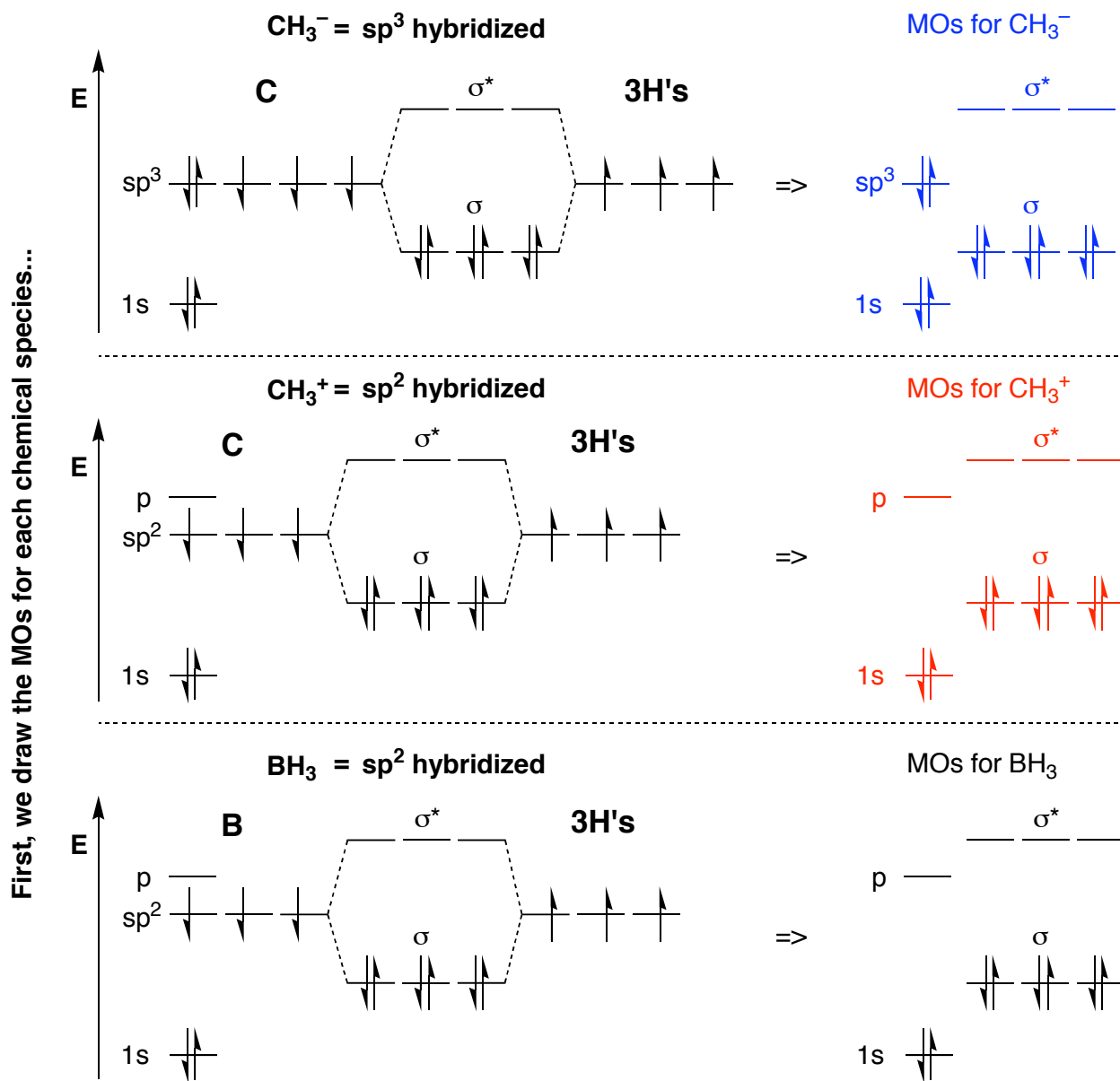
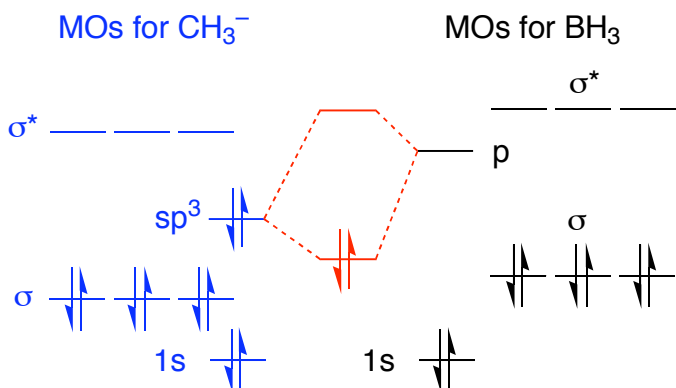


1. Using MO theory, explain why  $\text{CH}_3^-$  reacts with  $\text{BH}_3$  while  $\text{CH}_3^+$  does not react with  $\text{BH}_3$ .  
**Note:** the VESPR model may help you to think about the problem, but you *must* use MO energy diagrams to solve the problem.

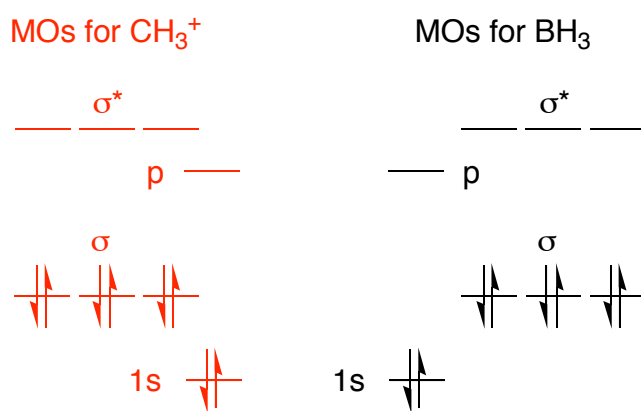


Solution cont'd on next page....

Next, we try to see what would happen if we combined them...

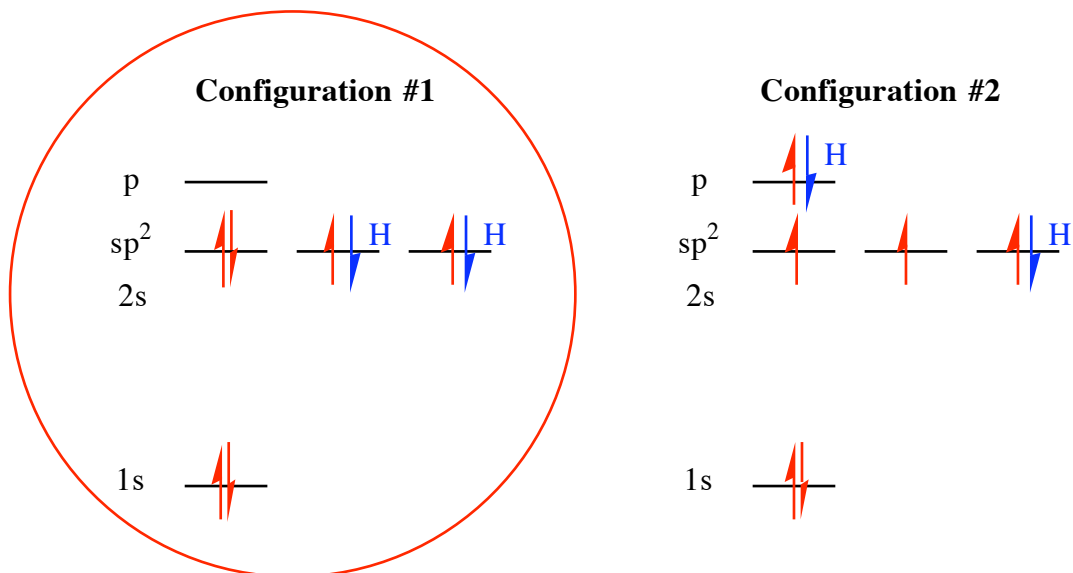


The  $sp^3$  orbital of  $CH_3^-$  can combine with the p orbital of  $BH_3$  to yield a filled orbital and to give a favorable energy situation.



There are no orbitals suitable for mixing between  $CH_3^+$  and  $BH_3$ . The difference in energy between the p orbital of  $BH_3$  and the s orbital of  $CH_3^+$  is too great. Besides, the  $\sigma$  orbital is already participating in bonding.

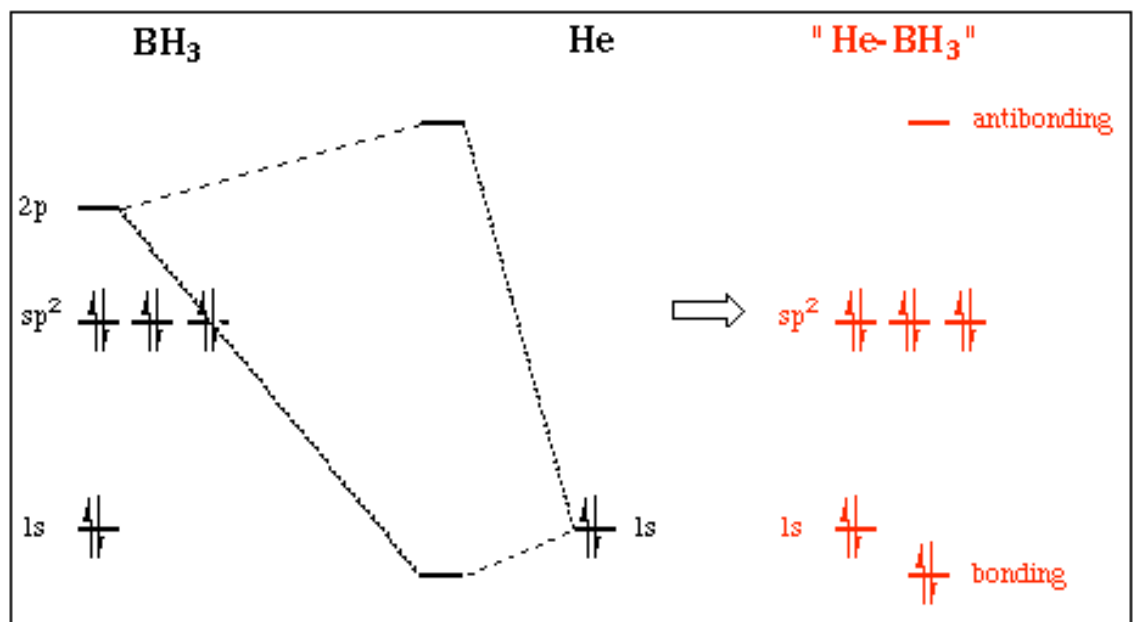
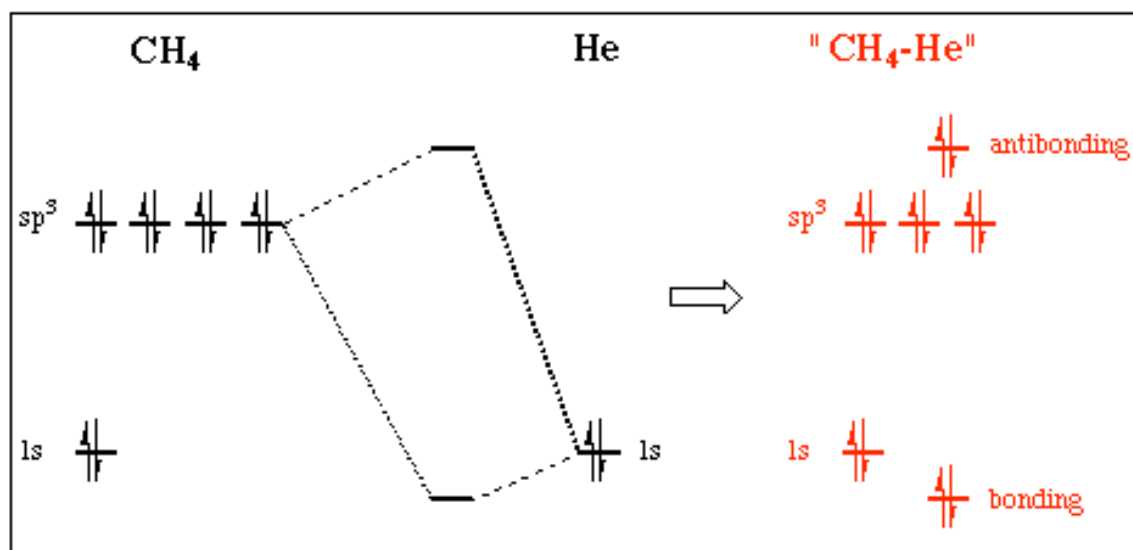
2. The molecule known as methylene has the formula  $\text{CH}_2$ , is  $\text{sp}^2$  hybridized, and is uncharged. There are two possible ways to complete its Molecular Orbital energy diagram. Show these two possibilities below and *circle the more favorable configuration*. Provide an explanation for your choice.



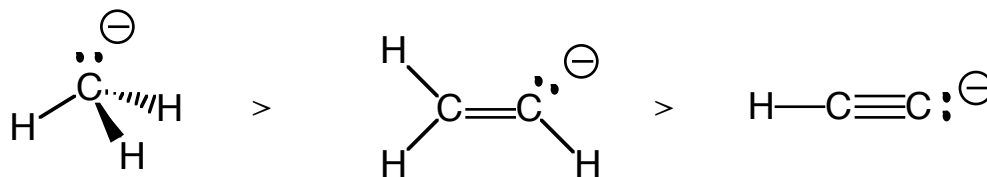
The circled configuration appears to be more favorable because of the occupation of the lower energy levels. In reality, the situation is much more complicated and **both** configurations are possible!

3. Use MO theory to explain why Helium cannot form a bond with any of the atoms in methane,  $\text{CH}_4$ , while it can theoretically form a bond with boron in the molecule  $\text{BH}_3$ . *Hint: you will need to draw MO energy diagrams for He and for each of the molecules.*

The theoretical MO energy diagrams are shown below. Notice that in the theoretical  $\text{He-BH}_3$  molecule, electrons are not placed into the antibonding MO, while in the theoretical  $\text{CH}_4\text{-He}$ , two electrons are forced into an antibonding MO. This produces a more stable energy situation for " $\text{He-BH}_3$ " than for " $\text{CH}_4\text{-He}$ ."

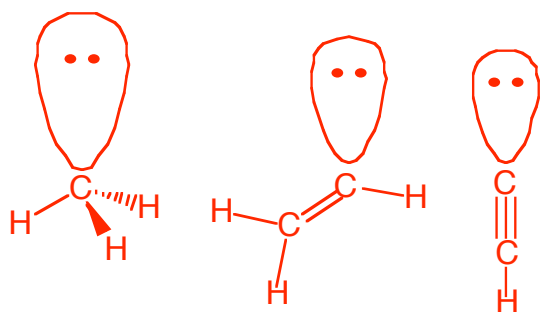


4. Provide *two* explanations for the following trend in reactivity. One of your explanations *must* use MO theory.

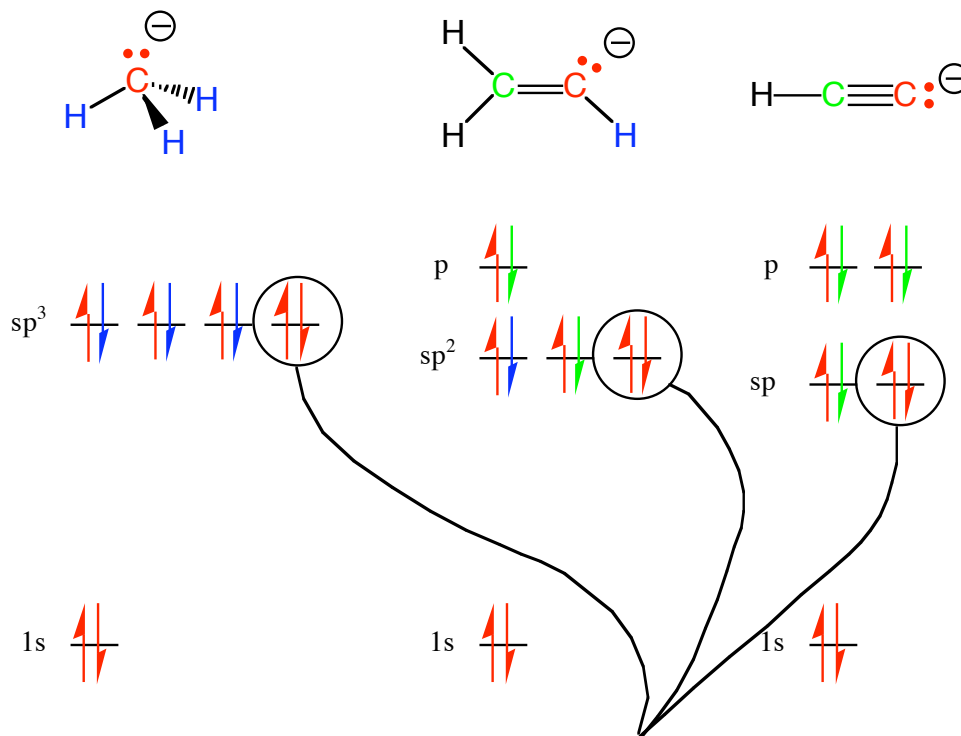


Most Basic

Least Basic

**Explanation #1**

The greater s character in the sp hybridized carbanion makes the orbital much smaller in volume. The converse is true for the  $\text{sp}^3$  hybridized carbanion. The greater distance spanned by the  $\text{sp}^3$  orbital allows it to reach out and grab a proton more easily than a smaller orbital. This makes it a better and thus stronger base.

**Explanation #2**

The energy level of the orbital in which each lone pair resides will determine the stability (and thus reactivity) of the base. Notice that the  $\text{sp}^3$  orbitals are highest in energy. Therefore the reactivity of the lone pairs in the  $\text{CH}_3^-$  anion is greatest. This is what causes it to be the strongest base.