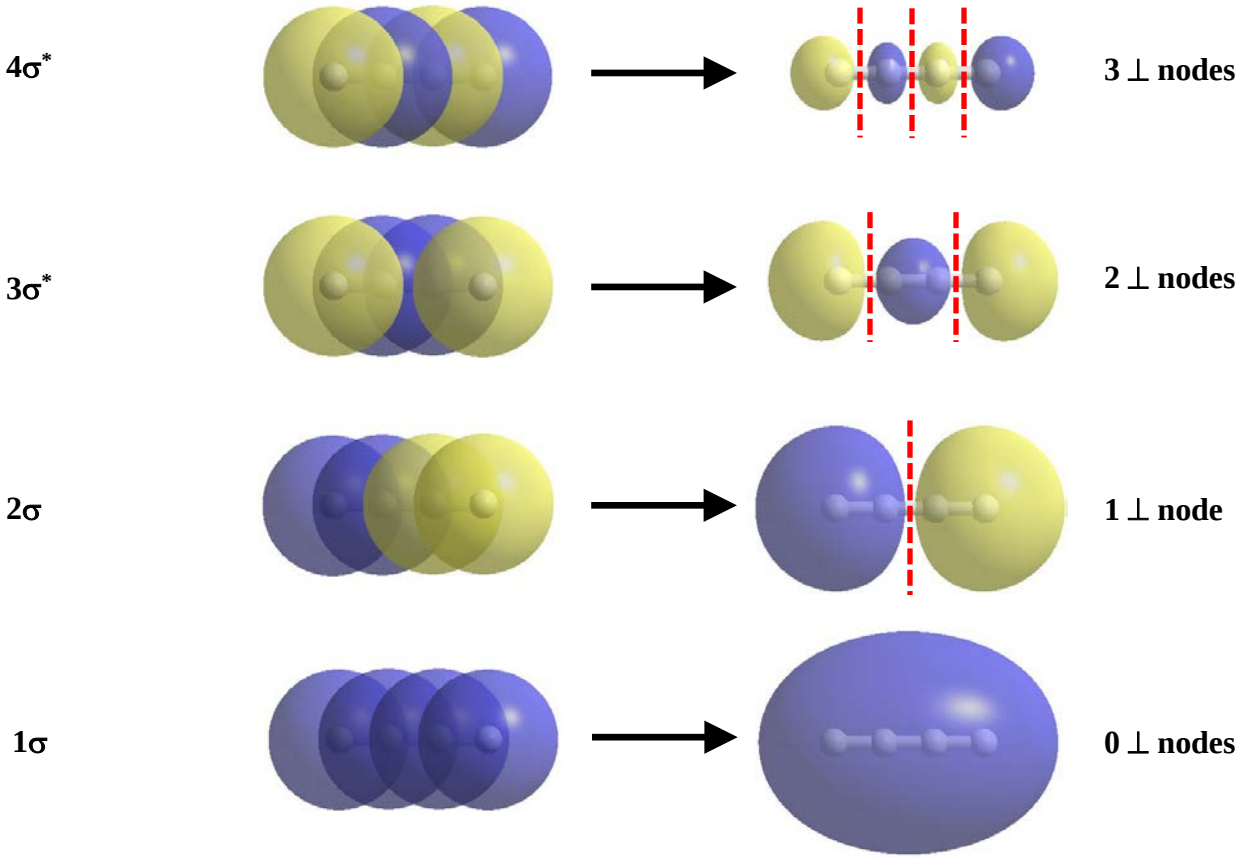
Answers to Exercise 4.1
Linear Combination of Atomic Orbitals: Linear Polyatomic Molecules

The atomic orbitals are shown on the left so that you can see how each molecular orbital is constructed. Your answer does not need to include them. If you have correctly drawn the set of molecular orbitals, that is sufficient.

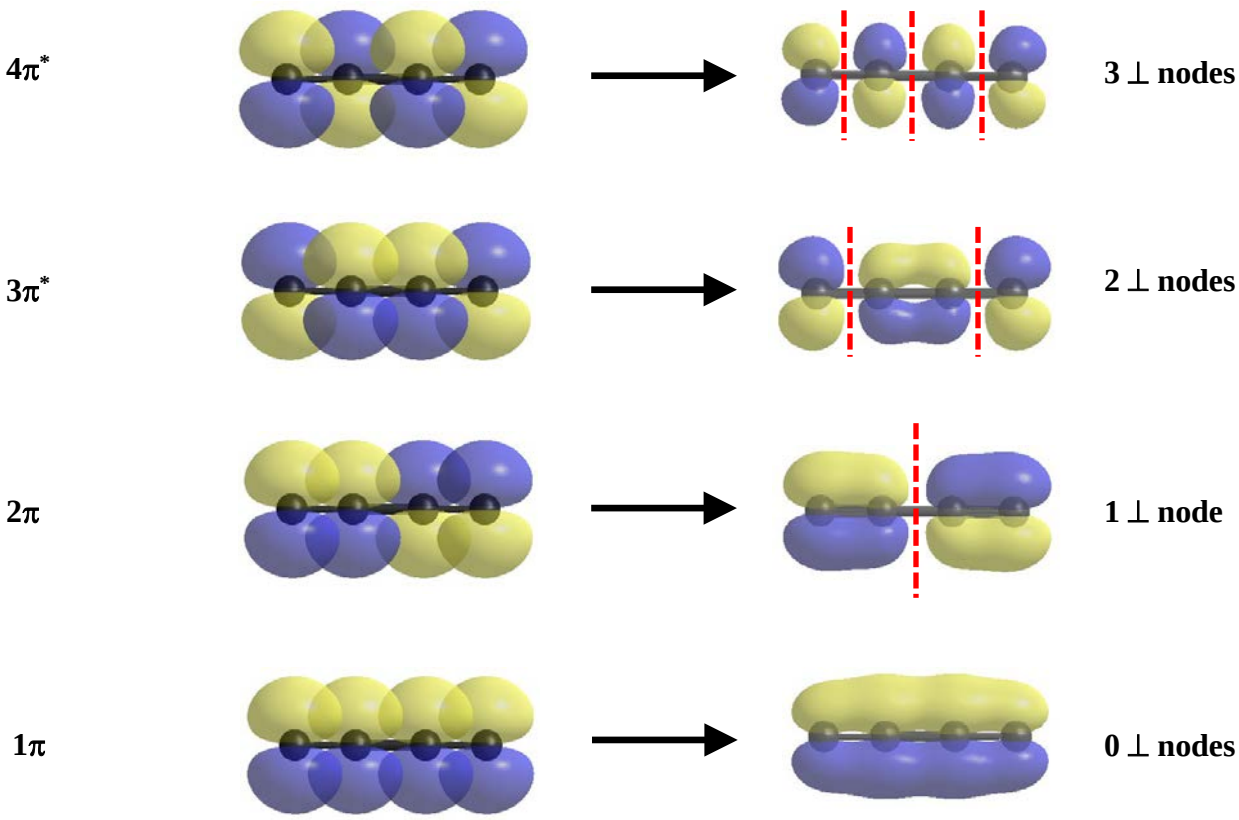
You are only required to draw the nodes if the question asks for them. These questions did not. They are shown for clarity.

1.



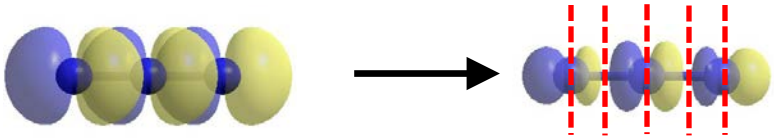
Lowest energy to highest energy: $1\sigma < 2\sigma < 3\sigma^* < 4\sigma^*$

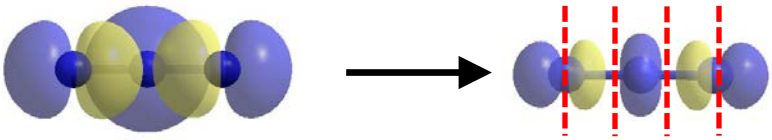
2.

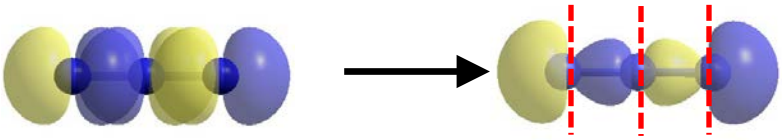


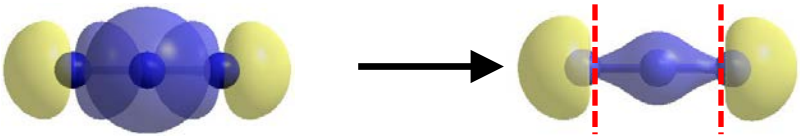
Lowest energy to highest energy: $1\pi < 2\pi < 3\pi^* < 4\pi^*$

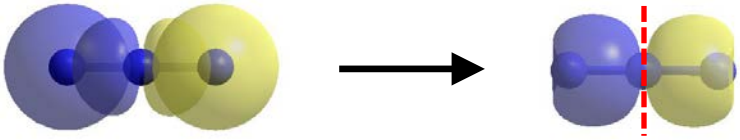
3.

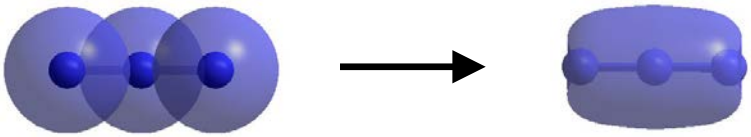
$6\sigma^*$  **5 ⊥ nodes**

$5\sigma^*$  **4 ⊥ nodes**

$4\sigma^*$  **3 ⊥ nodes**

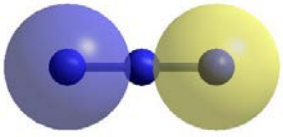
3σ  **2 ⊥ nodes**

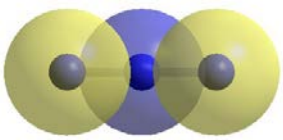
2σ  **1 ⊥ node**

1σ  **0 ⊥ nodes**

Lowest energy to highest energy: $1\sigma < 2\sigma < 3\sigma < 4\sigma^* < 5\sigma^* < 6\sigma^*$

Alternative AO combinations:

 *is an alternative way to combine AOs to give 2σ.*

 *is an alternative way to combine AOs to give 3σ.*

4. Ethyne is linear: H—C≡C—H

(a) two $1s(H)$, one from each hydrogen atom
two $2s(C)$, one from each carbon atom
two $2p_x(C)$, one from each carbon atom
two $2p_y(C)$, one from each carbon atom
two $2p_z(C)$, one from each carbon atom

(b) The following AOs are π-symmetric:

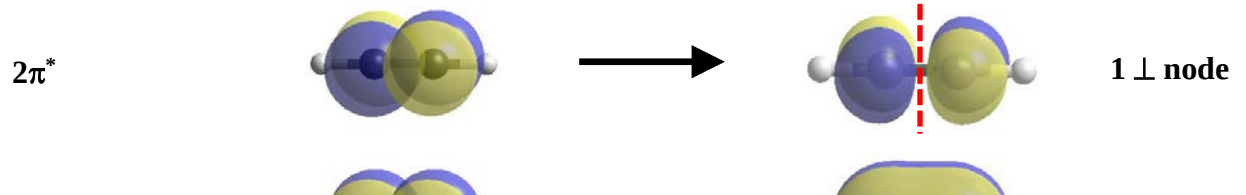
- two $2p_x(C)$, one from each carbon atom
- two $2p_y(C)$, one from each carbon atom

They cannot all combine.
They must be divided into two groups: the $2p_x$ orbitals and the $2p_y$ orbitals.

(c) The following AOs are σ-symmetric:

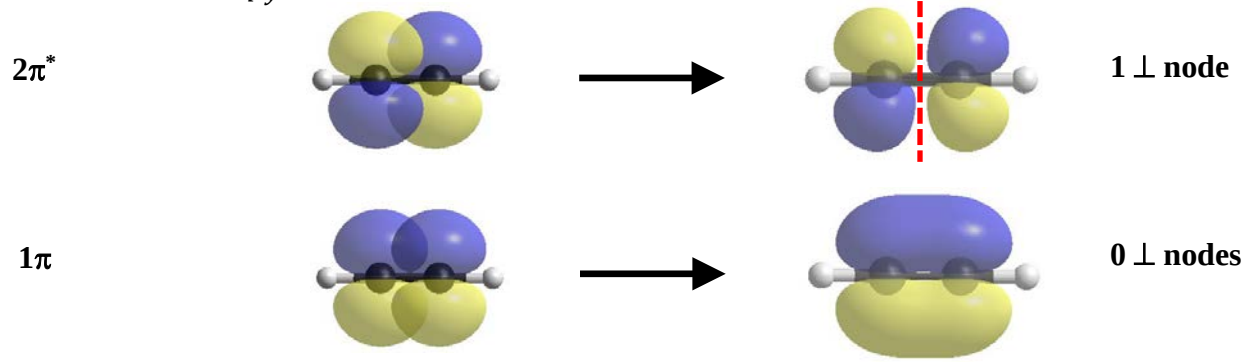
- two $1s(H)$, one from each hydrogen atom
- two $2s(C)$, one from each carbon atom
- two $2p_z(C)$, one from each carbon atom

(d) MOs from $2p_x$ orbitals:



1 ⊥ node
0 ⊥ nodes

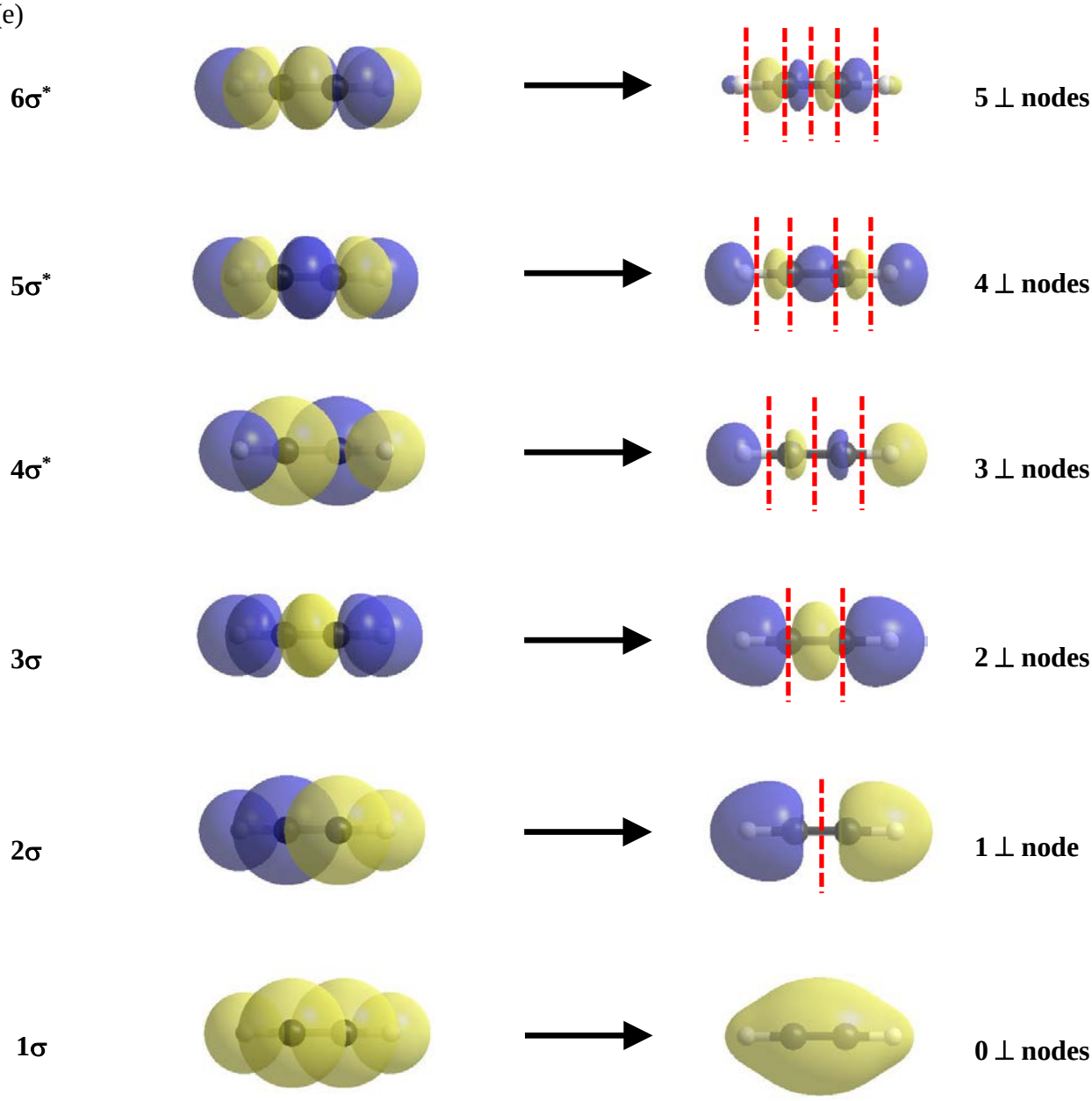
MOs from $2p_y$ orbitals:



1 ⊥ node
0 ⊥ nodes

Lowest energy to highest energy: $1\pi = 1\pi < 2\pi^* = 2\pi^*$

(e)



Lowest energy to highest energy: $1\sigma < 2\sigma < 3\sigma < 4\sigma^* < 5\sigma^* < 6\sigma^*$