Welcome to Chemistry 154!

Please make sure to sync your iClicker Cloud to Chem154 Section 113

Reminders

- **Worksheet: Unit 2**
- Due September 19th at 11:59pm

- **Worksheet: Unit 3 (Qs 1-10)**
- Due September 26th at 11:59pm

- **Achieve Assignment #3**
- Due Oct. 2nd at 11:59pm

Worksheet →
All Lectures Canvas Site
Submission link →
Section 113 Canvas Site

Instructor Office Hours
Monday and Friday 7-8pm via Zoom (All Lectures Site)

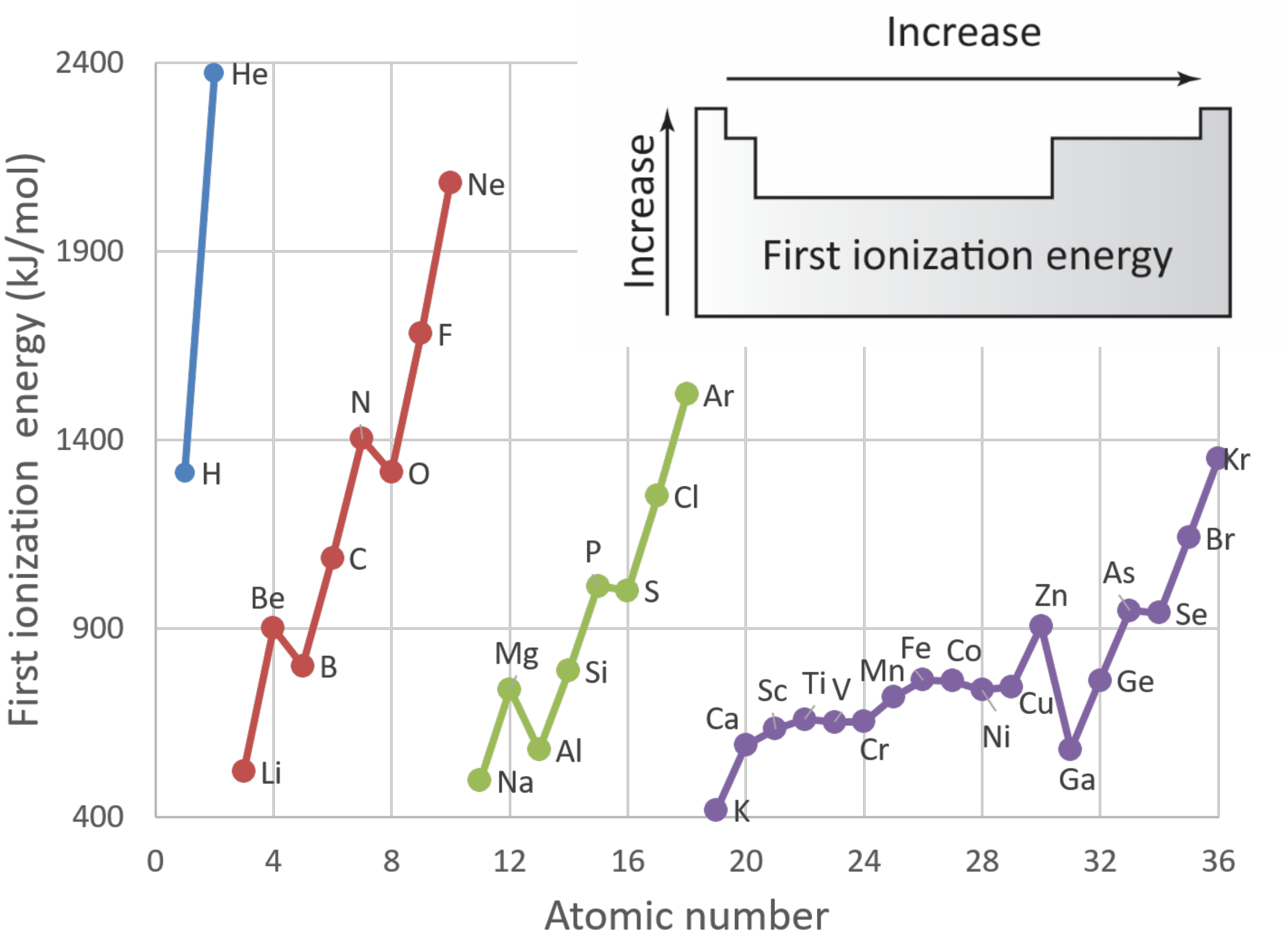
Ionization Energy (IE)

<u>For atoms, molecules or ions</u>: the minimum energy required to remove a single electron from an atom, molecule or ion in its gaseous state.

$$X(g) \rightarrow X^{+}(g) + e^{-}$$

<u>For solids</u>: the minimum energy required to remove an electron from the valence band of the solid.

As many elements are solids, values may be available for both, and differ due to the nature of bonding in solids. The elemental values always refer to the gas phase.



First ionization energy (kJ/mol)
2400
1900
1400
900
400
0
4
8
12
16
20
24
28
32
36
Atomic number
H
He
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Sc
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn
Ga
Ge
As
Se
Br
Kr
Increase
Increase
First ionization energy

Exercise

	Element M	Ionization Energy (kJ/mol)
IE_1	$M \rightarrow M^+ + e^-$	800
IE_2	$M^+ \rightarrow M^{2+} + e^-$	2426
IE_3	$M^{2+} \rightarrow M^{3+} + e^-$	3659
IE_4	$M^{3+} \rightarrow M^{4+} + e^-$	25020
IE_5	$M^{4+} \rightarrow M^{5+} + e^-$	32820

Rationalize the trend in ionization energies and determine the identity of M.

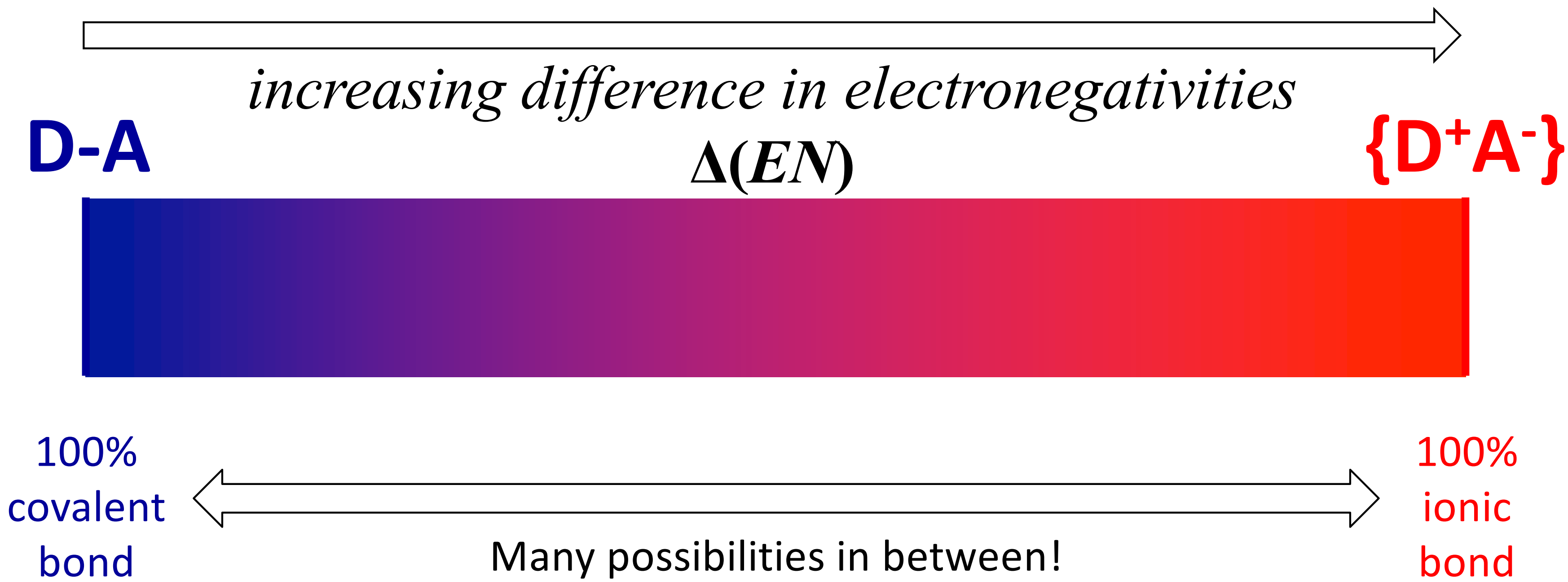
M is Boron

https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Physical_Properties_of_Matter/Atomic_and_Molecular_Properties/Ionization_Energy

What type of bond will form?

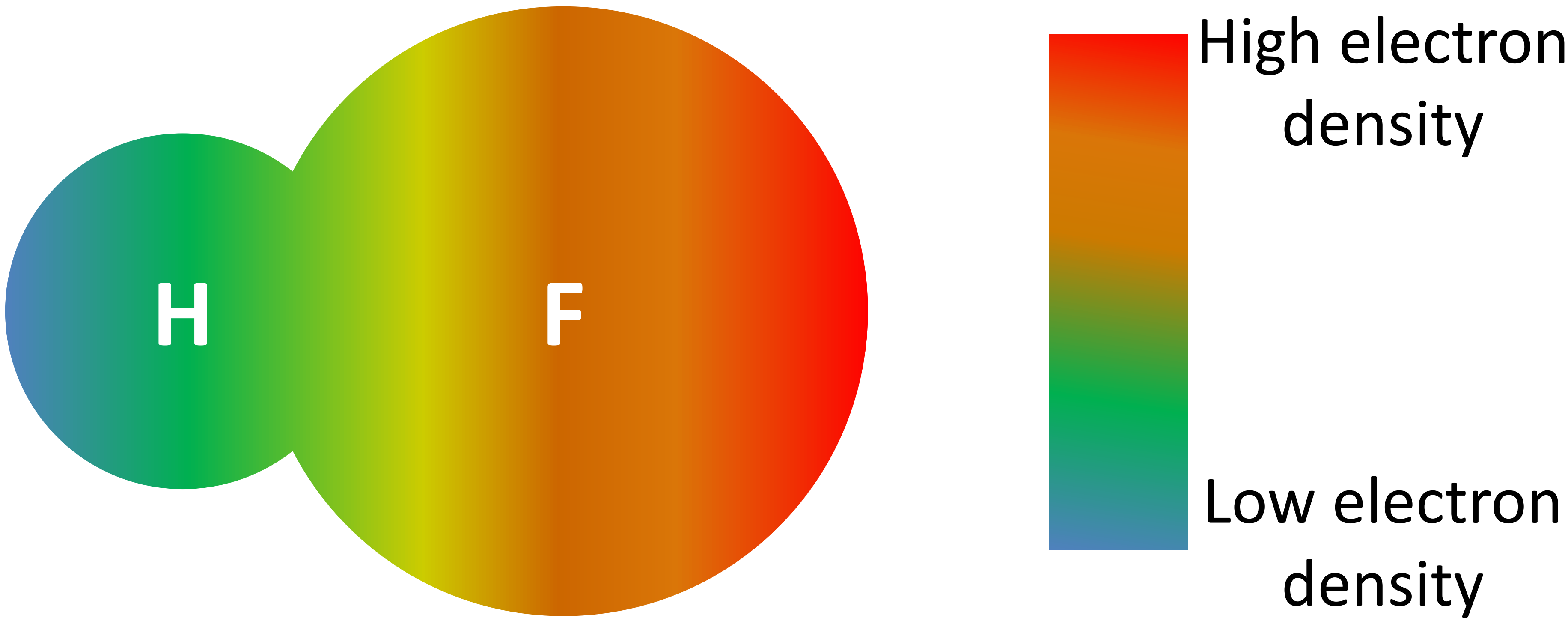
Can range from <u>covalent</u> (where a pair of electrons are <u>shared</u> between two atoms with no net charge) to <u>ionic</u> (where an electron is transferred from a donor to acceptor)

D ⇔ A



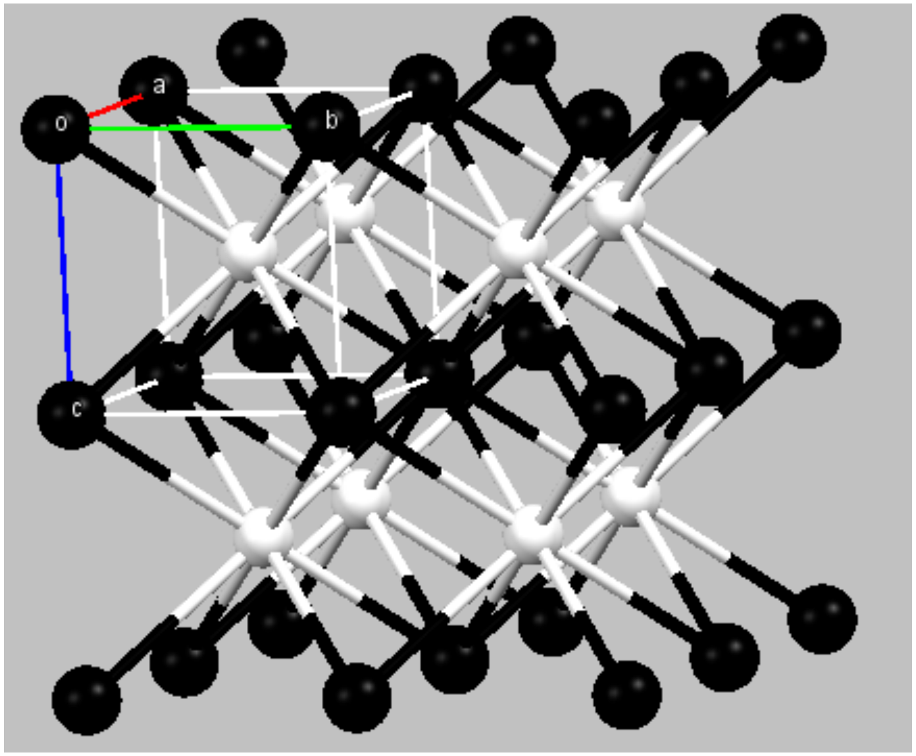
Polar covalent bonds

In some covalent bonds electrons are not equally shared (electron density is higher in one atom than in another) due to differences in electronegativity.



Ionic Bonding

Cesium cations (white) are electrostatically attracted to chloride anions (black). In a crystalline state, the ions form an "infinite", 3D array or lattice.



Rule of Thumb:

$\Delta(EN) \gtrsim 1.7$

for ionic bonding

Worksheet Question #10

Rationalize the trend in lattice energies for the compounds given in the table.

Compound	Lattice Energy (kJ/mol)
NaCl	787
NaF	923
$CaCl_2$	2528
MgO	3791
CaO	3401

How are you doing?

a) Great, fantastic!! 😃
b) Good! 🙂
c) Alright 😐
d) Nervous 🙁
e) Not good at all 😩

Unit 3

Molecular Structure

Learning Objectives (Part 1)

After mastering this unit you will be able to:

– Draw Lewis structures for a given chemical formula, or use the features of a Lewis structure to identify the unknown elements or chemical formula of a molecule.

– Draw resonance structures, or identify valid resonance structures, for a given molecule.

Bonding Theories

Molecular Orbital Theory (exact)

- Correct quantum mechanical description with orbitals extending over entire molecule

Valence Bond Theory (not quite exact)

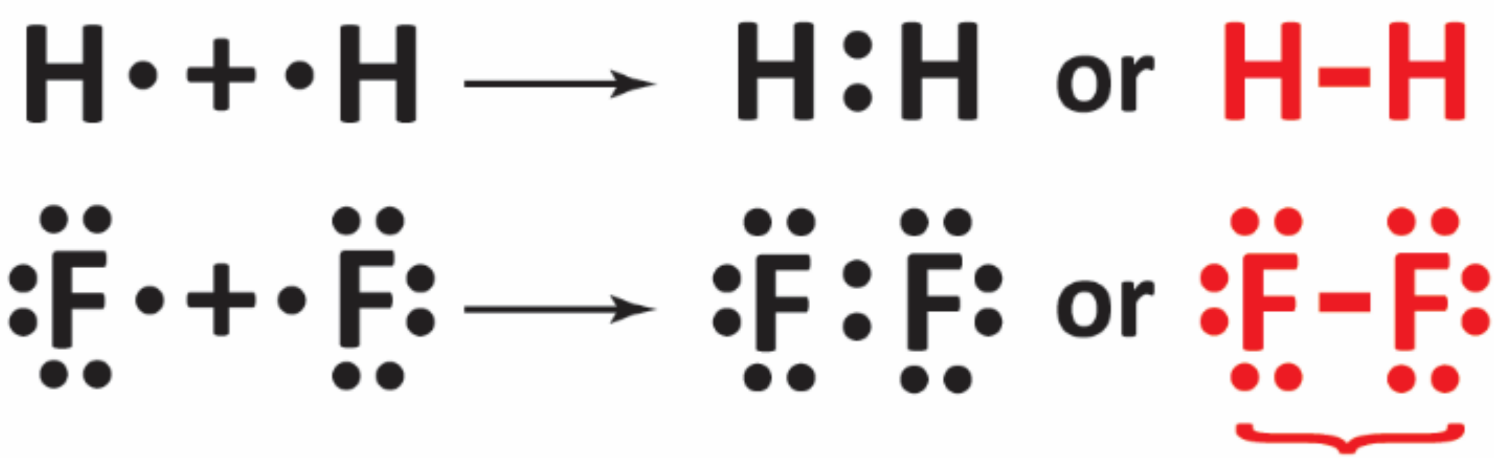
- Localized electron picture with bonds formed by the overlap of singly occupied atomic orbitals

Lewis Theory (approximate)

- Localized electron picture using rules based upon counting electrons

Representation of Covalent Bonds

A **Lewis structure** shows how valence electrons are shared in a molecule. Valence electrons that form a bond are called bonding pairs. Valence electrons that do NOT form a bond are called lone pairs.



Use this notation in CHEM 154

KEEP CALM

AND

DRAW LEWIS DOT STRUCTURES

Lewis Structures

Octet Rule

In forming chemical bonds, main group elements gain, lose, or share electrons to achieve a configuration in which they are surrounded by 8 valence electrons.

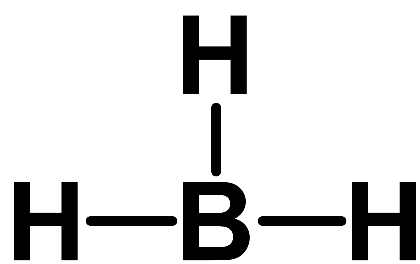
Duet Rule

For hydrogen only, surrounded by 2 electrons.

Note: exceptions can happen, e.g. Boron

Exceptions to the Octet Rule

Incomplete Octet: Elements in Group 13 sometimes follow a "sextet" rule. In other words they have only three electron groups surrounding them:



singly bonded to three H atoms.

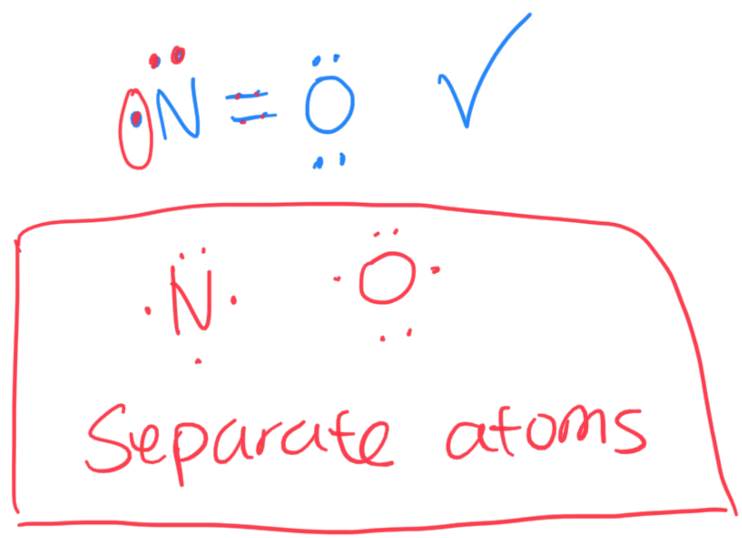
two electrons per bond

∴ B is surrounded by 6 electrons.

Exceptions to the Octet Rule

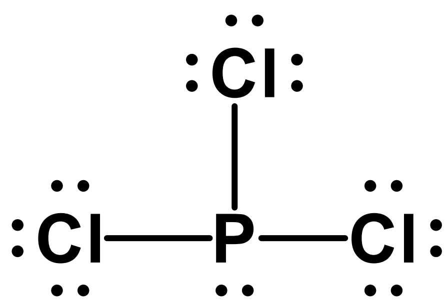
Radical species: Molecules with an odd number of electrons will have an unpaired electron. These species are called radicals.

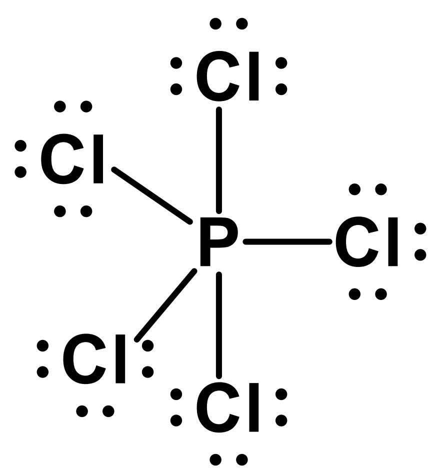
Example: NO $\quad 5 + 6 = \underline{\underline{11}}$ VE



Exceptions to the Octet Rule

Hypervalence (expanded octets): Elements on the third row of the periodic table and below can expand their octets. For example, although phosphorus obeys the octet rule in PCl_3, it has an expanded octet in PCl_5.





Hypervalence

Group

1	13	14	15	16	17	18	
H						He	Maximum duet
	B	C	N	O	F	Ne	Maximum octet, B may have 6 electrons (sextet)
	Al	Si	P	S	Cl	Ar	If central atom, can exceed octet
	Ga	Ge	As	Se	Br	Kr	If central atom, can exceed octet
	In	Sn	Sb	Te	I	Xe	If central atom, can exceed octet
	Tl	Pb	Bi	Po	At	Rn	If central atom, can exceed octet

Hypervalence Rules

- The octet rule will NOT be exceeded unless necessary to form bonds with more than four atoms or to minimize formal charges.
- Only atoms in the third row (period) of the periodic table and below can be hypervalent.
- Terminal atoms are not hypervalent.

Drawing Lewis Structures – Formal charge

Formal charge: Formal charge is the difference between the number of valence electrons and the number of electrons surrounding an atom in a particular Lewis structure.

$$FC = VE – LPE - 1/2(BE)$$

VE = number of valence electrons

LPE = number of lone pair electrons

BE = number of bonding electrons

The overall molecular charge is the SUM of the formal charges.

Electron Bookkeeping and Reality

Several different methods are used in chemistry for electron bookkeeping, each with their own particular application and philosophy. The table below contrasts formal charges and oxidation states with reality for the molecule HCl.

$1+7=8$

$1-\frac{1}{2}(2) = \emptyset$ H—Cl $7-6-\frac{1}{2}(2) = \emptyset$

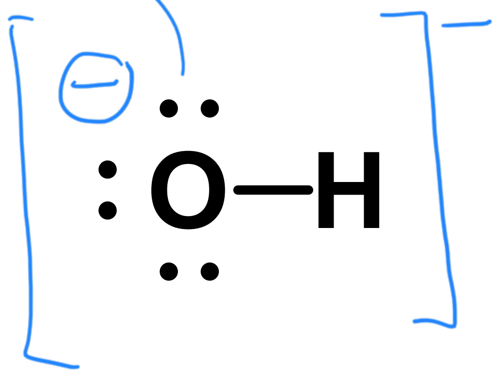
Method	Charge on H	Charge on Cl	Description
Formal Charge	0	0	Bonding e^- shared equally
Oxidation State	+1	-1	Bonding e^- to atom with highest EN
Reality	δ^+	δ^-	Polarized bonds with fractional charges

Worksheet Question #1

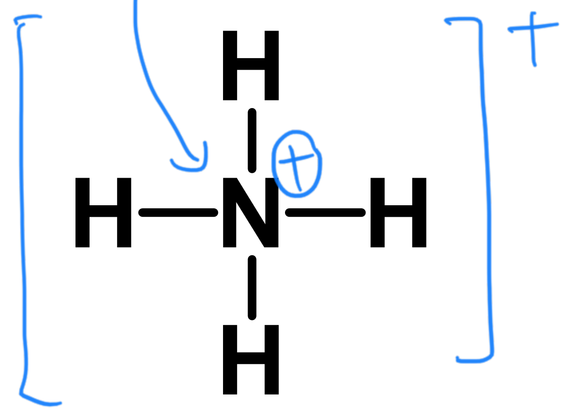
Calculate the formal charge of each atom in the following structures:

$6-6-\frac{1}{2}(2)$

$= -1$



$5-\emptyset-\frac{1}{2}(8) = +1$

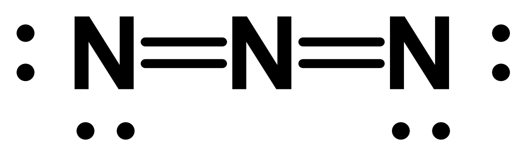


The overall molecular charge is NOT given in these structures. It is the SUM of the formal charges!

Click any answer on your clicker when you have finished this worksheet question!

Worksheet Question #1

The formal charges in the nitrogen atoms in the azide below are:



1 2 3

	N_1	N_2	N_3
A	0	0	0
B	0	+1	0
C	-1	0	-1
D	-1	+1	-1
E	None of the above		

Drawing Lewis Structures

1. Count the number of valence electrons (#ve$^-$) in the molecule or ion
2. Draw the skeletal structure of the molecule
   a) The least electronegative atom is generally the central atom
   b) Hydrogen is ALWAYS a terminal atom
   c) Unless told otherwise, do NOT form rings
3. Place two electrons in each bond of the skeletal structure (represented by single lines)

Drawing Lewis Structures

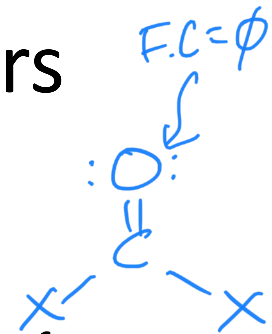
4. Place the remaining valence electrons not accounted for in Step 3 as lone pairs on individual atoms until the octet rule is satisfied
5. Form multiple bonds as needed to complete octets and account for all valence electrons
6. Label the formal charges (FCs)
   - The sum of FCs is equal to the overall molecular charge.

Remember

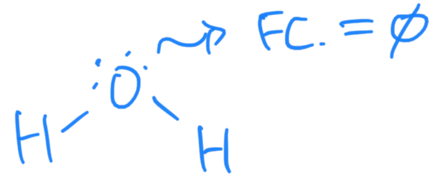
- Hydrogen atoms are always terminal
- The most stable Lewis structure is the one with the least non-zero formal charges
- The most stable Lewis structure is the one that, when possible, places the negative charge on the most electronegative atom and the positive charge on the least electronegative atom

Lewis Structure Tips

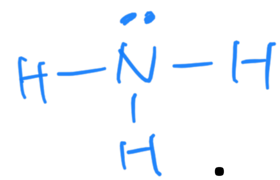
Carbon – always has 4 bonds and no lone pairs



Hydrogen – always has 1 bond



Oxygen – has 2 bonds + 2 lone pairs if FC = 0, 1 bond + 3 lone pairs if FC = -1, and 3 bonds + 1 lone pair if FC = +1 (rare)



Nitrogen – has 3 bonds + 1 lone pair if FC = 0, 4 bonds + 0 lone pairs if FC = +1

These patterns also apply to other elements in the same groups (unless hypervalency is used).

note: X is some atom

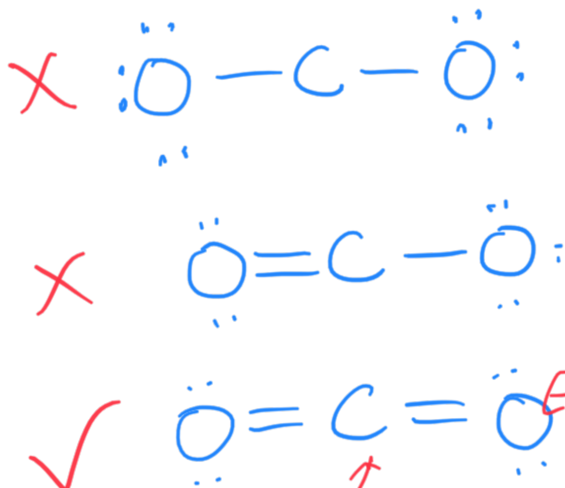
Evaluating Lewis structures - what's best?

1. Do all atoms have full octets?
2. Are formal charges **minimized**?
   - Can't always make them zero, but we want to minimize them
   - Minimize total number of formal charges – charge separation takes energy
3. Put charges on right atoms
   - Negative charges on most electronegative atoms
   - Positive charges on least electronegative atoms

Clicker Question: CO_2

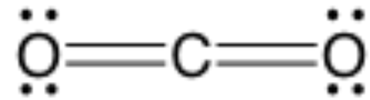
Which of the following represents the **best** Lewis structure for CO_2?

$4 + 6 \times 2 = 16$ VE

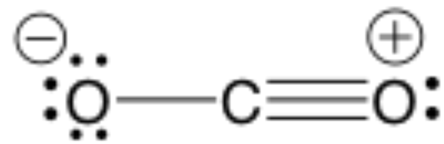


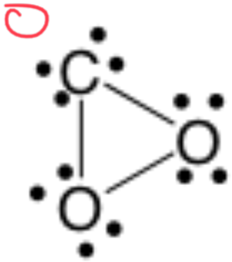
$6 - 4 - \frac{1}{2}(4) = 0$

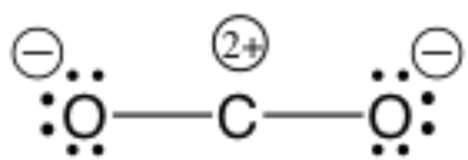
$4 - 0 - \frac{1}{2}(8) = 0$

A 

all atoms are octet fulfilled. and minimized formal charge

B 

C 

D 

Worksheet Question #2b – Clicker

In the N_2O structure you drew, the central atom is:

$(5 \times 2 + 6 = 16 \text{ VE})$

A) Nitrogen

B) Oxygen

C) It is a ring structure without a central atom.