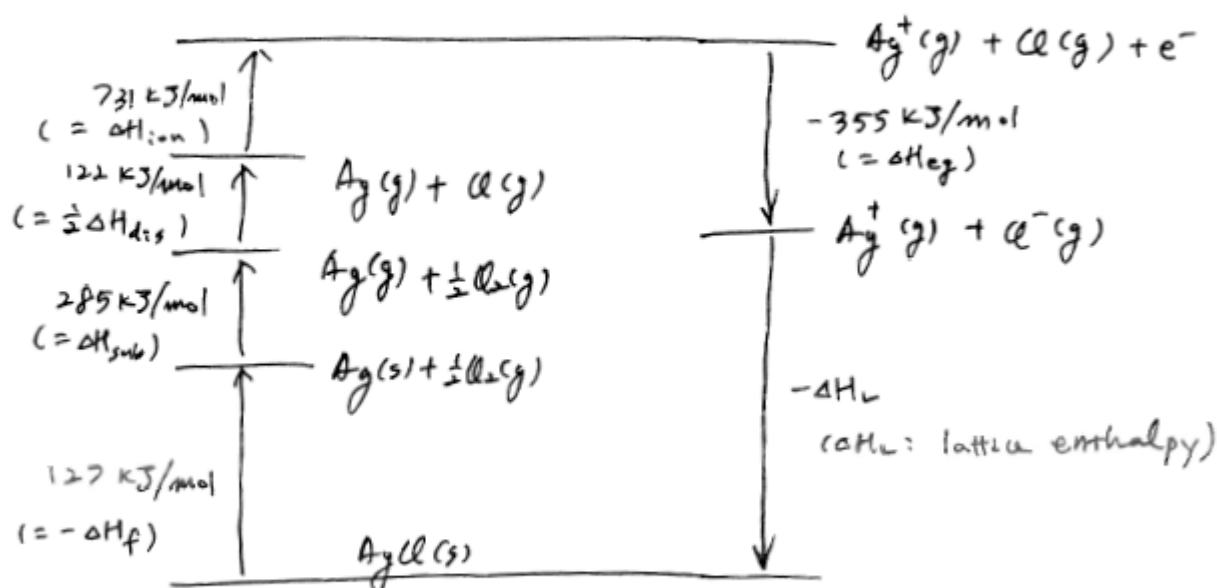
(b)

$$V = \frac{(6.022 \times 10^{23} / \text{mol}) (1.602 \times 10^{-19} \text{C})^2}{1.13 \times 10^{-10} \text{C}^2 / \text{Jm}} \cdot \frac{1}{2.514 \times 10^{-10} \text{m}} \cdot \left(1 - \frac{0.345 \text{\AA}}{2.514 \text{\AA}} \right) \cdot 1.744$$

$$= 833 \text{ kJ/mol}$$

4. (cont'd)

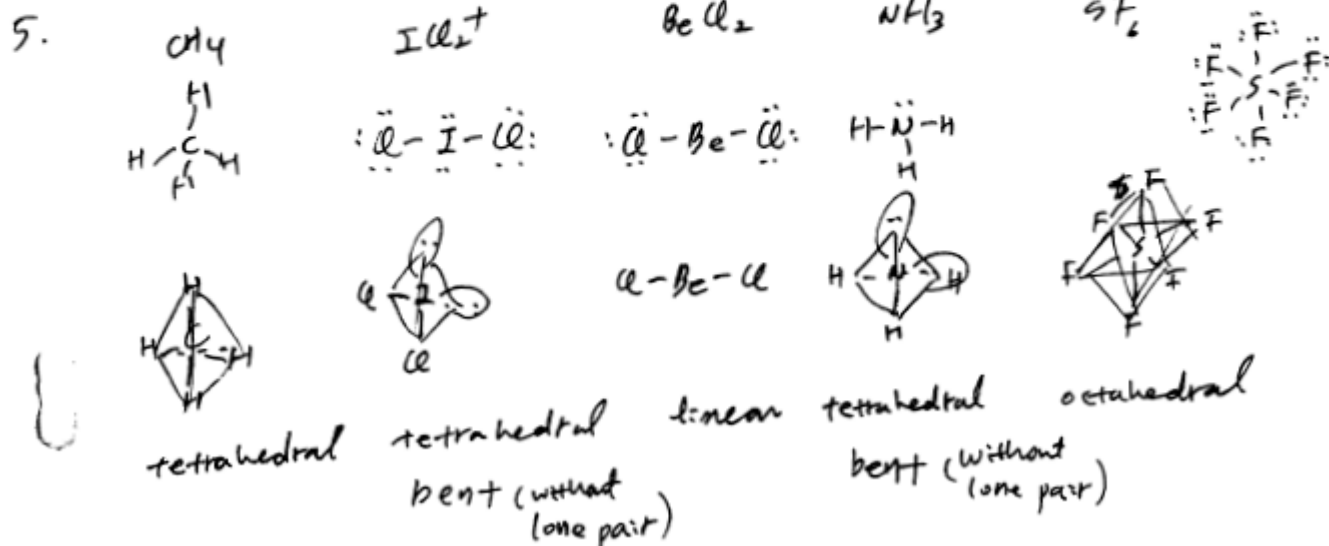
(c)



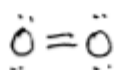
$$\therefore [127 + 285 + 122 + 731 - 355] \text{ kJ/mol} - \Delta H_L = 0$$

$$\therefore \Delta H_L = 910 \text{ kJ/mol}$$

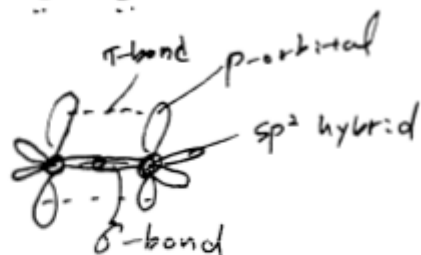
(d) Born-Mayer Eq. was derived from the assumption of ionic model. calculated value (833 kJ/mol) / experimental value ($= 910 \text{ kJ/mol}$) is 91.5%. we can predict AgCl includes pretty much bond covalent character.



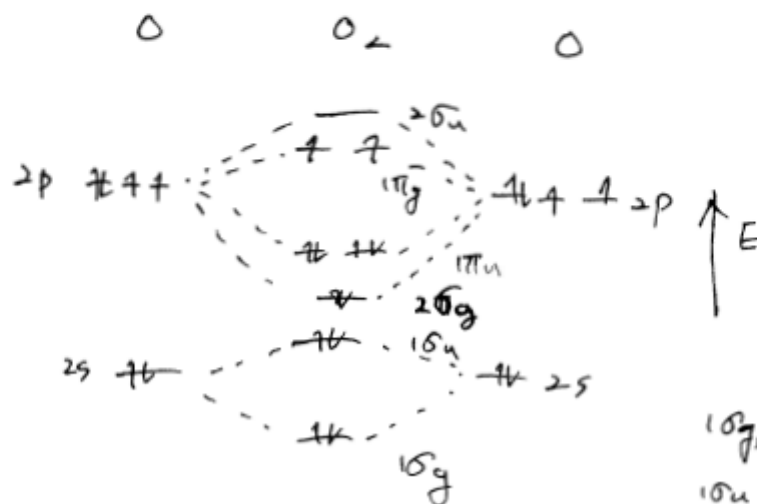
6. (a)



(b)



(c)

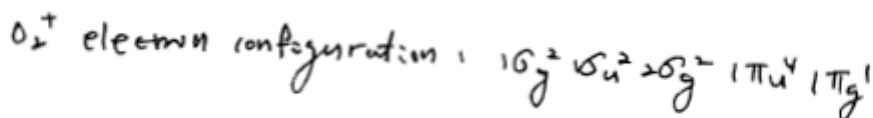
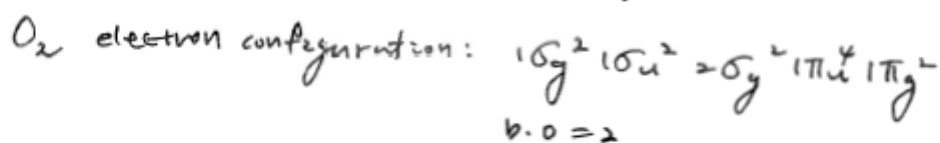


$1\sigma_g, 2\sigma_g, 1\pi_u$: bonding orbital
 $1\sigma_u, 1\pi_g, 2\sigma_u$: anti-bonding orbital

$$\text{bond order} = \frac{8 - 4}{2} = 2$$

two unpaired electrons in $1\pi_g$ anti-bonding orbital
 $\Rightarrow$ paramagnetic

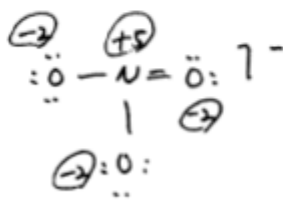
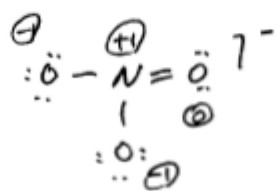
(d)



$$\therefore \text{b.o} = \frac{8 - 3}{2} = 2.5$$

$\therefore$ Bond length increases.

7.



formal charge

oxidation number