

ACS INORGANIC CHEMISTRY STUDY GUIDE

1. Period 2: O₂, F₂ etc, why not Ne₂?: difference is MO diagram's relative energies of the bonding orbitals π_u and π_g
2. H-X: H is something that bonds through 2p and 2s orbitals, relative energies of the atomic orbitals are taken into account because there are two separate atoms, H 1s is usually higher in energy, 4 atomic orbitals of X will mix with 1s of H to give 5 molecular orbitals. Anti bonding is mostly H in character while the other 4 are mostly X
3. X-Y: relative energies are taken into account, more electronegative=lower energy of orbitals
4. Relative energies of MOs: $4\sigma > 2\pi > 3\sigma > 1\pi > 2\sigma > 1\sigma$
5. Polyatomic MO: must use approximations of MO theory. Linear combinations of Atomic orbitals create a cumulative approximation of the atomic orbitals of its constituent atoms, compare orbitals to determine what will mix
6. LCAO notation: a,b=nondegenerate, e=doubly degenerate, t=triple degenerate
7. LCAO energies: lowest=a (nondegenerate) intermediate=e
highest=t
8. LCAO: linear combinations of atomic orbitals
9. Bond order: a method to assessing overall bond strength between two atoms in a molecule, higher bond order=stronger bond, assesses net number of bonds between two atoms
10. Calculating bond order: $(\text{bonding} - \text{antibonding})/2$
11. How to assign bonding character-bonding: a bonding orbital will lie lower in energy than its substituent atomic orbitals
12. How to assign bonding character-nonbonding: a nonbonding orbital will be equal in energy to its corresponding atomic orbitals
13. How to assign bonding character-antibonding: an antibonding orbital will lie higher in energy than its substituent atomic orbitals
14. HOMO interactions: highest occupied molecular orbital, highest energy electrons reside
15. LUMO interactions: lowest unoccupied molecular orbital, it is the energy level directly above the HOMO
16. Importance of HOMO/LUMO: critical to electron structure, when excited an electron is promoted from HOMO to LUMO, bonding and anti bonding characteristics determine stability, the frontier orbitals are the point of interaction and basis of understanding for molecular

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James Coy-Dibley



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