

Homework III

Introduction to Physical Chemistry

Basil R. Yap 1001690

2018 February 08

1 Question 1

$$\begin{aligned} E &= -(2.18 \times 10^{-18}) \frac{Z^2}{n^2} \\ \text{(a)} \quad &= -(2.18 \times 10^{-18}) \frac{3^2}{1^2} \\ &= -1.96 \times 10^{-17} J \end{aligned}$$

(b) **Figure 1:**



Figure 1: Line Spectrum

2 Question 2

(a) $1s^1$

$$E = -(2.18 \times 10^{-18}) \frac{Z^2}{n^2}$$

$$\begin{aligned} \text{(b)} \quad &= -(2.18 \times 10^{-18}) \frac{4^2}{3^2} \\ &= -3.876 \times 10^{-18} J \end{aligned}$$

$$E = hv$$

$$\begin{aligned} v &= \frac{E}{h} \\ \text{(c)} \quad &= \frac{3.876 \times 10^{-18}}{6.626 \times 10^{-34}} \\ &= 5.849 \times 10^{15} \text{Hz} \end{aligned}$$

$$E = -(2.18 \times 10^{-18}) \frac{Z^2}{n^2}$$

$$\begin{aligned} \text{(d)} \quad &= -(2.18 \times 10^{-18}) \frac{1^2}{3^2} \\ &= -9.69 \times 10^{-19} J \end{aligned}$$

The binding energy of a H electron is higher than that of a Be electron. This is because the nuclear charge of a beryllium ion is higher than the nuclear charge of a hydrogen ion, requiring more energy to remove an electron from the second excitation level.

(e) This is an emission of a photon, as the electron goes from a lower potential energy level to a higher potential energy level.

$$\begin{aligned} \Delta E &= -(2.18 \times 10^{-18}) \left(\frac{Z^2}{n_1^2} - \frac{Z^2}{n_2^2} \right) \\ &= -(2.18 \times 10^{-18}) \left(\frac{4^2}{3^2} - \frac{4^2}{1^2} \right) \\ &= 3.1 \times 10^{-17} \end{aligned}$$

$$E = \frac{hc}{\lambda}$$

$$\begin{aligned} \lambda &= \frac{hc}{E} \\ &= \frac{6.626 \times 10^{-34} \times 2.99 \times 10^8}{3.1 \times 10^{-17}} \\ &= 6.39 \times 10^{-9} m \end{aligned}$$

3 Question 3

$$\begin{aligned}
 KE &= \frac{hc}{\lambda} - \Phi \\
 \text{(a)} \quad &= \frac{6.626 \times 10^{-34} \times 2.99 \times 10^8}{9.89 \times 10^{-10}} - \Phi \\
 &= 2 \times 10^{-16} - \Phi
 \end{aligned}$$

Energy levels	Φ	KE
2s	273 eV	1.563×10^{-16}
2p	205 eV	1.672×10^{-16}
3s	21 eV	1.966×10^{-16}
3p	10 eV	1.984×10^{-16}

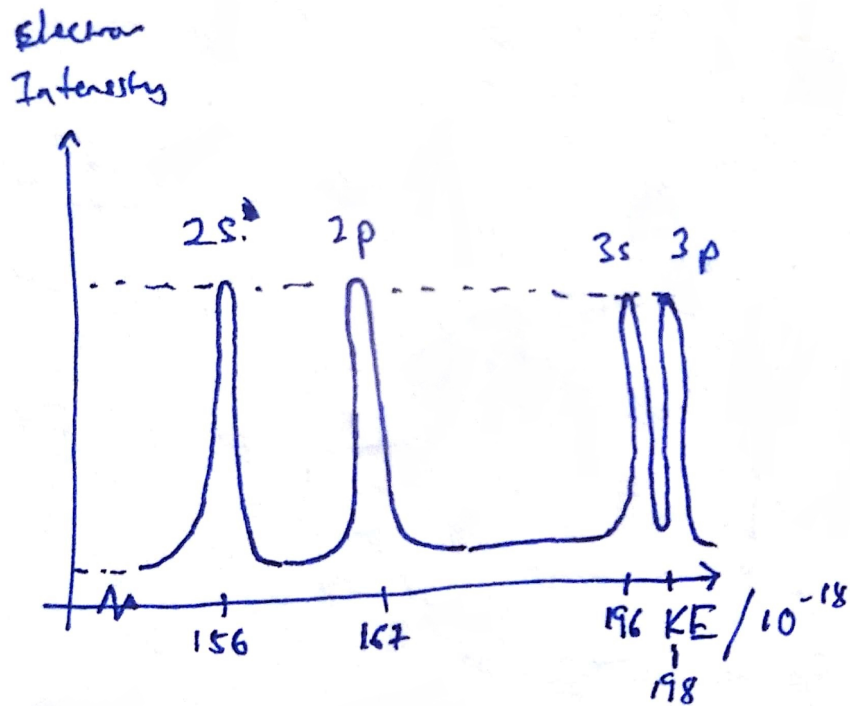


Figure 2: Stick Spectrum

$$\begin{aligned}
 Z_{eff} &= Z - S \\
 \text{(b)} \quad &= 17 - 10 \\
 &= +7
 \end{aligned}$$

4 Question 4

(a) Figure 3

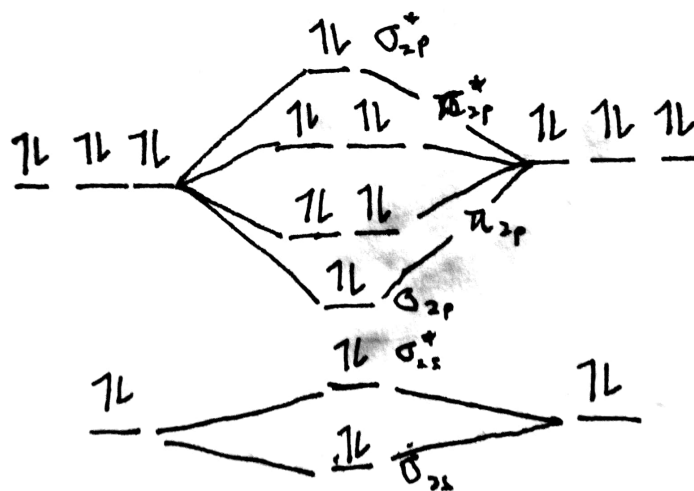
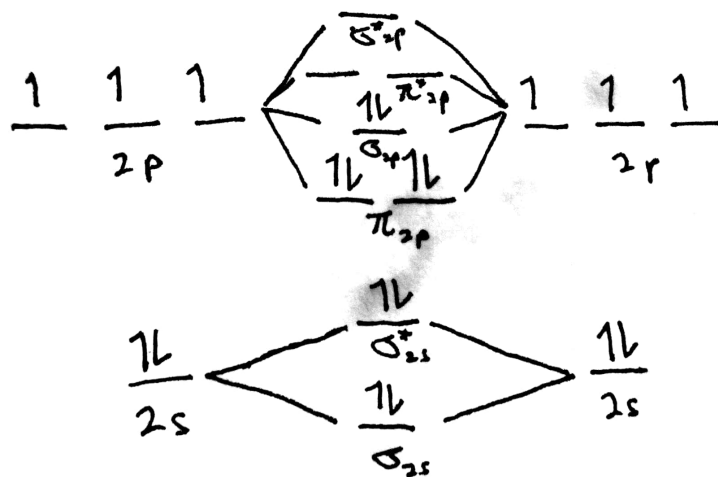


Figure 3: Molecular Orbital Diagram of N_2 (above) & Ne_2 (below)

- (b)
- N_2 : $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2px})^2(\pi_{2py})^2(\sigma_{2pz})^2$
 - Ne_2 : $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2pz})^2(\pi_{2px})^2(\pi_{2py})^2(\pi_{2px}^*)^2(\pi_{2py}^*)^2(\sigma_{2pz}^*)^2$
- (c) From the the MO Diagram,
- N_2 : 3
 - Ne_2 : 0

N_2 is more stable than Ne_2 because it has a higher bond order. This is because both molecules have the same number of bonding orbitals but N_2 has fewer anti-bonding orbitals.

- (d) Yes, there is a difference between the positions of the σ_{2p} and π_{2p} orbitals of the two molecules. In N_2 , the π_{2p} orbital is at a lower energy level than σ_{2p} , and the opposite is true for Ne_2 . This is due to a phenomena called s-p mixing, where molecules made of elements with lower nuclear charge have small differences in energy level between σ_{2p} and π_{2p} . At higher nuclear charges, such as Ne, the difference becomes significant enough for the energy level of π_{2p} to be higher than that of σ_{2p} .

5 Question 5

- (a)
- A: B
 - Bond order = 1.5
- (b)
- D: Be
 - Bond order = 0
- (c)
- E: F
 - Bond order = 2

6 Question 6

(a) Figure 4:

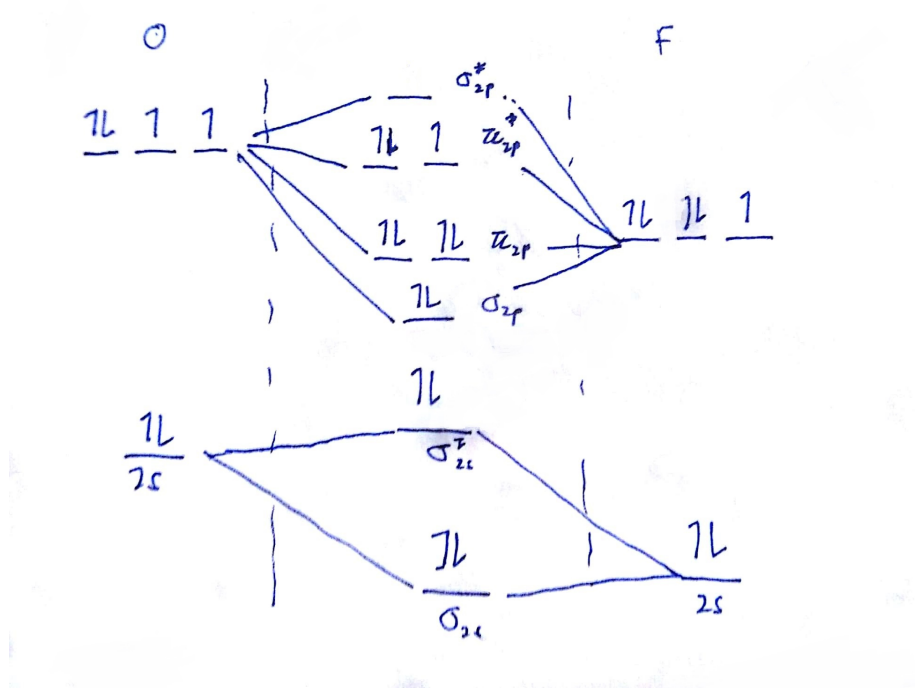


Figure 4: MO Diagram of FO

- (b) The MO bond order of OF = 1.5
- (c) The MO bond order of OF^+ = 2
The bond shortens because the electron in the π_{2px}^* orbital is removed, reducing the number of electrons populating the anti-bonding orbitals by one, thereby increasing the bond order and decreasing the bond length.
- (d)
- HOMO: π_{2px}^*
 - LUMO: σ_{2pz}^*
- (e) Paramagnetic