CHEM 1410 Homework 8 Solutions

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P11.19

A

For d^5:

$$\begin{aligned} l &= 2 \\ m_l &= \{-2,-1,0,1,2\} \quad \Rightarrow \quad m_{l_{max}} = -2-1+0+1+2 = 0 \quad \Rightarrow \quad S \\ m_s &= \frac{5}{2} \quad \Rightarrow \quad \frac{5}{2}(2)+1 = 6 \end{aligned}$$

The term symbol is then $^{\mathbf{6}}\boldsymbol{S}$.

B

For f^3:

$$\begin{aligned} l &= 3 \\ m_l &= \{-3,-2,-1,0,1,2,3\} \quad \Rightarrow \quad m_{l_{max}} = 1+2+3 = 6 \quad \Rightarrow \quad I \\ m_s &= \frac{3}{2} \quad \Rightarrow \quad \frac{3}{2}(2)+1 = 4 \end{aligned}$$

The term symbol is then $^{\mathbf{4}}\boldsymbol{I}$.

C

For p^4:

$$\begin{aligned} l &= 1 \\ m_l &= -1,0,1 \quad \Rightarrow \quad m_{l_{max}} = 1+0-1+1 = 1 \quad \Rightarrow \quad P \\ m_s &= \frac{2}{2} \quad \Rightarrow \quad \frac{2}{2}(2)+1 = 3 \end{aligned}$$

The term symbol is then $^{\mathbf{3}}\boldsymbol{P}$.

P11.36

Ground-state term symbol for d^5 is $^{\mathbf{6}}\boldsymbol{S}$ from the previous problem. There are 5 m_l values and 2 m_s values, leading to $n = 10$. There are 5 electrons, leading to $m = 5$. Then

$$\frac{n!}{m!(n-m)!} = \frac{10!}{5!5!} = \mathbf{252}$$

Since $S = 5/2$ and $L = 0$, there are $(5+1)(0+1) = \mathbf{6}$ states.

Q12.21

The electrostatic potential shows a blue region on the H atoms. This means that electrons have left the H atoms, making the H atoms electron donors.

P12.5

A

$$BO_{Li_2} = \frac{4-2}{2} = \mathbf{1}$$
$$BO_{Li_2^+} = \frac{3-2}{2} = \mathbf{0.5}$$

B

$$BO_{C_2} = \frac{8-4}{2} = \mathbf{2}$$
$$BO_{C_2^+} = \frac{7-4}{2} = \mathbf{1.5}$$

C

$$BO_{O_2} = \frac{10-6}{2} = \mathbf{2}$$
$$BO_{O_2^+} = \frac{10-5}{2} = \mathbf{2.5}$$

D

$$BO_{F_2} = \frac{10-8}{2} = \mathbf{1}$$
$$BO_{F_2^-} = \frac{10-9}{2} = \mathbf{0.5}$$

P12.8

A

a	MO_6	bonding σ
b	MO_4	anti-bonding σ
c	MO_5	bonding π
d	MO_8	anti-bonding π
e	MO_7	bonding π
f	MO_3	bonding σ

B

MO's 5 and 7 should have equal energies since they are simply the x- and y- components of the π MOs.

P12.19

Anti-bonding LUMO and non-bonding HOMO. This diagram differs from the HF diagram in that the AO energies are shifted up for O, affecting the MO energies. This should not be enough to drastically change the MO energies and ordering.