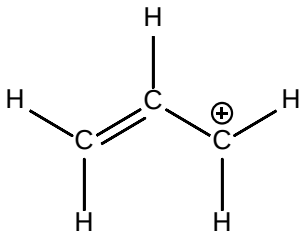
Answers to Exercise 4.4
Pi Molecular Orbital Energy Level Diagrams: Planar Molecules

1.

(a)



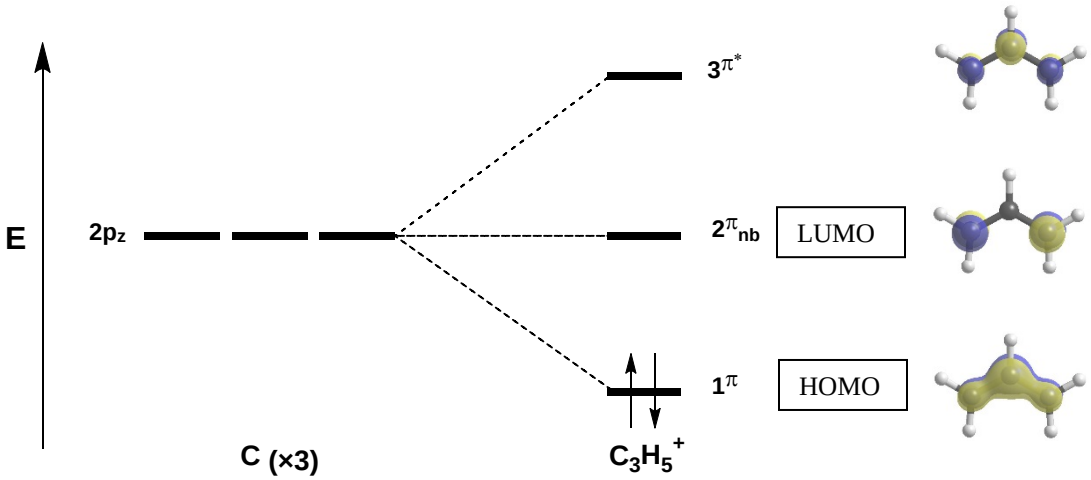
C_3H_5 would have 17 valence electrons, four from each C and one from each H, so $C_3H_5^+$ has 16 valence electrons

Grouping the AOs by symmetry and energy gives:

- **three pi-symmetric $2p_z$ orbitals: one from each C,**
- fourteen sigma-symmetric orbitals: three $2s(C)$, three $2p_x(C)$, three $2p_y(C)$, five $1s(H)$.

We count fourteen electrons in sigma-symmetric MOs and two electrons in pi-symmetric MOs.

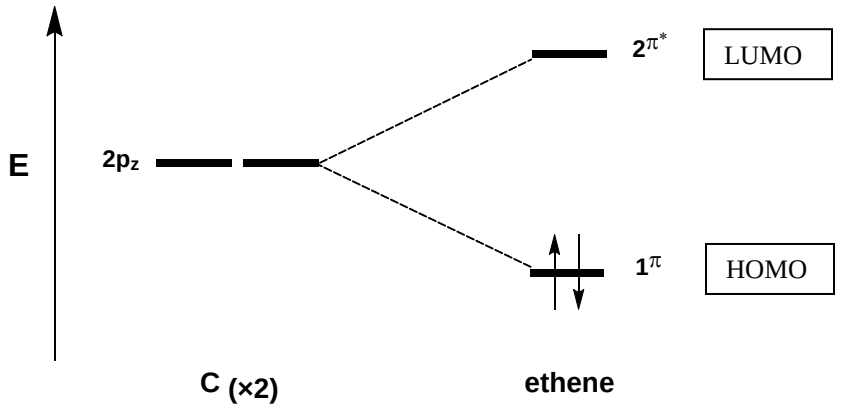
The molecular orbital energy level diagram for $C_3H_5^+$ therefore looks like:



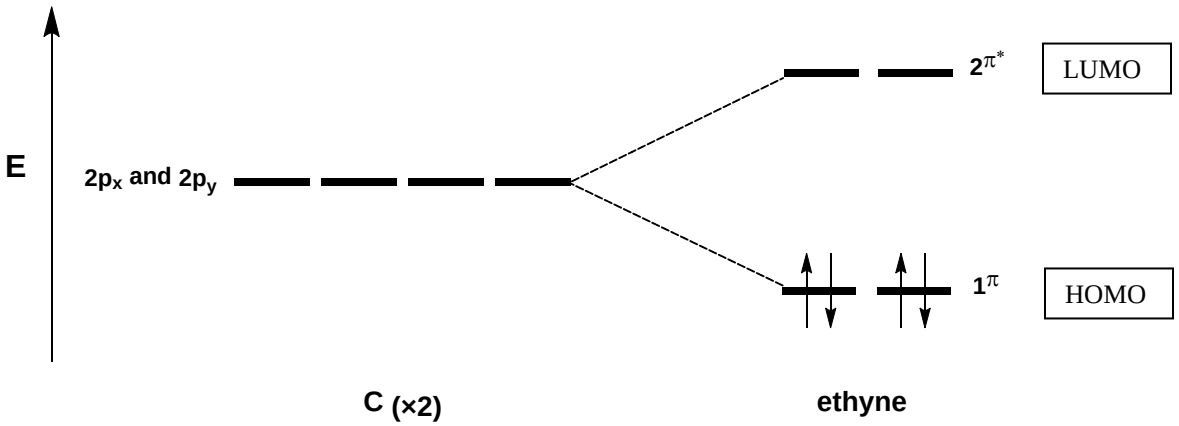
(b) Since this is a cation, it is more likely to accept electrons than to donate them. It will accept electrons into its LUMO ($2\pi_{nb}$). Since this is a nonbonding MO with the lobes distributed only between the two terminal carbon atoms, that means the electrons would be added to one or both terminal carbon atoms and that this addition would not affect C-C bond order.

2.

(a)



(b)



(c) Ethene is a planar molecule, so it only has one pi system (made from $2p_z(C)$). As such, it only has one π MO at each energy level.

Ethyne is a linear molecule, so it has two pi systems (one made from $2p_x(C)$ and one made from $2p_y(C)$). As such, it has two degenerate π MO at each energy level