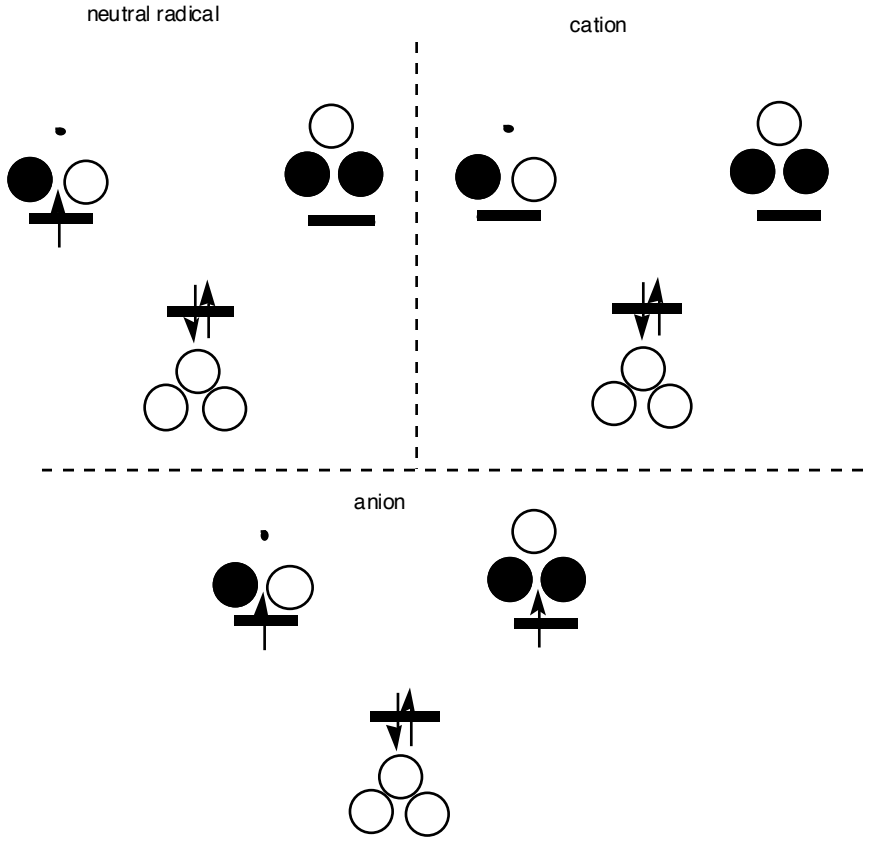
Answers to Problem 9, Chemistry 301X - 2006

Distort (bend) the MO's of linear HHH to make the MO's of triangular H_3. How will the energy of each MO change in forming the triangle?

See answers to Problem 1.52 and 1.53, Study Guide, pp 34-35.

Place electrons for the cation, anion, and radical.



Now do the same thing for allyl (Problem 5) - transform the MOs into the MOs for the cyclic version, called “cyclopropenyl.”

The answer looks almost exactly like that for HHH transforming into the triangular version. Indeed, as seen from above, it is exactly the same. Just replace the *s* orbitals with 2*p* orbitals.

Which is more stable, linear or triangular H_3?

Only the lowest MO matters, because only that MO is occupied in H_3^+. So the trianglar version, in which the occupied MO is lower in energy, is better.