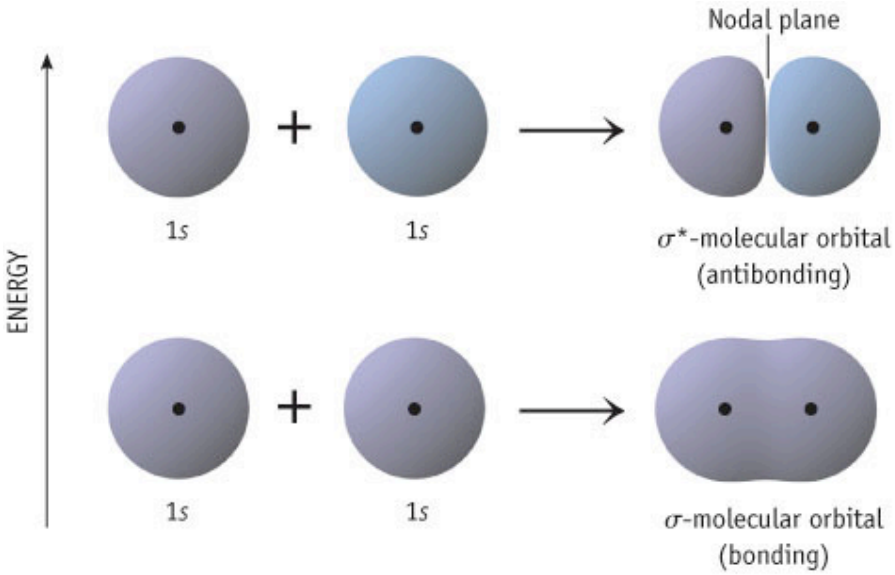
Back to H_2

Conserve energy when “mixing” orbitals



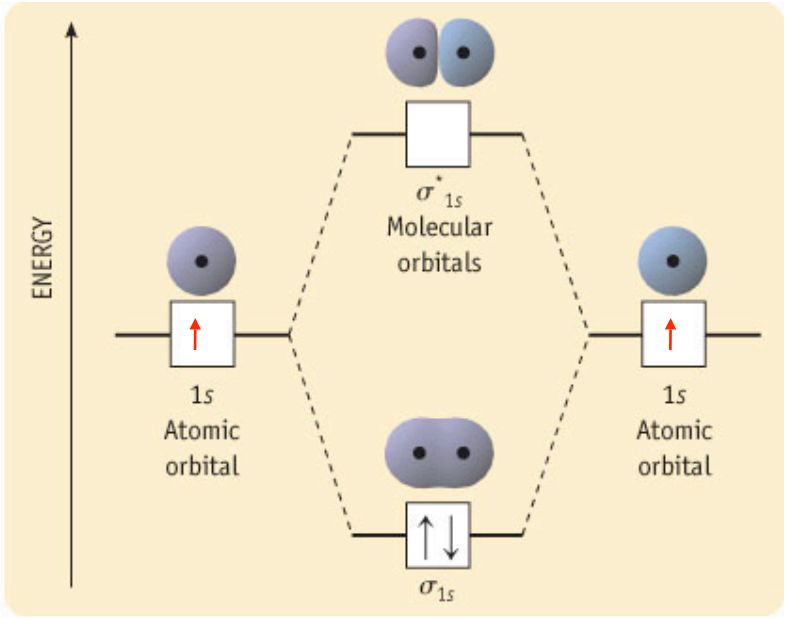


Fig. 9-16, p. 424

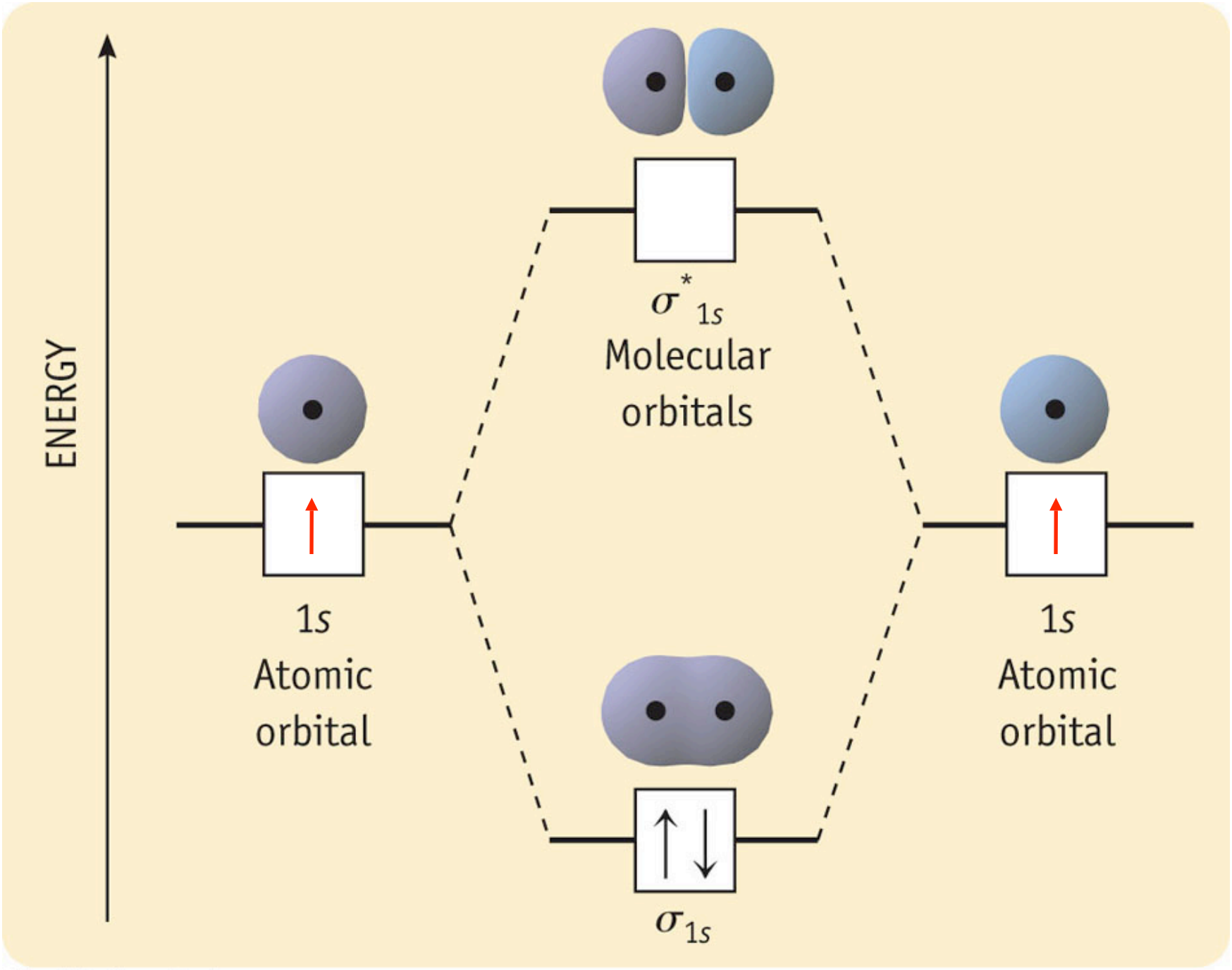


Fig. 9-16, p. 424

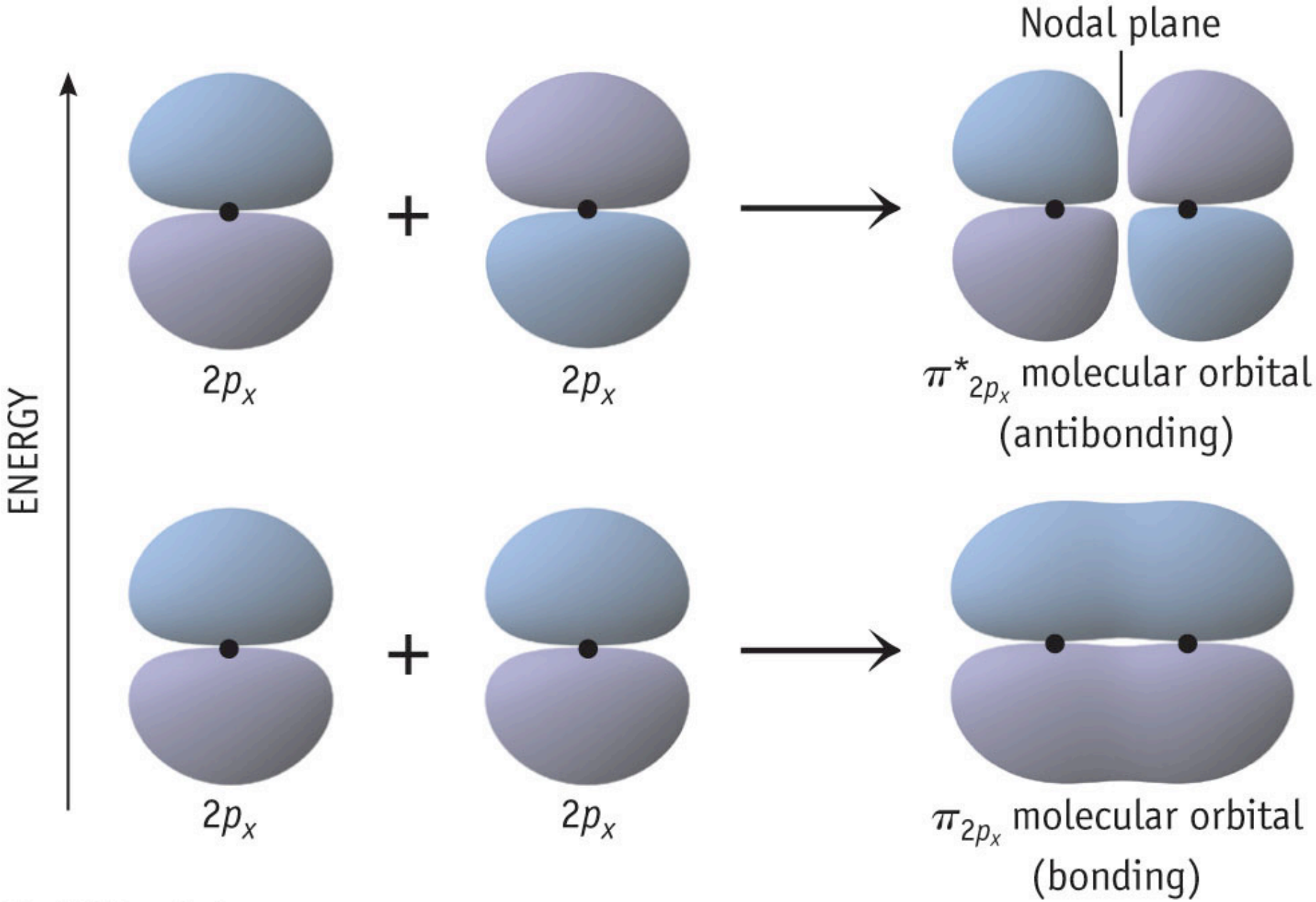


Fig. 9-20, p. 427

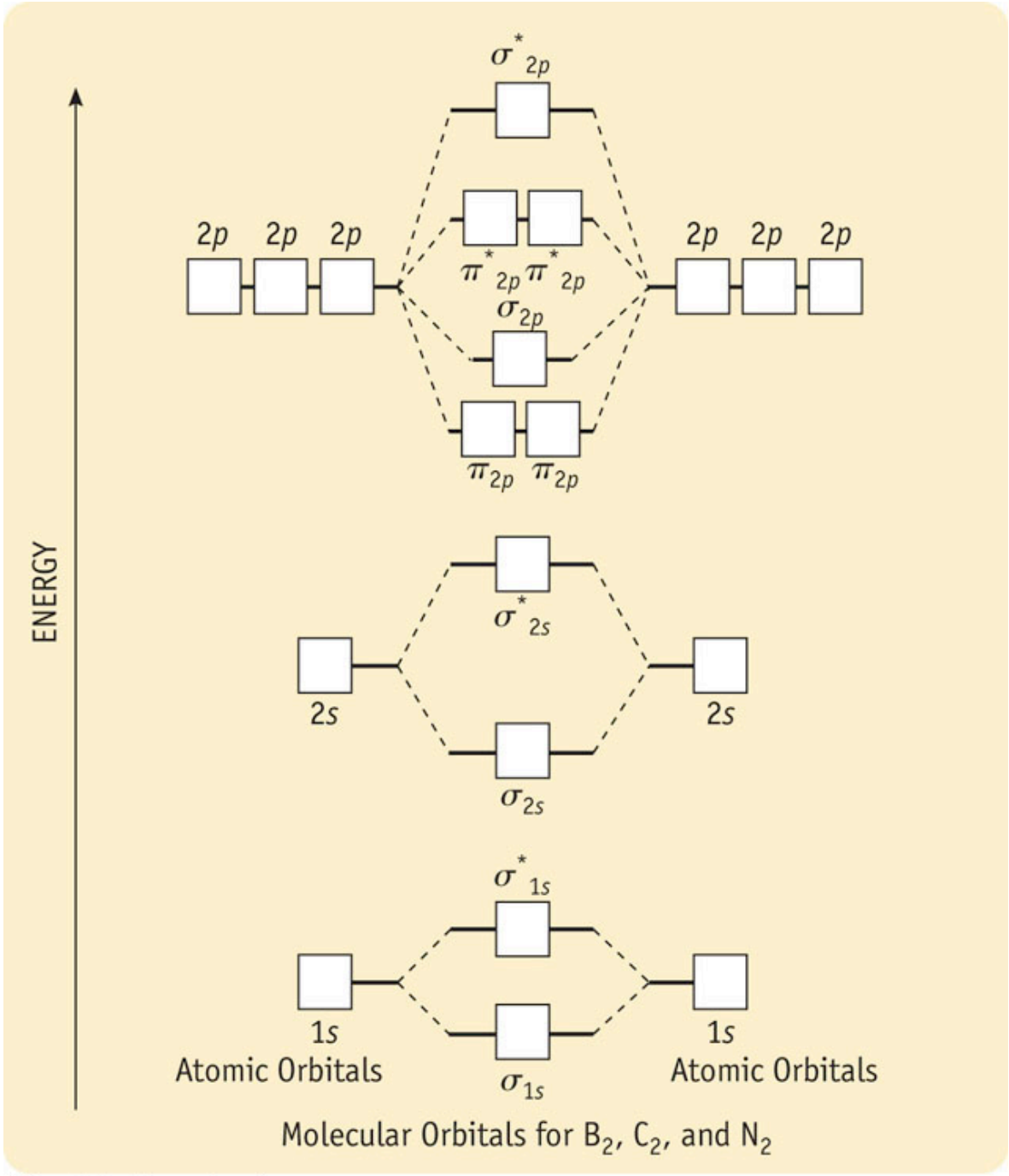
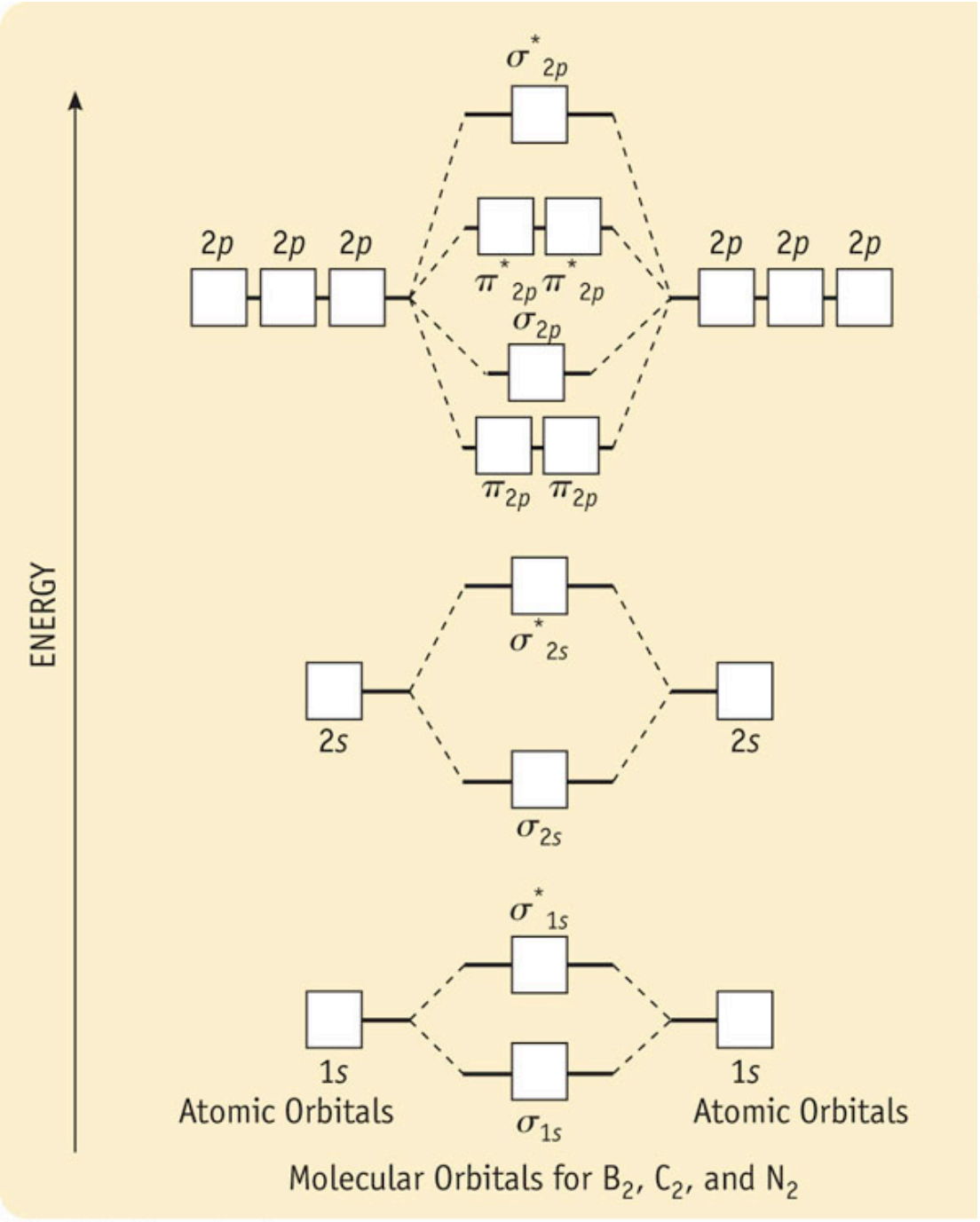
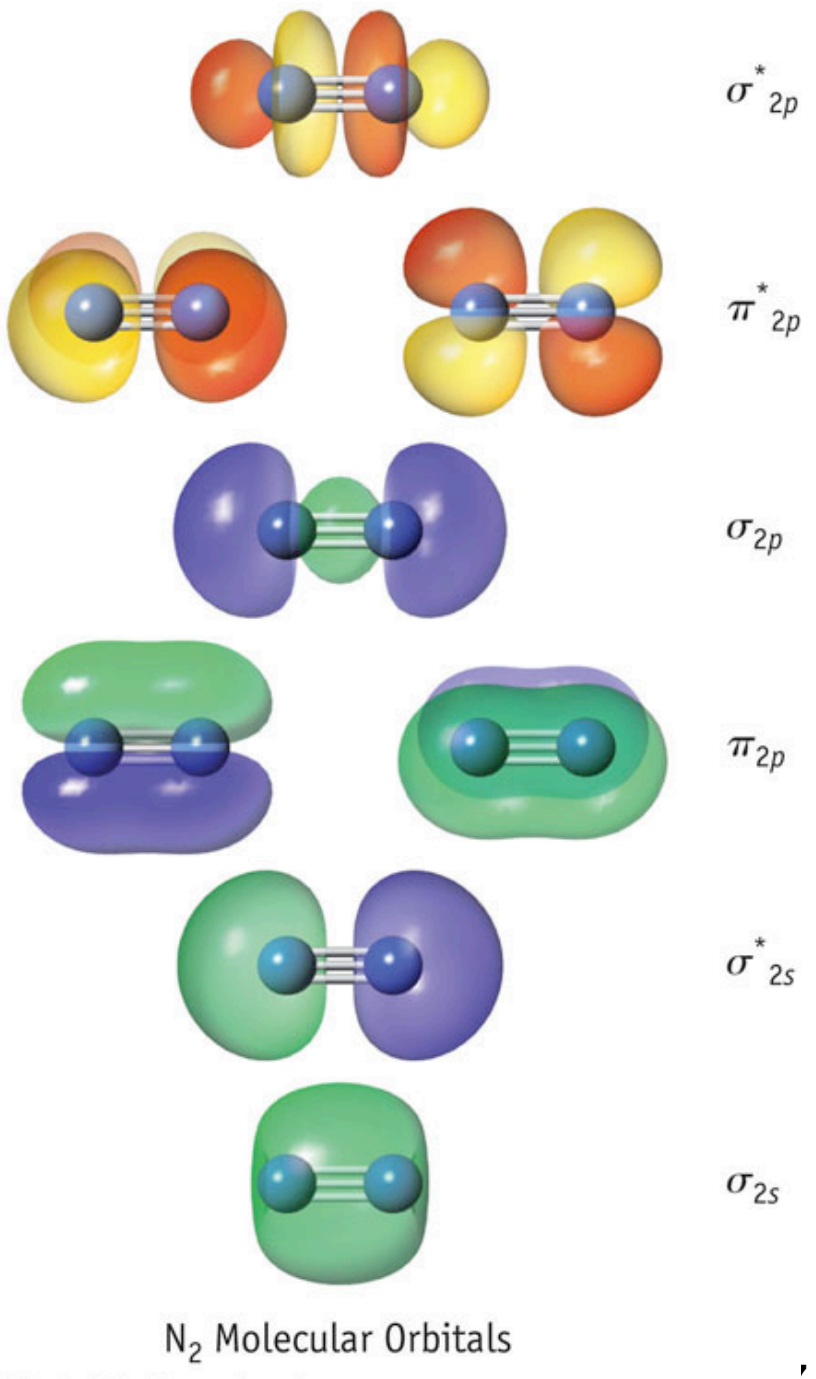


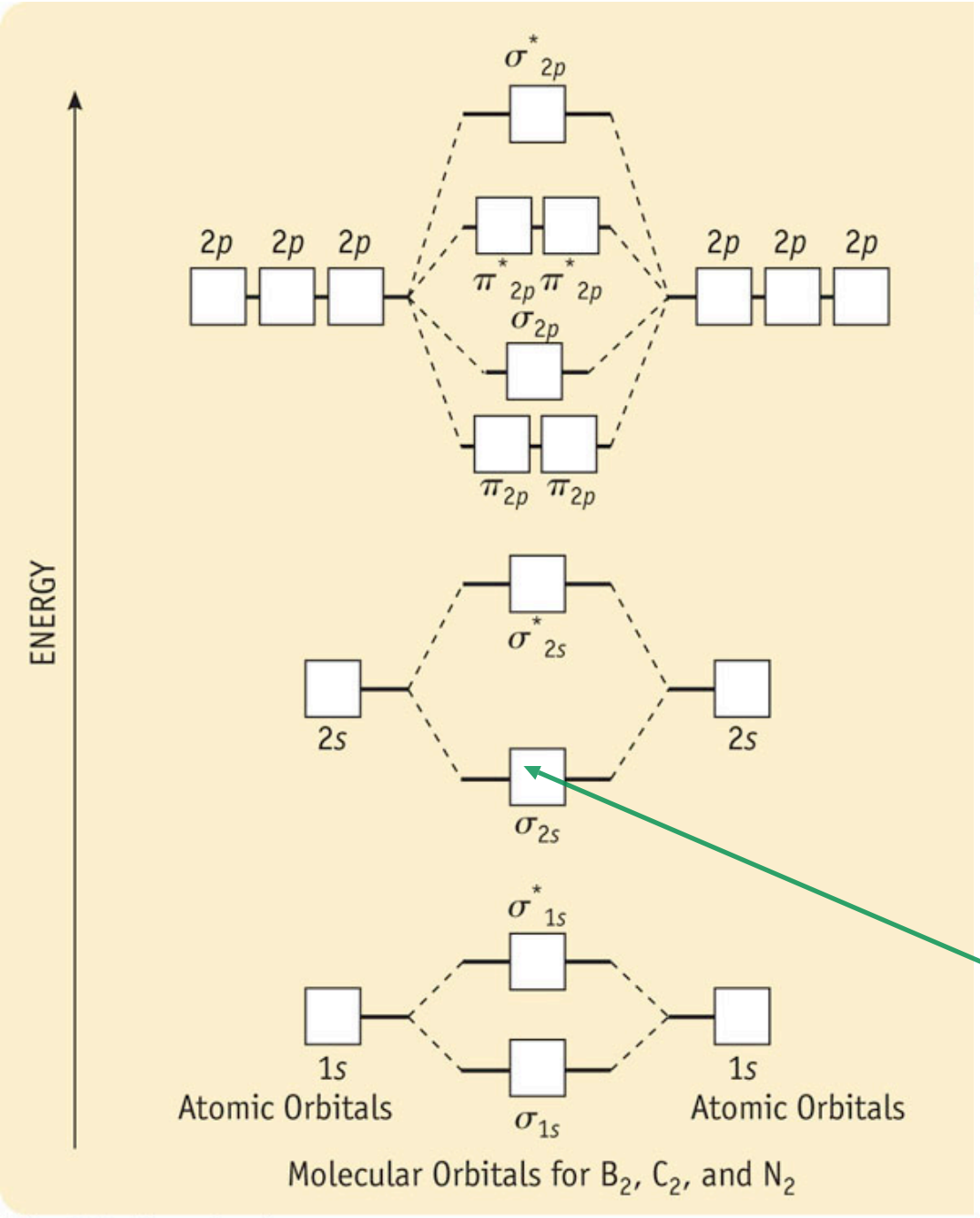
Fig. 9-21a, p. 427



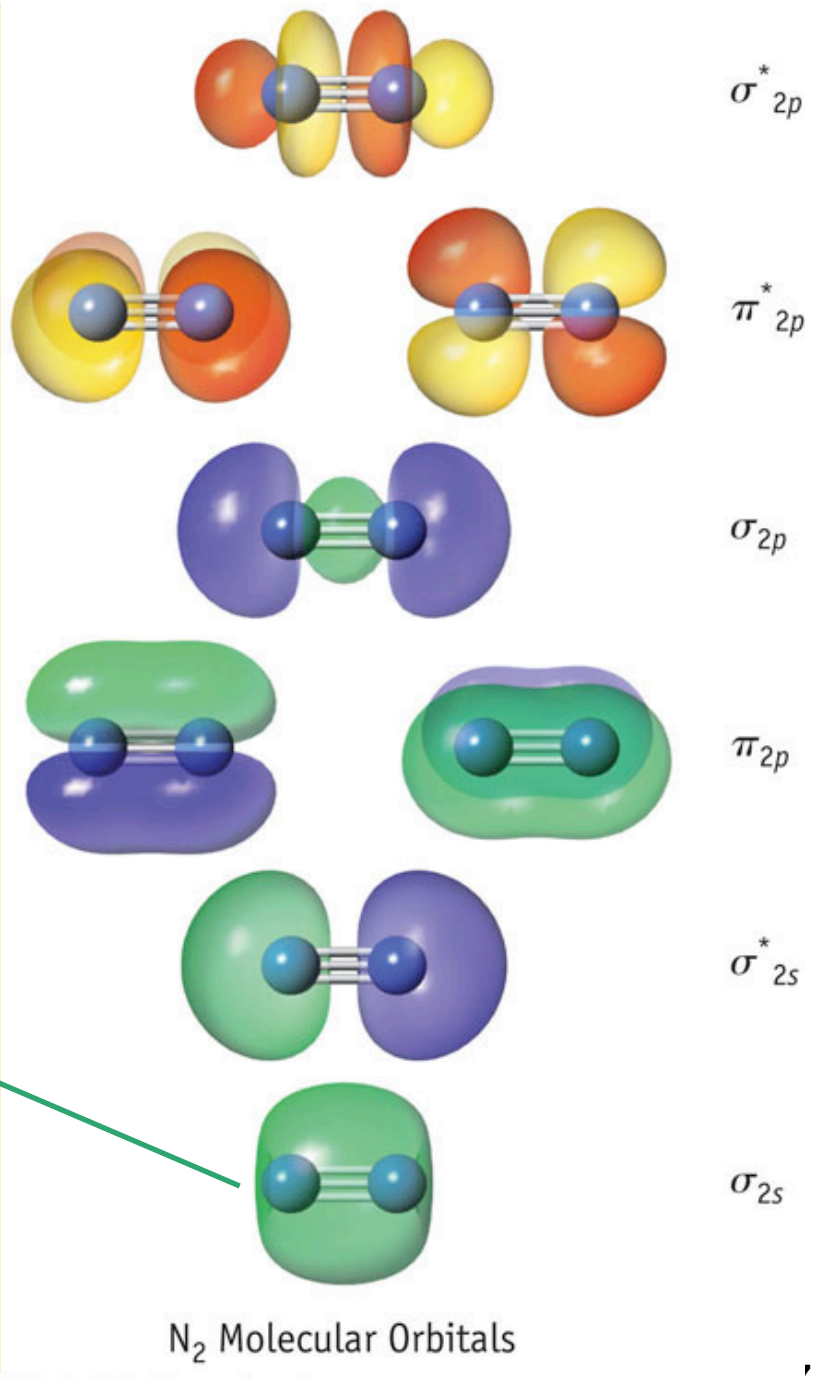
Molecular Orbitals for B_2, C_2, and N_2



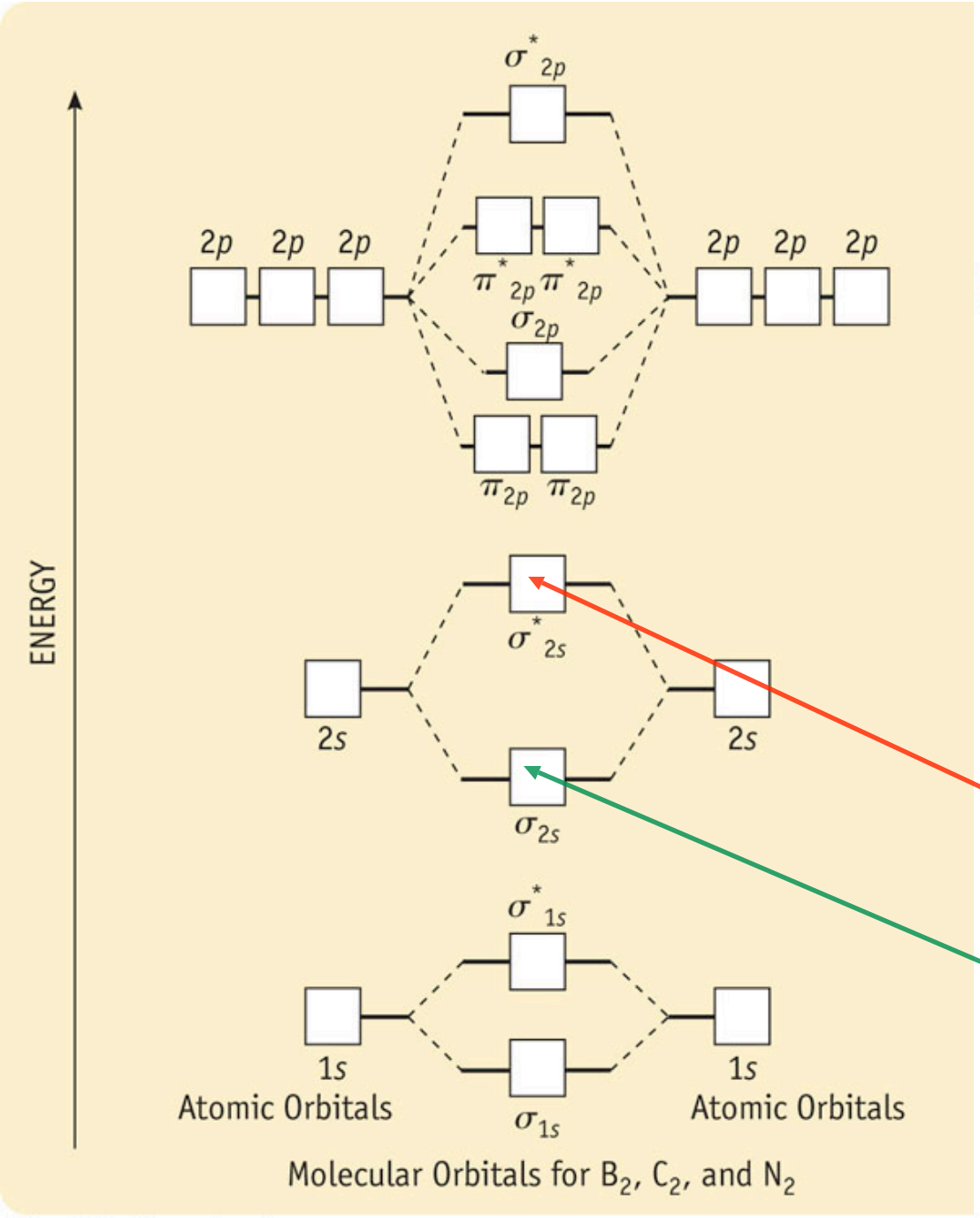
N_2 Molecular Orbitals



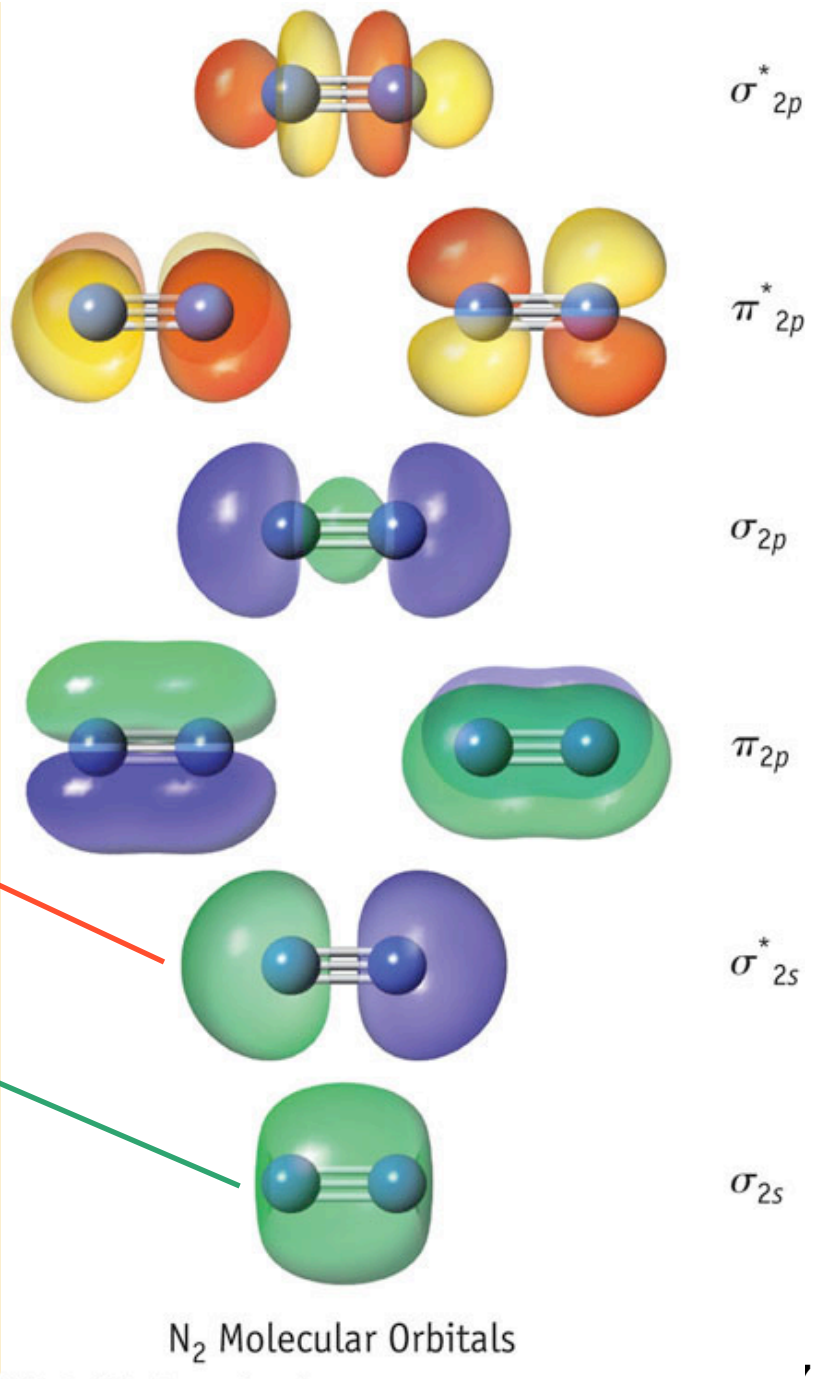
Molecular Orbitals for B_2, C_2, and N_2



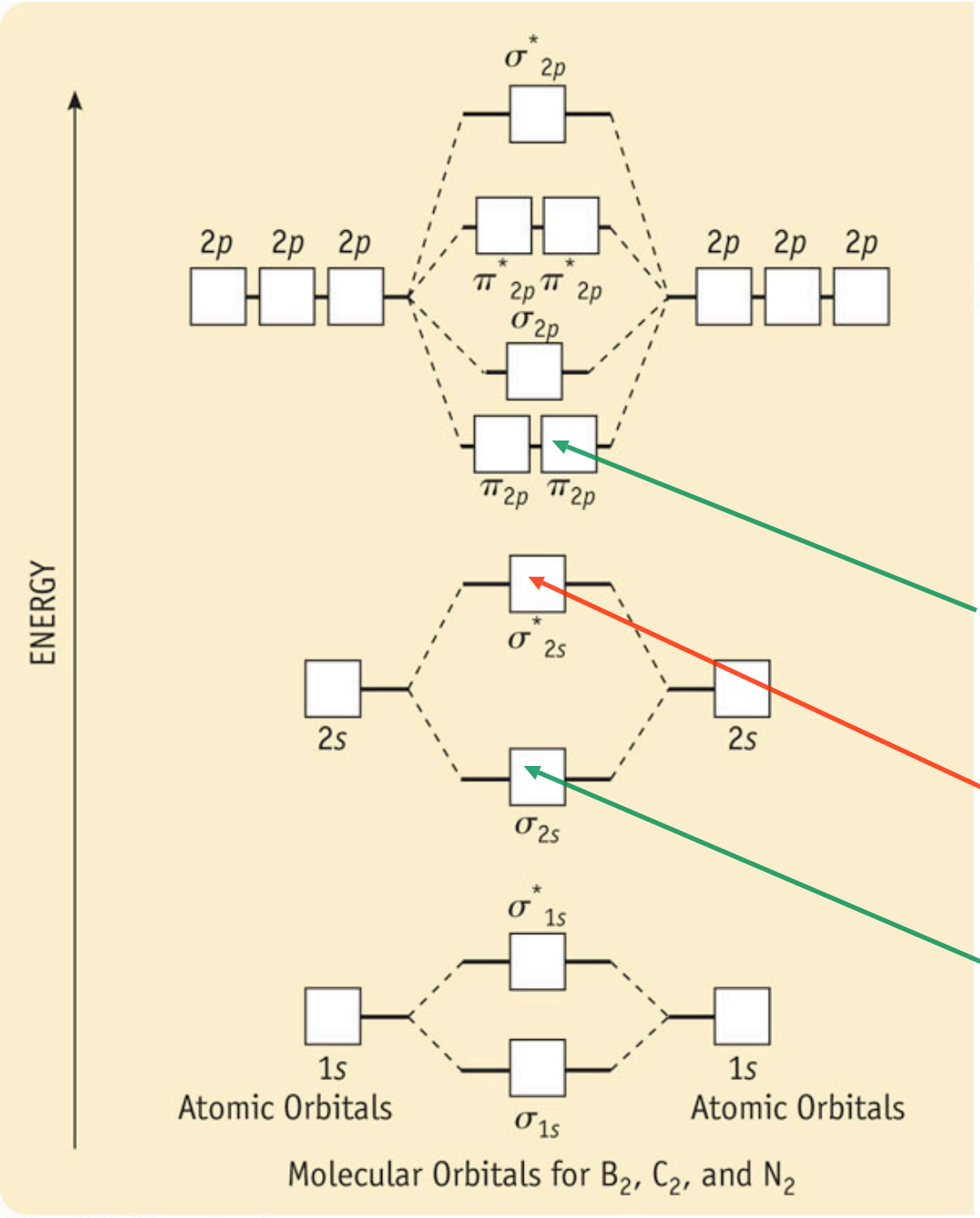
N_2 Molecular Orbitals



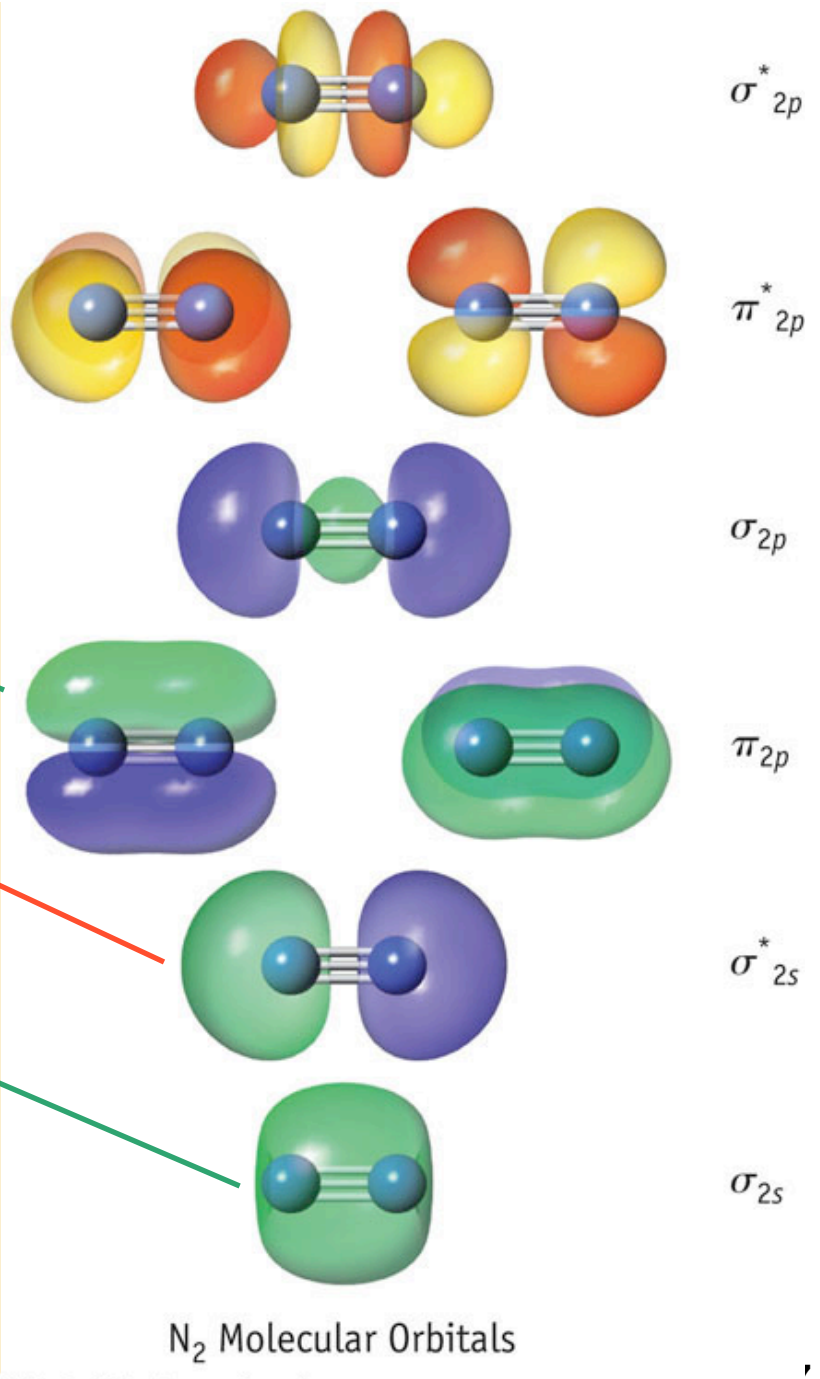
Molecular Orbitals for B_2, C_2, and N_2



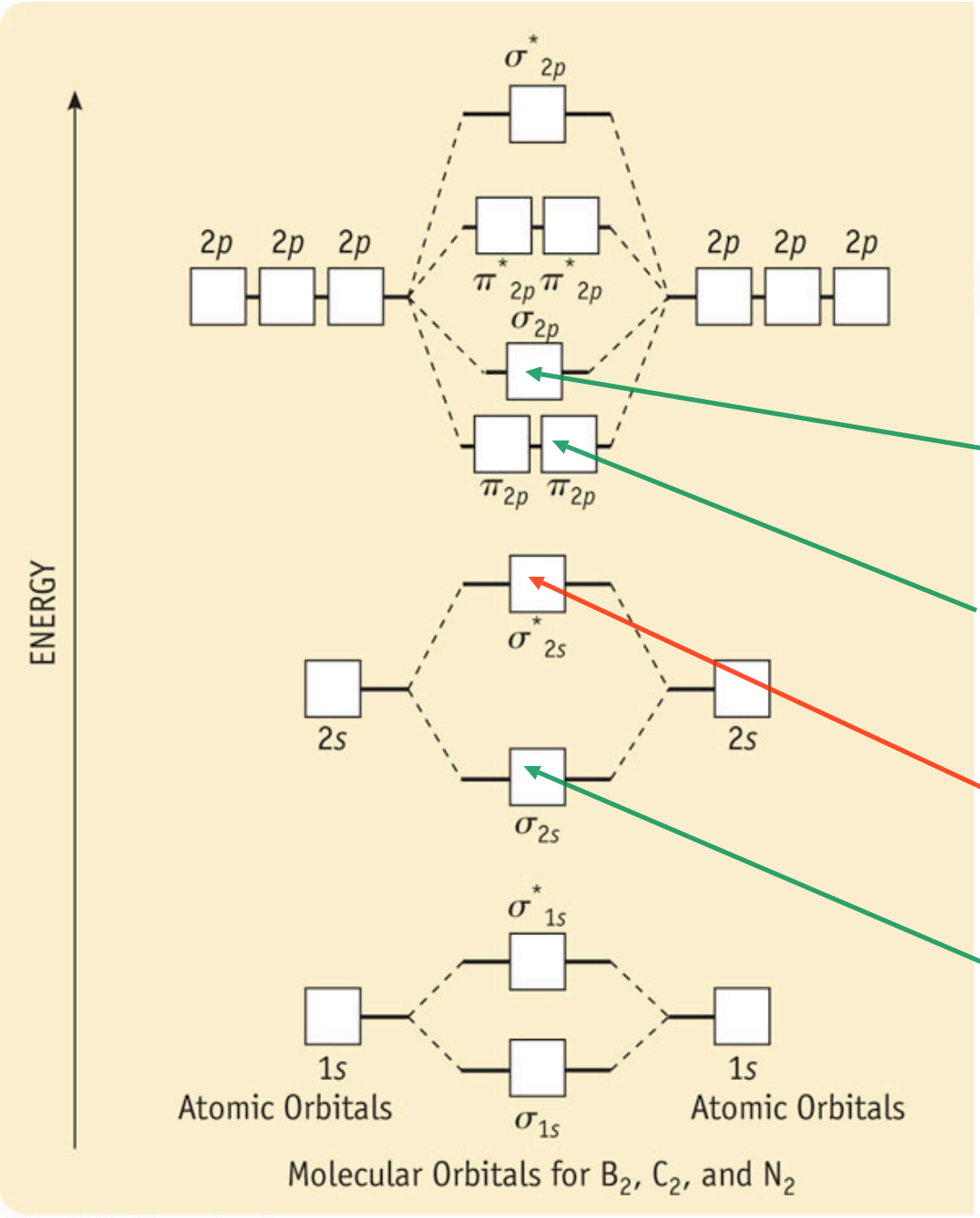
N_2 Molecular Orbitals



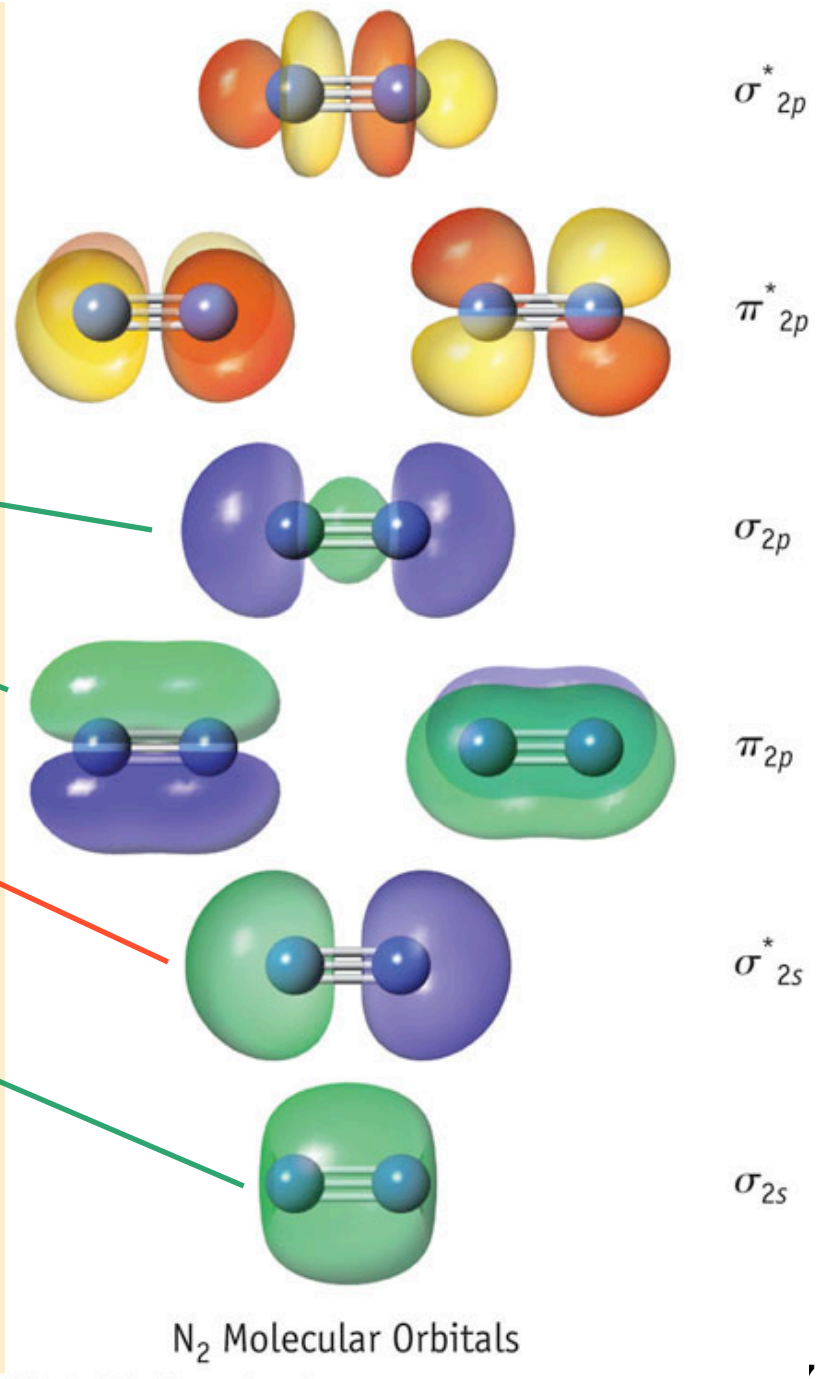
Molecular Orbitals for B_2, C_2, and N_2



N_2 Molecular Orbitals



Molecular Orbitals for B_2, C_2, and N_2



N_2 Molecular Orbitals

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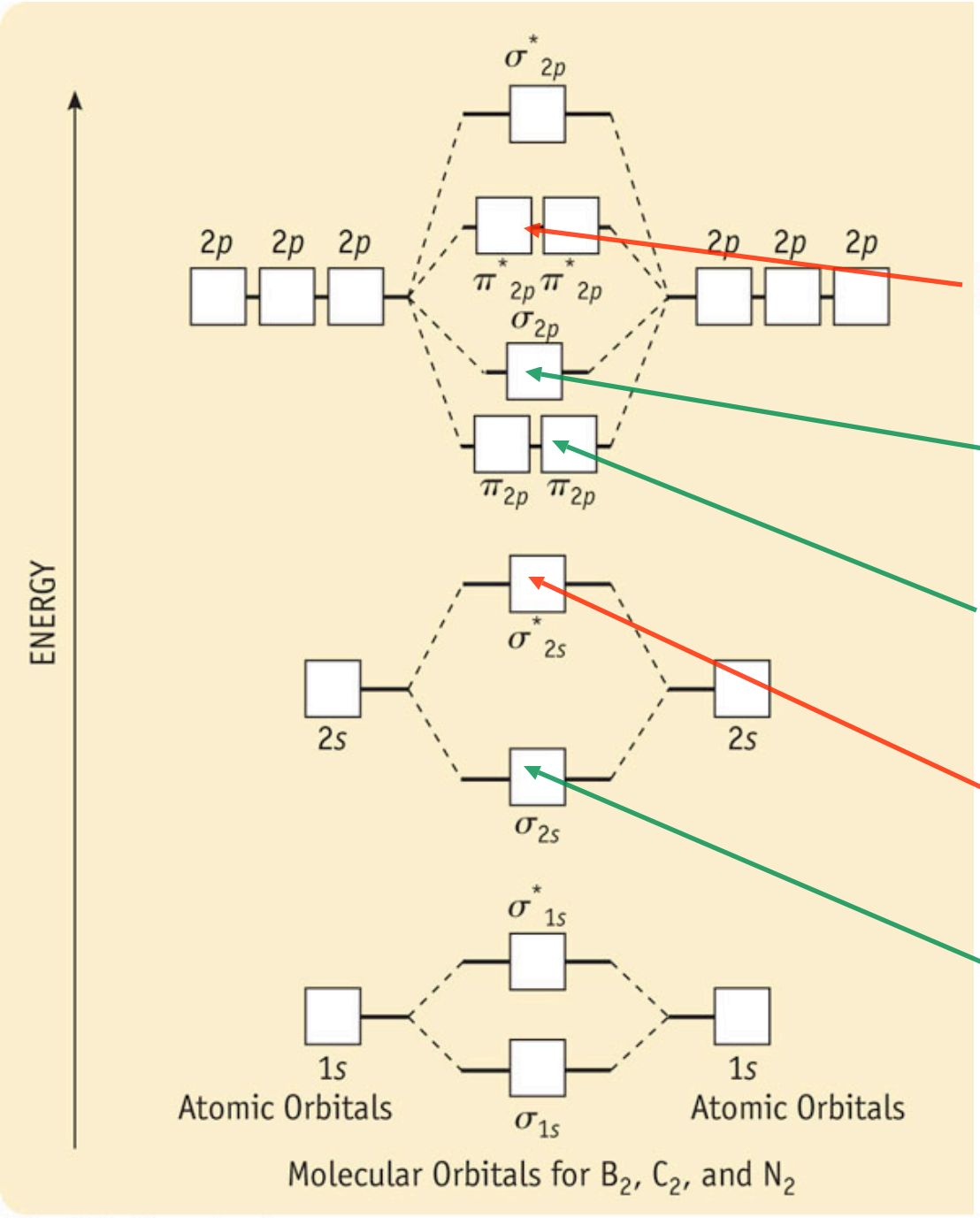
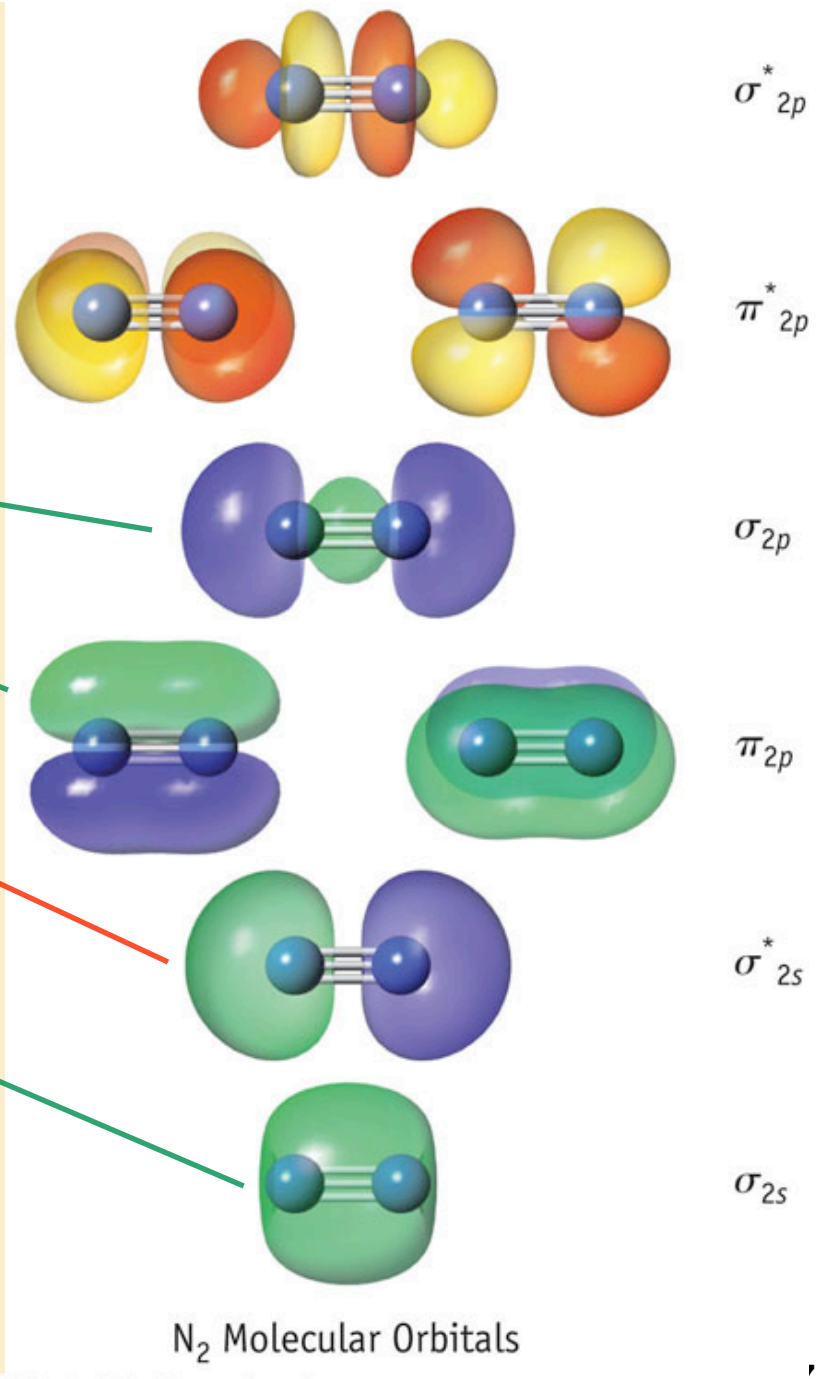


Molecular Orbitals for B_2, C_2, and N_2



N_2 Molecular Orbitals

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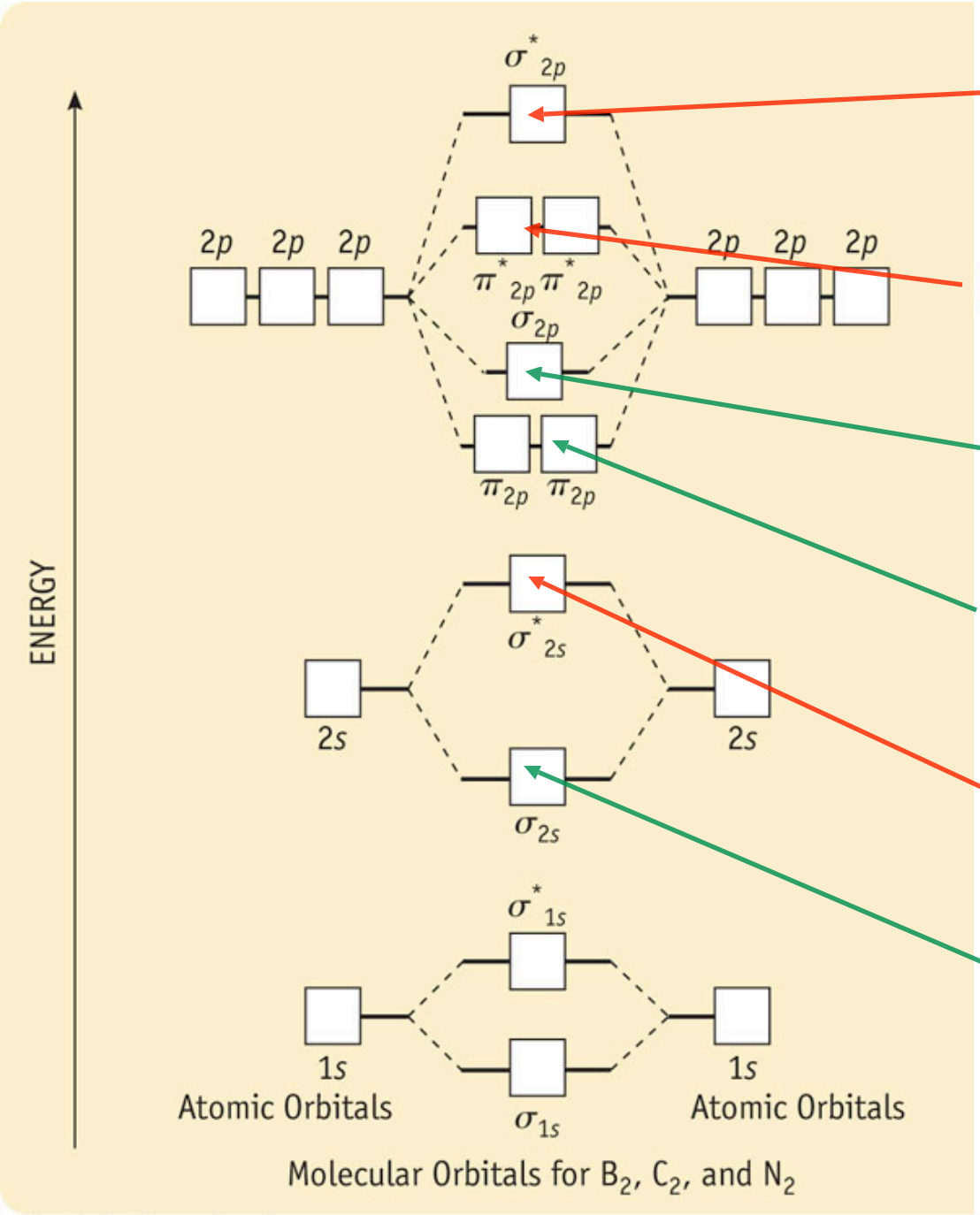
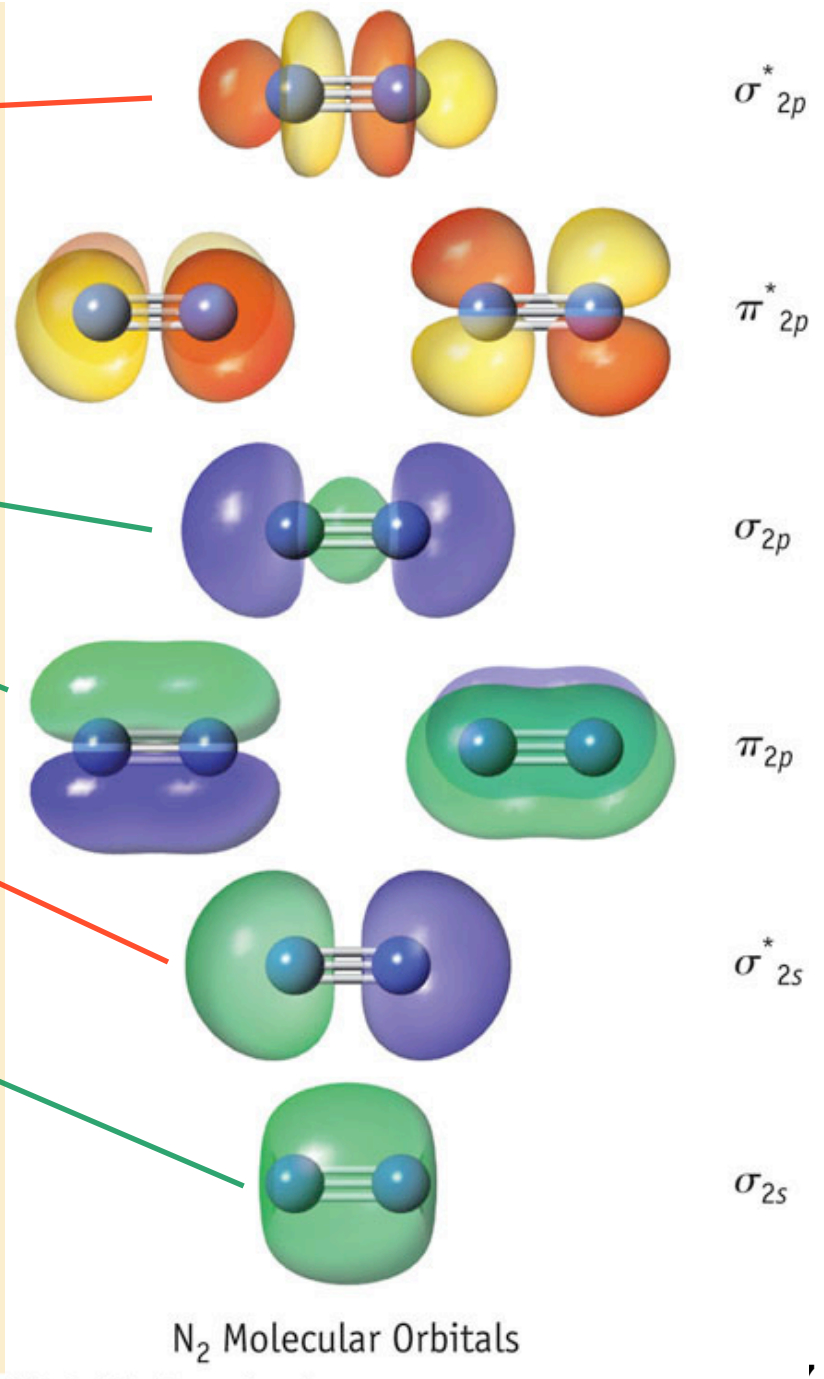


Molecular Orbitals for B_2, C_2, and N_2



N_2 Molecular Orbitals

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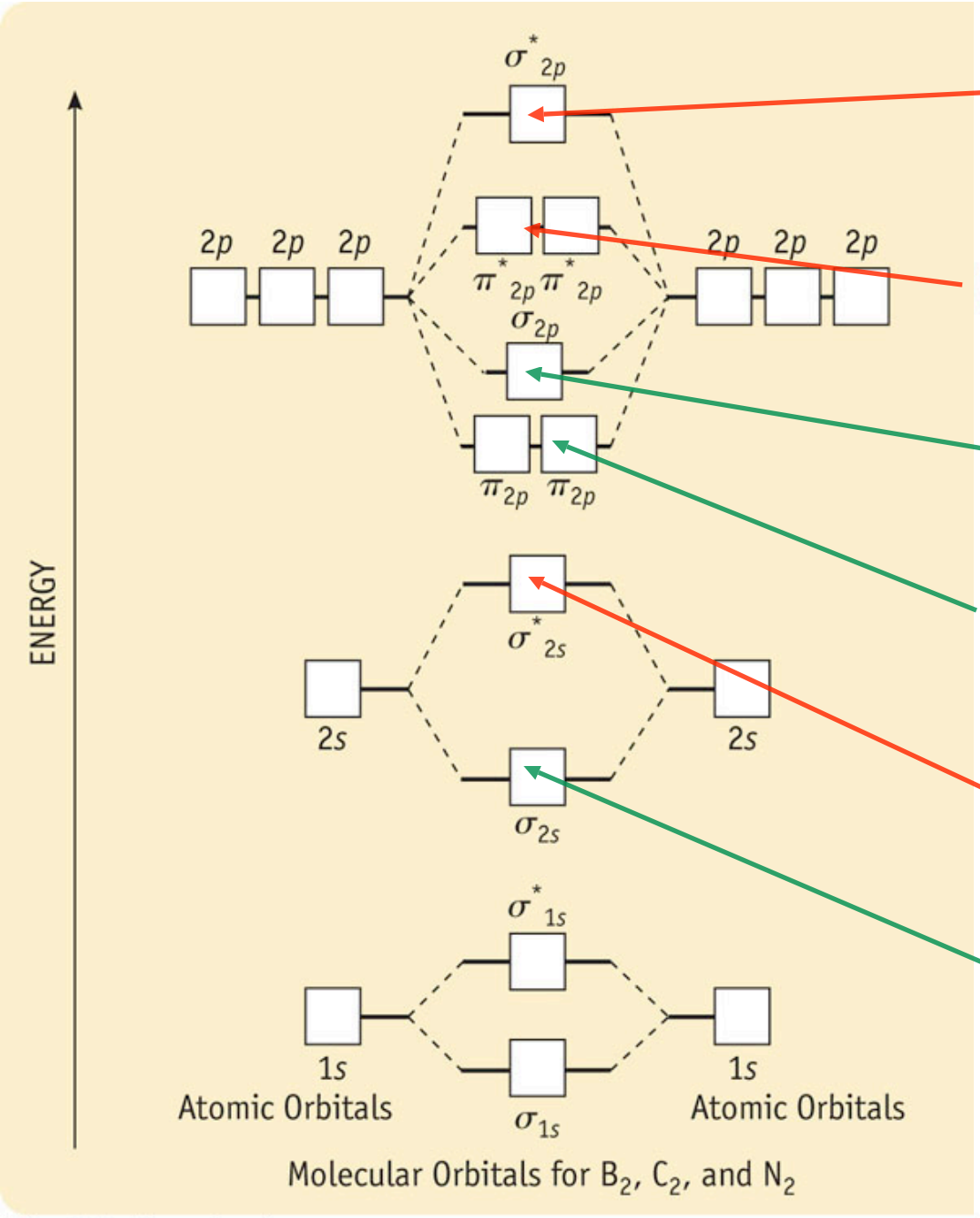
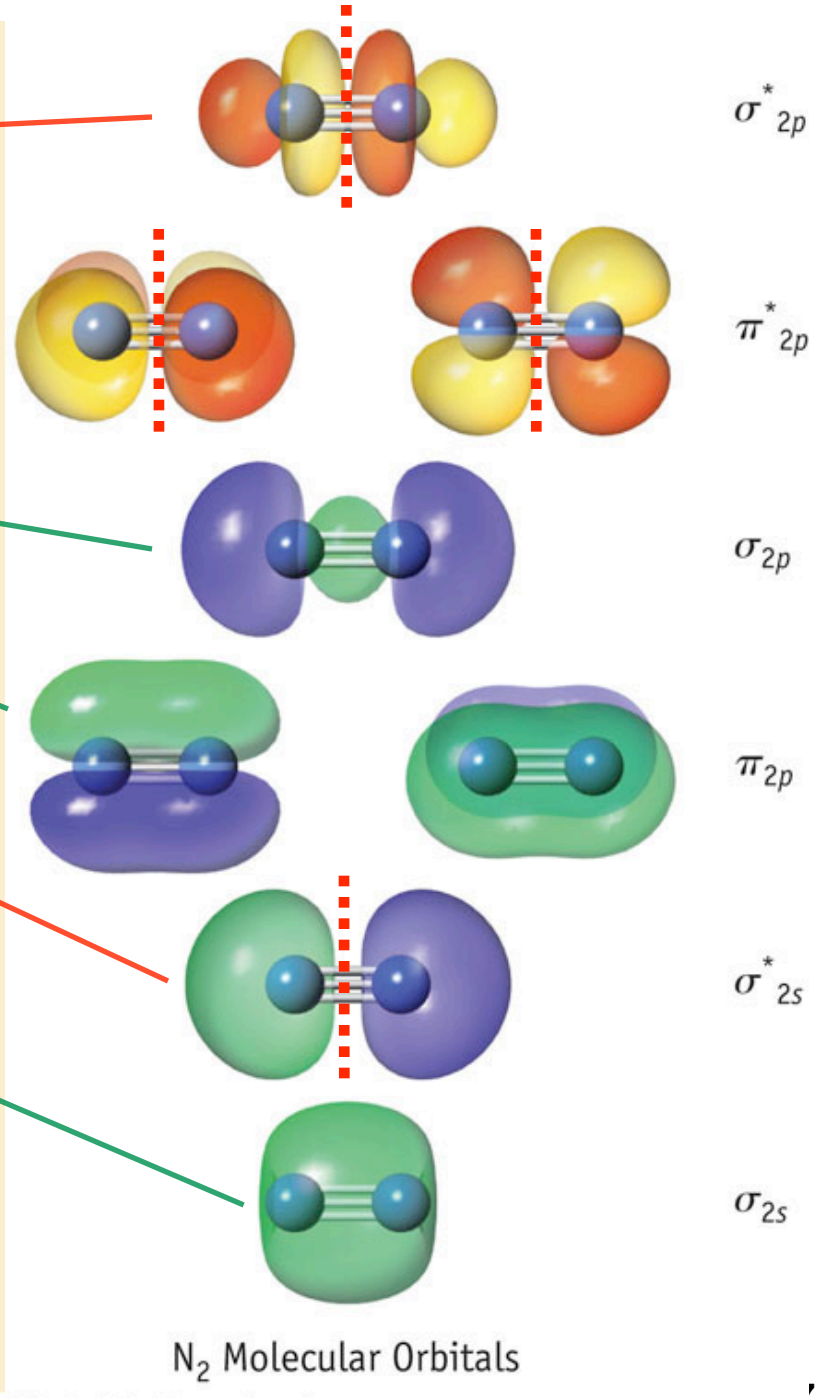


Molecular Orbitals for B_2, C_2, and N_2



N_2 Molecular Orbitals

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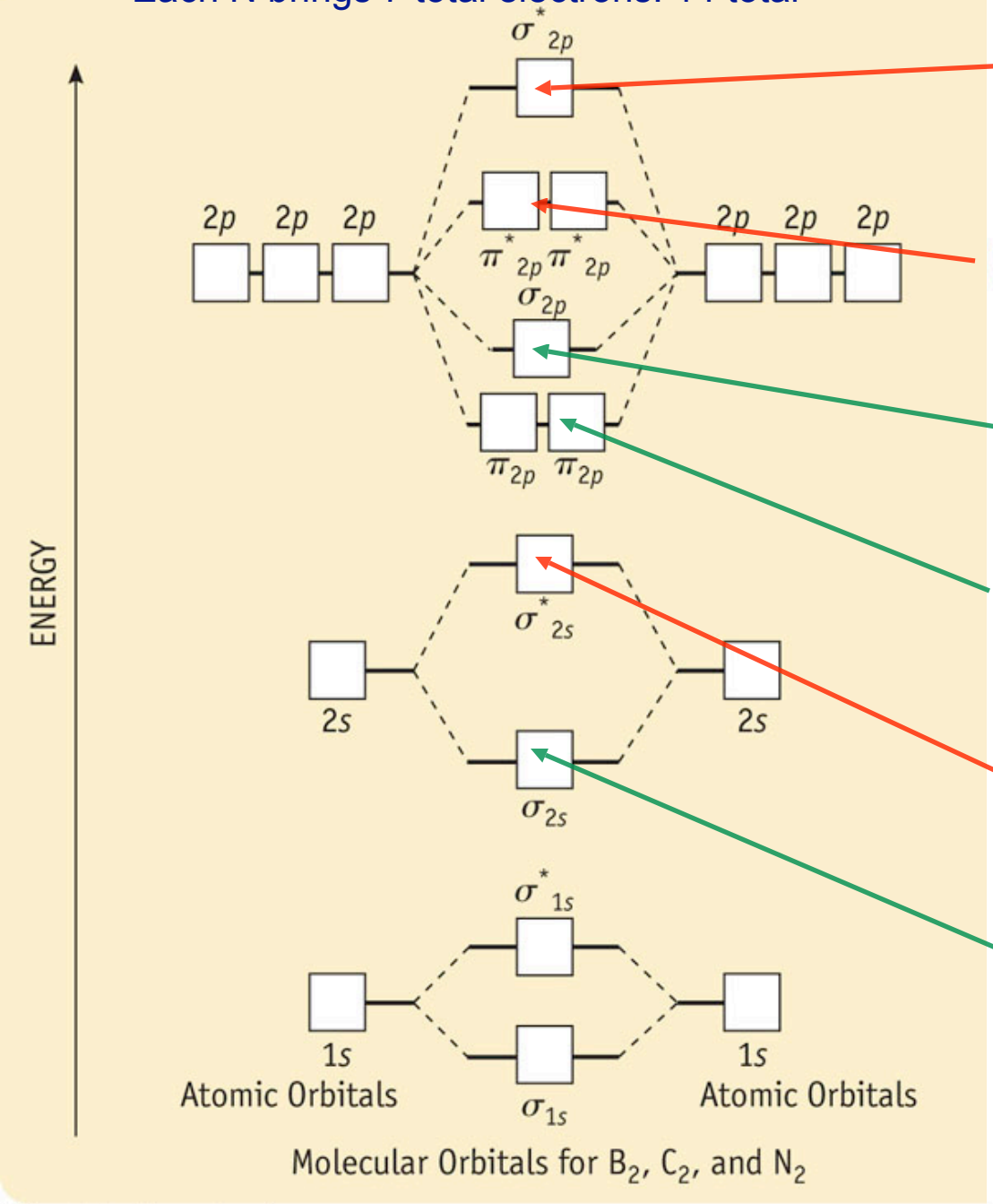
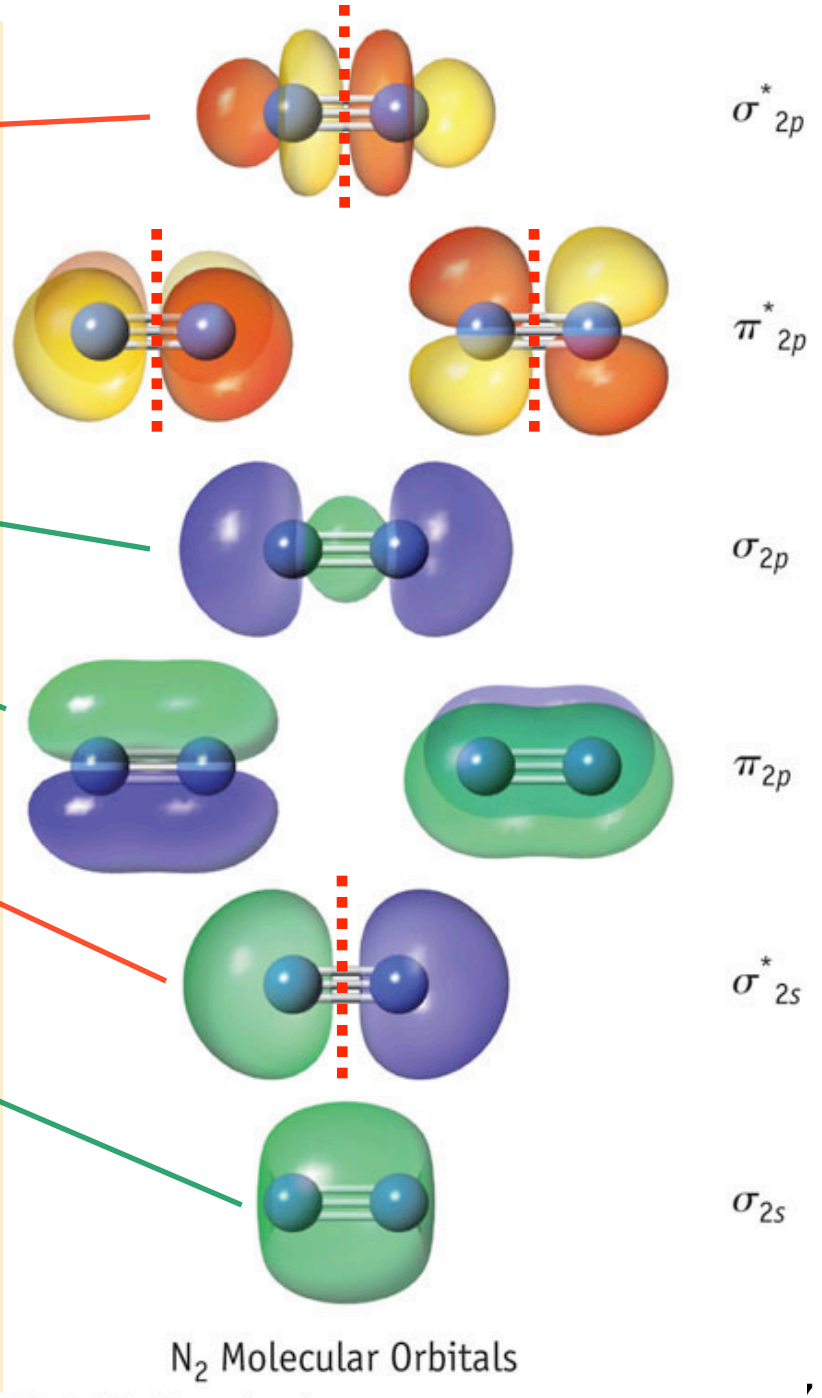
Each N brings 7 total electrons: 14 total



Molecular Orbitals for B_2, C_2, and N_2



N_2 Molecular Orbitals

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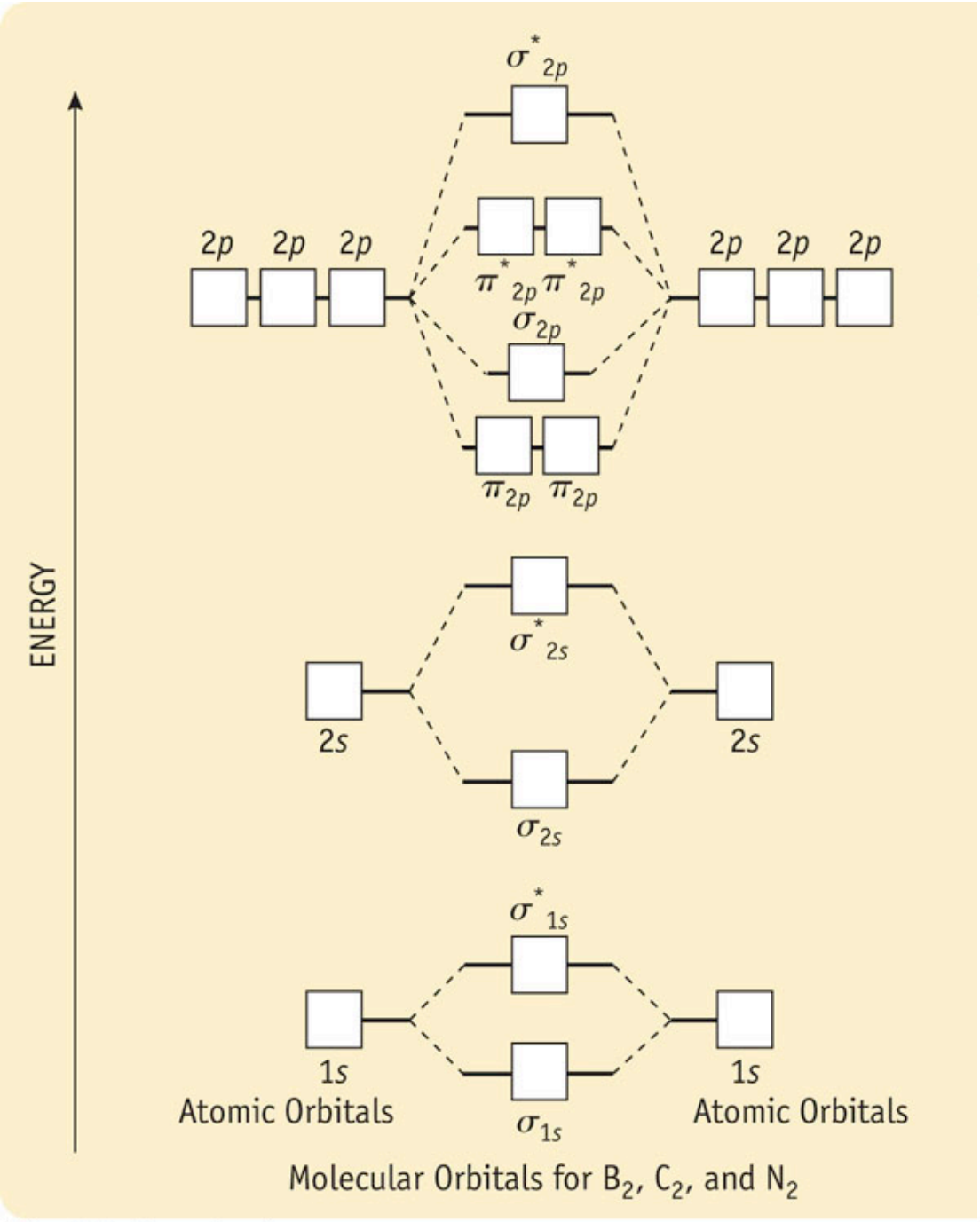
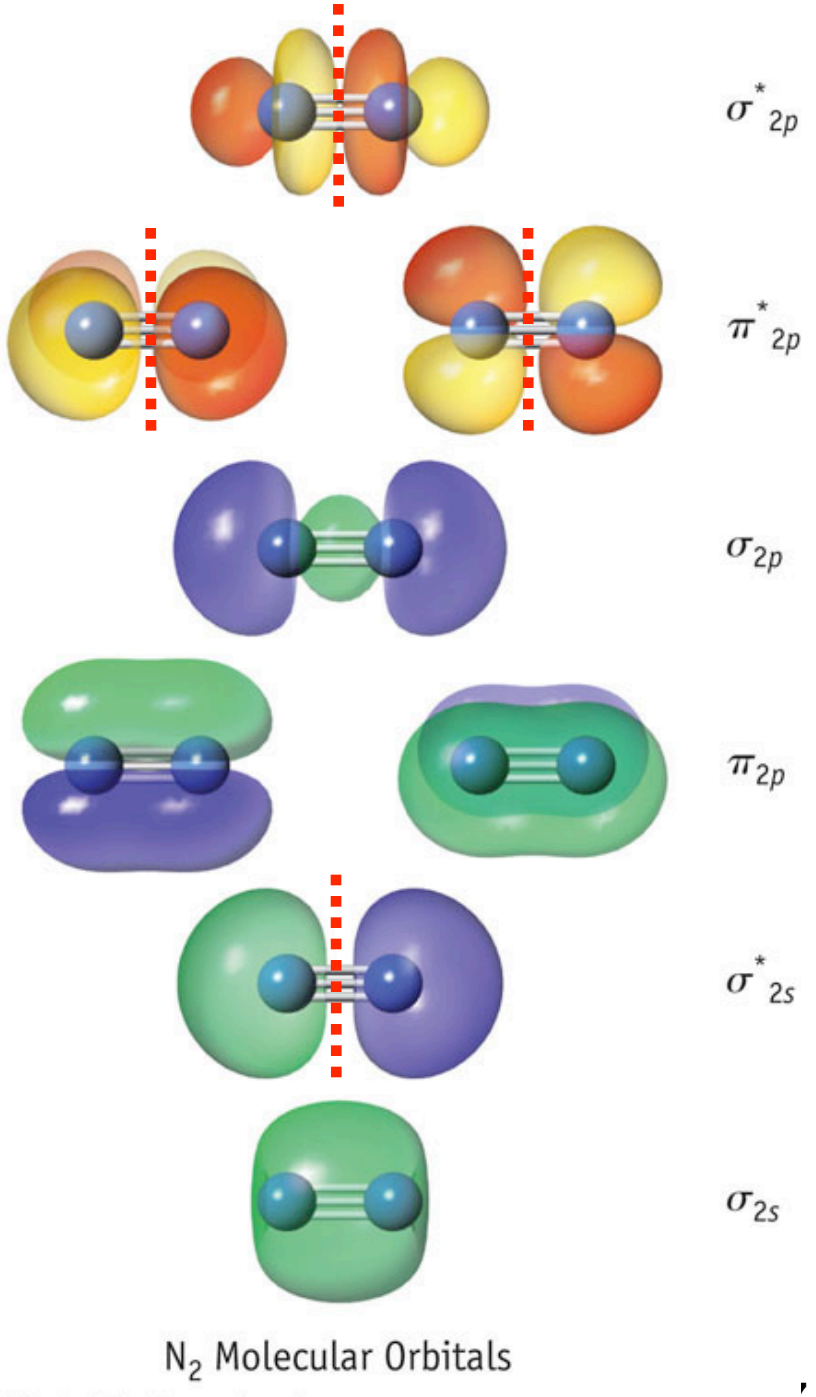


Molecular Orbitals for B_2, C_2, and N_2



N_2 Molecular Orbitals

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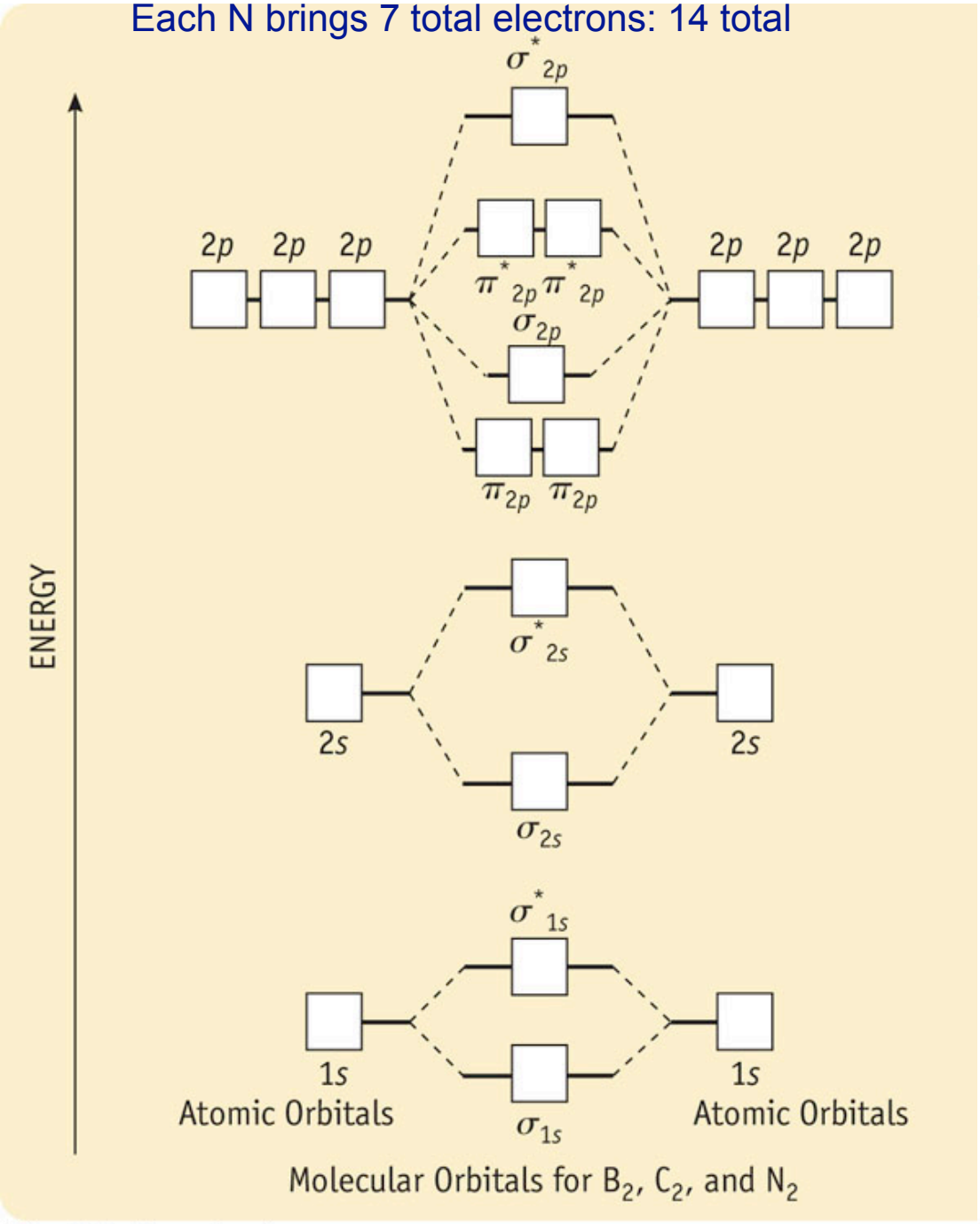
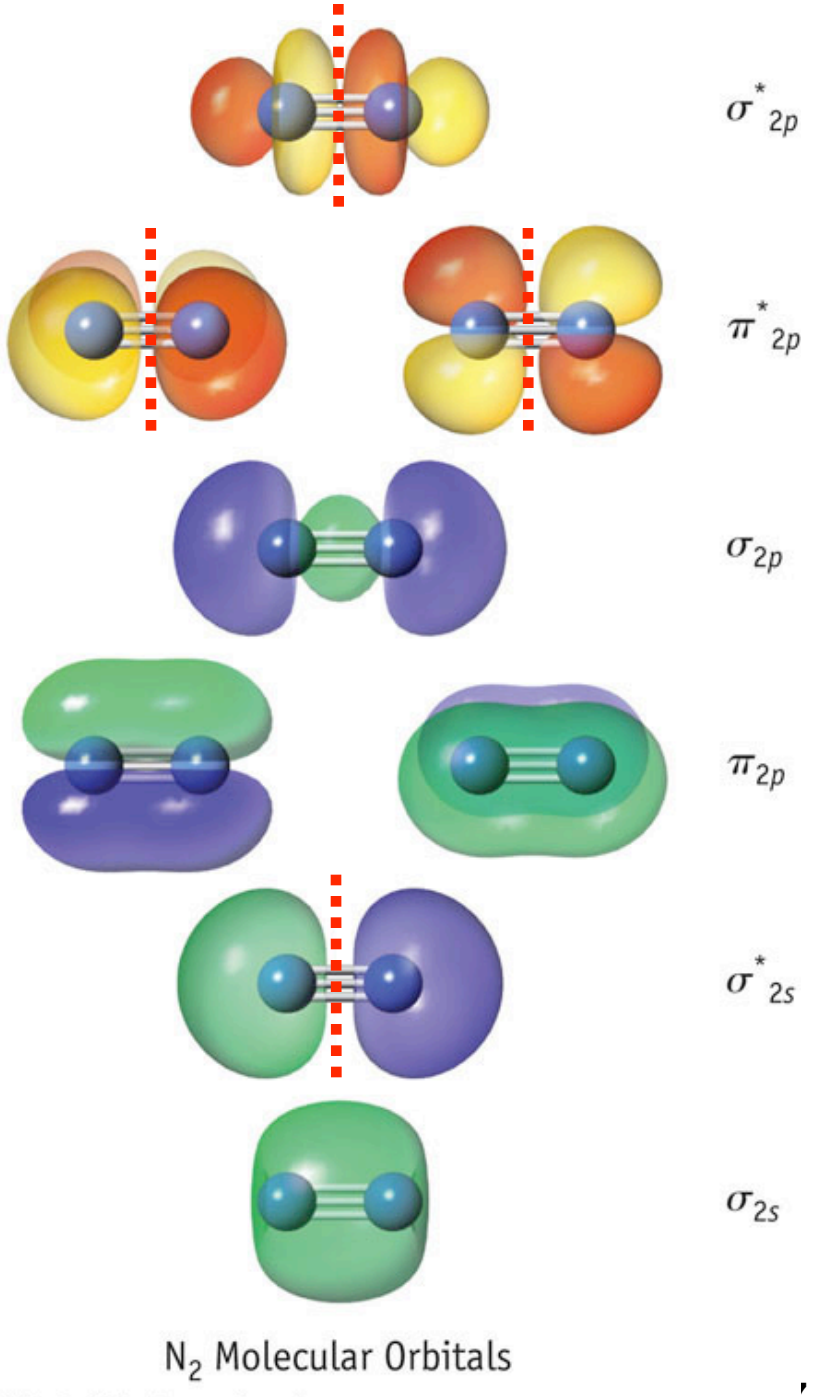


Molecular Orbitals for B_2, C_2, and N_2



N_2 Molecular Orbitals

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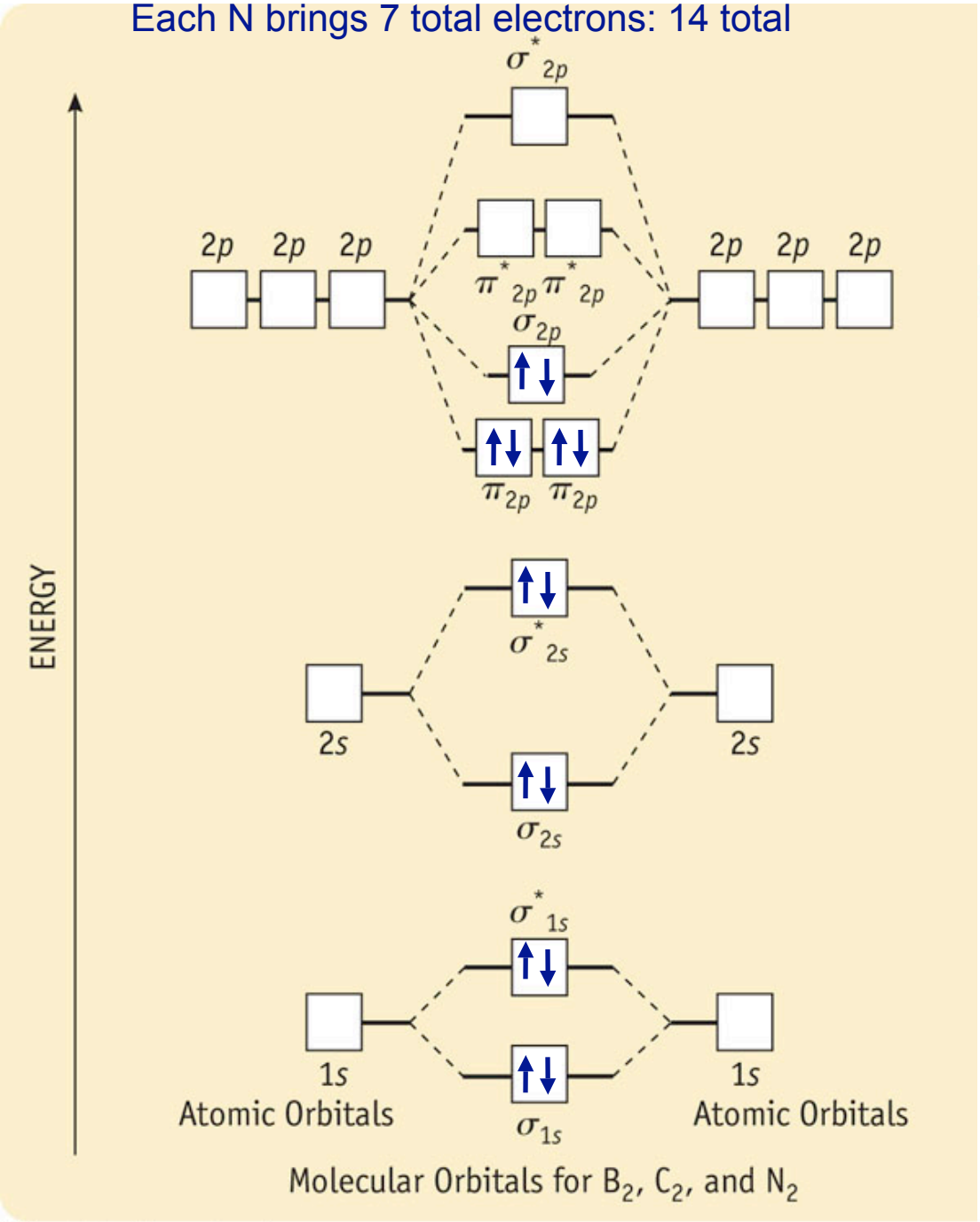
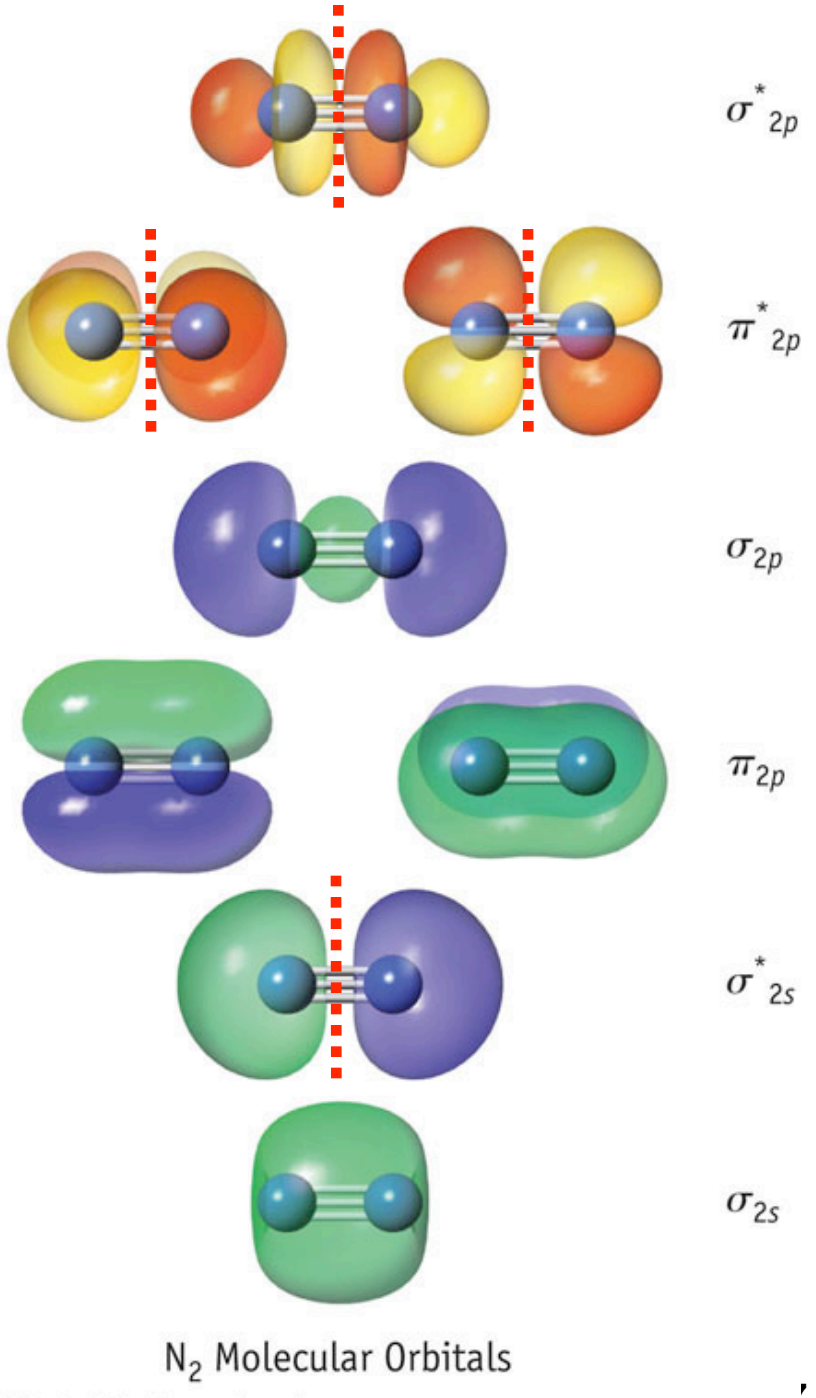
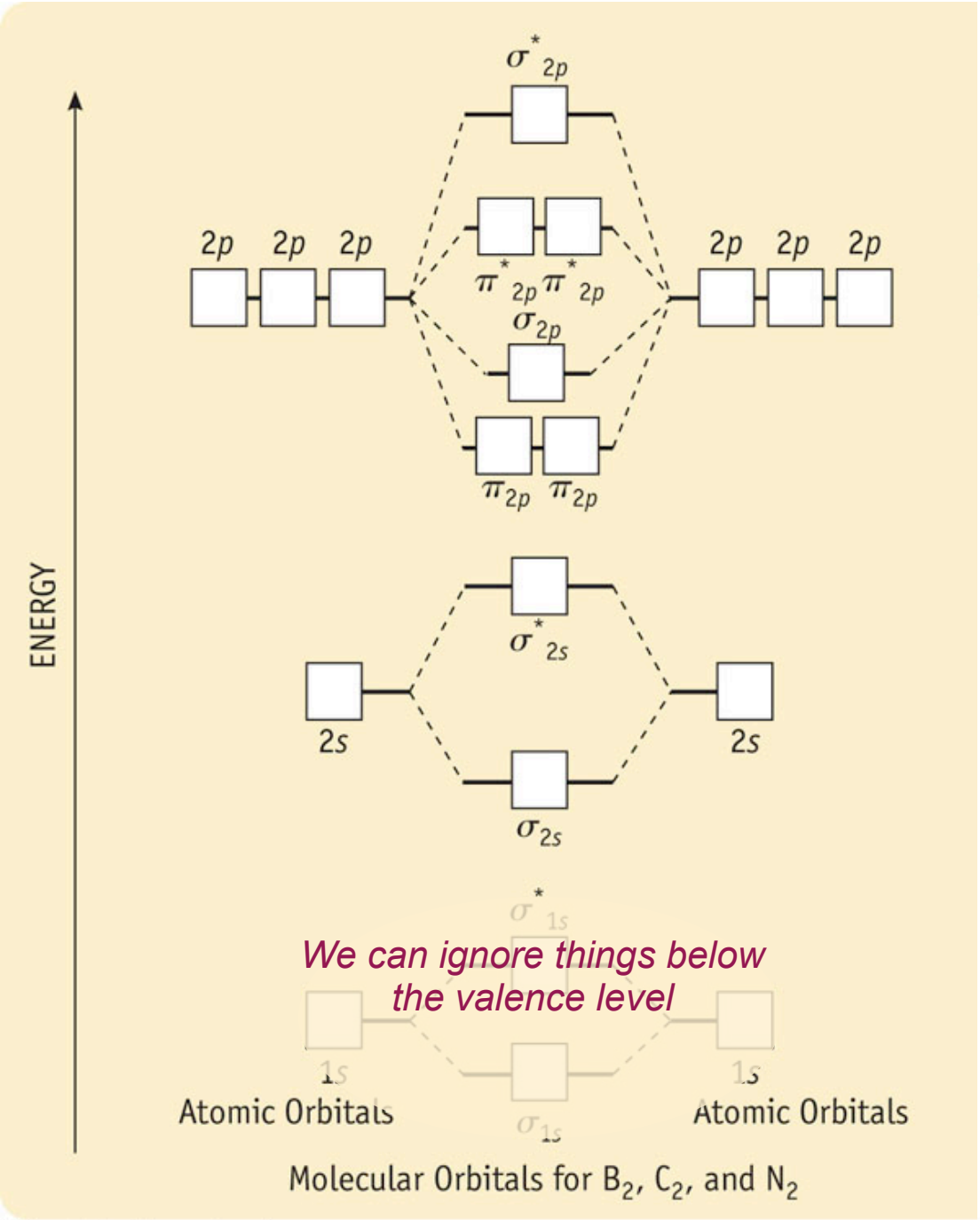


Molecular Orbitals for B_2, C_2, and N_2

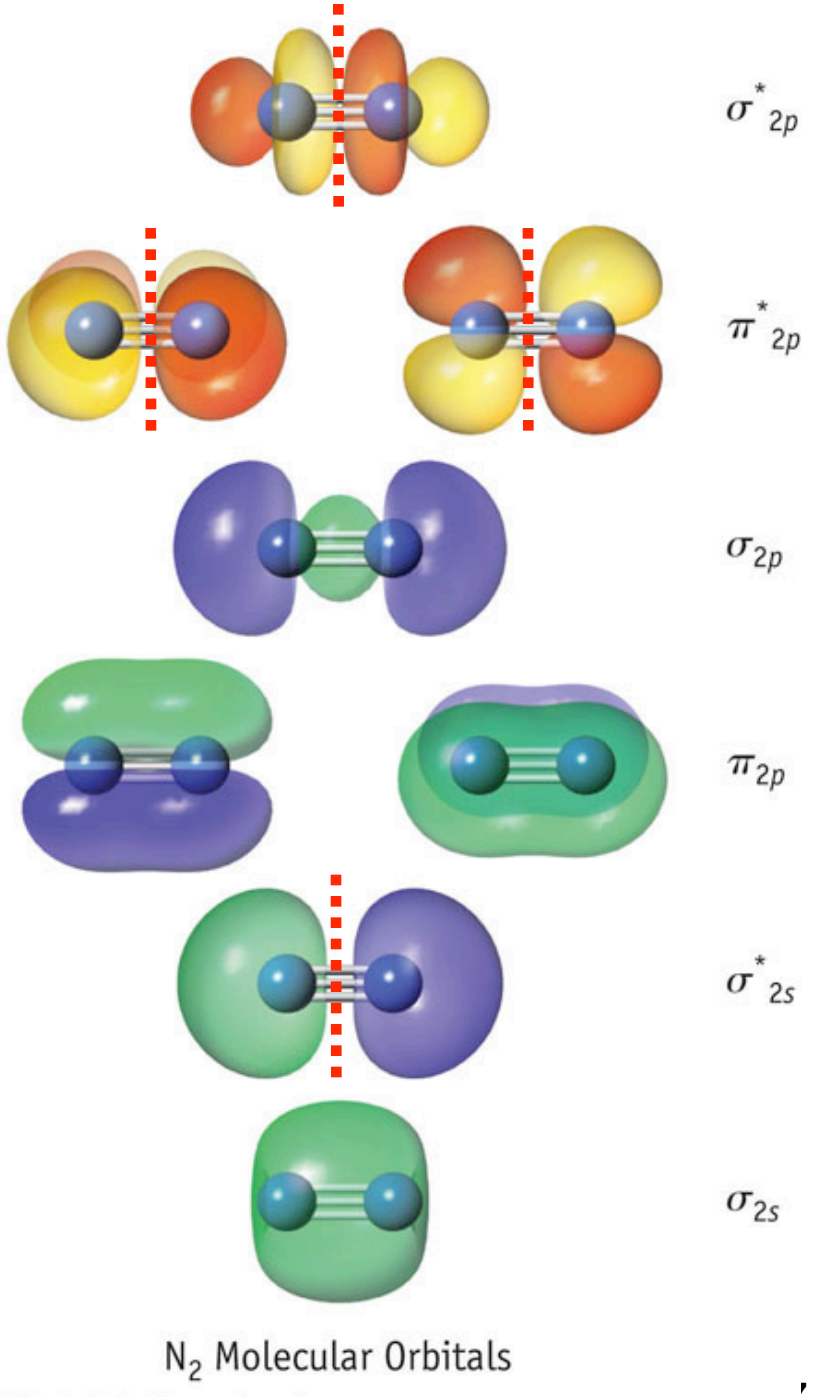


N_2 Molecular Orbitals



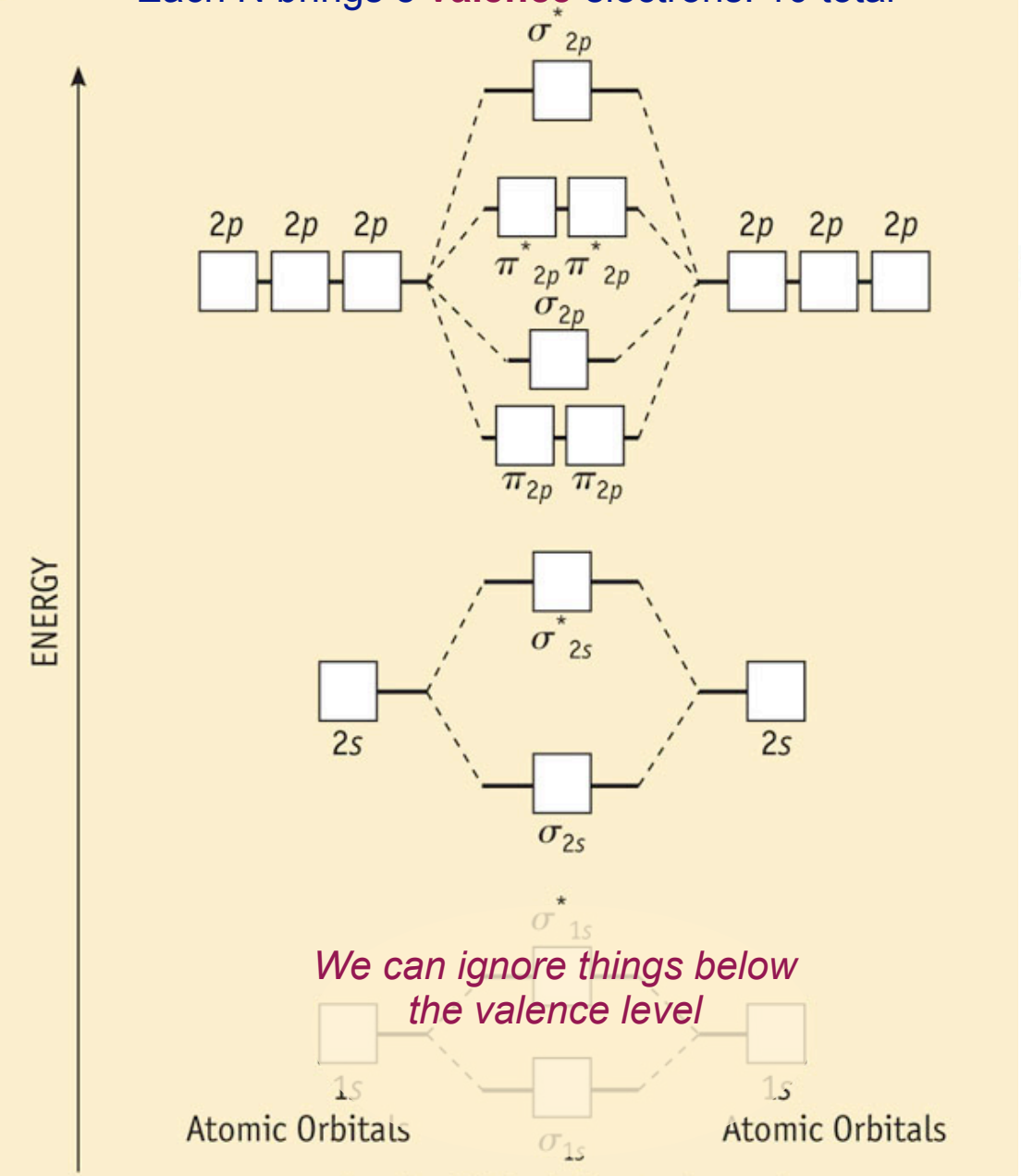
We can ignore things below the valence level

Molecular Orbitals for B_2, C_2, and N_2



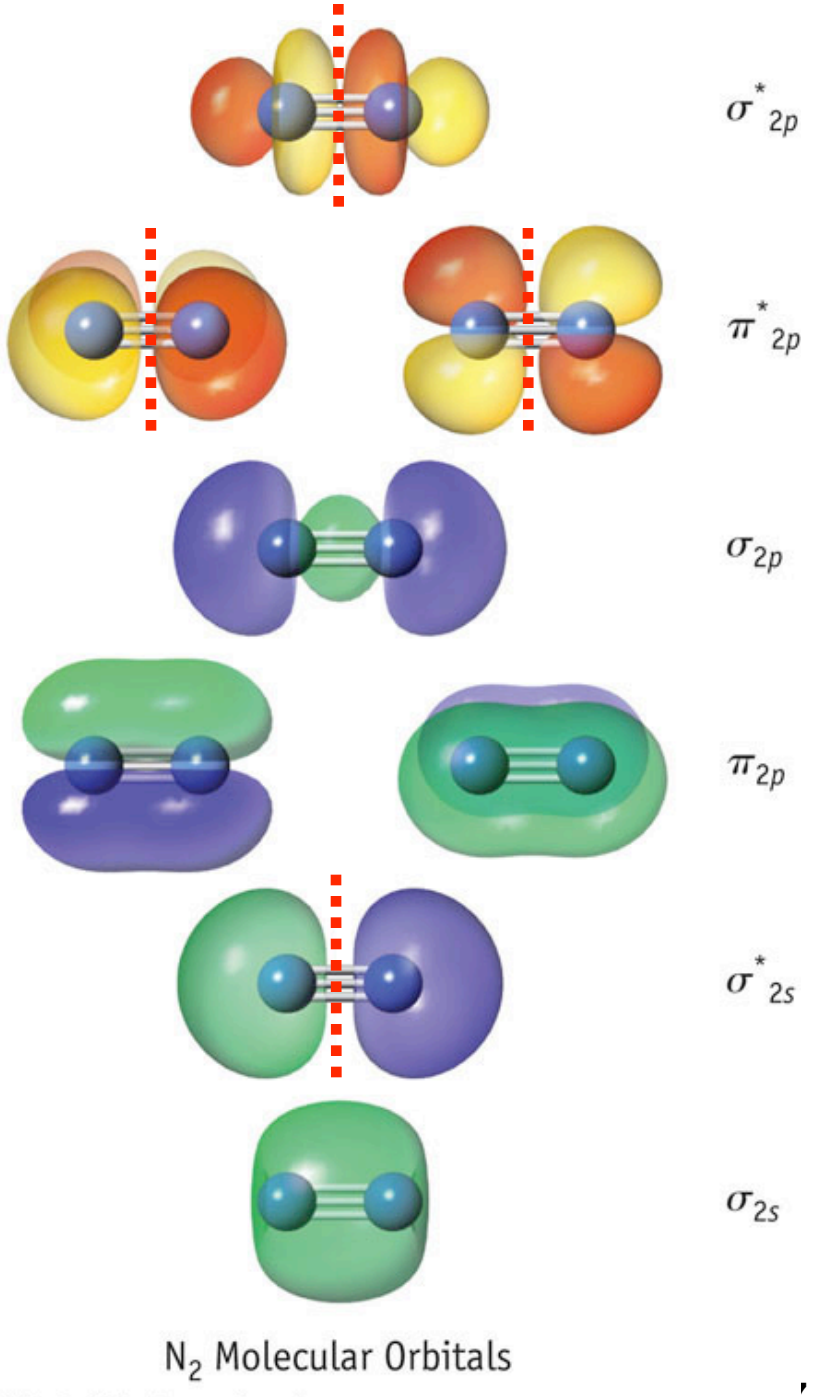
N_2 Molecular Orbitals

Each N brings 5 **valence** electrons: 10 total



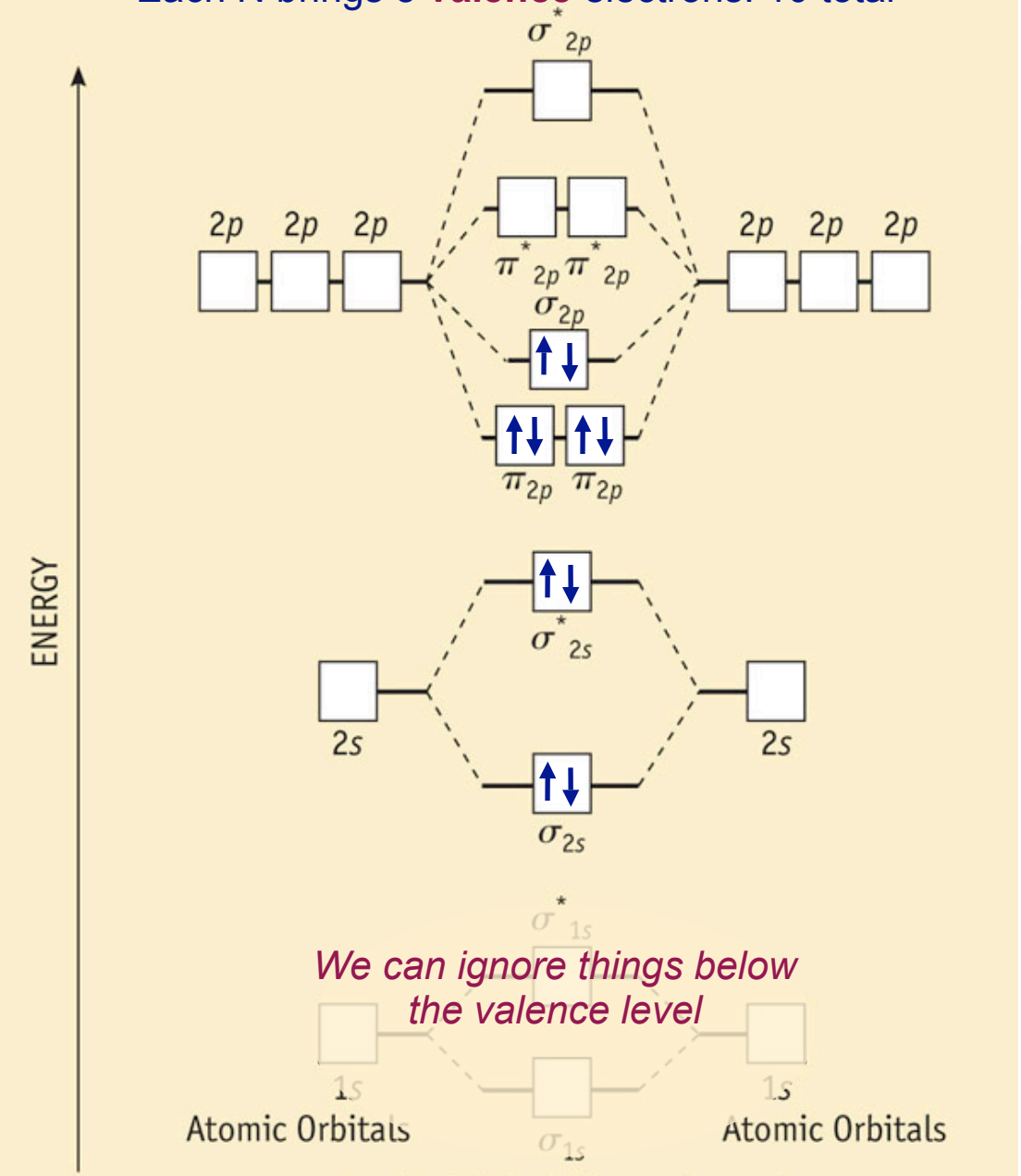
We can ignore things below the valence level

Molecular Orbitals for B_2, C_2, and N_2



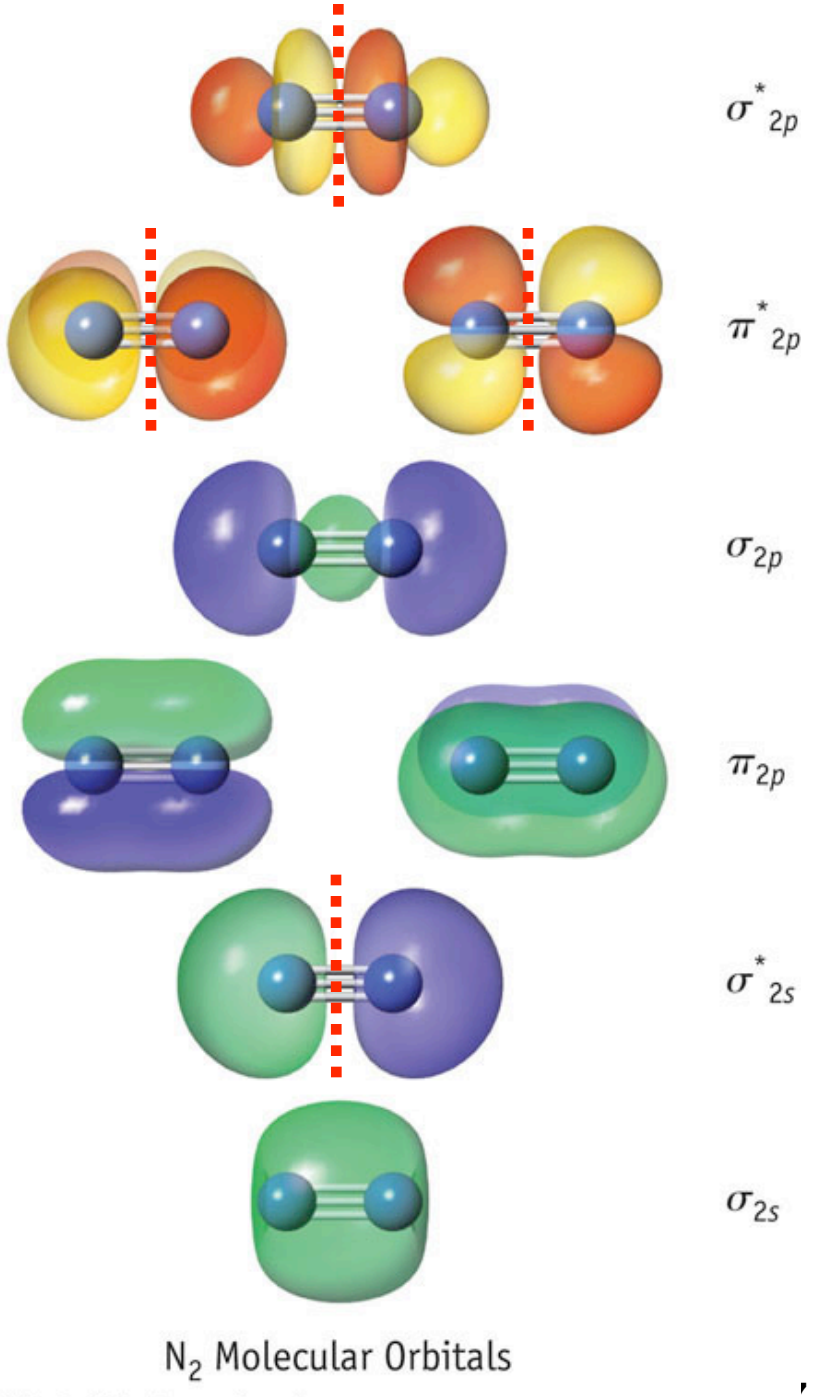
N_2 Molecular Orbitals

Each N brings 5 **valence** electrons: 10 total



We can ignore things below the valence level

Molecular Orbitals for B_2, C_2, and N_2



N_2 Molecular Orbitals

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear Diatomic Molecules of Second-Period Elements

	B_2	C_2	N_2	O_2	F_2
σ^*_{2p}	☐	☐	☐	☐	☐
π^*_{2p}	☐☐	☐☐	☐☐	↑☐↑	↑↓☐↑↓
σ_{2p}	☐	☐	↑↓	↑↓↑↓	↑↓↑↓
π_{2p}	↑↑	↑↓↑↓	↑↓↑↓	↑↓	↑↓
σ^*_{2s}	↑↓	↑↓	↑↓	↑↓	↑↓
σ_{2s}	↑↓	↑↓	↑↓	↑↓	↑↓
Bond order	One	Two	Three	Two	One
Bond-dissociation energy (kJ/mol)	290	620	945	498	155
Bond distance (pm)	159	131	110	121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia	Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear Diatomic Molecules of Second-Period Elements

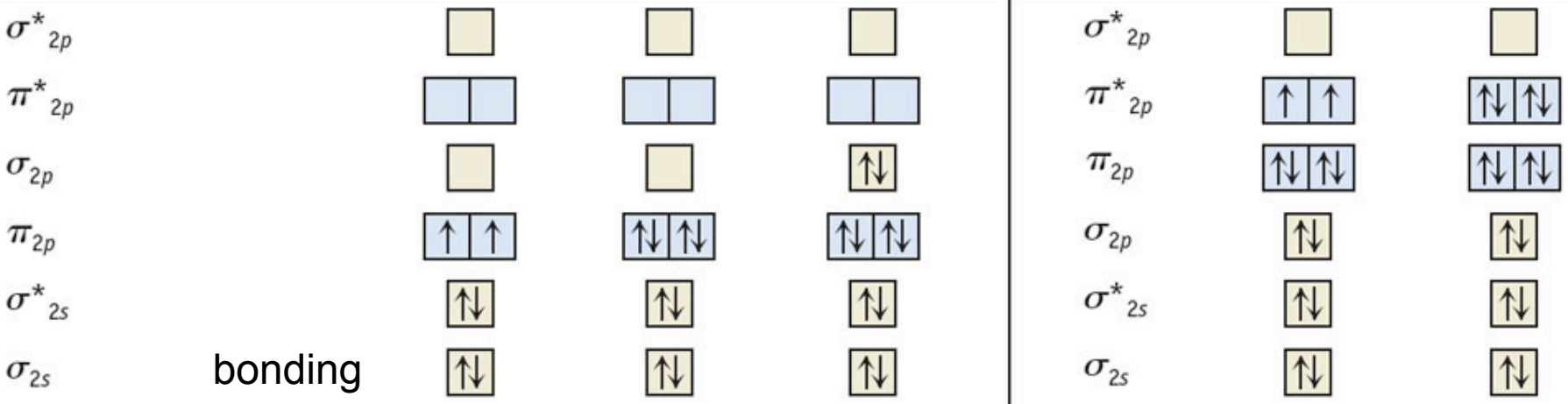


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TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear Diatomic Molecules of Second-Period Elements

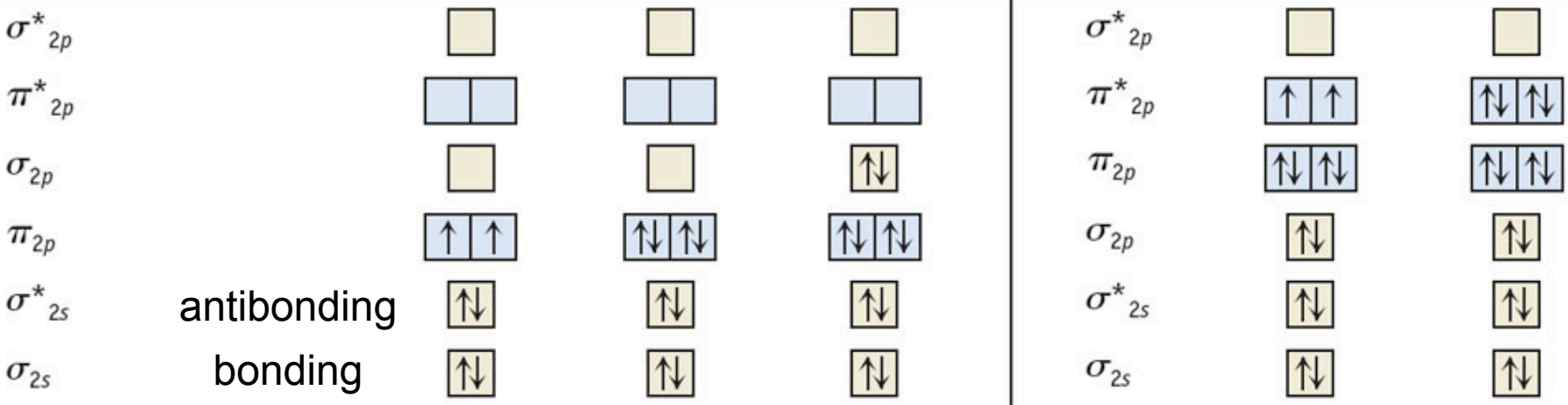

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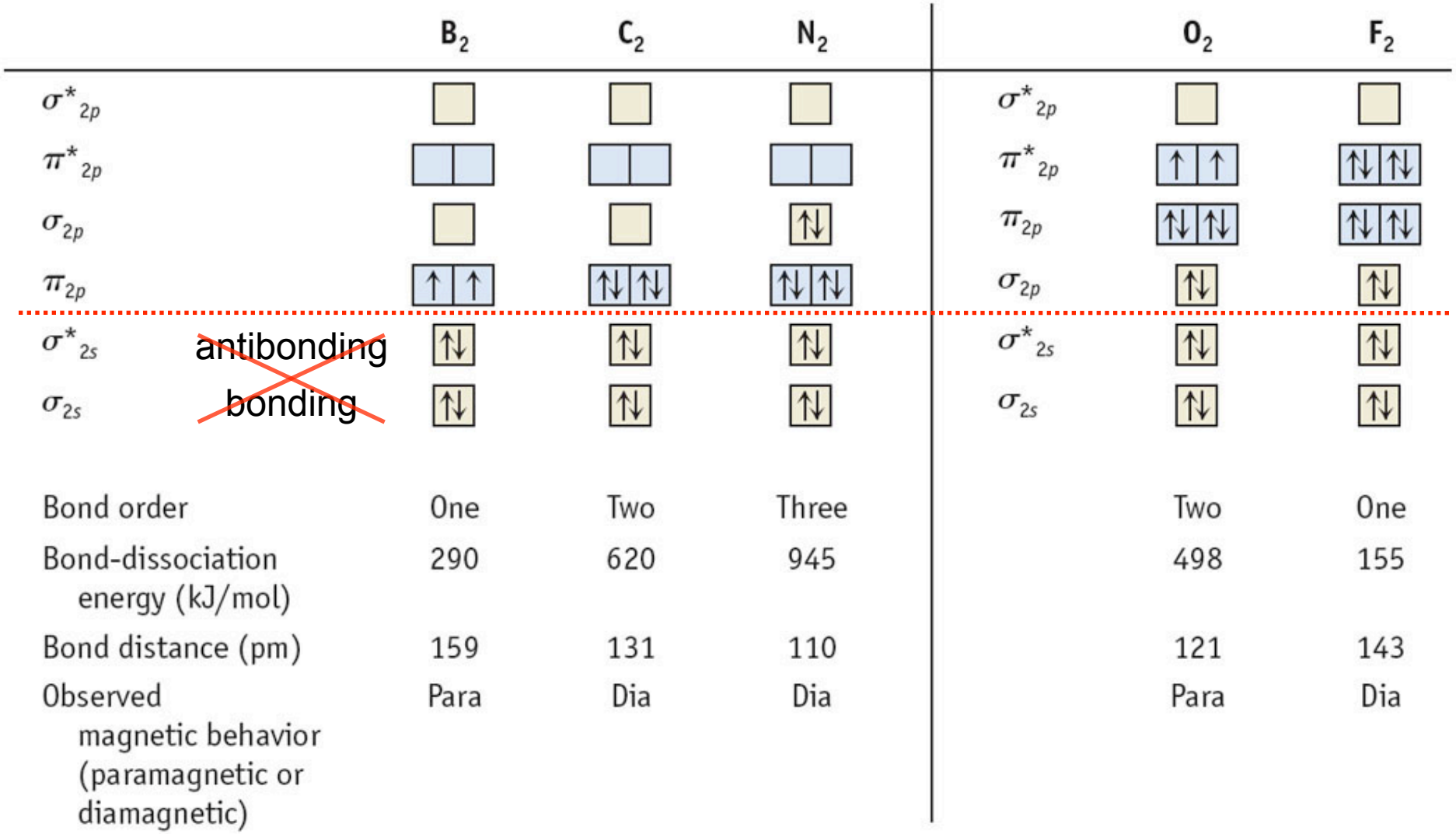
TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear Diatomic Molecules of Second-Period Elements



	B_2	C_2	N_2	O_2	F_2
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Bond distance (pm)	159	131	110	121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia	Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

1 bond

	B_2	C_2	N_2	O_2	F_2
σ^*_{2p}					
π^*_{2p}					
σ_{2p}					
π_{2p}					
σ^*_{2s}					
σ_{2s}					
Bond order	One	Two	Three	Two	One
Bond-dissociation energy (kJ/mol)	290	620	945	498	155
Bond distance (pm)	159	131	110	121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia	Para	Dia

~~antibonding~~ ~~bonding~~

Table 9-1, p. 428

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

1 bond 2 bonds

	B_2	C_2	N_2	O_2	F_2
σ^*_{2p}					
π^*_{2p}					
σ_{2p}					
π_{2p}					
σ^*_{2s}					
σ_{2s}					
Bond order	One	Two	Three	Two	One
Bond-dissociation energy (kJ/mol)	290	620	945	498	155
Bond distance (pm)	159	131	110	121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia	Para	Dia

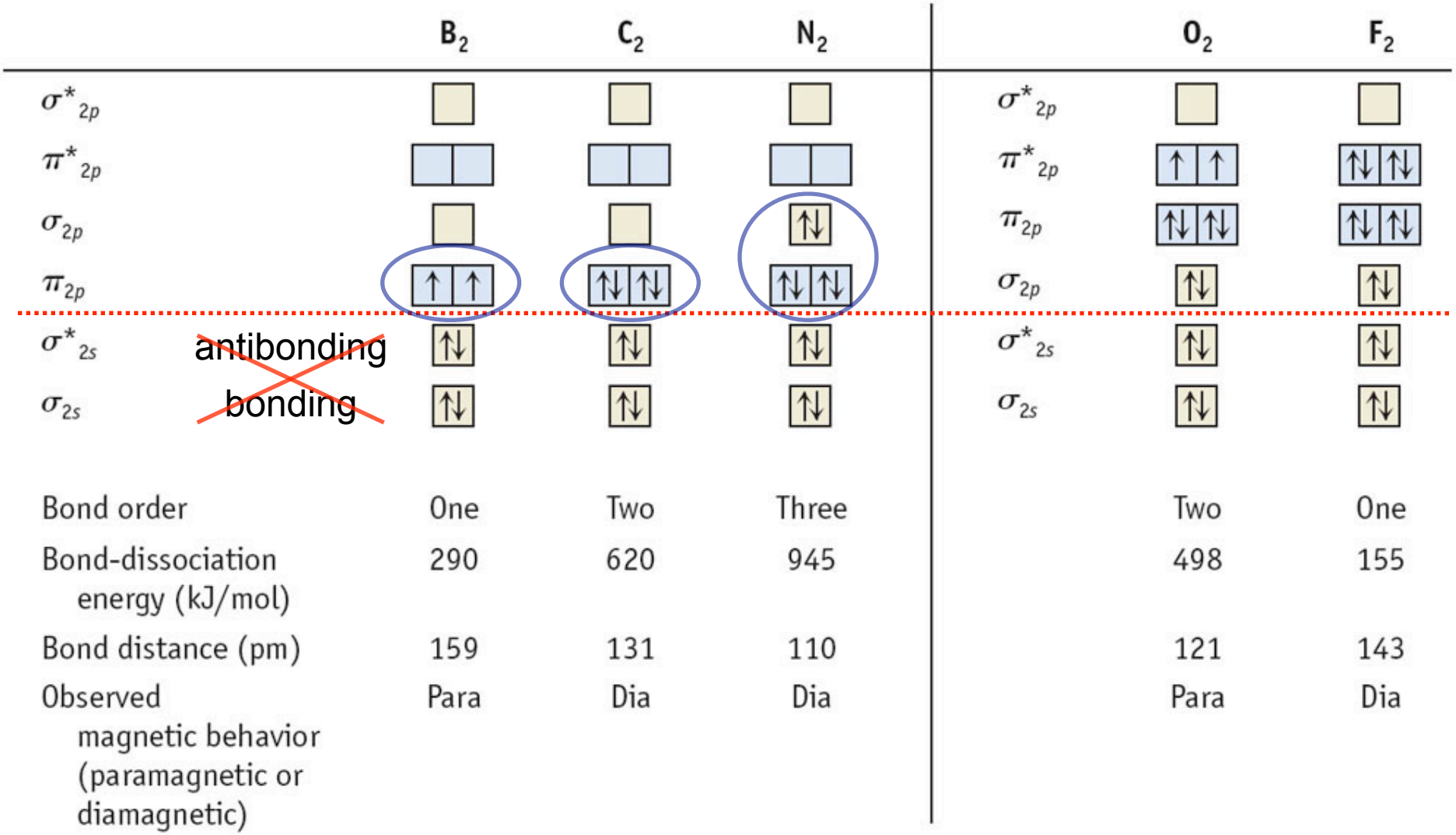
antibonding

bonding

Table 9-1, p. 428

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

1 bond 2 bonds 3 bonds

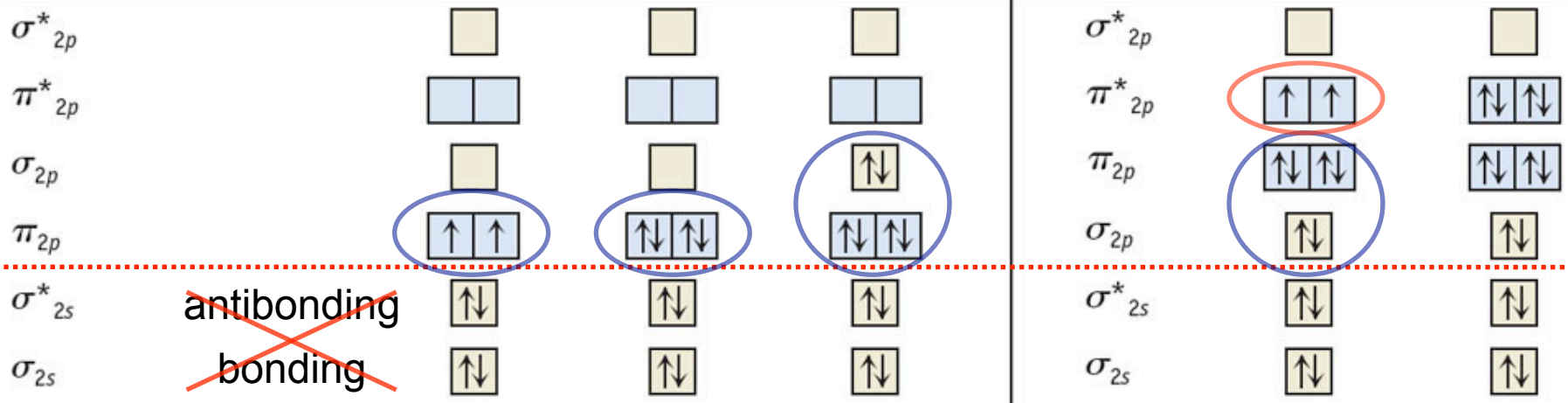


	B_2	C_2	N_2	O_2	F_2
Bond order	One	Two	Three	Two	One
Bond-dissociation energy (kJ/mol)	290	620	945	498	155
Bond distance (pm)	159	131	110	121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia	Para	Dia

Table 9-1, p. 428

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

1 bond 2 bonds 3 bonds 3-1=2

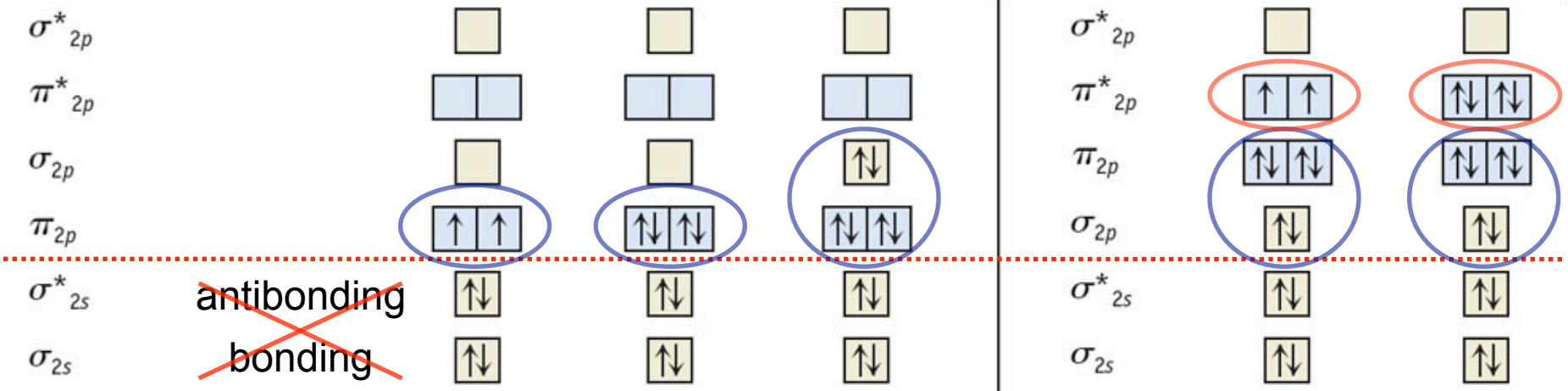


	B_2	C_2	N_2	O_2	F_2
Bond order	One	Two	Three	Two	One
Bond-dissociation energy (kJ/mol)	290	620	945	498	155
Bond distance (pm)	159	131	110	121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia	Para	Dia

Table 9-1, p. 428

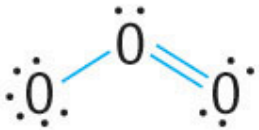
TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

1 bond 2 bonds 3 bonds 3-1=2 3-2=1

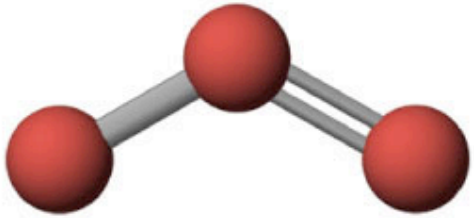


	B_2	C_2	N_2	O_2	F_2
Bond order	One	Two	Three	Two	One
Bond-dissociation energy (kJ/mol)	290	620	945	498	155
Bond distance (pm)	159	131	110	121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia	Para	Dia

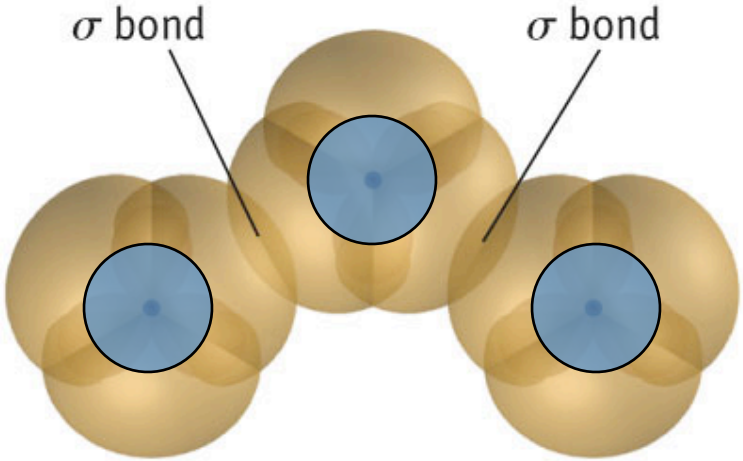
Table 9-1, p. 428



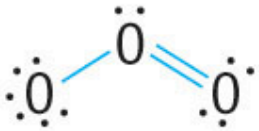
Lewis structure of O_3. All O atoms are sp^2 hybridized.



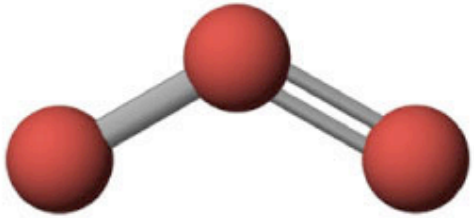
Molecular model



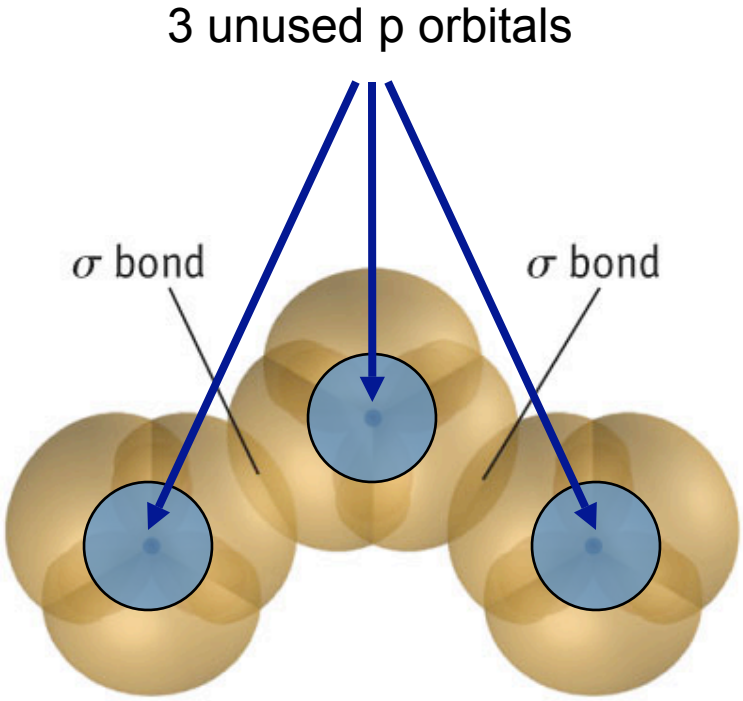
A representation of the sigma bonding framework of O_3 using sp^2 hybrid orbitals



Lewis structure of O_3. All O atoms are sp^2 hybridized.

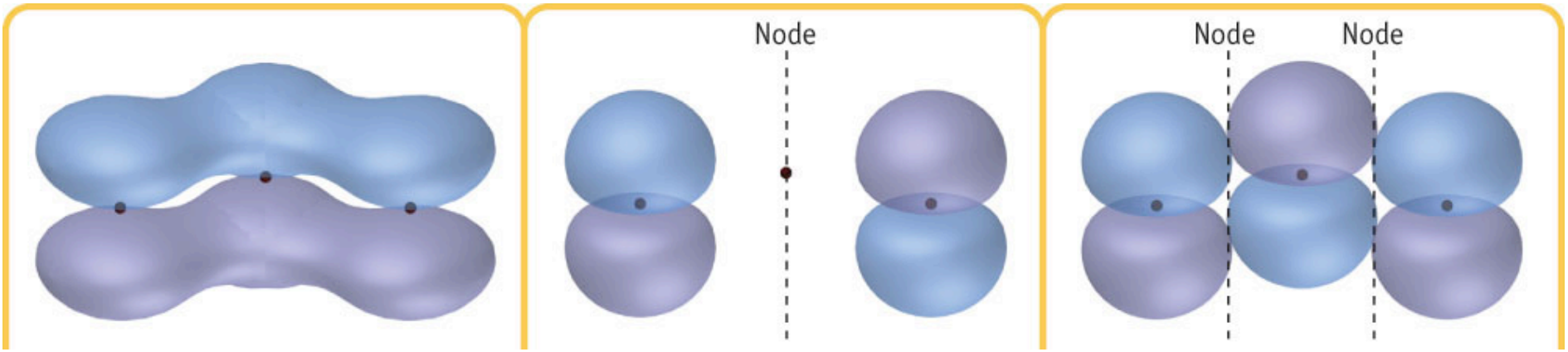


Molecular model



A representation of the sigma bonding framework of O_3 using sp^2 hybrid orbitals

3 atomic p orbitals combine to form 3 molecular π orbitals



(1) (2) (3)

Which molecular orbital is lowest in energy?

3 atomic p orbitals combine to form 3 molecular π orbitals

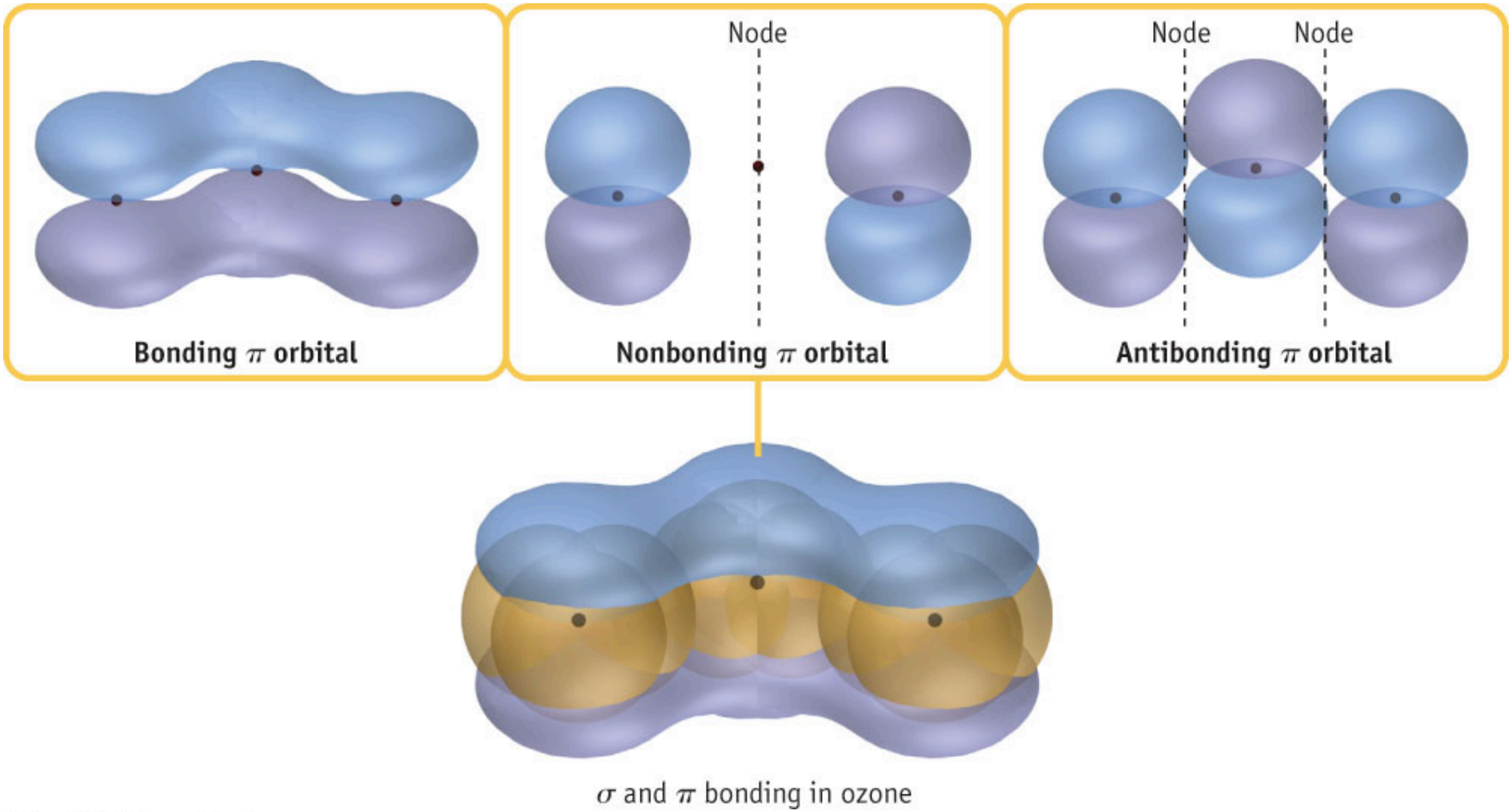


Fig. 9-22, p. 431

Note the symmetry - there is no double bond side or single bond side

3 atomic p orbitals combine to form 3 molecular π orbitals

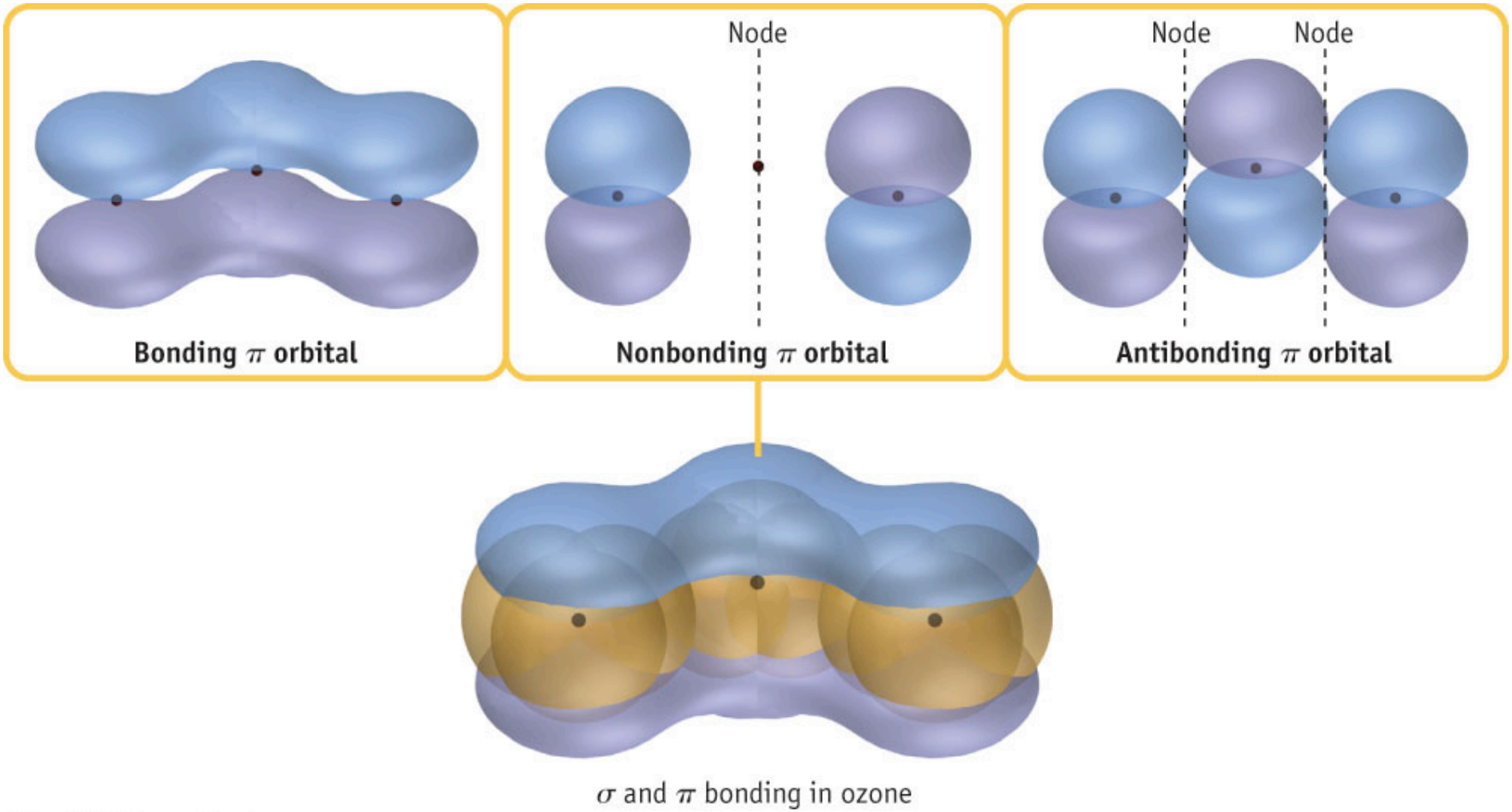


Fig. 9-22, p. 431

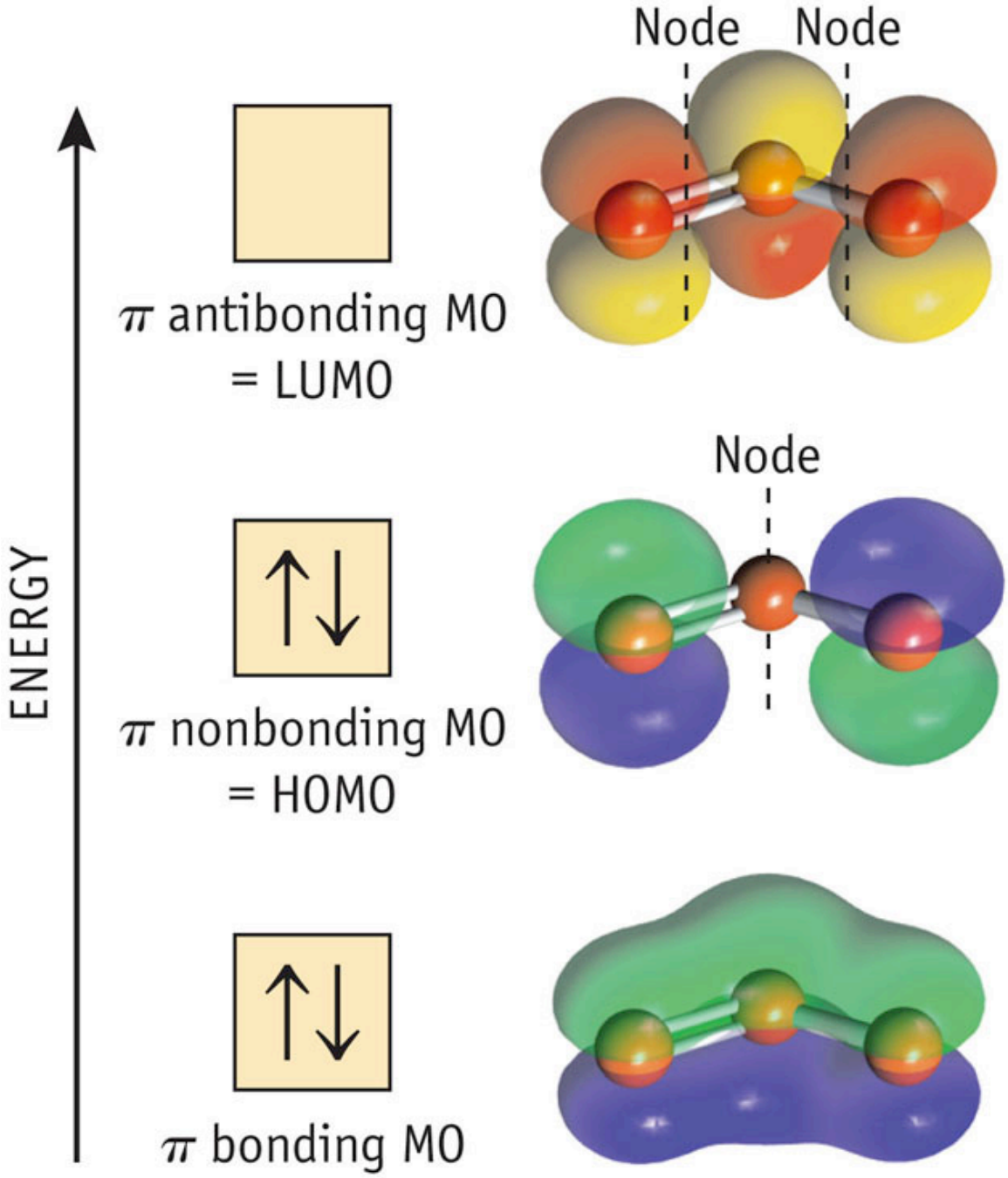
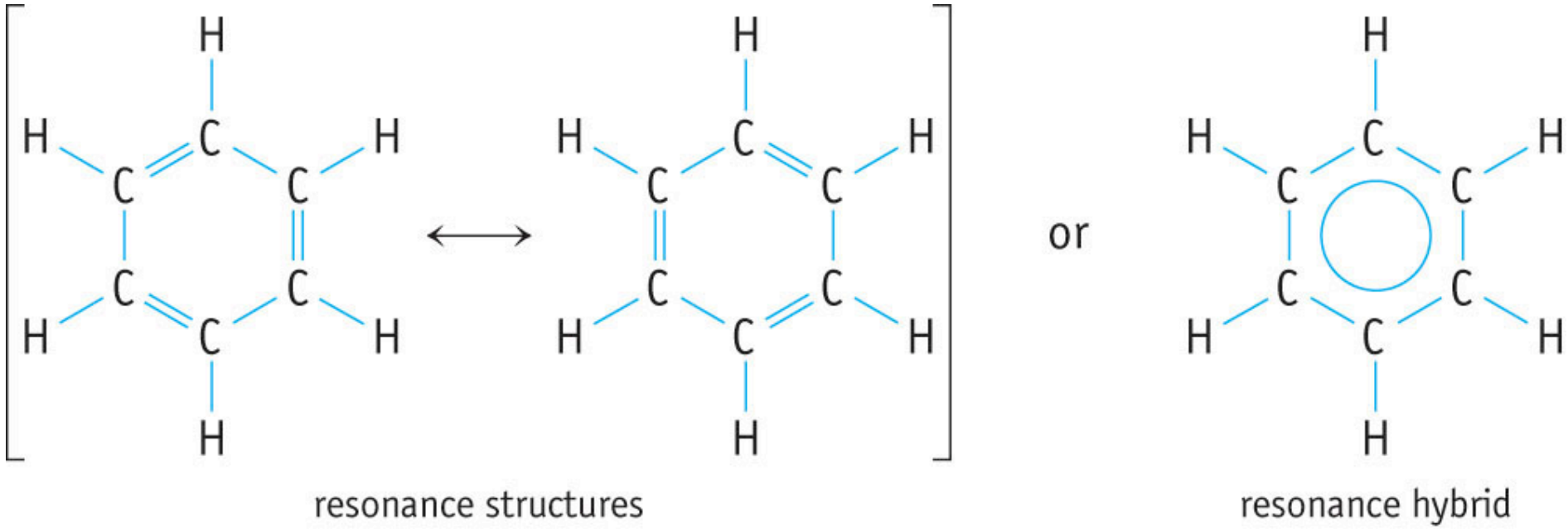
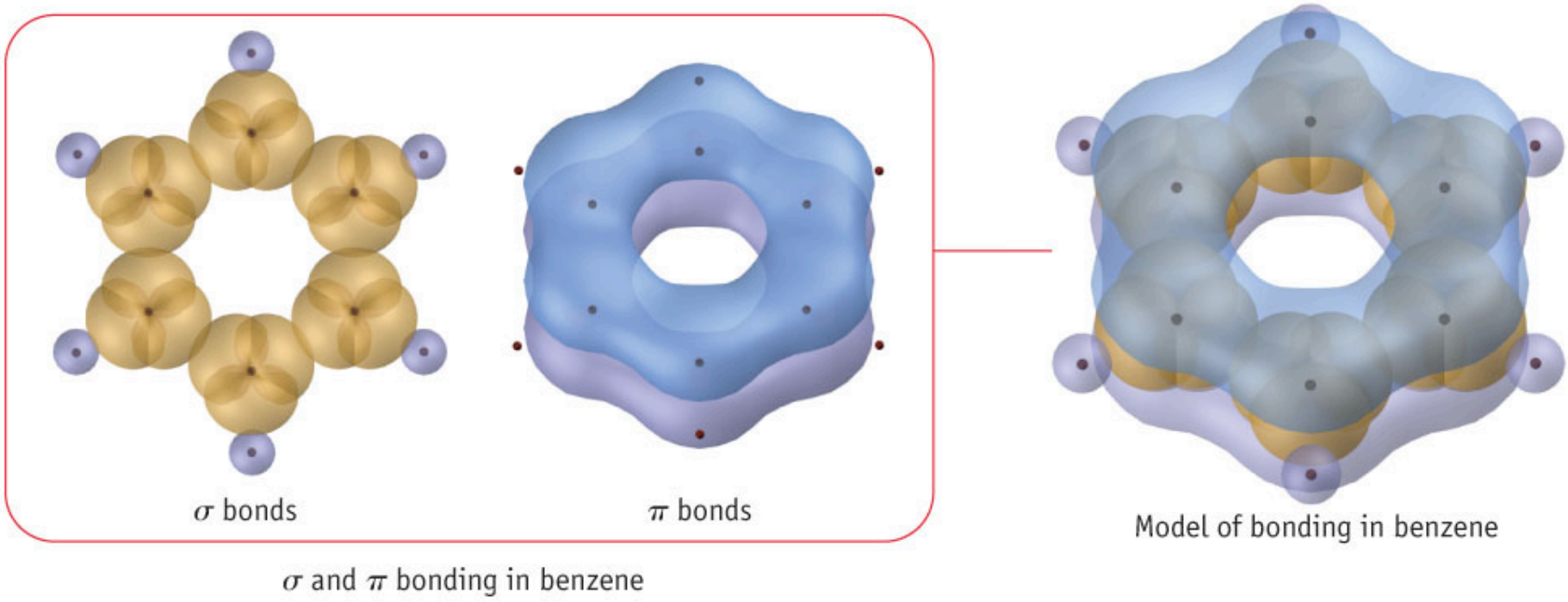


Fig. 9-23, p. 432

Benzene

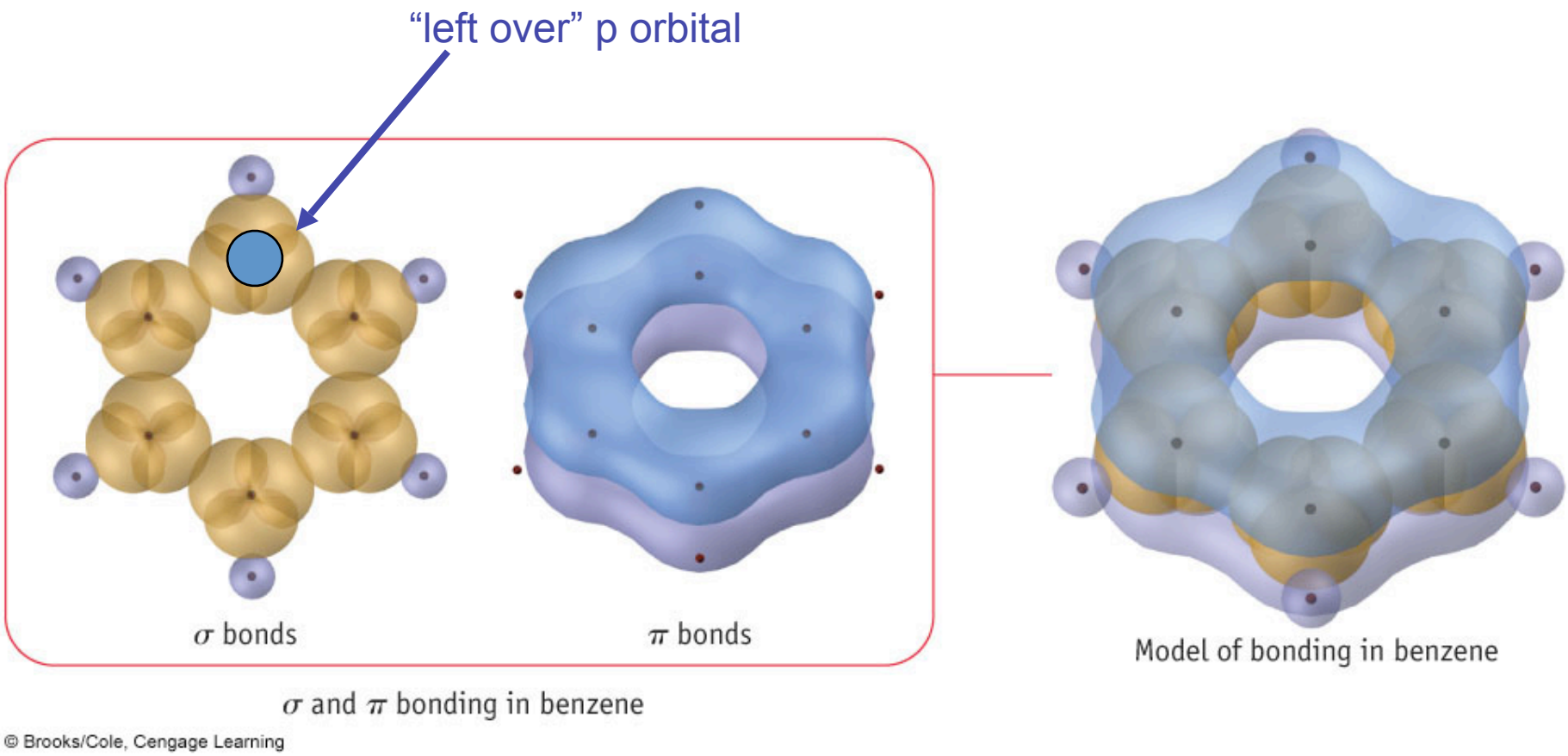
Represented by two resonance structures





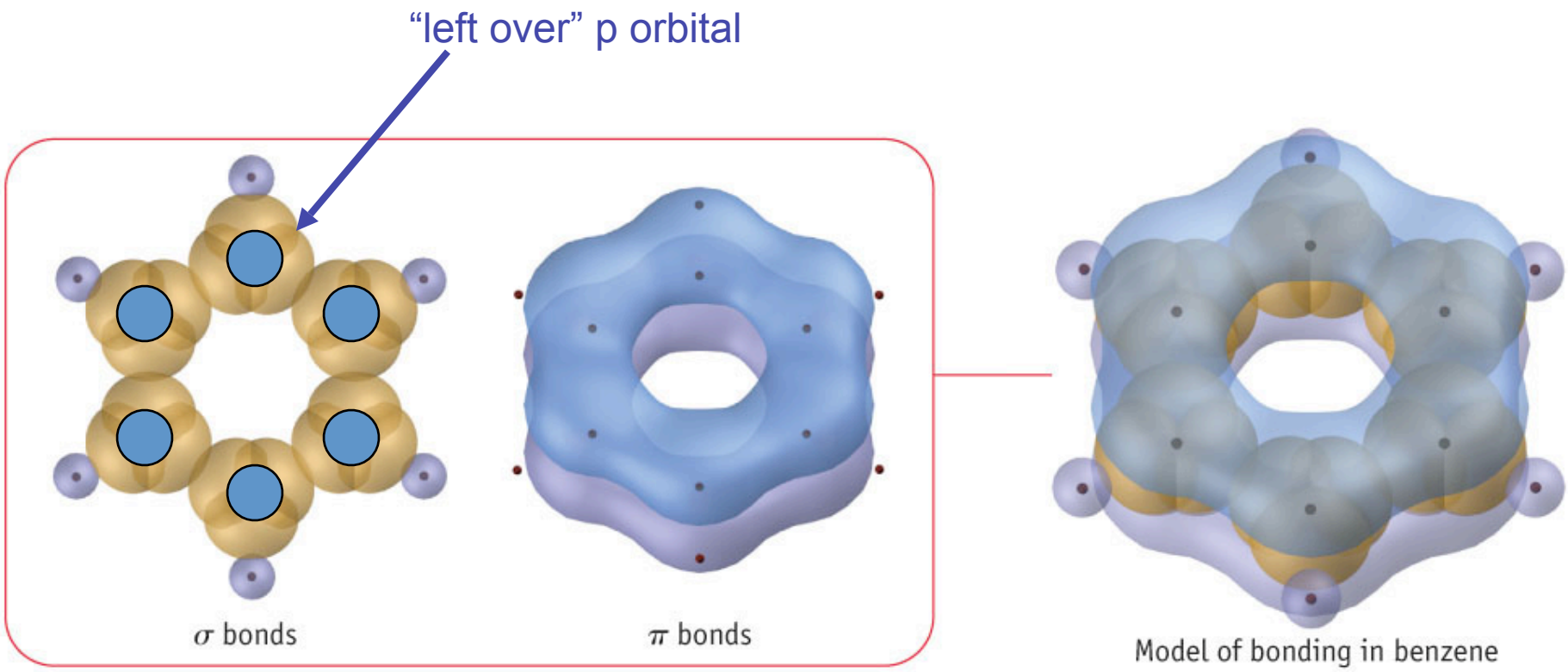
σ and π bonding in benzene

Fig. 9-14, p. 422



σ and π bonding in benzene

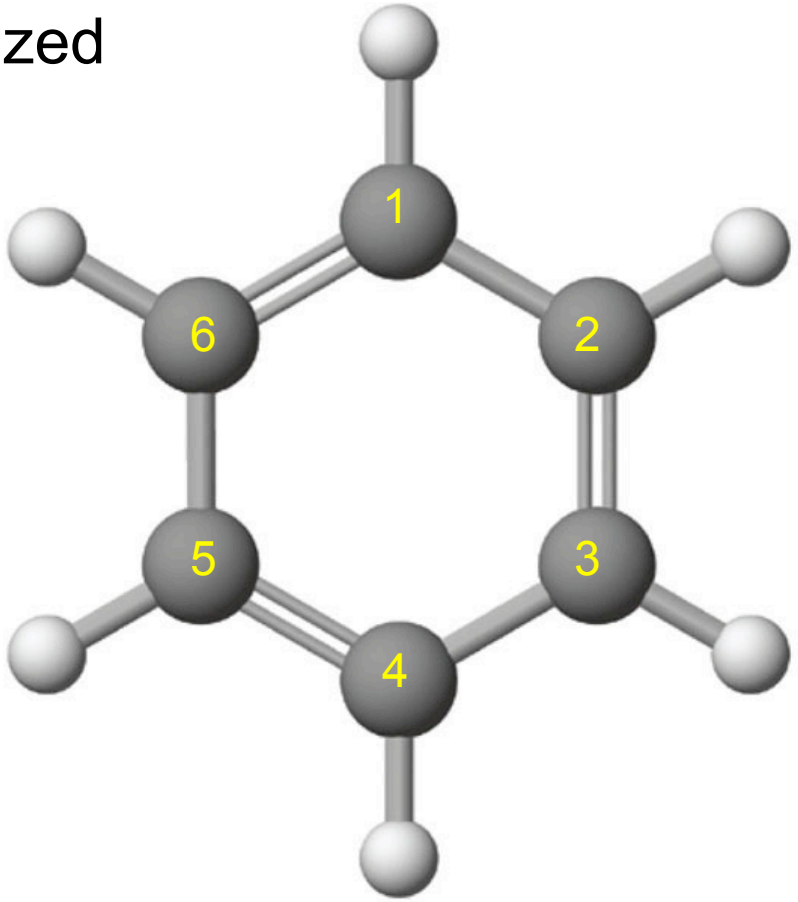
Fig. 9-14, p. 422



σ and π bonding in benzene

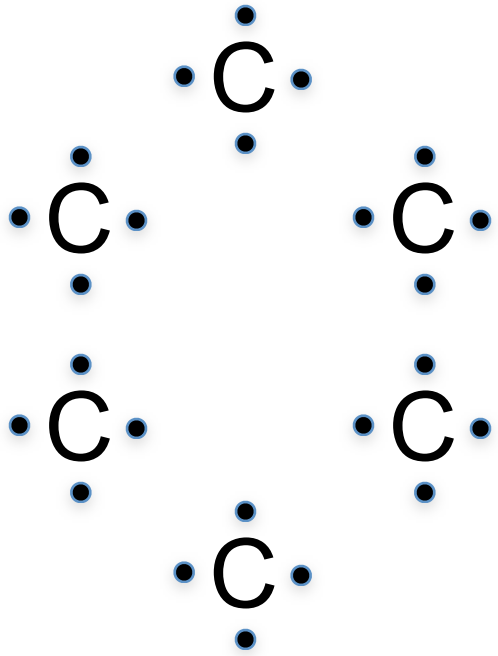
Fig. 9-14, p. 422

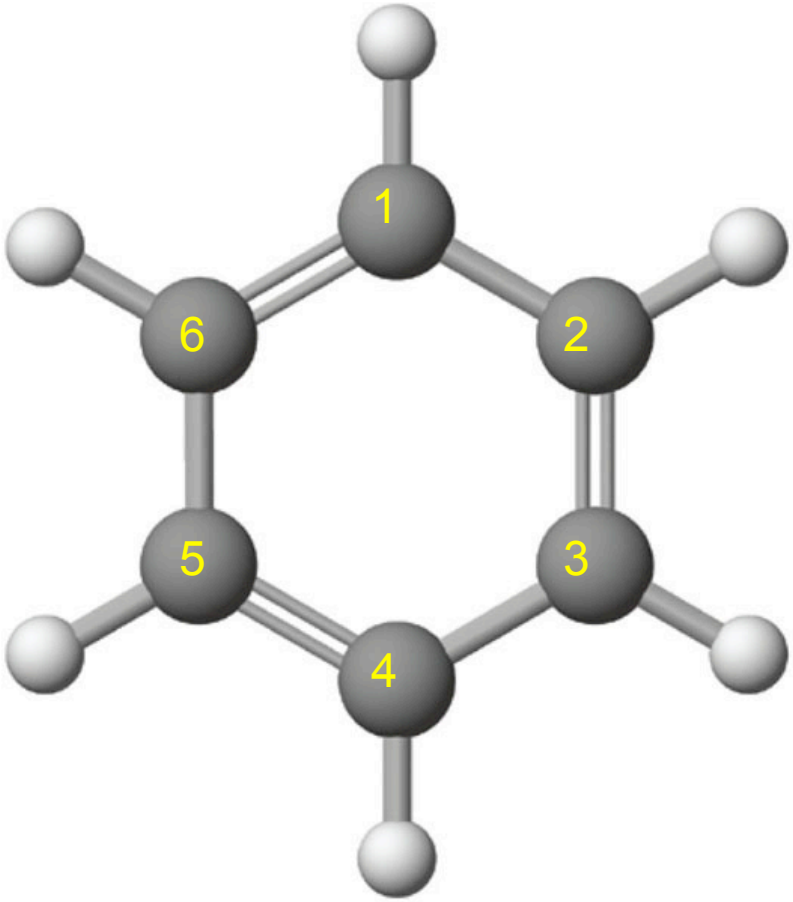
All six C centers are sp^2 hybridized



Benzene, C_6H_6

From Lewis dot structure to molecular orbitals





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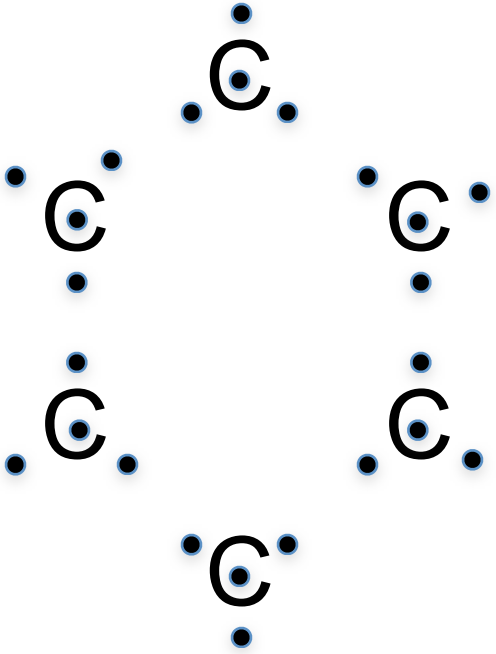

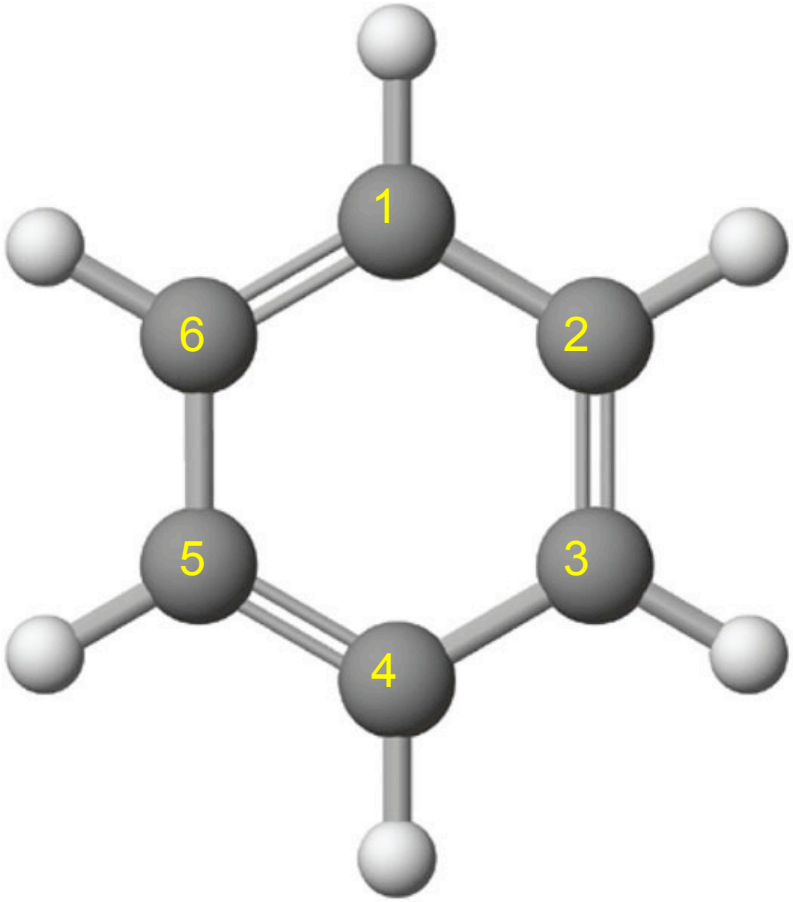

Benzene, C_6H_6

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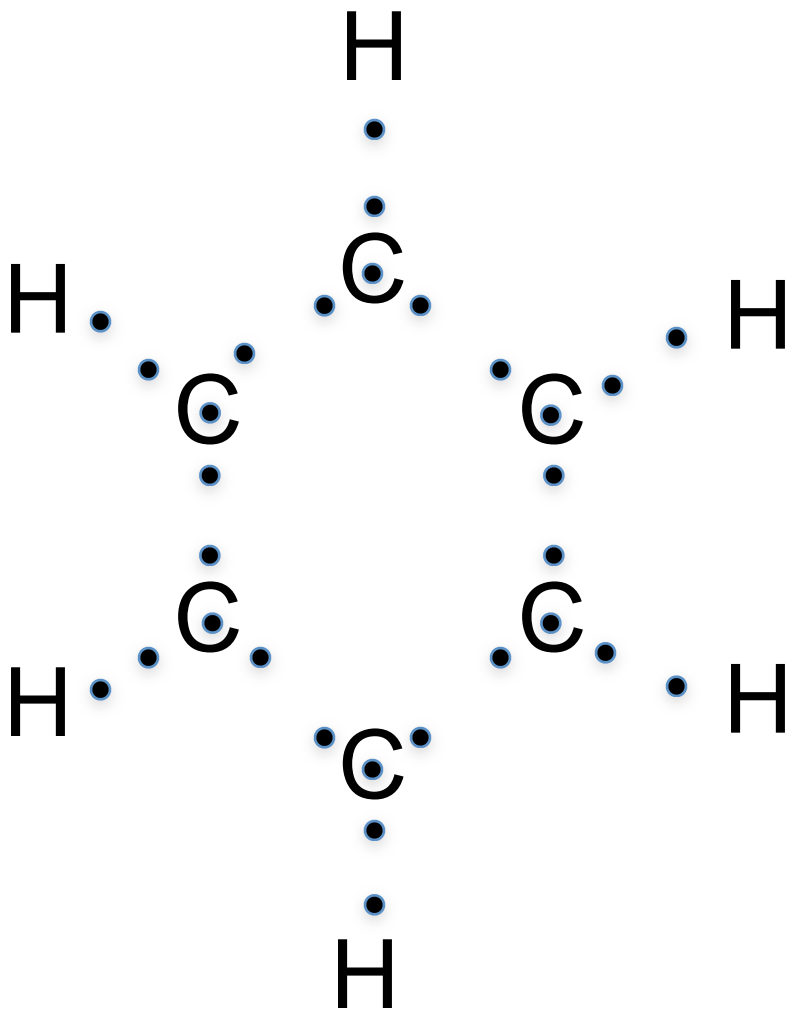
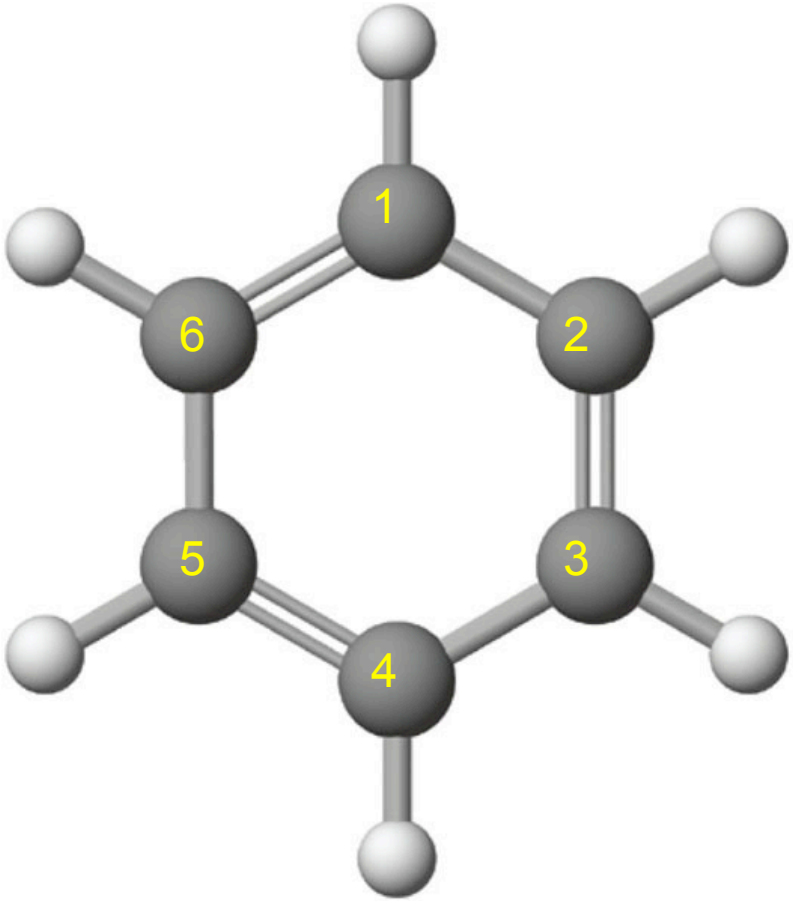
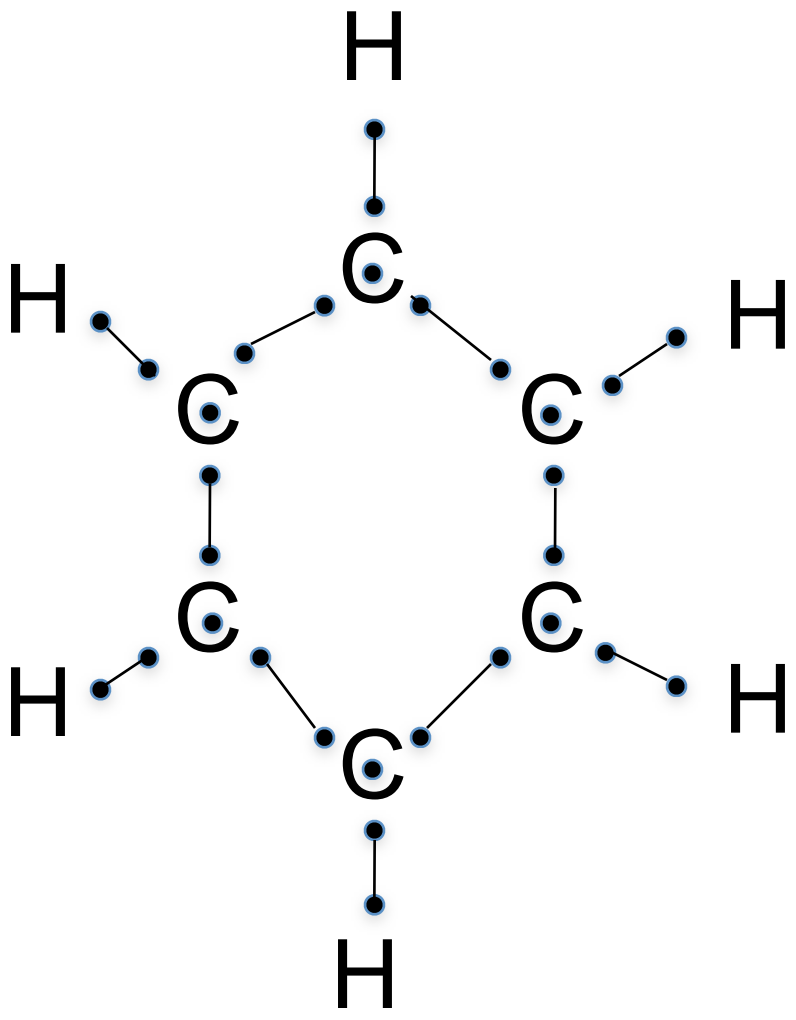
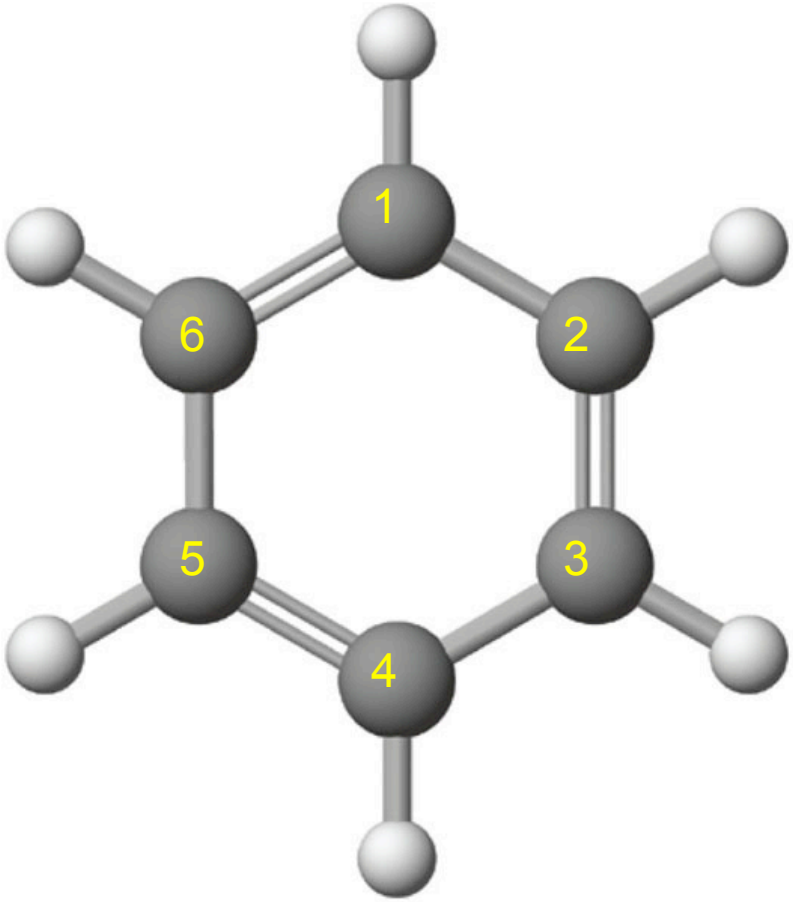




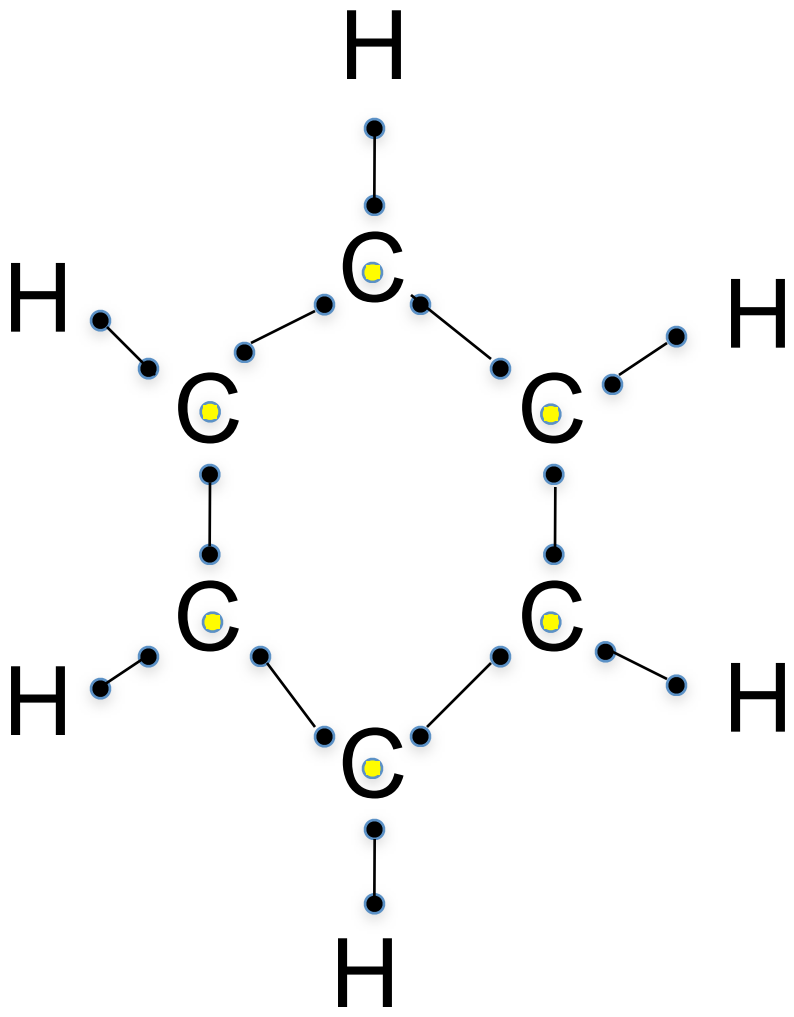
Benzene, C_6H_6

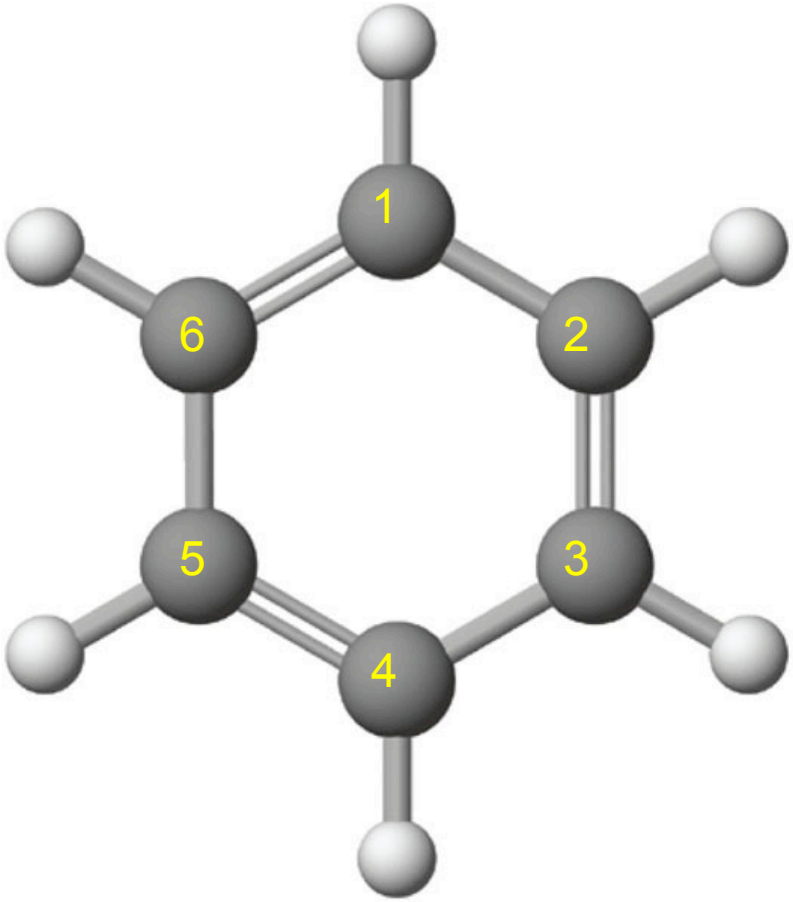
From Lewis dot structure to molecular orbitals





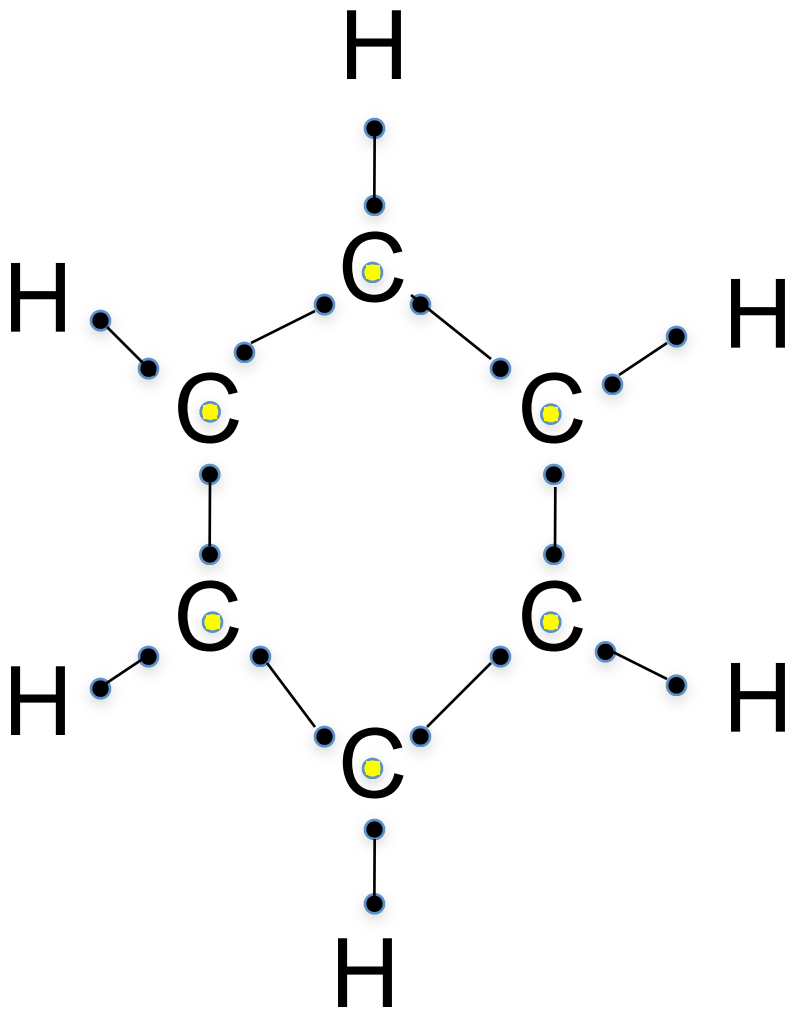
Benzene, C_6H_6

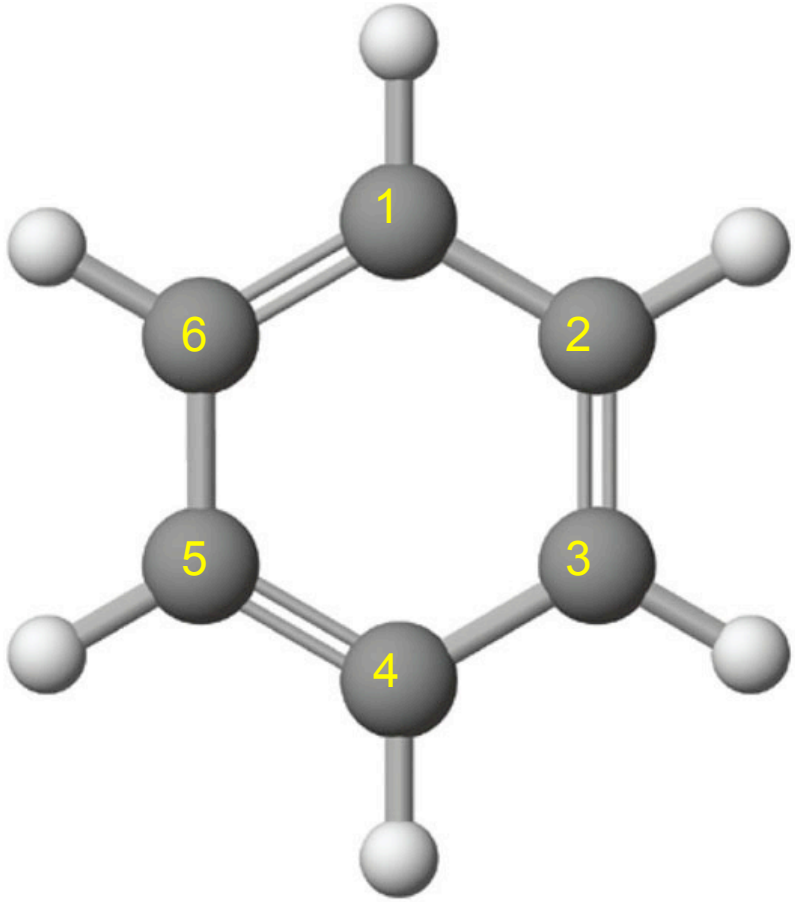




Benzene, C_6H_6

Six p orbitals => Six molecular orbitals (3 bonding + 3 antibonding)

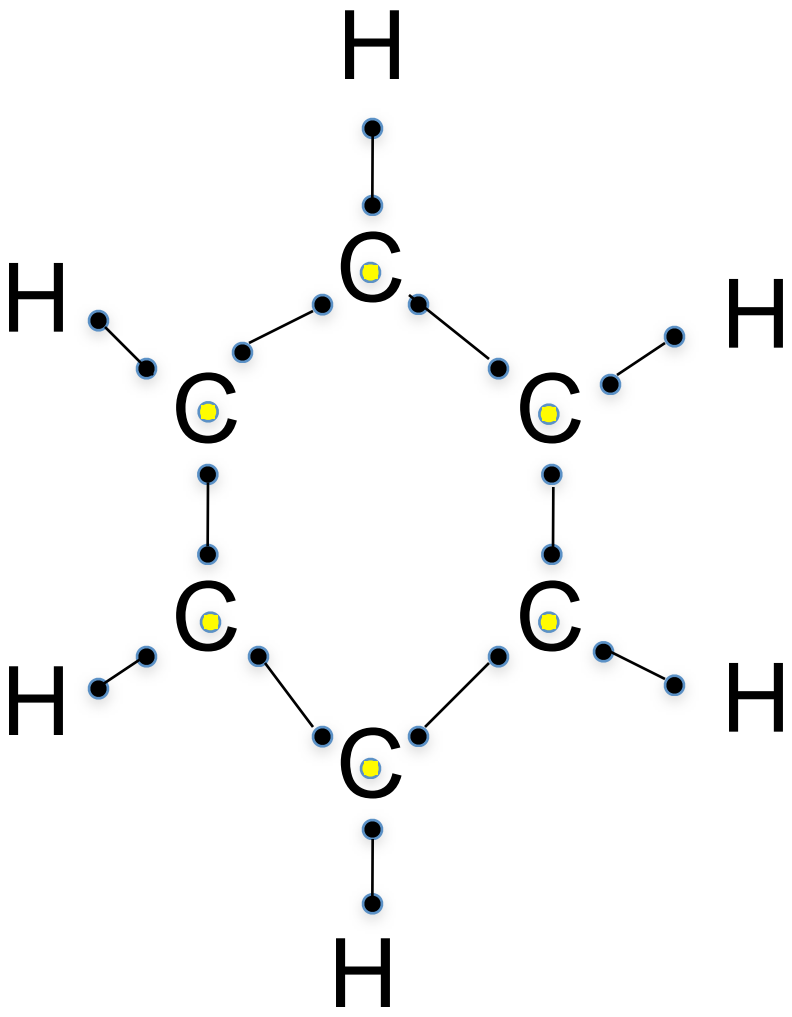


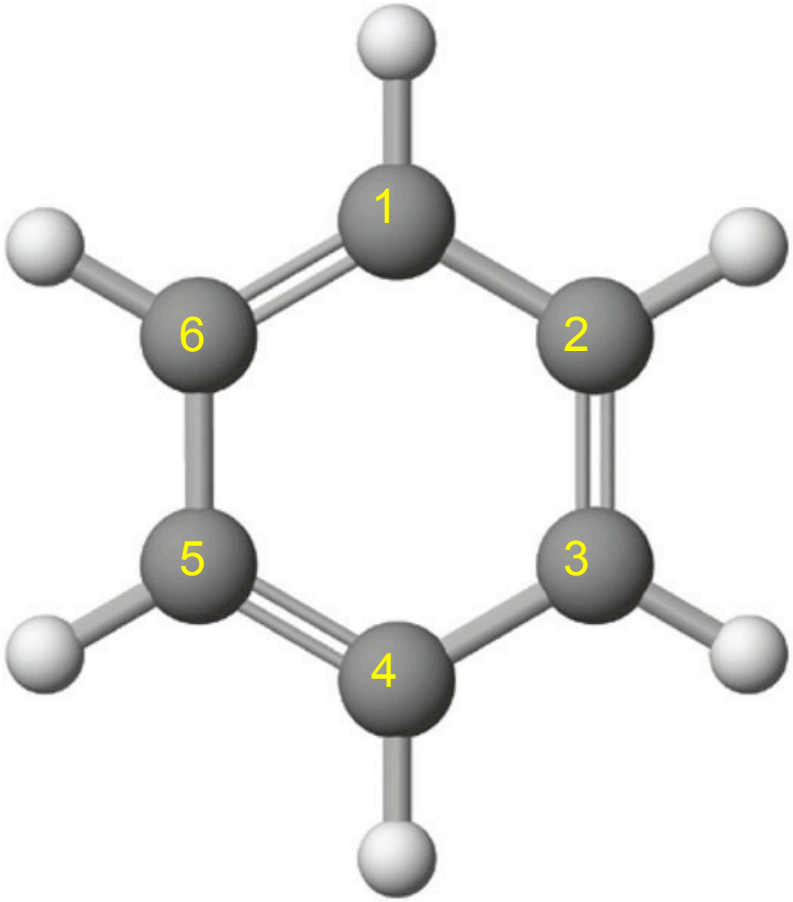


Benzene, C_6H_6

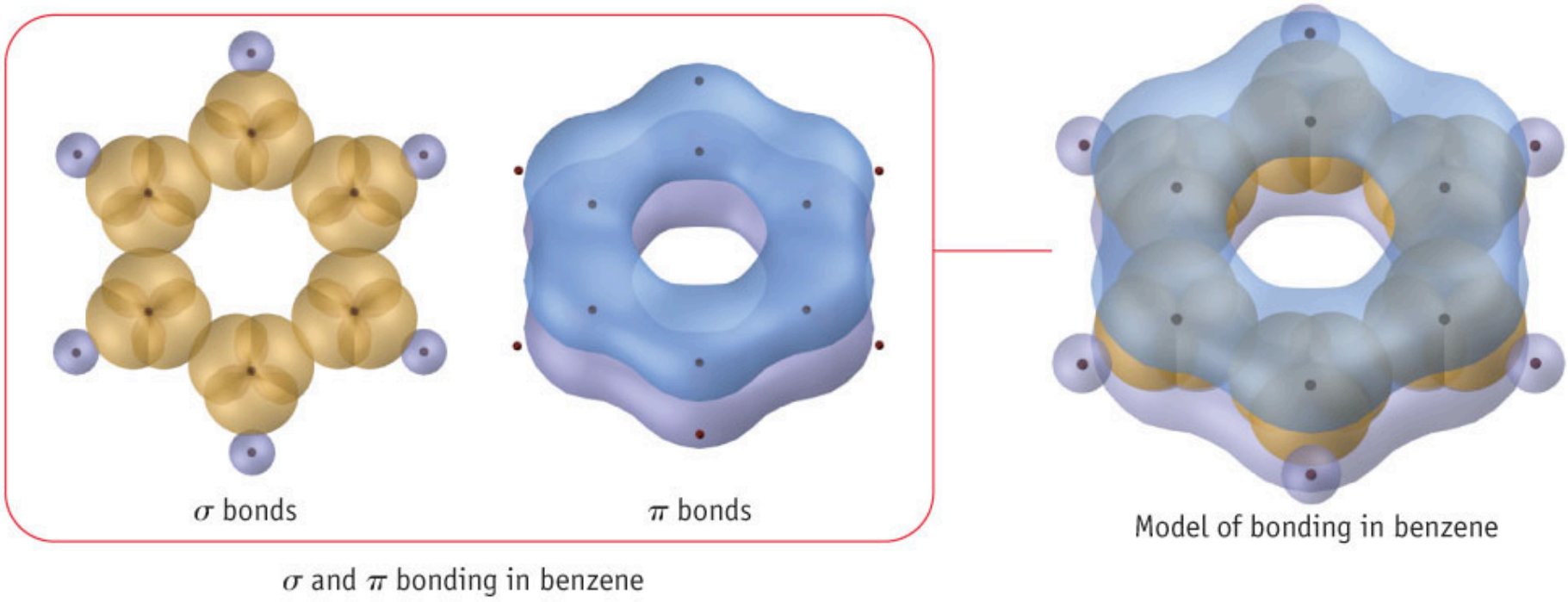
Six p orbitals => Six molecular orbitals (3 bonding + 3 antibonding)

Six electrons go here



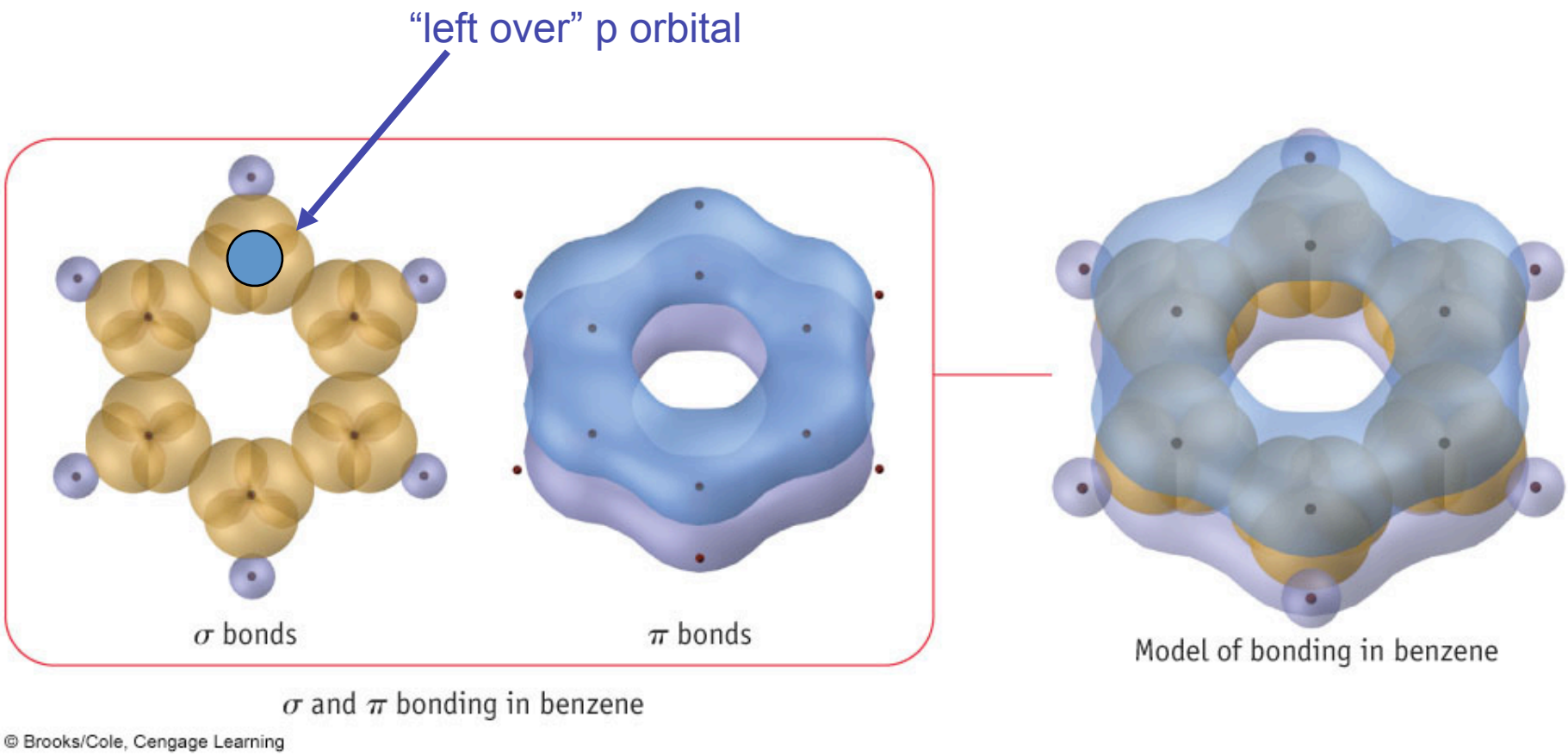


Benzene, C_6H_6



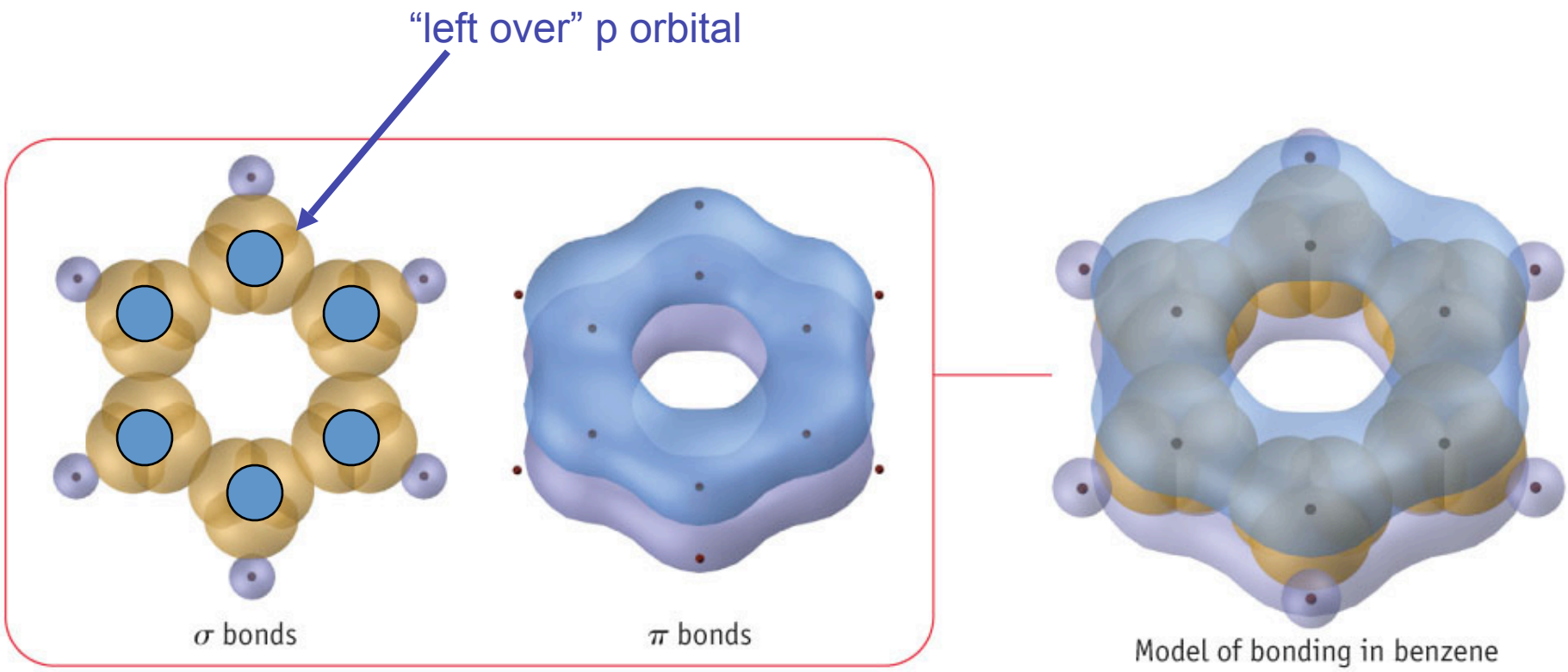
σ and π bonding in benzene

Fig. 9-14, p. 422



σ and π bonding in benzene

Fig. 9-14, p. 422



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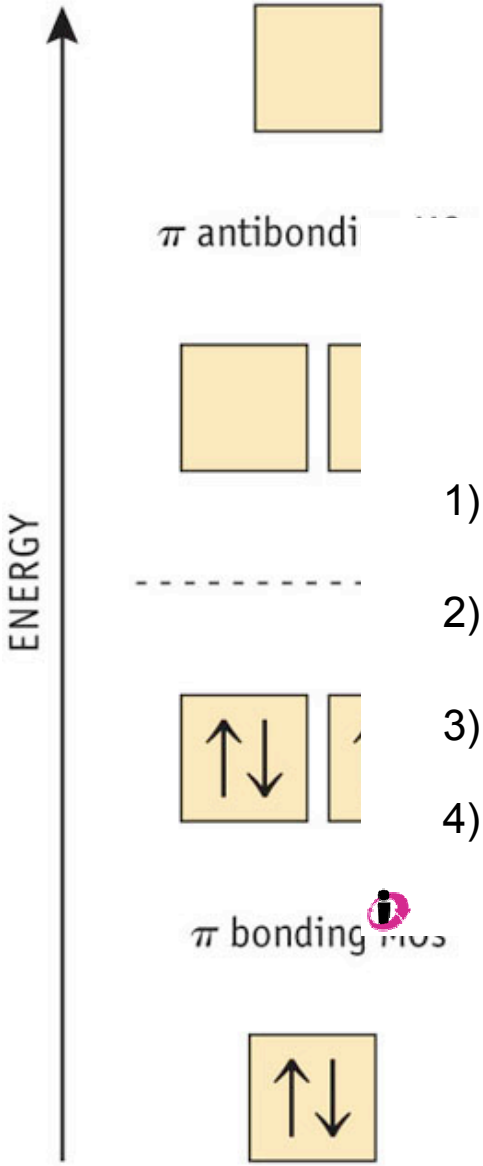
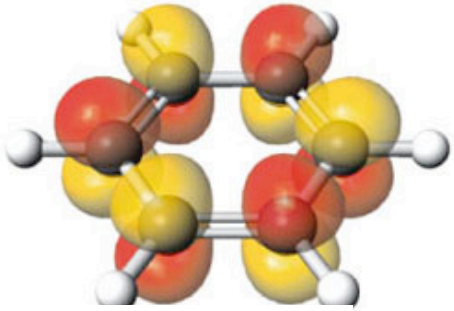
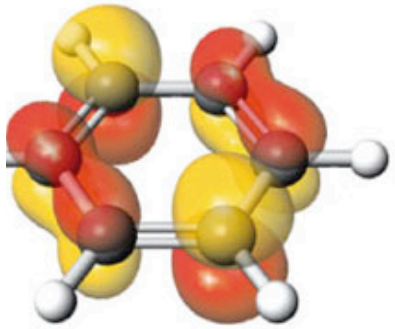
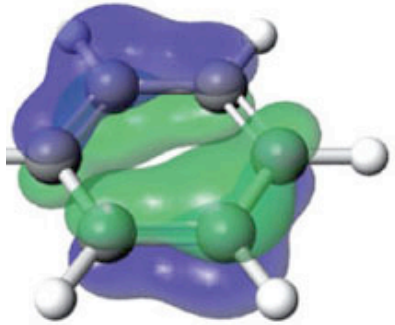
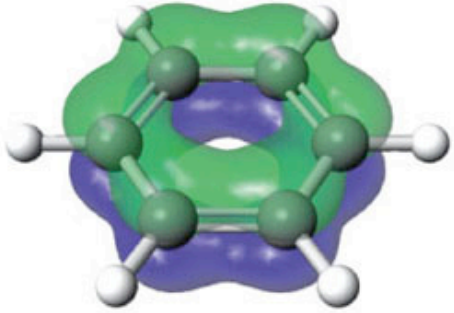










Rank boiling points
Lowest ⟶ Highest

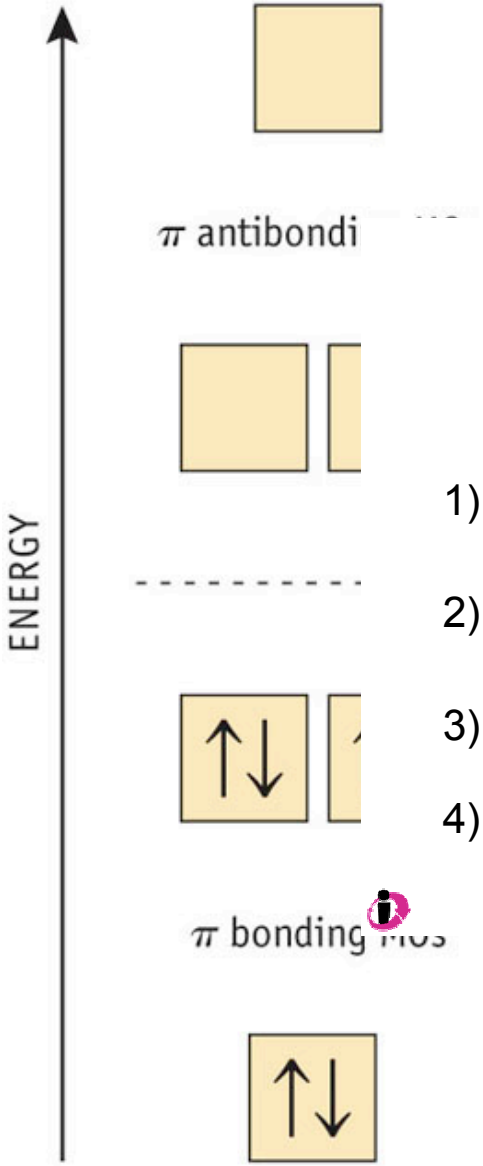
1) CH_3CH_3 CH_3NH_2 CH_3OH

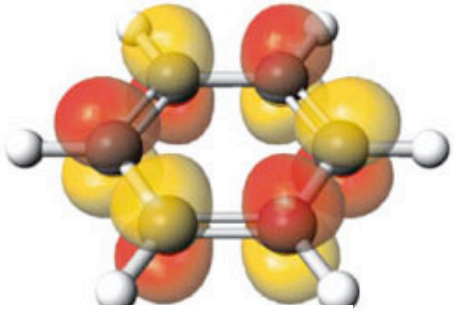
2) CH_3CH_3 CH_3OH CH_3NH_2

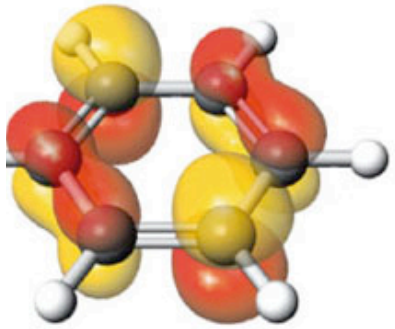
3) CH_3NH_2 CH_3OH CH_3CH_3

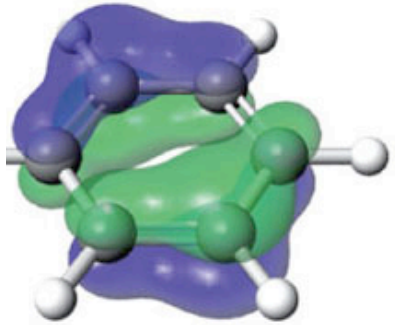
4) They are all about the same

Fig. 9-24, p. 432









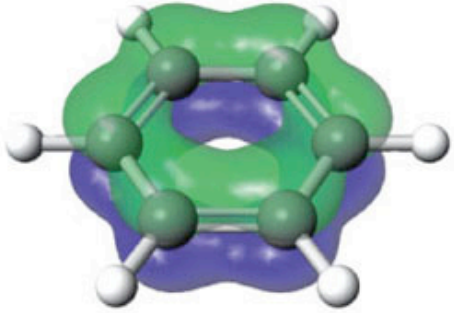


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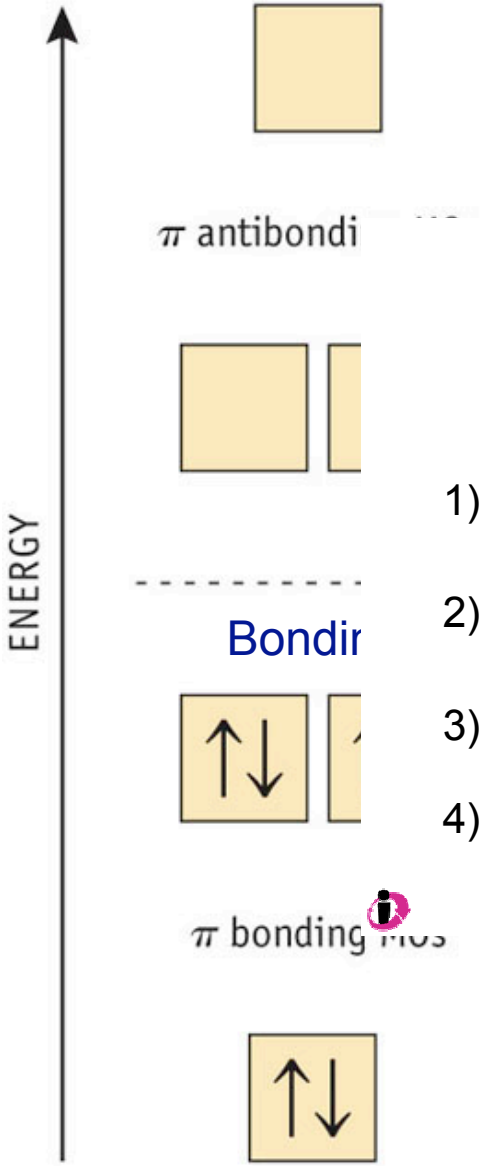
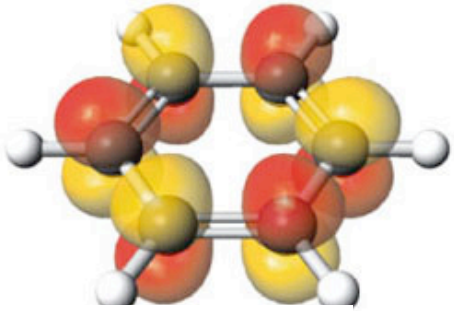
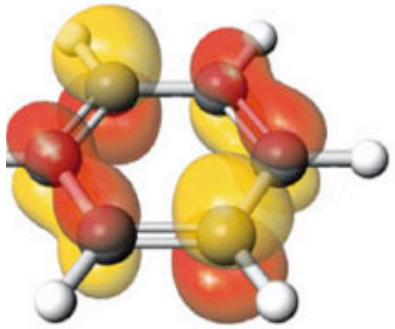
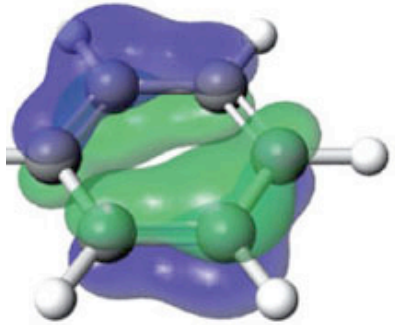
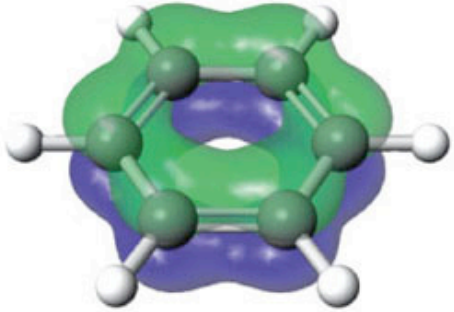
Fig. 9-24, p. 432











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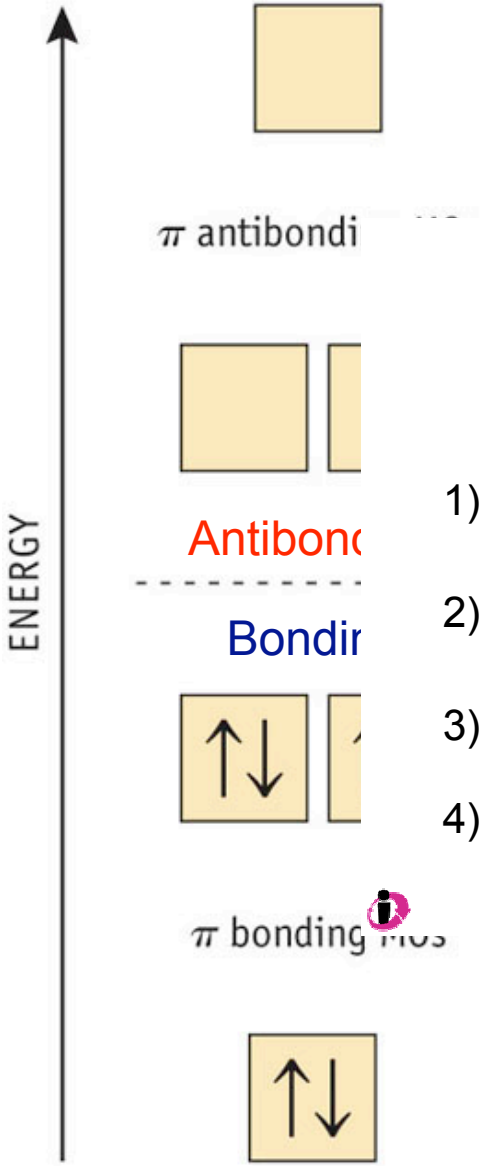

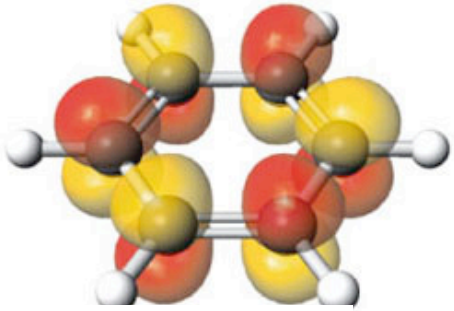

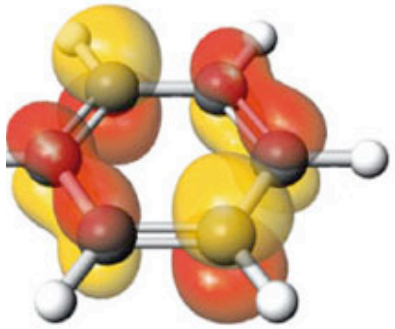

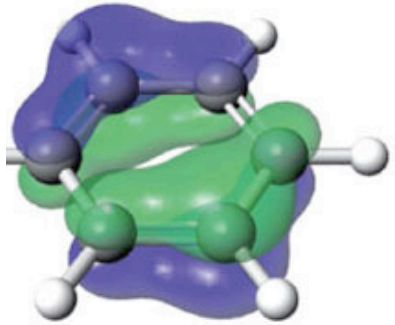

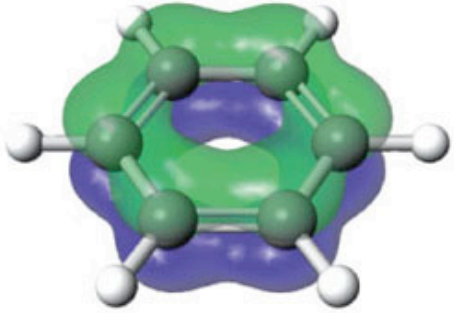

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