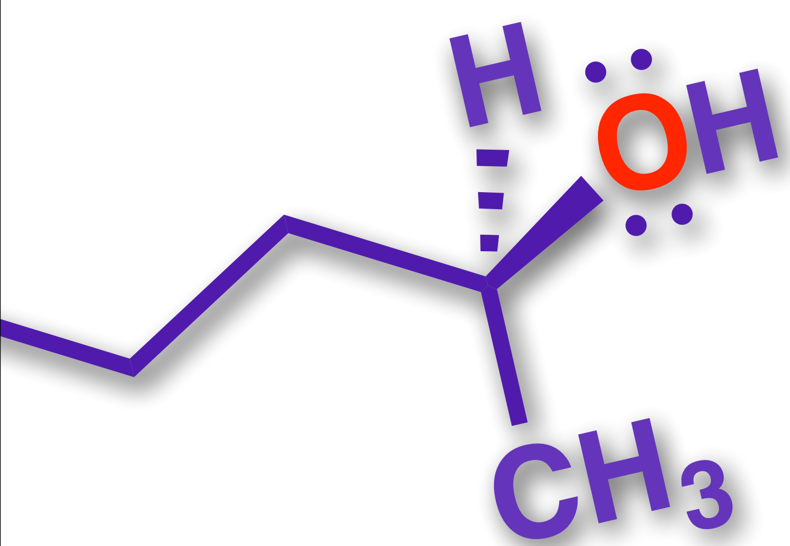
Models of Chemical Bonding



Chemistry Lecture 1

Outline I

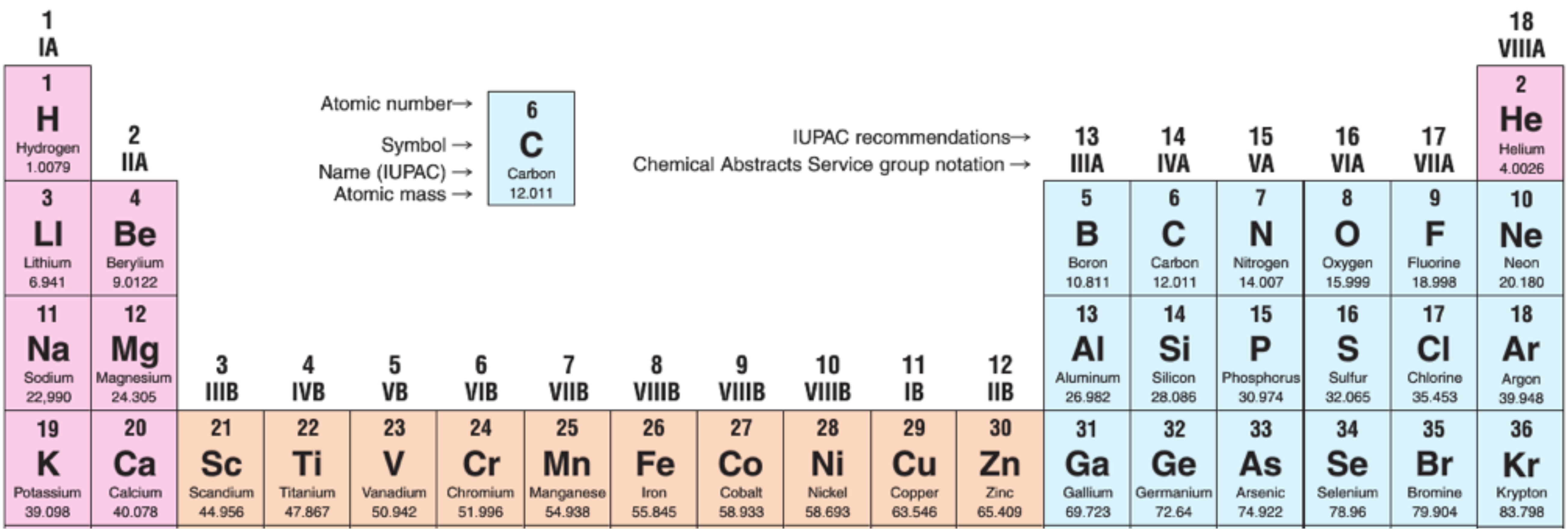
- Valence Electrons and the Octet Rule
- Bonds- Ionic vs. Covalent
- Lewis Structures - Dashes and Dots
- Formal Charge
- Resonance Structures

Outline II

- Structural Formulas- Condensed and Bond-Line
- Three-Dimensional Formulas
- VSEPR Theory
- Polar Covalent Bonds
- Dipole Moments

Valence e$^-$ and the Periodic Table

- Valence electrons - Electrons in the outermost electronic level of an atom
  - Group # on the Periodic Table indicates how many an element possesses (Roman numeral)

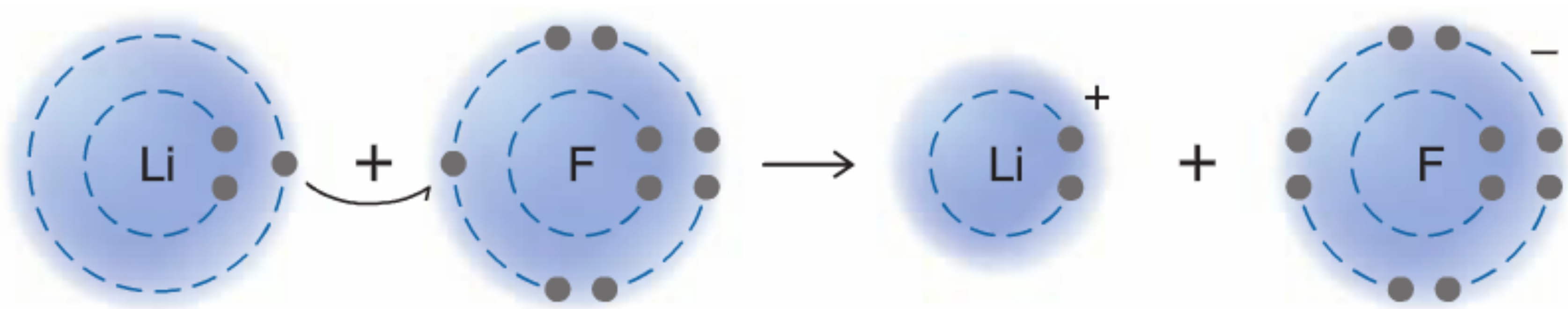


The Octet Rule

- Octet Rule - The tendency for an atom to achieve a configuration where its valence level contains 8 e^-
  - Based on the idea that atoms without the configuration of a noble gas would react to attain such a configuration
    - Noble gases have full valence levels and are, for the most part, unreactive
    - Atoms of the first row, H and He, usually have 2 e^-
    - Atoms of the 2nd row, B, C, N, etc., can have 8 e^-

Types of Bonding

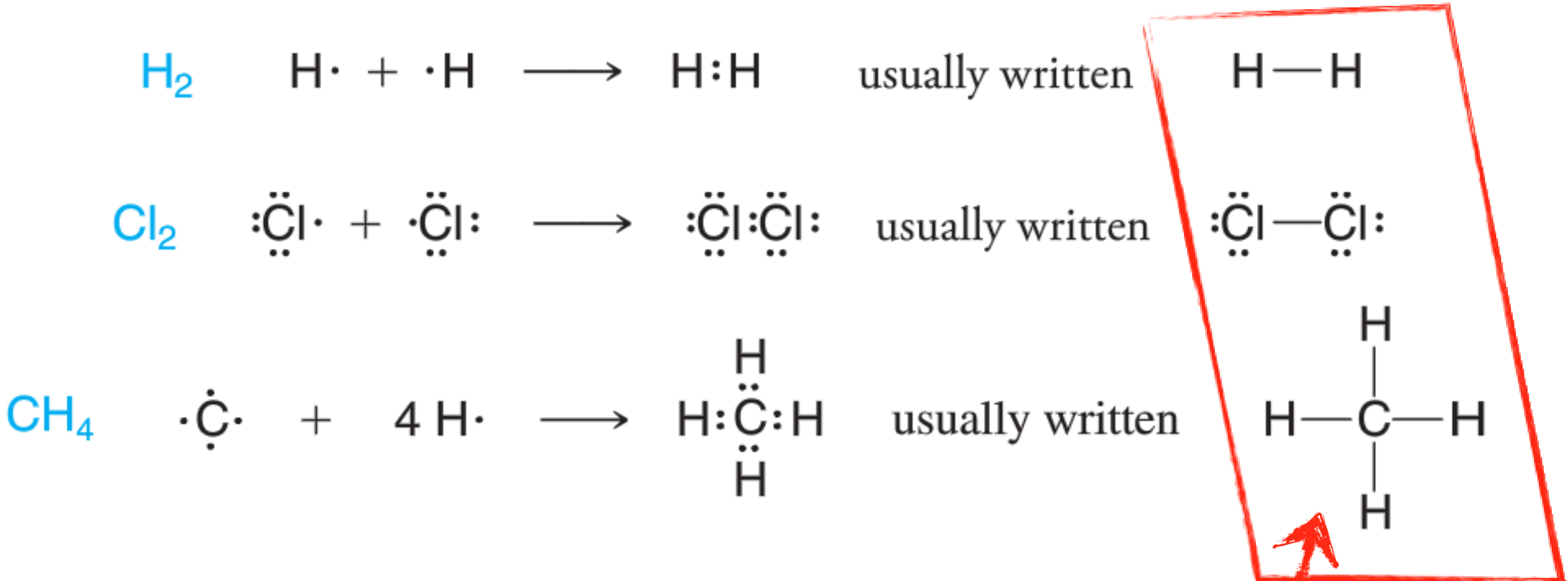
- Atoms may lose or gain valence electrons to become charged species called ions
- Ions may arise from the interaction of atoms of widely differing electronegativities.



- The very electronegative F attracts an e^- from the weakly electronegative Li (called electropositive) to form an ion pair referred to as a salt
- Ionic Bond - The attractive force between oppositely charged ions

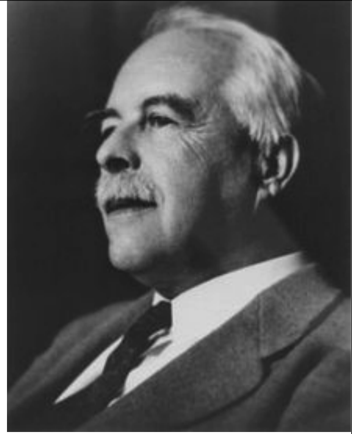
Covalent Bonds

- Covalent bonds form by the sharing of e- between atoms



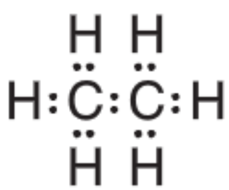
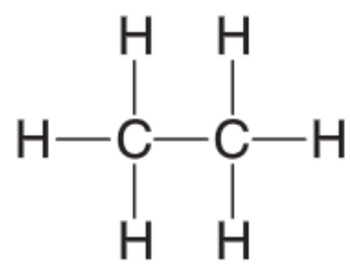
- Molecules are composed of atoms joined exclusively or primarily by covalent bonds

Dash structural formulas



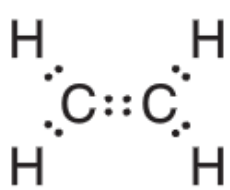
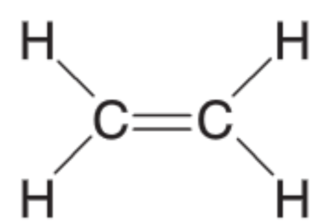
Dash Structural Formulas

- Dash structural formulas show *shared* e^- pairs as dashes and show the elements using their symbols
  - These are often called Lewis Structures

C_2H_6  and as a dash formula 

Ethane

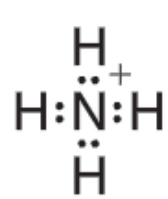
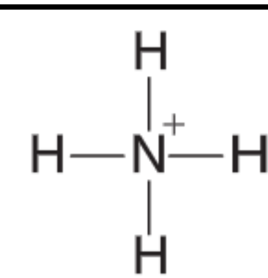
N_2  and as a dash formula 

C_2H_4  and as a dash formula 

Ethene

C_2H_2  and as a dash formula 

Ethyne

NH_4^+  and as a dash formula 

Lewis Structure Rules

- Lewis structures only use valence e^-
- The # of valence e^- of a neutral atom is equal to its group number in the periodic table (Carbon has 4)
- If the structure is an anion (negatively charged ion), add an e^- for each negative charge
- If the structure is a cation (positively charged ion), subtract an e^- for each positive charge
- Give each element the configuration of a noble gas
    - C, N, O, F want 8 (octet rule!)
    - H needs 2 e^- to have configuration of He

- Let's try CH_3F

Lewis Structure Problems

- CH_3NH_2
- CH_3CH_2OH
- CO_3^{2-}
- H_2C_2
- $HOCl$
- OCl_2
- NO_3^-
- BH_4^-
- C_6H_6

Formal Charge

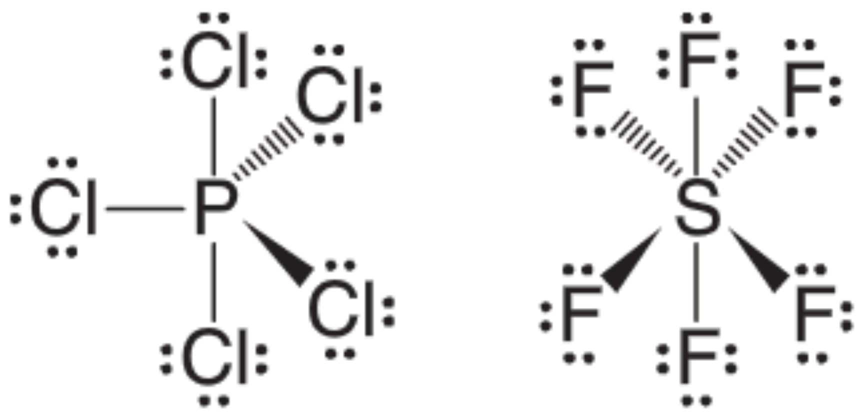
- Many Lewis structures are incomplete until we assign a formal charge to the atoms
- There are a few ways to do this. I use the formula:
    - FC = Group# – 1/2 shared e^- – unshared e^-
- The sum of charges on the atoms must equal the overall charge of the molecule
    - Let's try NH_4^+

Formal Charge Problems

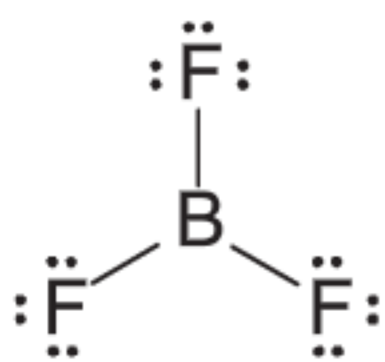
- NO_3^-
- I_3^- (does F3- exist???)
- CO
- SCN^-
- H_3C^+
- HF_2^-
- O_3

Octet Rule Exceptions

- Atoms in the third row or higher can have >8 e^-
  - They have access to higher orbitals
  - Cl, Br, I, P and S often do this:



  - Trivalent boron is electron deficient and only has 6 e^- around it

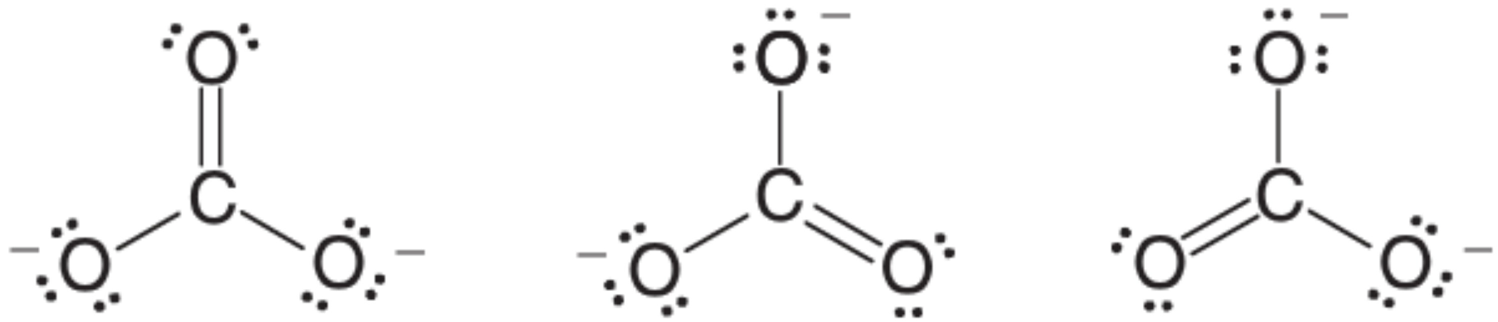


Octet Rule Exceptions Problems

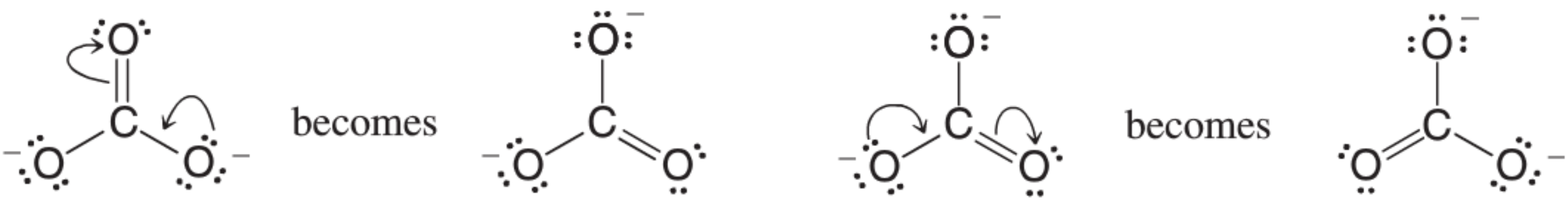
- H_2SO_4
- $H_3CB(OH)_2$
- $P(O)(OH)_3$

Resonance Structures

- Often more than one equivalent Lewis structure can be written for one molecule
- The only difference between these structures is the position of e^-.... The connectivity remains constant



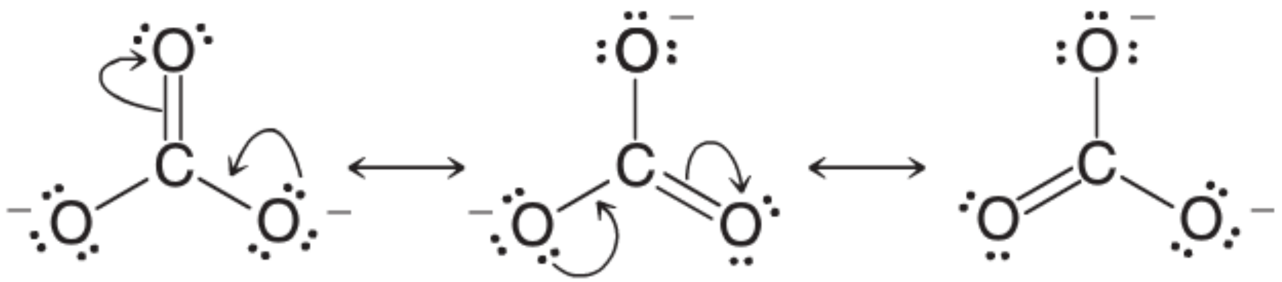
1 2 3



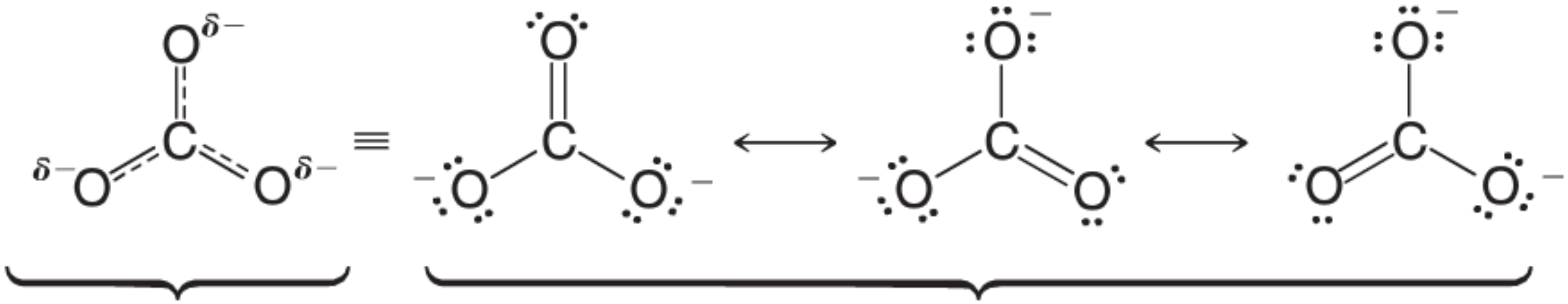
1 2 2 3

Resonance Structures

- An X-RAY of the carbonate ion reveals that all of the C/O bonds are the same length
- One wouldn't predict this by looking at individual Lewis structures



- Resonance theory states that all of these structures contribute to the actual molecule, which is represented by the hybrid wherein the bond lengths are part way between single and double bond lengths



Hybrid

Contributing resonance structures

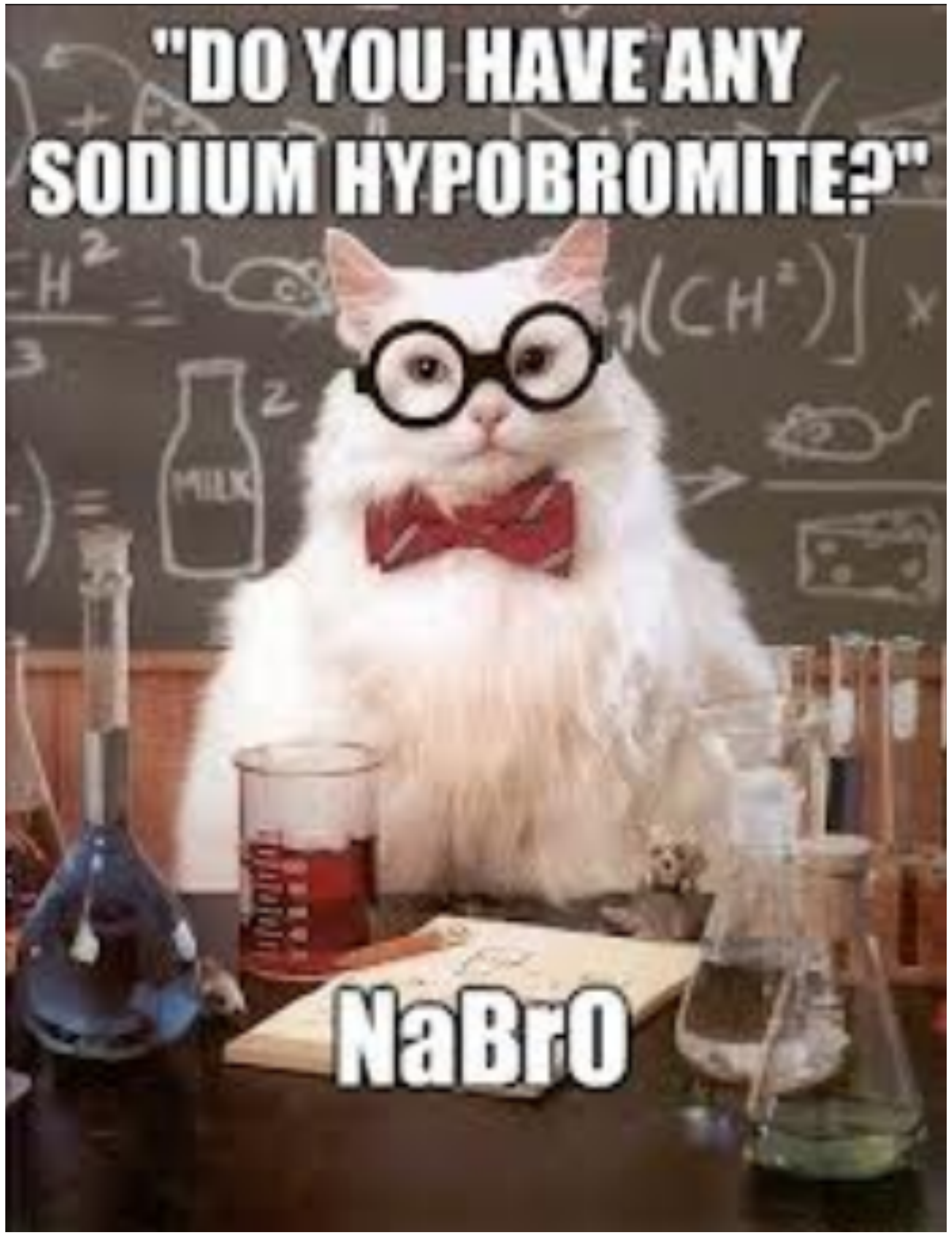
Resonance Structure Rules

- Resonance structures exist only on paper (or iPads)
- Only electrons may be moved in drawing new RSs
- All must be proper Lewis structures
- The resonance hybrid is lower in energy than any one contributing resonance structure
  - The more covalent bonds the better
  - More filled valances the better
  - The less charge separation the better

- Lets draw resonance structures and the resonance hybrid for NO_3^-, SCN-, CO, C_6H_6

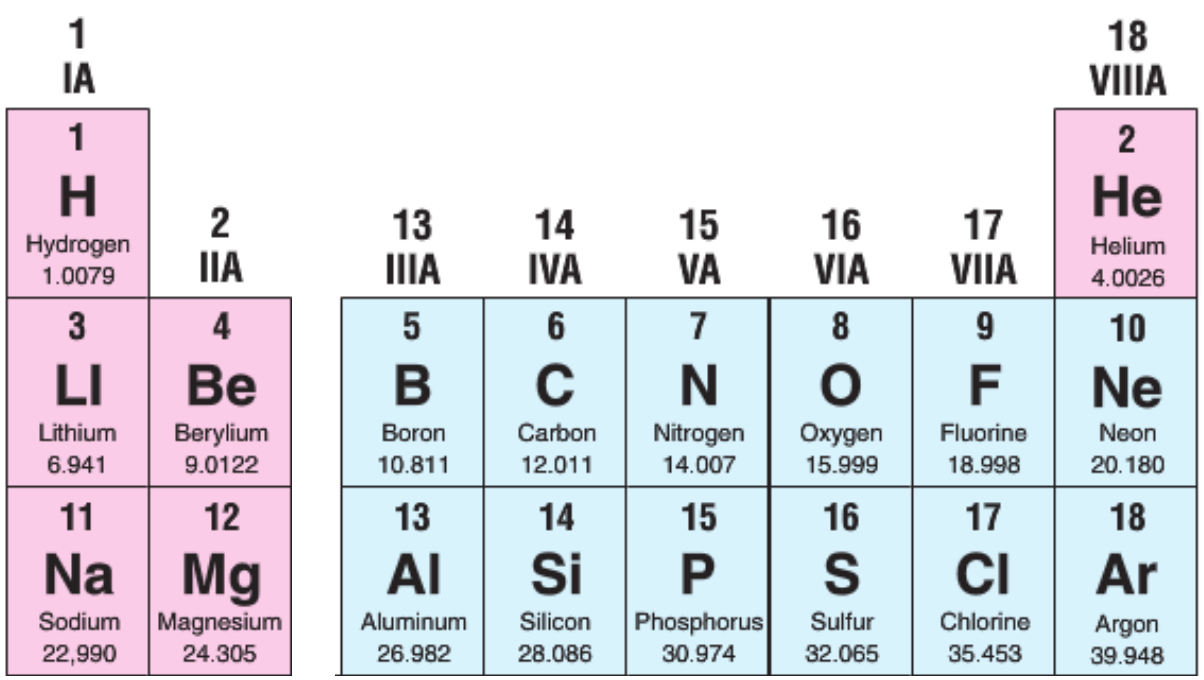
Lewis Structures, Formal Charge & Resonance

- Let's draw the Lewis structures and resonance structures for ClO3-



Valence e^- and Electronegativity

- Electronegativity - The measure of the ability of an atom to attract electrons
    - Trend apparent on the Periodic Table



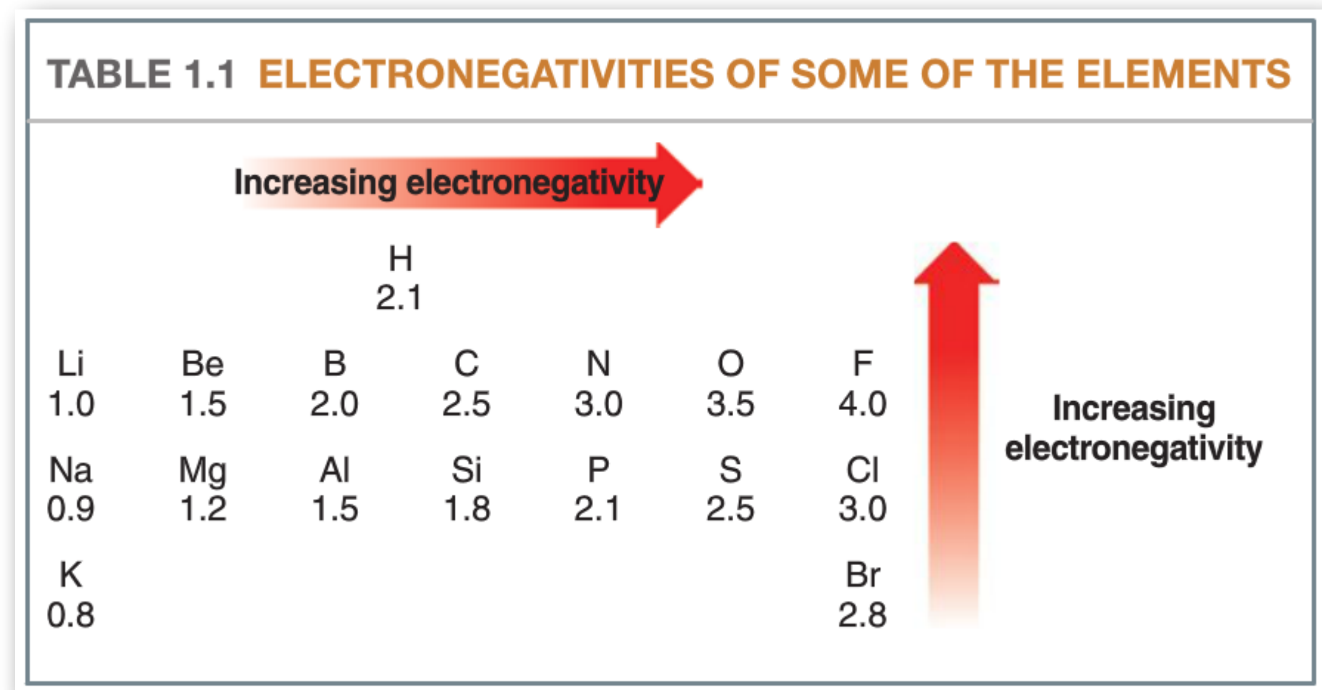


TABLE 1.1 ELECTRONEGATIVITIES OF SOME OF THE ELEMENTS

Increasing electronegativity

		H 2.1				
Li 1.0	Be 1.5	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8						Br 2.8

Increasing electronegativity