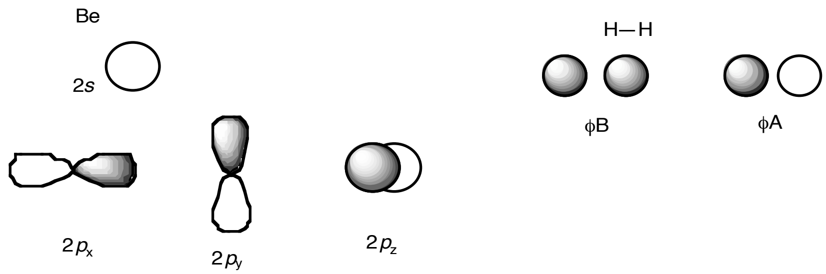
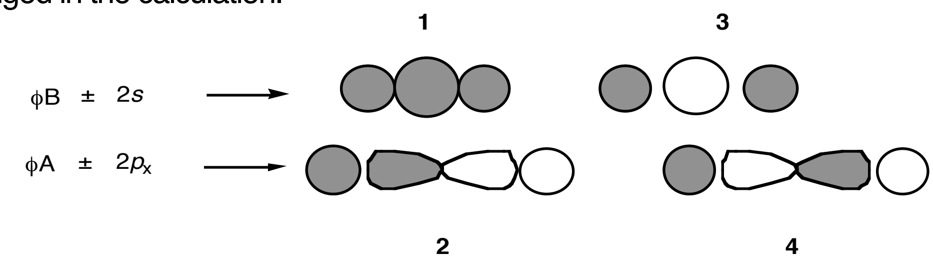
Answers to Problem 6, Chemistry 301X - 2006

(a) there will be six MOs
(b)

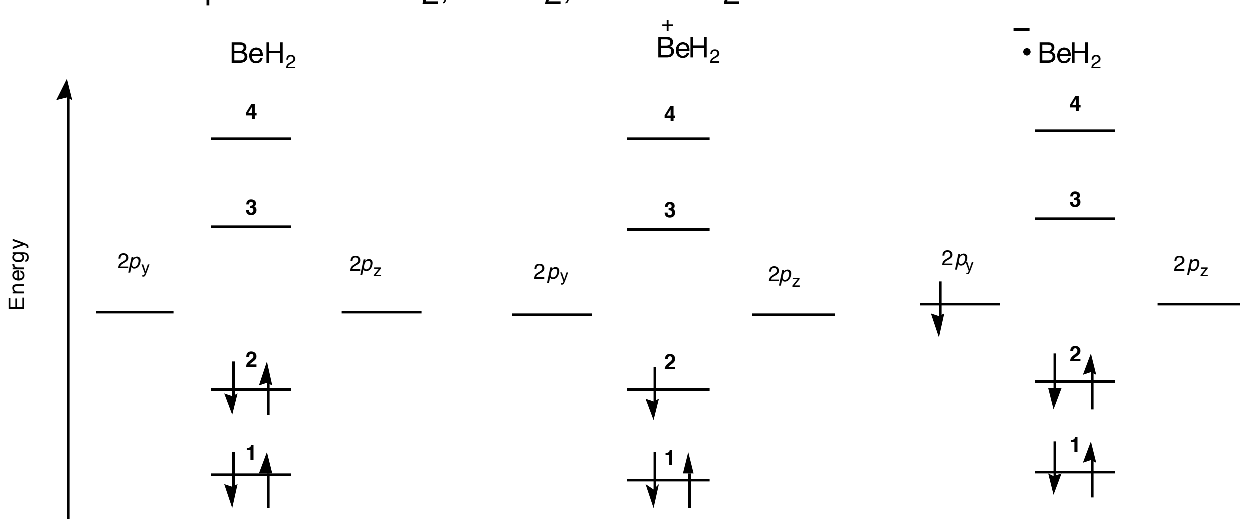


(c)The bonding MO of H_2 interacts with 2*s* to give MOs **1** and **3**. The antibonding MO of H_2 interacts with $2p_x$ to give MOs **2** and **4**. Neither the $2p_y$ nor the $2p_z$ orbital interacts with either the bonding or antibonding MO of H_2 (net zero, orthogonal interactions), and so are unchanged in the calculation.



(d) Order the MOs by counting the nodes. MO **1** and **2** are net bonding, **3** and **4** are antibonding, and the residual 2*p* orbitals are nonbonding.

Neutral BeH_2 will have four electrons, two from the pair of hydrogens and two from Be. The cation will have one fewer electron and the anion one more electron. Here are the electronic occupancies for BeH_2, $^{+}BeH_2$, and $^{-}BeH_2$.



People often have trouble on this one. That's OK (for now) because we are right at the beginning. General problems:

1. Never mix and match models - this is not a hybridization problem, it is a MO/AO

problem. Use the MO method.

2. Watch out for orthogonal interactions.

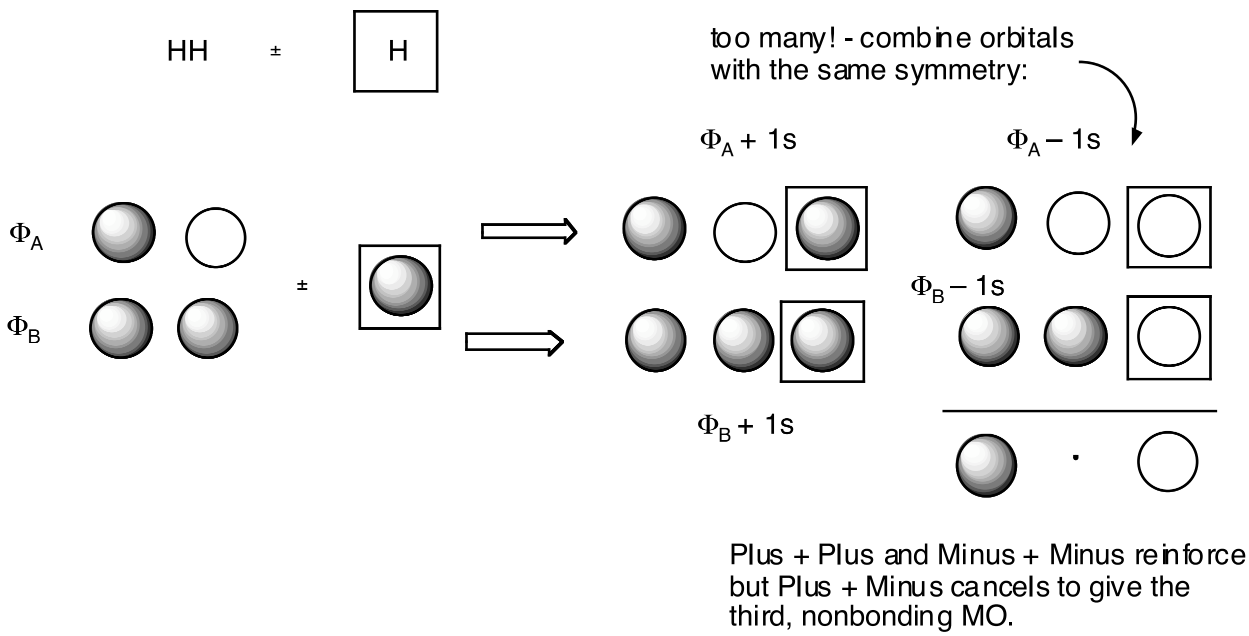
You can either use the following assumption:

At this level of “theory” you only need interact the orbitals closest in energy.

Or watch carefully for orthogonal interactions. If you are a computer, you can write out all the combinations, thus getting far too many (remember “n” in, “n” out) orbitals. You will then have to combine all the ones of like symmetry (very very hard). Or, you can drop out all orthogonal interactions. Or you can use the assumption above:

Here is a very quick treatment of HHH made as a computer would do it (sort of). This molecule is small enough so we can get away with this method, but essentially nothing bigger works easily:

We’ll make HHH by adding an H to the end of HH to make linear HHH.



Want to see if you “got it? Try Problem 1.57 in the book.