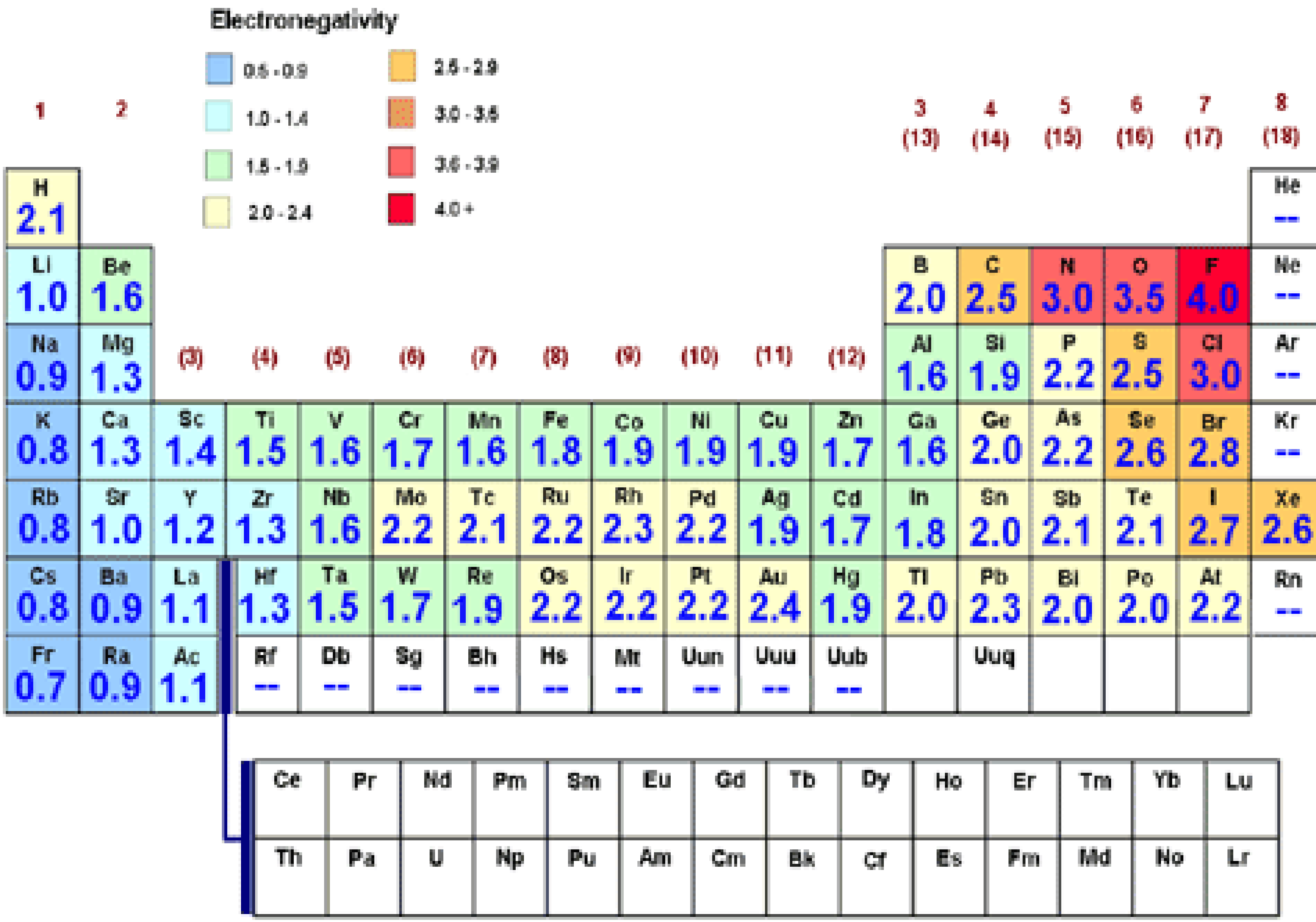
POLARITY

Polarity – main concepts

1. A polar molecule has opposite charged ends (+ & -)
2. The polarity of a bond is the result of a difference in electronegativity between the two bonded atoms
3. A molecule can have polar bonds but the entire molecule still be nonpolar
4. Polarity is largely determined by molecular geometry

electronegativity

- The measure of the attraction an atom has for the electrons in a bond
  - Higher electronegativity = greater pull on e^-'s
- Periodic trend parallels electron affinity
- Pauling scale:
  - Fluorine assigned a value of 4.0
  - All other elements listed relative to (less than) this value
  - Nonmetals ≥ 2
  - Metals ≤ 2



http://www.green-planet-solar-energy.com/electronegativity-values.html

Increasing electronegativity →

Decreasing electronegativity ↓

- electronegativity < 1.0
- 1.0 ≥ electronegativity < 2.0
- 2.0 ≥ electronegativity < 3.0
- 3.0 ≥ electronegativity < 4.0

1 **H** 2.20																	2 **He**
3 **Li** 0.98	4 **Be** 1.57											5 **B** 2.04	6 **C** 2.55	7 **N** 3.04	8 **O** 3.44	9 **F** 3.98	10 **Ne**
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87 **Fr** 0.70	88 **Ra** 0.90	89 **Ac** 1.1	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**	110 **Ds**	111 **Uuu**	112 **Uub**	113 **Uut**	114 **Uuq**	115 **Uup**	116 **Uuh**		118 **Uuo**

Electronegativity Values in Paulings

electronegativity

- Atoms with different electronegativities pull on the bonding electrons differently
- This results in an uneven distribution of the electrons…

…which then results in a polar bond…

…which **may** then result in a polar molecule.

When is a ***BOND*** polar?

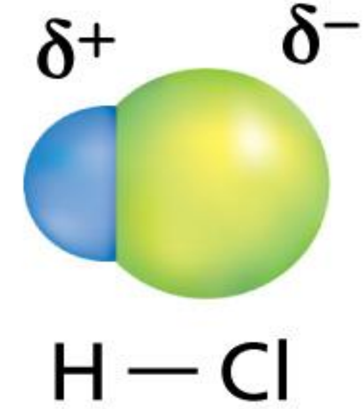
Polar bonds

- If the bonding atoms have $\Delta \mathrm{EN} \geq 0.4$, the resulting covalent bond will be ***polar***
- The bond is called a polar covalent bond, and is often referred to as a "dipole"

Polar bonds

ElectronegativityCl = 3.16
ElectronegativityH = 2.20

Difference = 0.96



Nonpolar bonds

- If both bonding atoms have identical or very similar EN's ($\Delta\text{EN} \leq 0.4$), the bonds will be ***nonpolar***
- Ex: C-S bonds
  - (both atoms have an EN=2.5, so ΔEN=0.0)

When is a ***MOLECULE*** polar?

2 atom molecules (diatomics)

Polar **molecules**

- If there are only two atoms in the molecule, and they are *different* elements, the molecule is **polar**
- Examples would include HCl, HF, CO, among others

Nonpolar molecules

- If there are only two atoms in the molecule, and they are *the same* element, the molecule is **nonpolar**
- Examples of this are the diatomic elements
  - H_2, N_2, O_2, F_2, Cl_2, Br_2, I_2

Molecules with MORE than 2 atoms

Polar molecules

- If there are *more than* two atoms in the molecule, a bond being polar may or may not result in the entire molecule being polar
- The entire geometry of the molecule must be considered

"Assymetric" molecules tend to be polar

Molecular content and polarity: If…

1. all the atoms covalently bonded to the central atom are the same,
2. and there are no lone pairs on the central atom,

the molecule will be ***nonpolar***

- They are "symmetrical" - even if the bonds are polar, the individual dipoles will cancel each other out.
- Example: $CH_{4,}$ CO_2

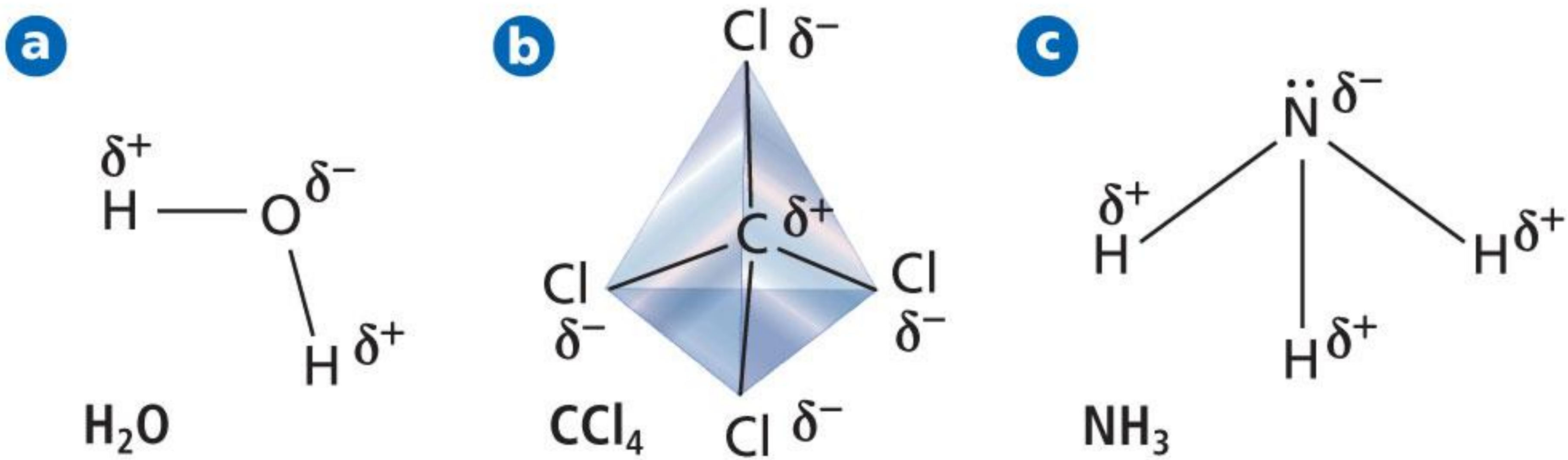
Molecular content and polarity: If…

- all the atoms bonded to the central atom are not the same, they will not have the same EN, and therefore…
  - the molecule will be ***polar***
- They are "asymmetric" - the individual dipoles will not cancel each other out equally
- Example: CH_3F, HCN

Molecular shape and polarity

- Lone pairs on the central atom tend to result in a polar molecule
- The lone pair distorts the symmetry of the molecule
- The individual dipoles will not cancel each other out equally
- Example: H_2O, NH_3
- Exceptions: linear (XeF_2) and square planar (XeF_4) geometries

Molecular shape and polarity



The bent shape of a water molecule makes it polar.

The symmetry of a CCl_4 molecule results in an equal distribution of charge, and the molecule is nonpolar.

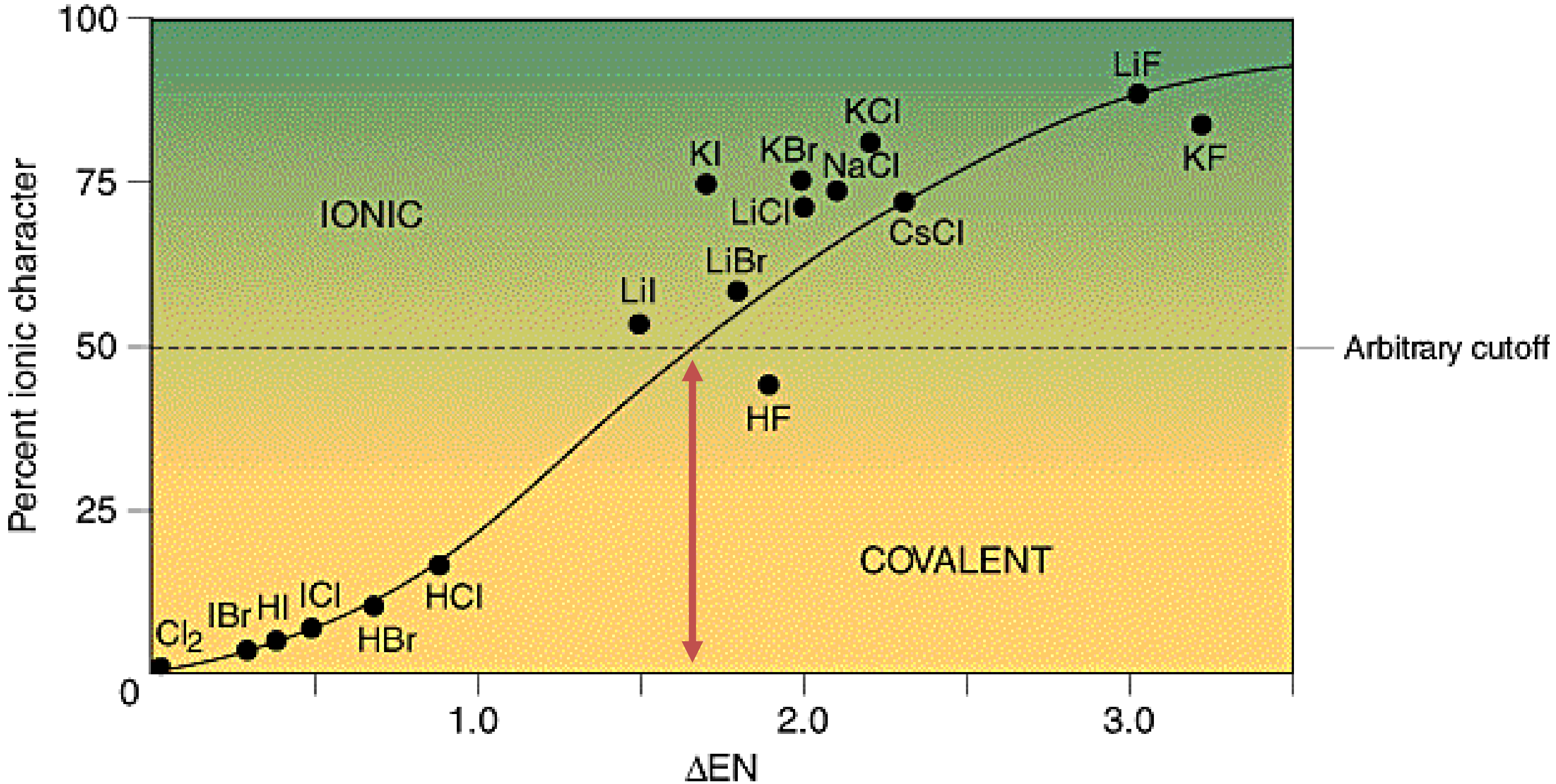
The asymmetric shape of an ammonia molecule results in an unequal charge distribution and the molecule is polar.

Molecular shape and polarity

- Hydrocarbons composed of only C and H are always NONPOLAR
  - CH_4, C_6H_6, $C_{12}H_{24}$, etc…
- "short chain" (1 – 3 carbon) alcohols are usually polar
  - CH_3OH, CH_3CH_2OH, C_3H_7OH, etc…
- The carbon chain portion of the alcohol is *nonpolar*, so as the chain grows longer, the polarity diminishes

What if…

- The truth: the polarity of a bond is a continuum rather than an either/or situation
- Bonds are classified as either covalent (nonpolar), polar covalent, or ionic
- A bond with ΔEN = 1.7 is considered 50% ionic in nature



www.chem.ufl.edu/~itl/2045/lectures/lec_13.html

Polarity continuum

- Examples…
- Cl_2: ΔEN = 0.0; this is considered nonpolar covalent
- Both of the Cl’s share the electrons equally

Polarity continuum

- Examples…
- HCl: ΔEN = 0.9; this is considered polar covalent
- The Cl has the electrons a majority of the time
- But, the H is not considered to have “lost” its valence electron

Polarity continuum

- Examples…
- NaCl: ΔEN = 2.1; this is considered ionic
- The Cl has the electrons the huge majority of the time
- The Na is considered to have “lost” its valence electron
- In an aqueous solution, the Na is indeed Na^+ and the Cl is Cl^-

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