Phy 491 HW 3

Problem 3.1 Given are the following electron configurations $1s^2 2s^2 2p^6 3s^2 3p^5$ and $[Ar] 4s^2 3d^6$

3.1.1 Find the elements corresponding to these electron configurations. (2 points)

3.1.2 What type of magnetism do you expect for both and why? (4 points)

3.1.1

Element 1: Chlorine
Element 2: Iron

3.1.2

We are considering either paramagnetism or diamagnetism. Our rule of thumb is that an element is paramagnetic unless $J = 0$, in which case it is diamagnetic.

Chlorine and Iron both have unpaired electrons in their outermost shells. Chlorine has one unpaired in its 3p orbital, and Iron has four unpaired electrons. As such, there is a net angular momentum $\neq 0$ for both resulting in paramagnetism

Problem 3.2 Assuming full shielding by all electrons in shells with $n < n_{valence}$,

3.2.1 Calculate the first ionization energy of S. (4 points)

3.2.2 Is this assumption realistic? Discuss. (3 points)

S aka Sulfur?

3.2.1

Sulfur has the electron configuration [Ne]$3s^2 3p^4$, and google reports it's first ionization energy is 10.36eV, but this result is found experimentally.

To calculate the first ionization energy, we need to make another strong assumption aside from full shielding: no $e^- e^-$ interactions. Using both of these, we can use our very simple ionization energy equation

$$E_n = -\frac{Z_{\text{eff}}^2}{n^2} R$$

For electrons in the outermost orbital $3p$, we have $n = 3$. Since there are 12 electrons in the inner orbitals, $Z_{\text{eff}} = 16 - 12 = 4$, yielding

$$\begin{aligned} E_3 &= -\frac{4^2}{3^2}(13.6)eV \\ &= -24.2eV \end{aligned}$$

3.2.2

Well, based off the difference from the experimental value, I'd say no it is not. The electrons in lower shells do not necessarily shield out the valence electrons fully since there is overlap in their wave functions.

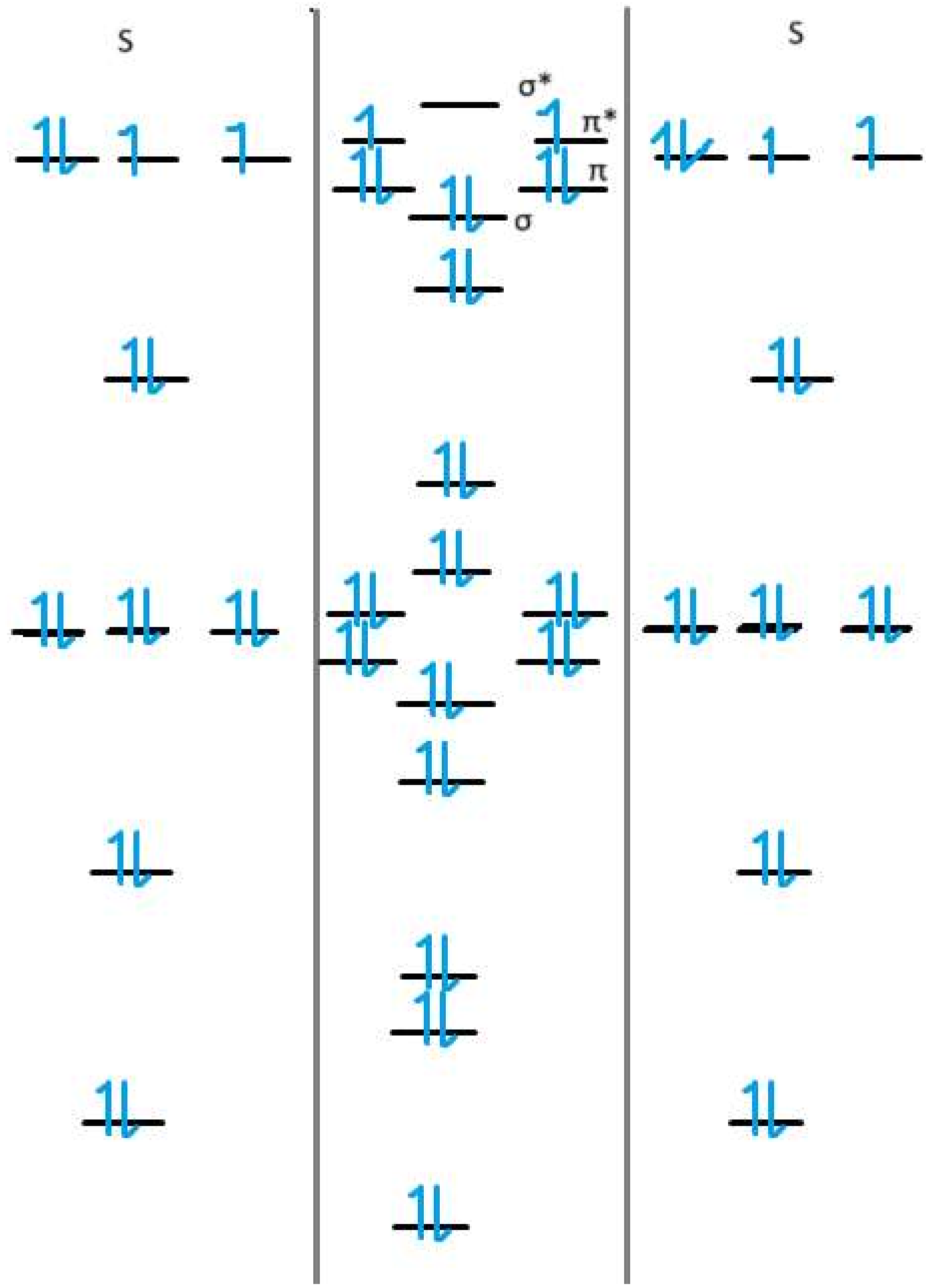
Problem 3.3 Disulfur is the diatomic molecule with the formula S_2. It is analogous to the dioxygen molecule but rarely occurs at room temperature.

3.3.1 Sketch the molecular orbital diagram for S_2 in its ground state. (4 points)

3.3.2 Calculate the bond order. What can you say about the stability of S_2 based on the result? (3 points)

3.3.1

Molecular orbital diagram:



3.3.2 Bond order formula:

$$B = \frac{(\text{bonding } e^-) - (\text{antibonding } e^-)}{2} = \frac{6-2}{2} = 2$$

According to bonding order, S_2 is a stable molecule