Principles of Qualitative Molecular Orbital Theory

1. The number of molecular orbitals = the number of atomic orbitals in the basis set from which they are generated.
2. Molecular orbitals are generated from valence atomic orbitals only.
3. A bonding combination involves a positive, constructive overlap of orbitals of like sign (coefficients); an antibonding combination involves destructive overlap of orbitals of opposite sign (coefficients)
4. Orbitals must be of the same symmetry to interact; atomic orbitals perpendicular to each other do not interact
5. **The energy of similar atomic orbitals (s or p) are lower for elements of higher electronegativity; the molecular orbitals to which they contribute will reflect this difference in energy**.
6. The relative energies of molecular orbitals in a molecule increases with increasing number of nodes.
7. Sigma-type orbitals are lower in energy than Pi-type orbitals
8. Orbital signs and sizes are indicated by the atomic coefficients
9. **In mixing two orbitals of unequal energy the bonding combination has a greater contribution from the lower energy AO (or MO); the antibonding combination has a greater contribution from the higher energy MO**.
10. **The out-of-phase or antibonding interaction between two starting orbitals always raises the energy more than the corresponding in-phase or bonding interaction lowers the energy.**
11. The smaller the initial energy gap between two interacting orbitals, the larger the interaction.
12. Hybrid orbitals are only formed if the two highest energy MO's of a given symmetry derive primarily from different kinds of AO's; then they can be mixed to form hybrids.