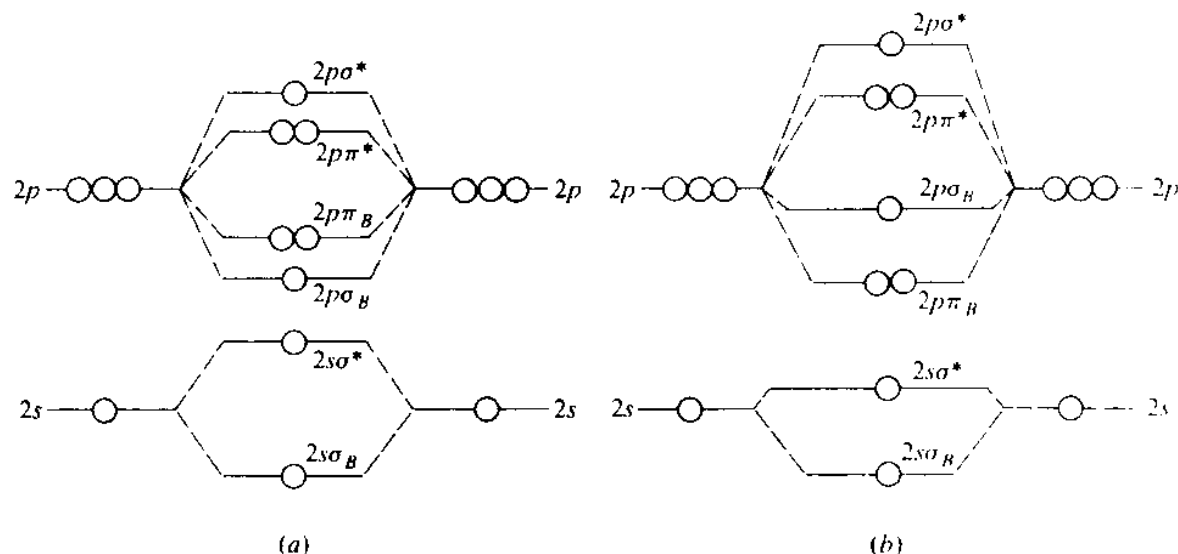


# Diatomic Species of the First Row Elements



**FIGURE 4.7**  
Valence-shell energy level diagrams for a homonuclear diatomic molecule containing first-row atoms. (a) corresponds to no interaction between  $2s$  and  $2p$  levels; (b) corresponds to substantial  $2s$ - $2p$  interaction.

## DIATOMIC SPECIES OF FIRST-ROW ELEMENTS

Species	Valence electron configuration	Unpaired electrons	Bond order	$D$ , kcal mol <sup>-1</sup> †	$r$ , Å
Li <sub>2</sub>	$(s\sigma_B)^2$	0	1	26	2.67
Be <sub>2</sub>	$(s\sigma_B)^2(s\sigma^*)^2$	0	0		
B <sub>2</sub>	$(s\sigma_B)^2(s\sigma^*)^2(p\pi_B)^2$	2	1	71	1.59
C <sub>2</sub>	$(s\sigma_B)^2(s\sigma^*)^2(p\pi_B)^4$	0	2	142	1.31
N <sub>2</sub>	$(s\sigma_B)^2(s\sigma^*)^2(p\pi_B)^4(p\sigma_B)^2$	0	3	226	1.10
O <sub>2</sub>	$(s\sigma_B)^2(s\sigma^*)^2(p\sigma_B)^2(p\pi_B)^4(p\pi^*)^2$	2	2	119	1.21
O <sub>2</sub> <sup>-</sup>	$(s\sigma_B)^2(s\sigma^*)^2(p\sigma_B)^2(p\pi_B)^4(p\pi^*)^3$	1	1.5	...	1.33
F <sub>2</sub>	$(s\sigma_B)^2(s\sigma^*)^2(p\sigma_B)^2(p\pi_B)^4(p\pi^*)^4$	0	1	38	1.42
Ne <sub>2</sub>	$(s\sigma_B)^2(s\sigma^*)^2(p\sigma_B)^2(p\pi_B)^4(p\pi^*)^4(p\sigma^*)^2$	0	0		

† 1 kcal = 4.1840 kJ