

CHAPTER 5: MOLECULAR ORBITALS

5.1 There are three possible bonding interactions:



- 5.2 a. Li_2 has a bond order of 1.0 (two electrons in a σ bonding orbital; see Figures 5.7 and 5.1). Li_2^+ has a bond order of only 0.5 (one electron in a σ bonding orbital). Therefore, Li_2 has the shorter bond.
- b. F_2 has a bond order of 1.0 (see Figure 5.7). F_2^+ has one less antibonding (π^*) electron and a higher bond order, 1.5. F_2^+ would be expected to have the shorter bond.
- c. Expected bond orders (see Figure 5.1):

	Bonding electrons	Antibonding electrons	Bond order
He_2^+	2	1	$\frac{1}{2}(2 - 1) = 0.5$
HHe^+	2	0	$\frac{1}{2}(2 - 0) = 1$
H_2^+	1	0	$\frac{1}{2}(2 - 1) = 0.5$

Both He_2^+ and H_2^+ have bond orders of 0.5. HHe^+ would therefore be expected to have the shortest bond because it has a bond order of 1.

- 5.3 a. These diatomic molecules should have similar bond orders to the analogous diatomics from the row directly above them in the periodic table:

P_2	bond order = 3 (like N_2)	
S_2	bond order = 2 (like O_2)	
Cl_2	bond order = 1 (like F_2)	Cl_2 has the weakest bond.

- b. The bond orders match those of the analogous oxygen species (Section 5.2.3):

S_2^+	bond order = 2.5	
S_2	bond order = 2	
S_2^-	bond order = 1.5	S_2^- has the weakest bond.

- c. Bond orders:

NO^+	bond order = 3 (isoelectronic with CO , Figure 5.13)
NO	bond order = 2.5 (one more (antibonding) electron than CO)
NO^-	bond order = 2 (two more (antibonding) electrons than CO)

NO^- has the lowest bond order and therefore the weakest bond.

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