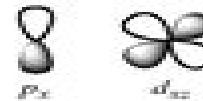
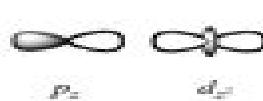


## CHAPTER 5: MOLECULAR ORBITALS

**5.1** There are three possible bonding interactions:



- 5.2** a. Li<sub>2</sub> has a bond order of 1.0 (two electrons in a  $\sigma$  bonding orbital; see Figures 5.7 and 5.1). Li<sub>2</sub><sup>+</sup> has a bond order of only 0.5 (one electron in a  $\sigma$  bonding orbital). Therefore, Li<sub>2</sub> has the shorter bond.
- b. F<sub>2</sub> has a bond order of 1.0 (see Figure 5.7). F<sub>2</sub><sup>+</sup> has one less antibonding ( $\pi^*$ ) electron and a higher bond order, 1.5. F<sub>2</sub><sup>+</sup> would be expected to have the shorter bond.
- c. Expected bond orders (see Figure 5.1):

	Bonding electrons	Antibonding electrons	Bond order
He <sub>2</sub> <sup>+</sup>	2	1	$\frac{1}{2}(2 - 1) = 0.5$
HHe <sup>+</sup>	2	0	$\frac{1}{2}(2 - 0) = 1$
H <sub>2</sub> <sup>+</sup>	1	0	$\frac{1}{2}(2 - 1) = 0.5$

Both He<sub>2</sub><sup>+</sup> and H<sub>2</sub><sup>+</sup> have bond orders of 0.5. HHe<sup>+</sup> 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 <sub>2</sub>	bond order = 3 (like N <sub>2</sub> )
S <sub>2</sub>	bond order = 2 (like O <sub>2</sub> )
Cl <sub>2</sub>	bond order = 1 (like F <sub>2</sub> )

Cl<sub>2</sub> has the weakest bond.

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

S <sub>2</sub> <sup>+</sup>	bond order = 2.5
S <sub>2</sub>	bond order = 2
S <sub>2</sub> <sup>-</sup>	bond order = 1.5

S<sub>2</sub><sup>-</sup> has the weakest bond.

- c. Bond orders:

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

NO<sup>-</sup> has the lowest bond order and therefore the weakest bond.

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