

**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  $F \propto \frac{q_1 q_2}{r^2}$

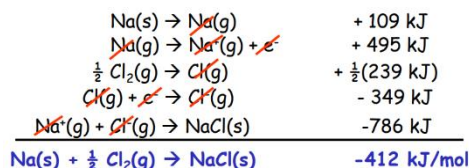
q = absolute value of charge on particles  
r = distance between particles

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

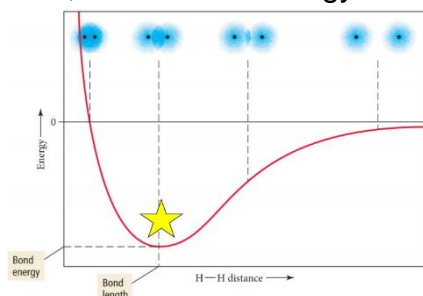
5. Lattice Formation Energy  
Five steps, example LiF

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.  $\Delta H_f$  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

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

Breaking bonds requires energy

Endothermic (+)

Forming bonds releases energy

Exothermic (-)

*“takes to break, free to form”*

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 =

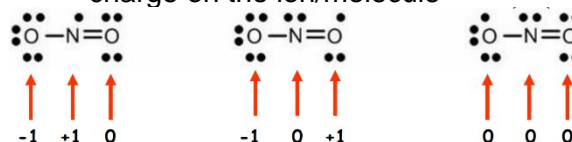
# valence electrons an atom should have

- # 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 <sub>2</sub>
3	Trigonal Planar	AX <sub>3</sub> , AX <sub>2</sub> E
4	Tetrahedral	AX <sub>4</sub> , AX <sub>3</sub> E, AX <sub>2</sub> E <sub>2</sub>
5	Trigonal Bipyramidal	AX <sub>5</sub> , AX <sub>4</sub> E, AX <sub>3</sub> E <sub>2</sub> , AX <sub>2</sub> E <sub>3</sub>
6	Octahedral	AX <sub>6</sub> , AX <sub>5</sub> E, AX <sub>4</sub> E <sub>2</sub>

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 (3<sup>rd</sup> 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.

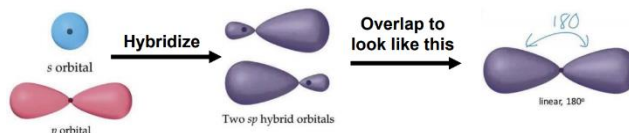
#### 19. Placement Suggestions:

- 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

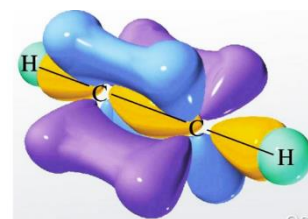
- Without hybridization some bonds would be longer/shorter than they are. Explains why CH<sub>4</sub> has four equal bonds.

#### 22. Which orbitals hybridize?

- sp = 1 s orbital and 1 p orbital
- sp<sup>2</sup> = 1 s orbital and 2 p orbitals
- sp<sup>3</sup> = 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 = sp<sup>2</sup>
- Steric #4 = sp<sup>3</sup>



#### 24. Sigma ( $\sigma$ ) and Pi ( $\pi$ ) 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

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

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

- 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