Chapter 2:

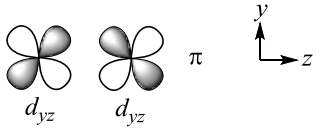
2-1 **a.** For $n = 3$, quantum number l can have values of **0**, **1**, and **2**.

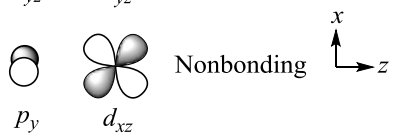
b. One electron in the orbital must have $m_s = \frac{1}{2}$, the other $m_s = -\frac{1}{2}$

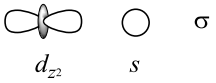
c. p electrons have quantum number $l = 1$; m_l can have the values: **–1**, **0**, **1**

d. In a d subshell ($l = 2$) m_l can have the values: **–2**, **–1**, **0**, **1**, **2**

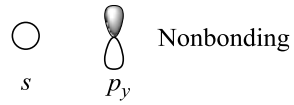
2-2

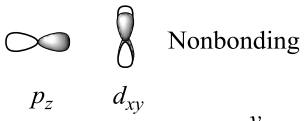
a. 

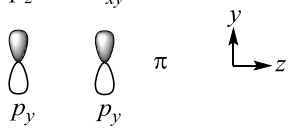
b. 

c. 

2-3

a. 

b. 

c. 

2-4 The molecular orbital diagram of NO is very similar to that of CO (Figure **2-5**).

In NO there is a single electron in a π_{2p}^{*} orbital. The bond order = $2(10-5)$ = **2.5**.

(Alternatively one can count only valence electrons; in that case bond order =

$2(8-3)$ = **2.5**)

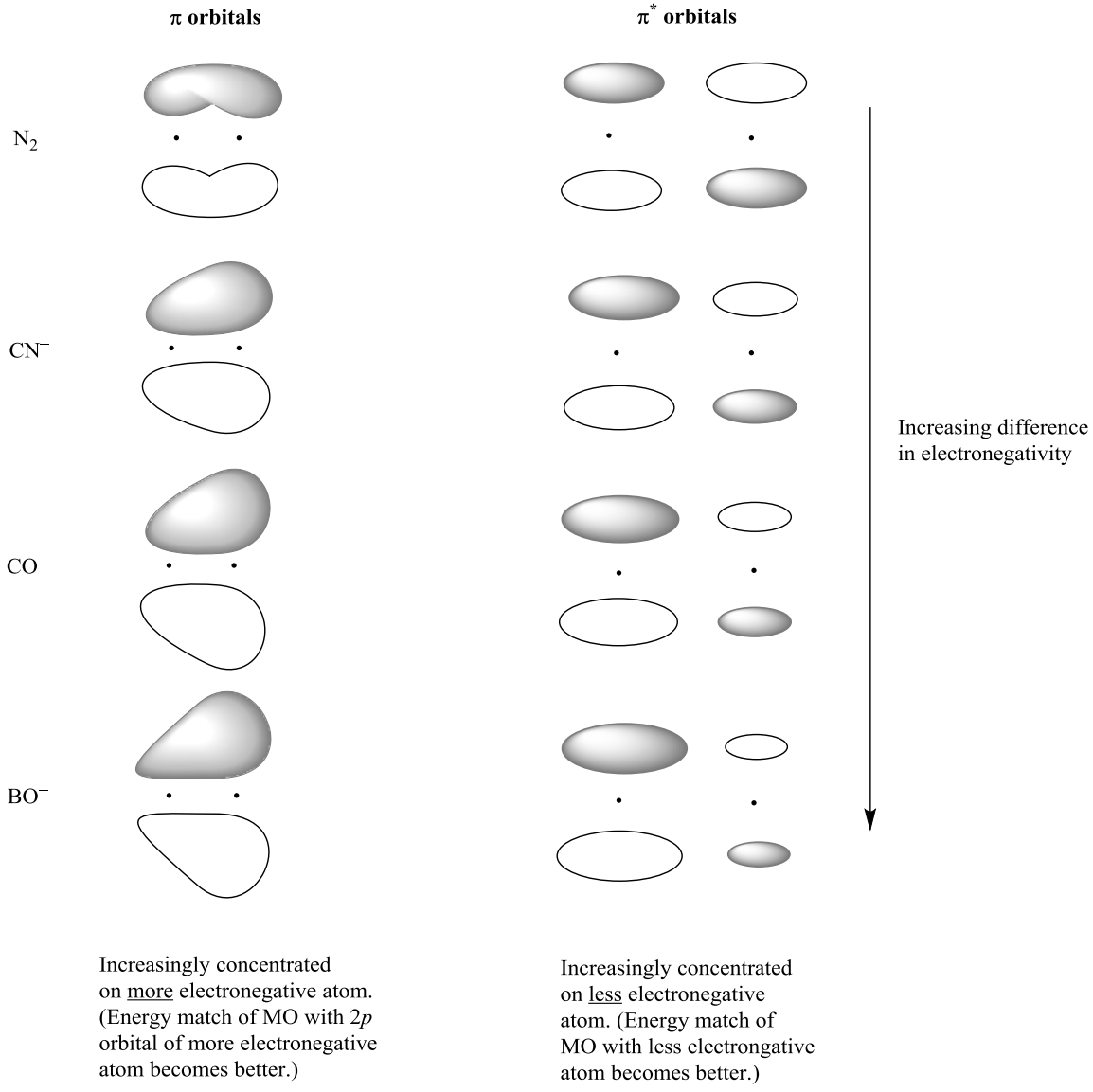
Bond orders for the three species:

	Bond order
NO^+	3
NO	2.5
NO^-	2

NO^+, with the highest bond order, has the shortest bond:

	Bond distance (pm)
NO^+	106
NO	115
NO^-	127

2-5



2-6 Calculations should give similar results to problem **2-5**: as the difference in electronegativity of the atoms increases, the lobes of the π orbitals should become increasingly concentrated on the more electronegative atom, and the lobes of the π* orbitals should become more concentrated on the less electronegative atom.

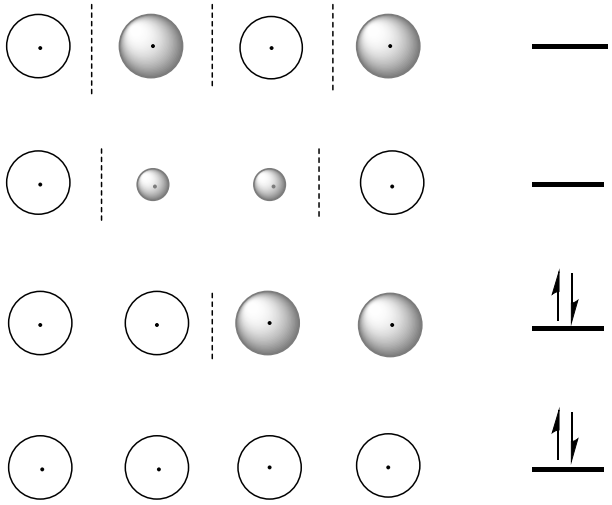
2-7 **a.** **H_2** (bond order = 1; bond order of H_2^+ = 0.5)

b. **NO^+** (bond order = 3; bond orders of NO and NO^- are 2.5 and 2, respectively)

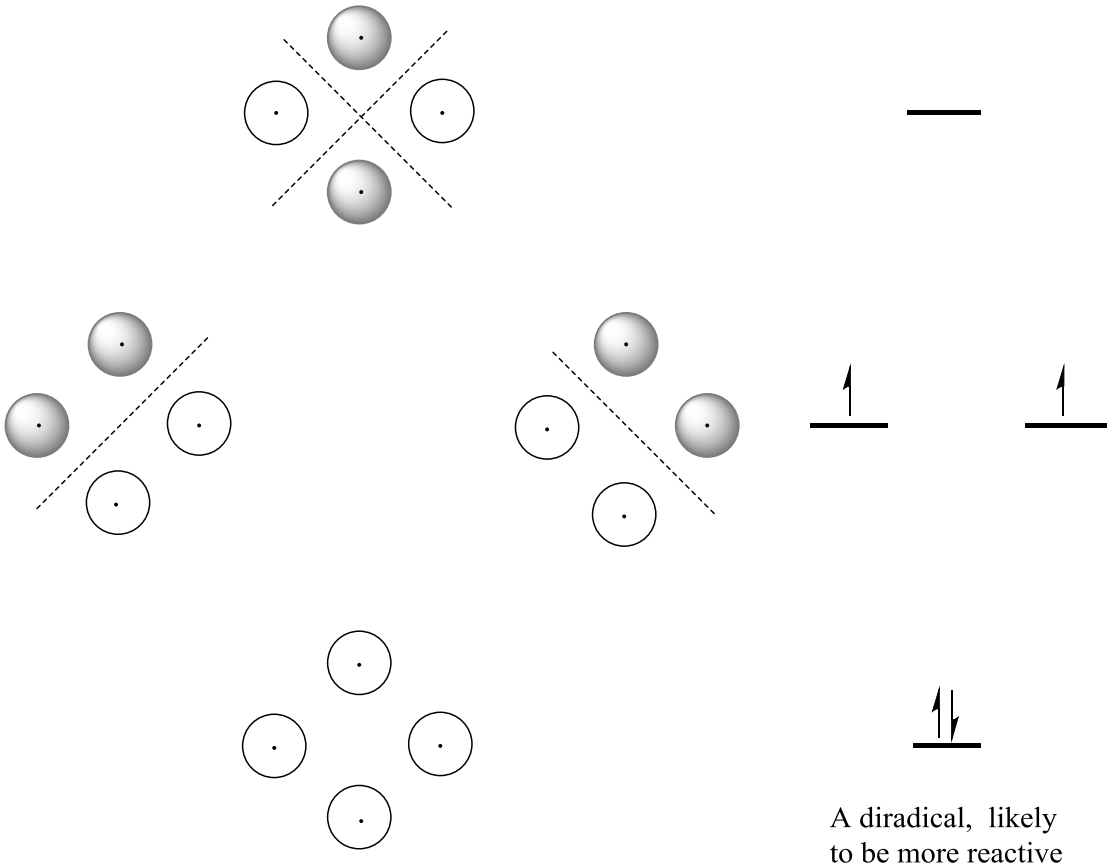
c. **CO** (bond order = 3; bond order of CO^+ = 2.5)

2-8

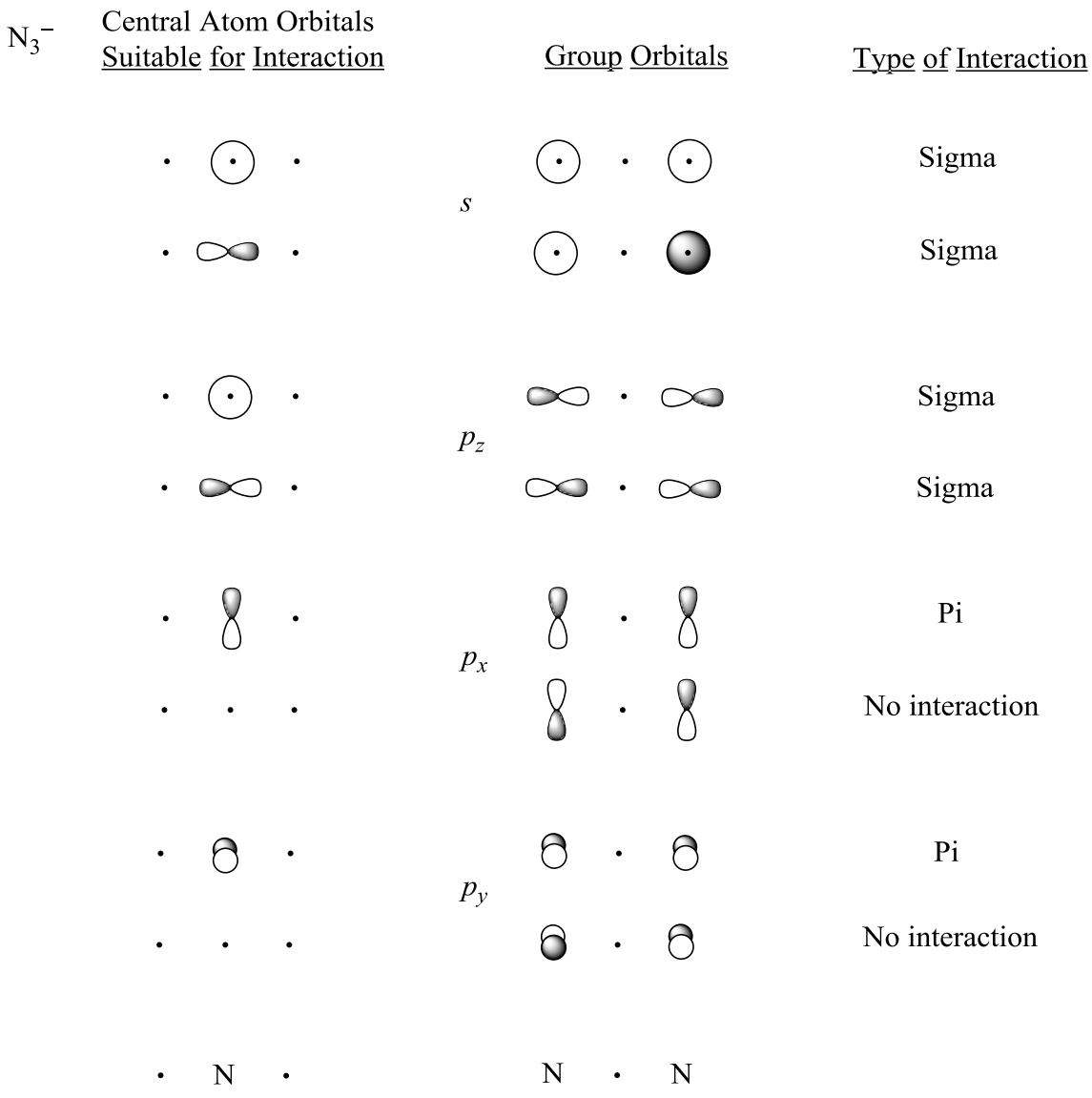
a. Linear:



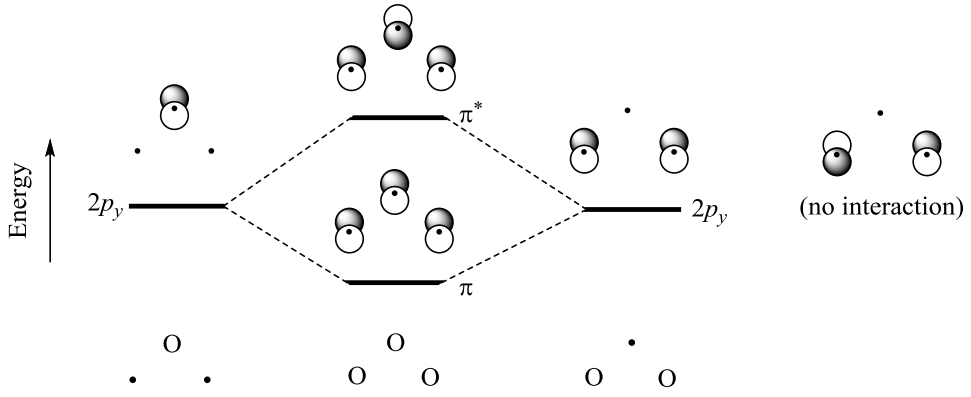
b. Square:

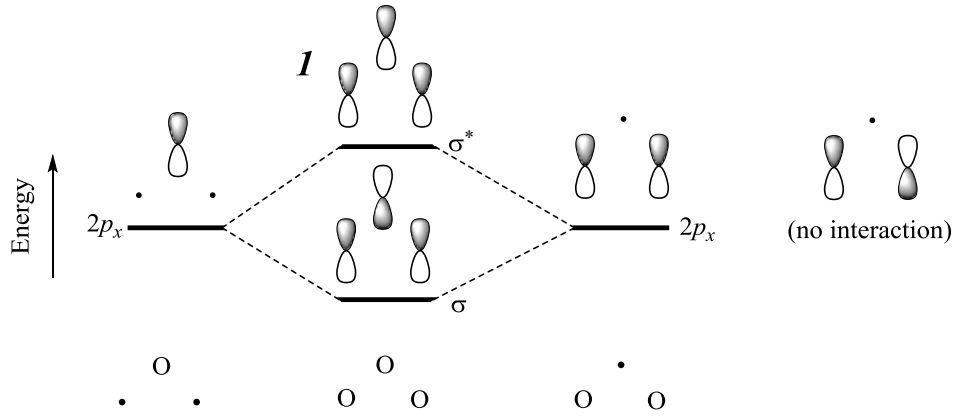


A diradical, likely to be more reactive than linear case.

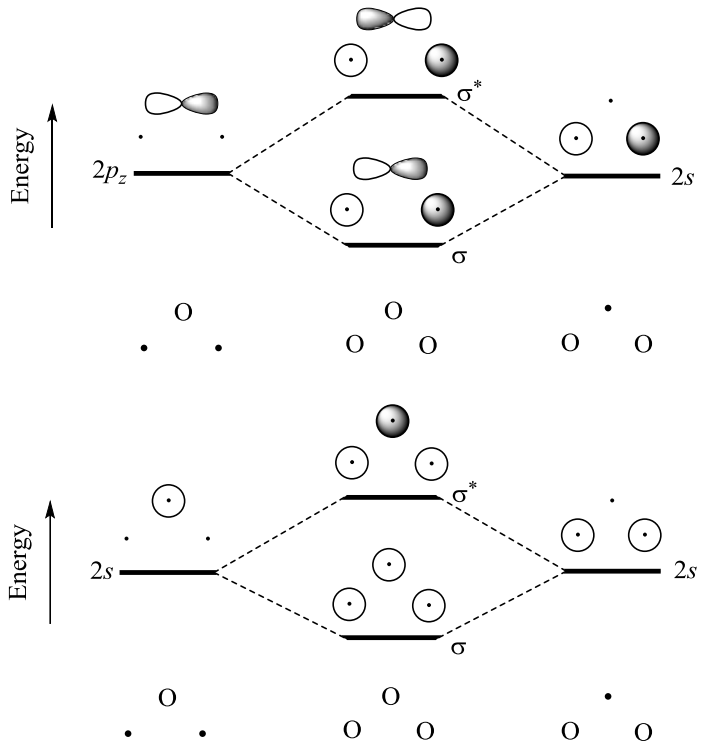

N_3^-
Central Atom Orbitals Suitable for Interaction
Group Orbitals
Type of Interaction
s
Sigma
Sigma
p_z
Sigma
Sigma
p_x
Pi
No interaction
p_y
Pi
No interaction
N
N
N

2-10 The MO diagram of O_3 will be similar to that for CO_2 (Figure **2-7**). However, the two degenerate π bonding and the two π antibonding MOs will convert to π-type bonding and antibonding MOs (resulting from interaction of the central oxygen atom's $2p_y$ atomic orbital and the group orbital composed of the $2p_y$ atomic orbitals from the outer oxygen atoms) and σ-type bonding and antibonding MOs (involving the combination of the $2p_x$ orbital of oxygen with the group orbital involving the $2p_x$ orbitals from the outer two oxygen atoms). These interactions are shown below:





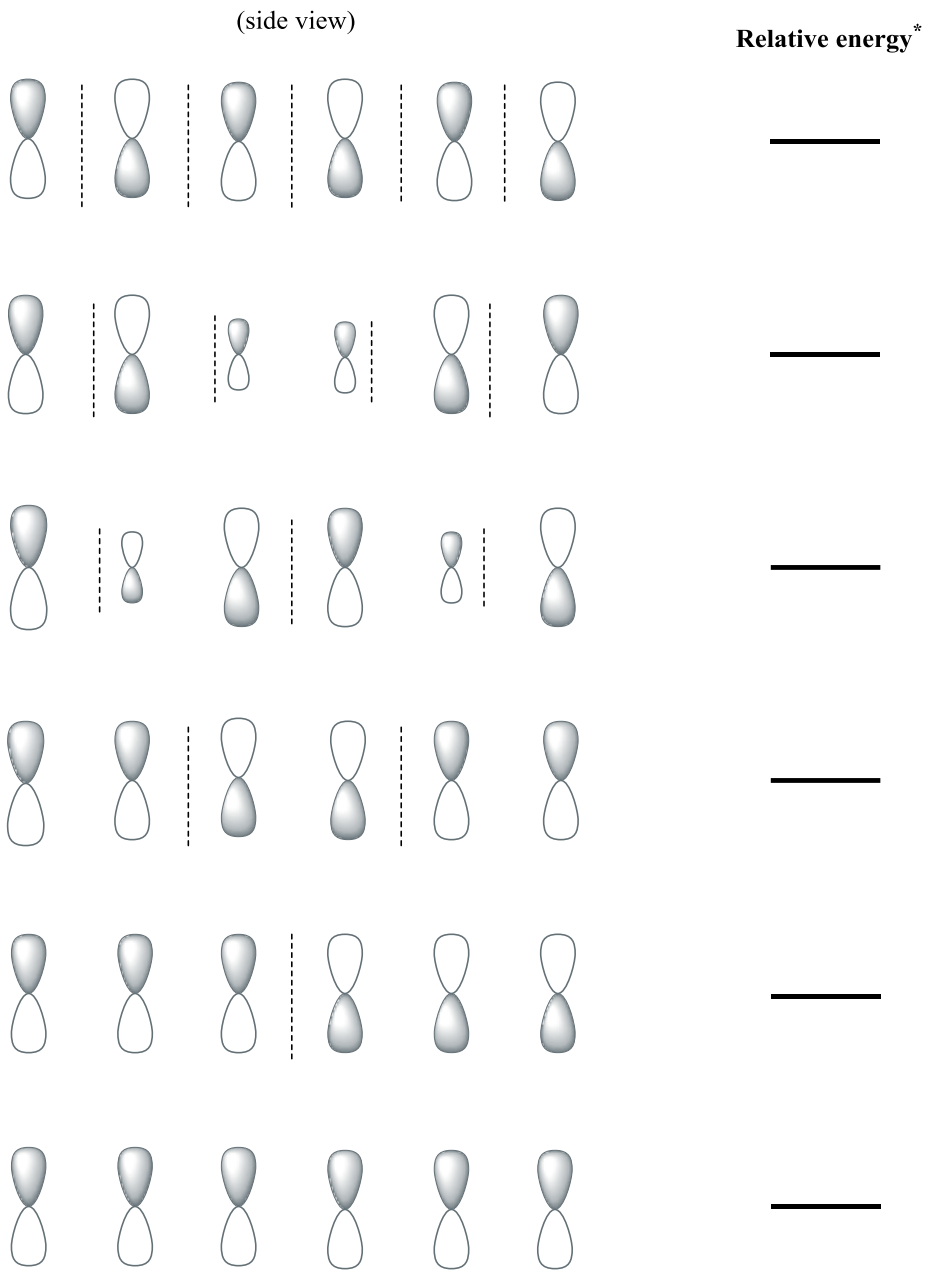
MOs resulting from combination of the 2*s* and 2p_z orbitals from the central oxygen atom and group orbitals comparable to 1 and 2 in Figure **2-7** yield the following MOs:



The remaining MOs of O_3 can be generated using the same procedure as above.

Since O_3 has two more electrons than CO_2, these extra electrons would likely reside in an MO that is antibonding (perhaps orbital ***1*** above). By placing two electrons in an antibonding orbital, the bond order of O_3 is decreased by one compared to CO_2. Thus, one would expect fewer than four bonds distributed among the three oxygen atoms, which is consistent with the Lewis structure of O_3.

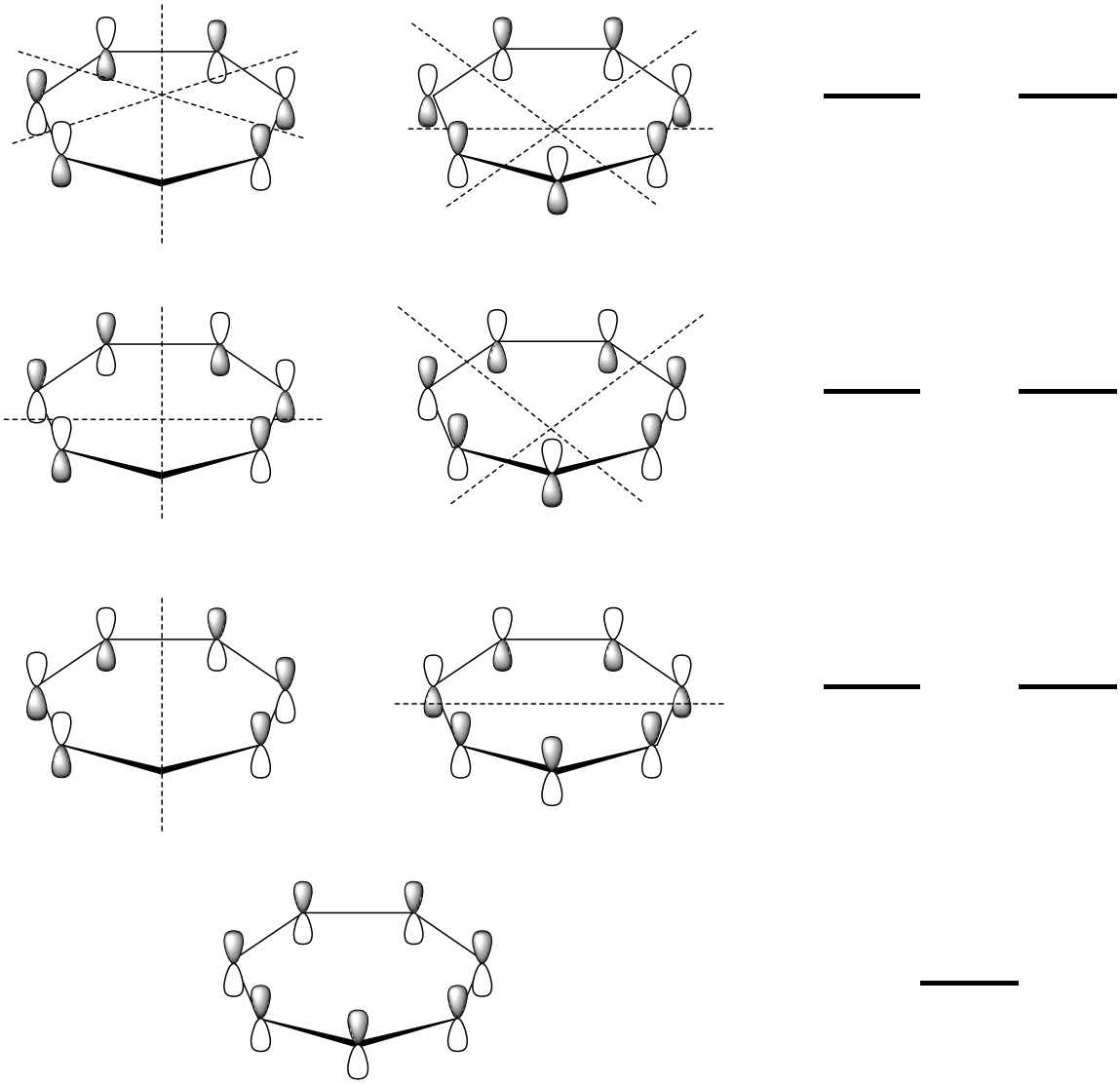
2-11



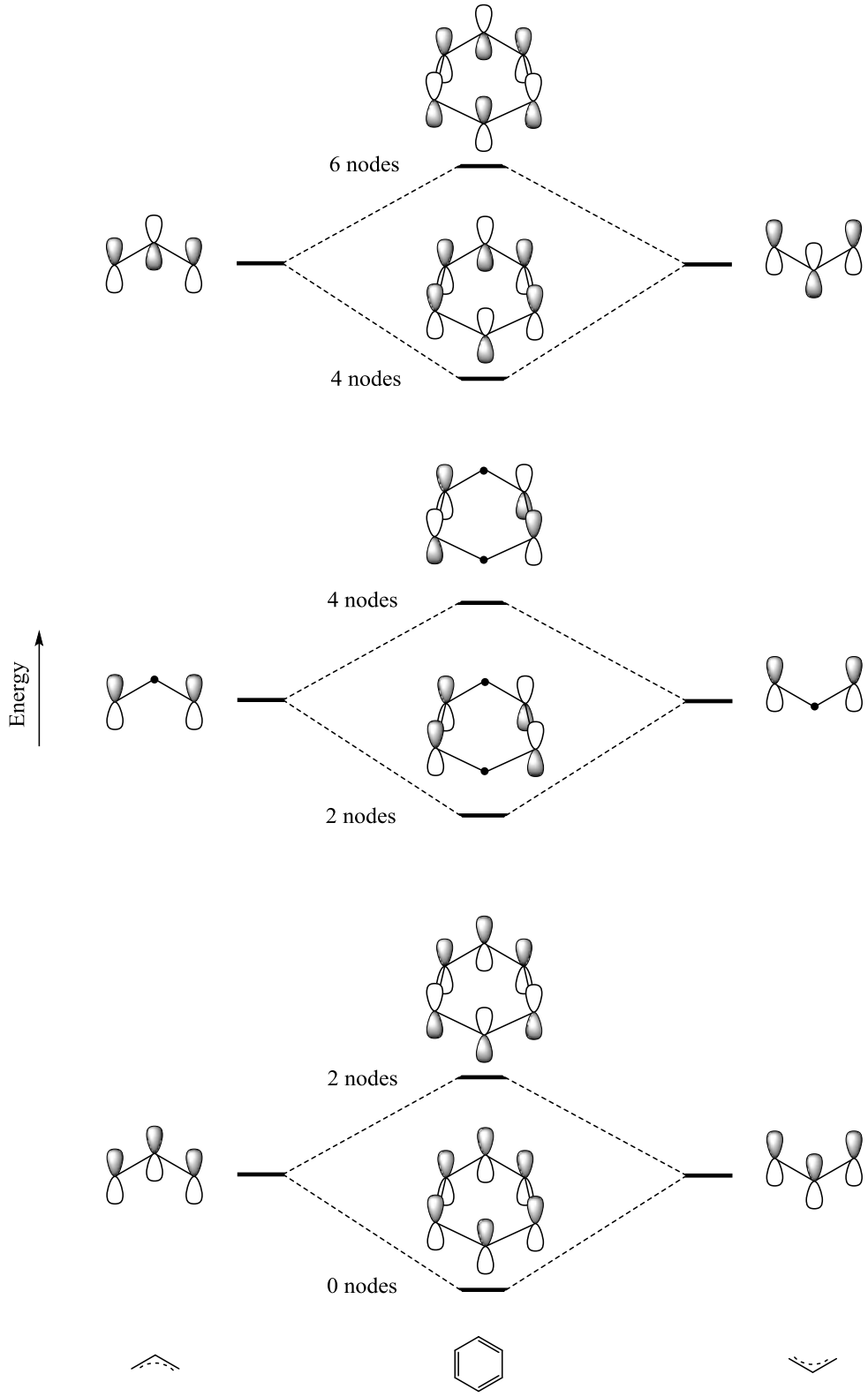
*Not all to scale; all are non-degenerate

2-12

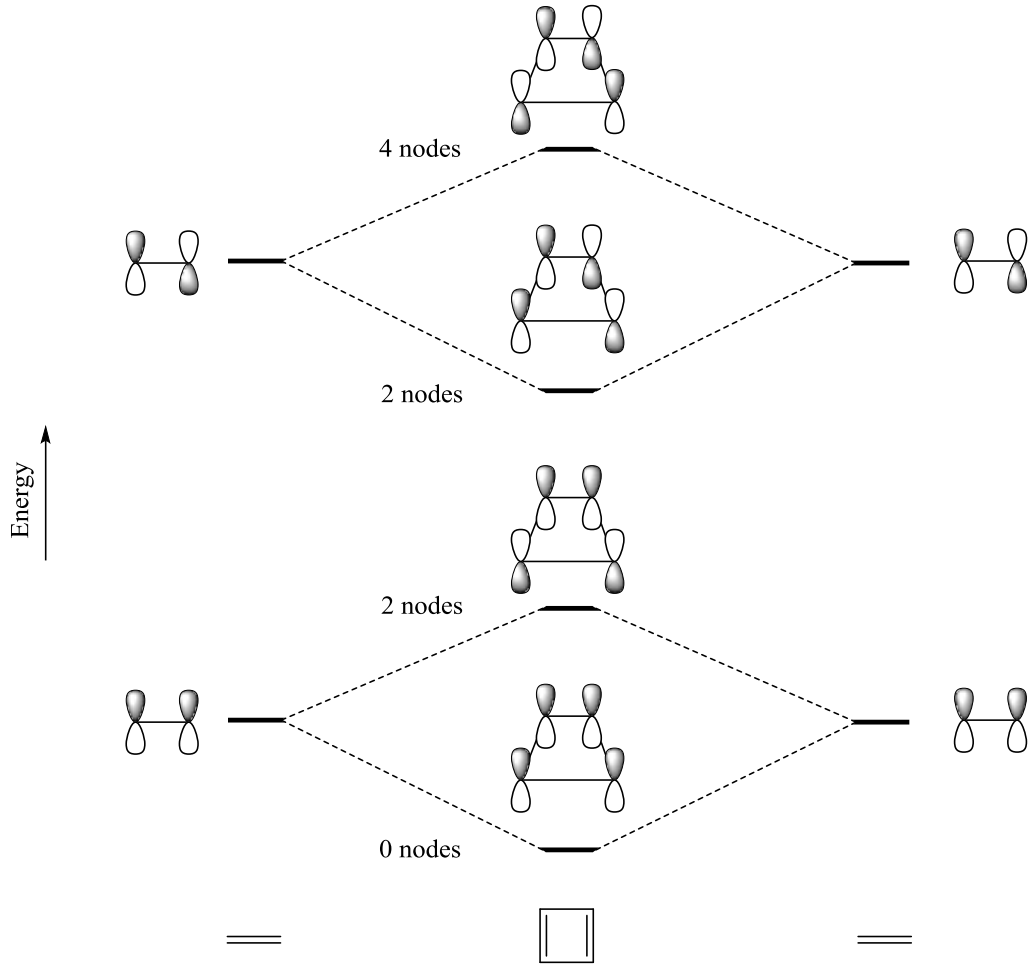
Relative energy



2-13



2-14



2-15 Generally the calculations should result in molecular orbitals that are similar to the sketches in the problems cited. It is instructive to observe the relative sizes of the orbital lobes, particularly in relation to how close the lobes are to the nodes; lobes closer to nodal surfaces are typically smaller.