

Bonding: Structure

Inspired by Paul Groves

A BLUFFER'S GUIDE

1. Electronegativity differences between bonded atoms results in a molecule being polar or nonpolar: **ranges can vary*

- Pure covalent = EN difference of 0
- Nonpolar covalent = EN diff. of 0.1 – 0.4
- Polar covalent = EN diff. of 0.5 – 1.9
- Ionic = EN diff. larger than or equal to 2.0

2. Electronegativity difference is not the final determination of whether a substance is ionic or not. It must also conduct electricity in its molten state.

3. Coulomb's Law $F \propto \frac{q_1 q_2}{r^2}$

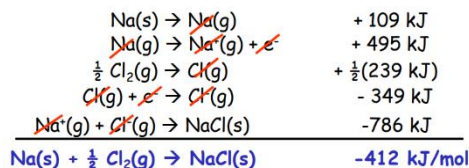
q = absolute value of charge on particles
r = distance between particles

4. Strongest ionic bond would be:
Large charge magnitude
Small ionic radius

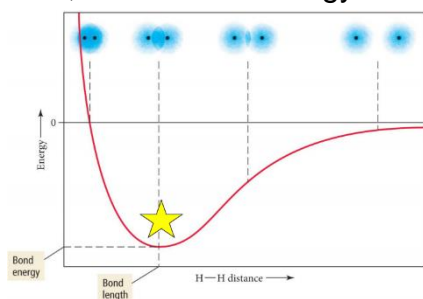
5. Lattice Formation Energy
Five steps, example LiF

1. Turn solid Li into gas *Sublimation energy*
2. Break the $F_{2(g)}$ bond *Bond energy*
3. Ionize Li $\rightarrow Li^+$ *Ionization energy*
4. Add an electron to F $\rightarrow F^-$ *Electron affinity*
5. Form the ionic bond *Lattice energy*

6. ΔH_f for sodium chloride example:



7. Atoms are considered "bonded" when at lowest, most stable energy.



8. Bond length and energy
Bonds become shorter and stronger as "multiplicity increases"

Length: single > double > triple
Strength: single < double < triple

9. Bond Energy and Enthalpy

$$\Delta H^\circ = \sum D_{\text{bonds broken}} - \sum D_{\text{bonds formed}}$$

"takes to break, free to form"

Breaking bonds requires energy
Endothermic (+)

Forming bonds releases energy
Exothermic (-)

10. Resonance – when more than one valid Lewis Structure can be made for a molecule.

11. Resonance bonds:

- Shorter and stronger than single bonds
 - Longer and weaker than double bonds
- When resonance we see the bond lengths ending up identical and intermediate compared to the single or double bond order (example: 1.5 vs 1 or 2). We know this from experimental data!

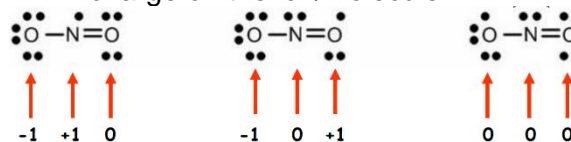
12. Formal charge can help predict which resonance structure is more stable/common.

13. Formal Charge =

- # valence electrons an atom should have
- # lone pairs on the atom
- $\frac{1}{2}$ the # of bonded e- (only $\frac{1}{2}$ b/c they are shared)

Guidelines:

- FC of 0 more stable
- Negative FC should be on most electronegative atoms
- Sum of all FC must equal the overall charge on the ion/molecule



14. Valence Shell Electron Pair Repulsion Model VSEPR

- The structure around a given atom is mostly determined by minimizing e⁻ pair repulsions.
- Allows us to predict the 3D structure and bond angles of molecules.

15. AXE Formulas can help you remember your geometries and bond angles

Steric # X+E	Electron Geometry	AXE Formula
2	Linear	AX ₂
3	Trigonal Planar	AX ₃ , AX ₂ E
4	Tetrahedral	AX ₄ , AX ₃ E, AX ₂ E ₂
5	Trigonal Bipyramidal	AX ₅ , AX ₄ E, AX ₃ E ₂ , AX ₂ E ₃
6	Octahedral	AX ₆ , AX ₅ E, AX ₄ E ₂

A = central atom

X = atoms bonded to A

E = nonbonding electron pairs on A

16. Octet "rule" – many atoms want to have 8 valence electrons.

Exceptions:

- H and He can only have 2 max
- Deficient Octets – B and Be
- Expanded Octets – P, S and other elements with d orbitals (3rd period and below) can have more than 8.

17. Lewis Structures – show the valence electrons involved in bonding.

18. "Rules" for Drawing Lewis Structures:

1. Count and sum valence electrons
2. Place your atoms
3. Bond all atoms w/ a single bond
4. Give all atoms a full shell
5. Re-count the electrons you used
6. Used too few? Put extras on the central atom.
7. Used too many? Try double or triple bonds to fix.

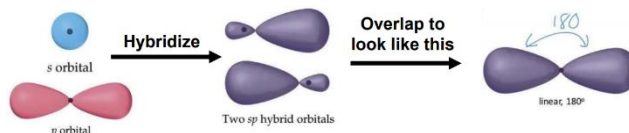
19. Placement Suggestions:

- Hydrogen always goes on the outside.
- Least electronegative atom in the center
- Symmetry is good
- Think about Formal Charges

20. Polarity – unequal distribution of electron density. Results in partial positive regions and partial negative regions on the molecule.

- Must have polar bonds
- Asymmetrical shape
- Bond dipole moment measured

21. Hybridization – the combining of two or more orbitals of similar energy into orbitals of equal energy and new shapes.



Explains bond angles and lengths better

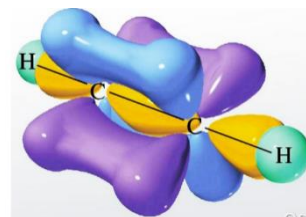
- Without hybridization some bonds would be longer/shorter than they are. Explains why CH₄ has four equal bonds.

22. Which orbitals hybridize?

- sp = 1 s orbital and 1 p orbital
- sp² = 1 s orbital and 2 p orbitals
- sp³ = 1 s orbital and 3 p orbitals
- No longer believed that d, f orbitals hybridize

23. Hybridization and AXE formulas

- Steric #2 = sp
- Steric #3 = sp²
- Steric #4 = sp³



24. Sigma (σ) and Pi (π) bonds – describes how the bonds are formed in 3D space, how the orbitals overlap.

Sigma Bonds – when orbitals of two atoms line up along the axis directly between the nuclei

Pi Bond – when the atomic orbitals of two atoms line up above and below the plane where the nuclei are.

- Can be normal orbitals or hybrids
- s-s, s-p, s-hybrid, p-hybrid, hybrid-hybrid, etc

Two unhybridized p orbitals are parallel to each other and the Pi bond forms above/below or front/back the plane of the nuclei.

- Two unhybridized p orbitals are parallel to each other and the Pi bond forms above/below or front/back the plane of the nuclei.

25. Sigma bonds are stronger than Pi bonds because the orbitals directly overlap between the nuclei. Because Pi bonds reach over/under they are further apart and less overlap, makes them weaker.

26. Single bond = 1 sigma

Double bond = 1 sigma, 1 pi

Triple bond = 1 sigma, 2 pi