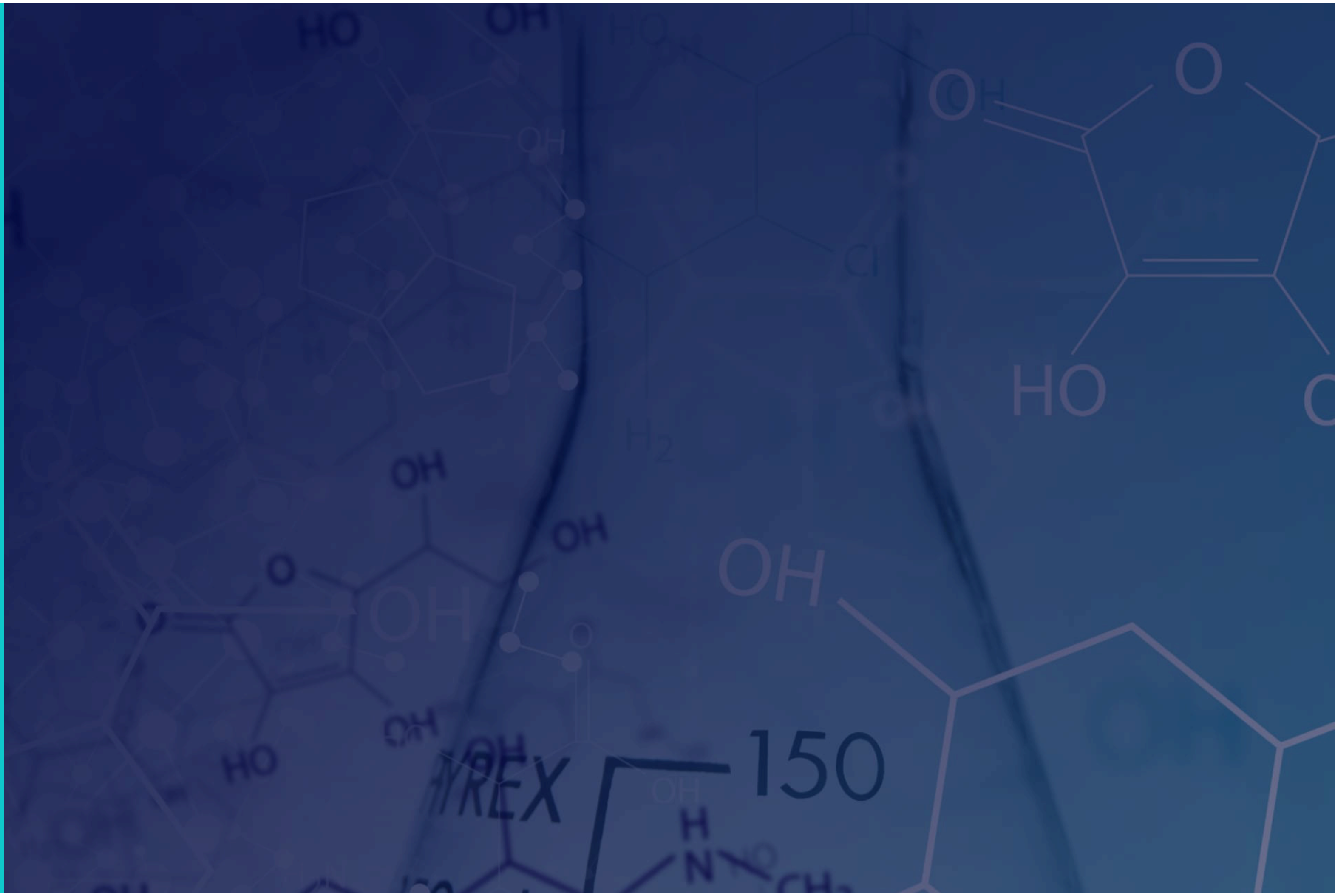

Mac

CHEM 1A03

Fall 2024, Chapter 4 Notes

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4. Unit 5: Chemical Bonding

4.1 Types of Bonds

4.1.1

Introduction to Intramolecular Bonds

Your university just had a poster sale! You bought a new poster to add to your collection and you were trying to decide what to use to stick the poster to the wall. You could have used:

Just like how we can use different things to stick the poster to the wall, there are different bonds that connect different atoms together.

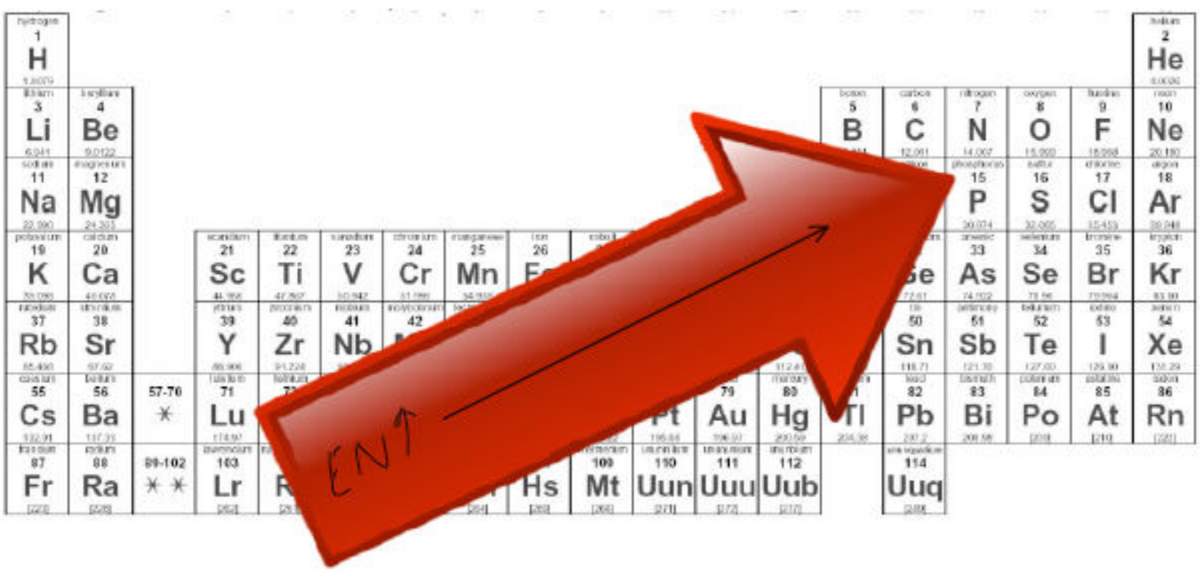
Intramolecular bond: a bond that connects two atoms within a molecule together

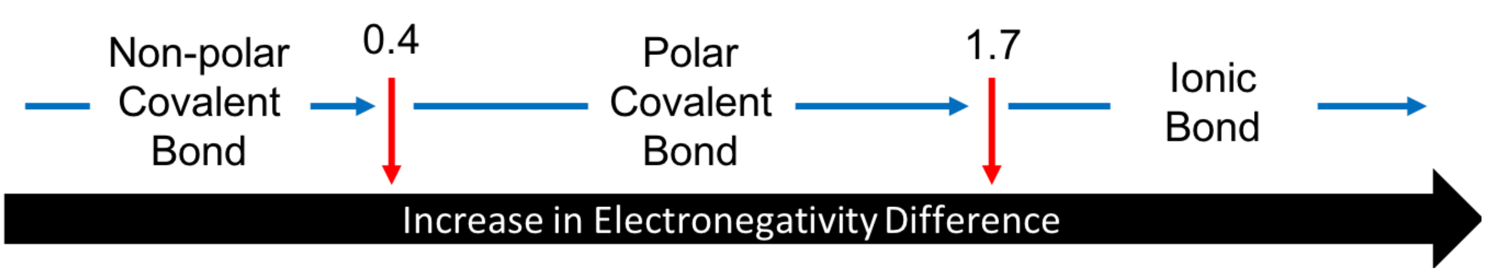
Before we take a look at the different types of intramolecular bonds, we will review electronegativity.

Electronegativity: is the tendency of an atom to pull bonding electrons towards itself

- Valence electrons are involved in chemical bonding
- The type of bond depends on the difference in electronegativity between the two atoms in the bond

> **WATCH OUT!**
>
> This is similar to electron affinity but not the same!
> Electron affinity involves a single atom/ion, whereas **electronegativity involves two bonded atoms**.





4.1.2

Types of Intramolecular Bonds

We will be discussing ionic bonds, covalent bonds (polar covalent bonds, non-polar covalent bonds, and coordination covalent bonds), as well as metallic bonds, which are tested on the least.

Ionic Bonds:

- Are between a **metal and a non-metal**
- You might see ionic compounds called **salts** like NaCl
- There is a **large difference in EN** ($\Delta EN > 1.7$) in these bonds
- The **metal gives electrons to the non-metal** (no sharing of electrons)

Example:

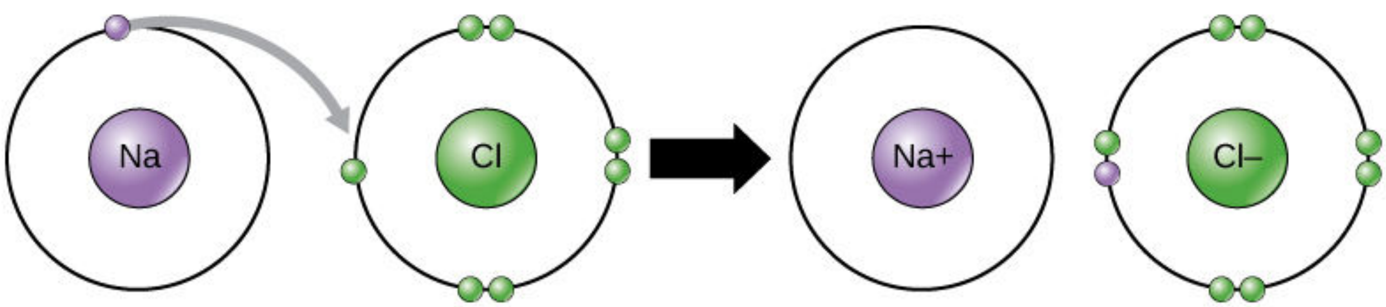


Photo by CNS Openstax/ CC BY

The **charges** that result are what allow ionic compounds to **conduct electric current**

Covalent Bonds:

- Bonds where electrons are **shared** between **two non-metals**
- We will consider 3 types of covalent bonds: i) Non-polar covalent bonds, ii) Polar covalent bonds iii) Coordination covalent bonds

Non-polar Covalent Bonds:

- Electrons are **shared equally** between **2 of the same non-metals**
- As a result there is a very small difference in EN, $0 < \Delta EN < 0.4$

Examples: H_2, O_2, N_2, Cl_2, ***S_8**, ***P_4**

Example: Shown below is an example of two hydrogen atoms sharing their single electron to form a covalent bond. This is specifically a non-polar covalent bond!

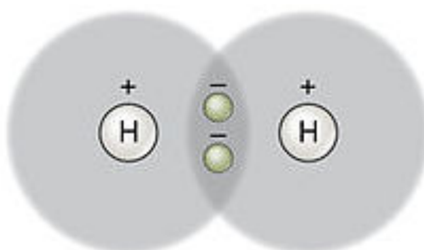


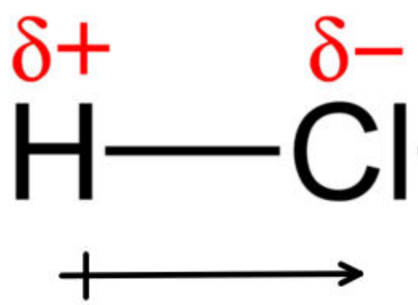
Photo by OpenStax College / CC BY

Polar Covalent Bonds:

- Electrons are shared **unequally** between **2 different non-metals**
- There is a difference in EN, $0.4 < \Delta EN < 1.7$

Since electrons are shared unequally in this bond, we say that there is a "**dipole moment**"

- The dipole moment is a vector with both magnitude and direction (more on this later!)
  - Partial negative charge (**δ-**) is assigned to the atom with the **higher EN**
  - Partial positive charge (**δ+**) is assigned to the atom with the **lower EN**
- **The greater the difference in electronegativity (EN), the greater the dipole moment!**

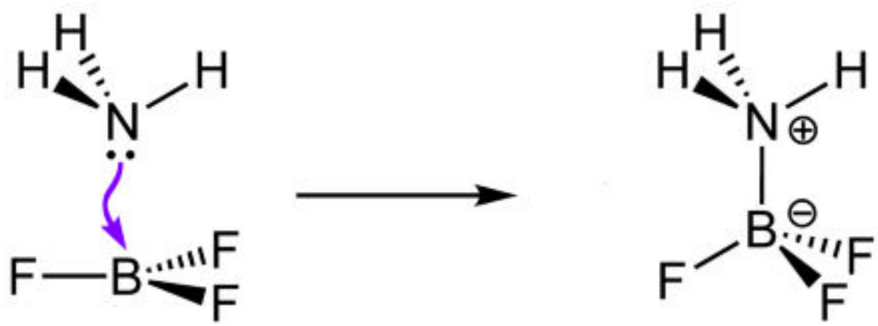


WIZE TIP

You can think of the dipole moment as a tug of war. The dipole moment (arrow) points towards the winner that is able to pull electrons more towards itself (is more electronegative!)

Coordination Covalent Bonds:

- These are covalent bonds (between 2 non-metals) where **both electrons in the bond are donated by one of the non-metals**
  Example: NH_3 reacting with BF_3



- The charges we see here as a result of the bond forming help the product **weakly conduct in solution**
  - **Note:** Ionic bonds conduct a much stronger electric current!

Metallic bond

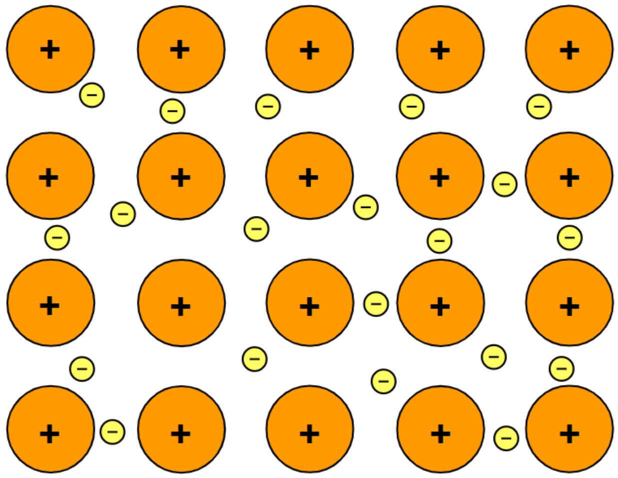


Photo by Muskid / CC BY

- The diagram is showing many atoms of a metal element and their inner shell electrons are surrounded by a **sea of electrons** that are free to move around (aka are delocalized)
  - The **circles with a "+"** inside of them represent a **metal atom + inner shell electrons** (recall nuclei are positively charged)
  - The **smaller circles with a "-"** inside of them represent **valence electrons**

- At least 1 VE/atom is free=**conduction electrons**

- These conduction electrons are what give the metal their properties!
  - Ductile, malleable, conduct thermal energy, conduct electricity, have lustre/shine

Examples: Aluminum metal, Iron, Zinc etc.

4.1.3

Example: Ionic *vs* Covalent Bonding

For the following list of compounds, determine which are mostly ionic and which are mostly covalent.

Cl_2, Li_2O, H_2, CO_2, Fe_2O_3, MgS

4.1.4

Example: Types of Intramolecular Bonds

Indicate what type of bond will be formed between the two atoms in the following compounds. Try to be specific. :)

a) CH_4

b) NH_3

c) LiBr

d) Br_2

e) Na_2SO_4

4.1.5

What type of bonding would be expected in the following compounds?

Part 1

Table salt (NaCl)

- Ionic bonding
- Polar covalent bond
- Non-polar covalent bond
- Metallic bond

What type of bonding would be expected in the following compounds?

Part 2

Ammonia (NH_3)

- Ionic bonding
- Polar covalent bond
- Non-polar covalent bond
- Metallic bond

What type of bonding would be expected in the following compounds?

Part 3

Nitrogen (N_2)

- Ionic bonding
- Polar covalent bond
- Non-polar covalent bond
- Metallic bond

4.1.6

Practice: Types of Intramolecular Bonds

For the three compounds: H_2, CCl_4 and MgF_2, indicate which types of bonds each molecule has.

A. ionic bond(s)

B. polar covalent bond(s)

C. non-polar covalent bond(s)

☐ H_2

☐ CCl_4

☐ MgF_2

4.2 Molecular Polarity

4.2.1

Molecular Polarity

How can we figure out if a molecule is polar or not?

Recall we talked about **polar covalent bonds** earlier, where **electrons are shared unequally between 2 elements**.

To figure out if a *molecule* is polar, we need to consider all of the bonds and use our knowledge of VSEPR.

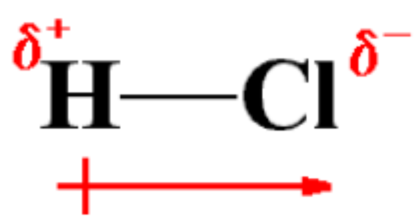
WIZE CONCEPT

If there are **no polar bonds** in the molecule-> it is **non-polar!**

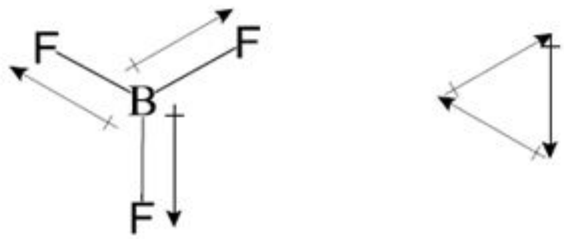
If they are **polar bonds but they are symmetrical**, their dipole moments will cancel each other out-> molecule is **non-polar!**

If there are **polar bonds that are not symmetrical**, the dipole moments don't cancel each other out and we are left with a **net dipole moment**-> molecule is **polar**!

Example: Polar Molecule



Example: Non-Polar Molecule



Non-Polar

Example #1: $AlCl_3$

Are there polar bonds? ________

Is there an overall dipole moment? ________

Therefore, $AlCl_3$ is (polar/non-polar): ______________

WIZE TIP

In order for a **MOLECULE to be considered polar**, then there must be a **<u>net</u> dipole moment** and the dipoles can't all cross out!

Example #2: Is H_2O a polar molecule?

Are there polar bonds? ______

Is there an overall dipole moment? ______

Therefore, H_2O is (polar/nonpolar): ______

Example #3: Is NH_3 polar or non-polar?

Are there polar bonds? ______

Is there an overall dipole moment? ______

Therefore, NH_3 is (polar/nonpolar) : ________

Example: Net Dipole Moment

Determine whether the following molecules have a net dipole moment (polar molecules). For the ones that do, draw the direction of the net dipole moment.

a) XeF_4

b) CCl_4

c) $CHCl_3$

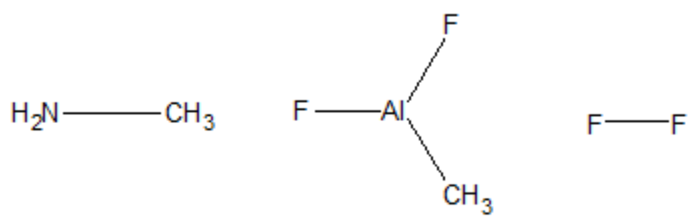
d) SCl_2

4.2.3

Practice: Polar Molecules

Which of the following are polar? (Select all that apply) and indicate the direction of polarity.

A) B) C)



- A)
- B)
- C)
- None of the above

Practice: Polar vs Non-Polar

Are the following compounds polar or non-polar?

Part 1

PF_5

- A) Polar molecule
- B) Non-polar molecule
- C) Is a mix of both polar and non-polar bonds so we cannot choose either.

Practice: Polar vs Non-Polar

Are the following compounds polar or non-polar?

Part 2

SF_4

- A) Polar molecule
- B) Non-polar molecule
- C) Is a mix of both polar and non-polar bonds so we cannot choose either

Practice: Polar vs Non-Polar

Are the following compounds polar or non-polar?

Part 3

CF_4

- A) Polar molecule
- B) Non-polar molecule
- C) Is a mix of both polar and non-polar bonds so we cannot choose either

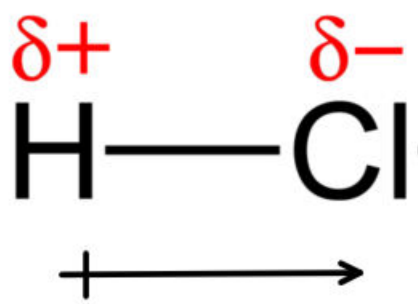
Polar Covalent Bonds

Polar Covalent Bonds:

- Electrons are shared **unequally** between **2 different non-metals**
- There is a difference in EN, $0.4 < \Delta EN < 1.7$

Since electrons are shared unequally in this bond, we say that there is a "**dipole moment**"

- The dipole moment is a vector with both magnitude and direction (more on this later!)
  - Partial negative charge (**δ-**) is assigned to the atom with the **higher EN**
  - Partial positive charge (**δ+**) is assigned to the atom with the **lower EN**
- **The greater the difference in electron density (EN), the greater the dipole moment!**



WIZE TIP

You can think of the dipole moment as a tug of war. The dipole moment (arrow) points towards the winner that is able to pull electrons more towards itself (is more electronegative!)

4.2.6

Properties of Covalent Bonds

Bonds can have various bond lengths and bond energies. There can also be a different number of bonds between different atoms. We will take a look at some of these terms and properties of bonds now.

Bond Length

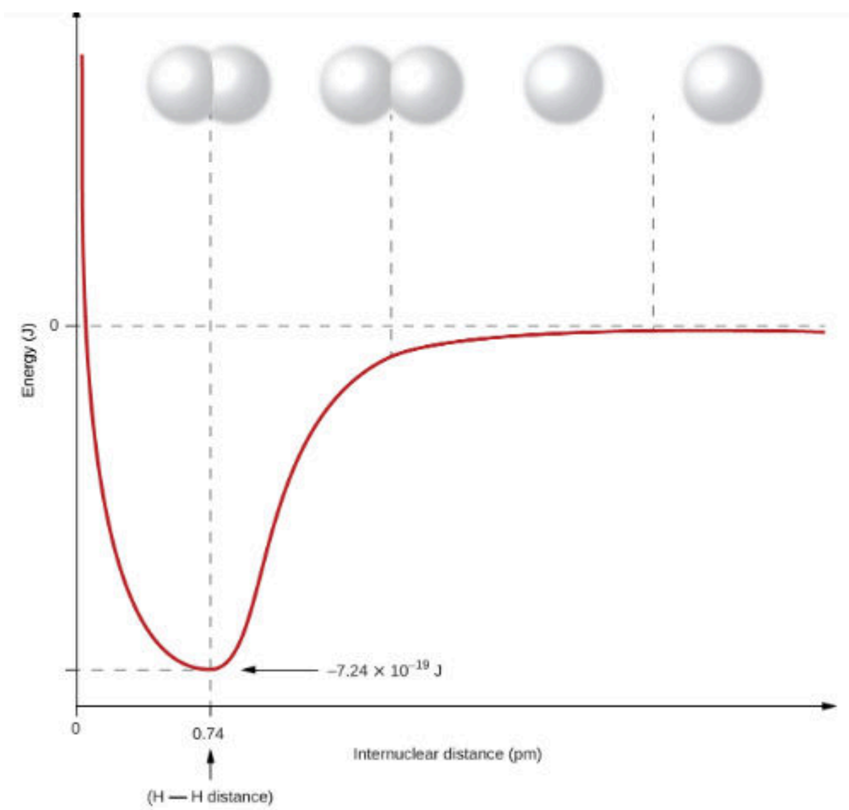


Photo by Rice University / CC BY

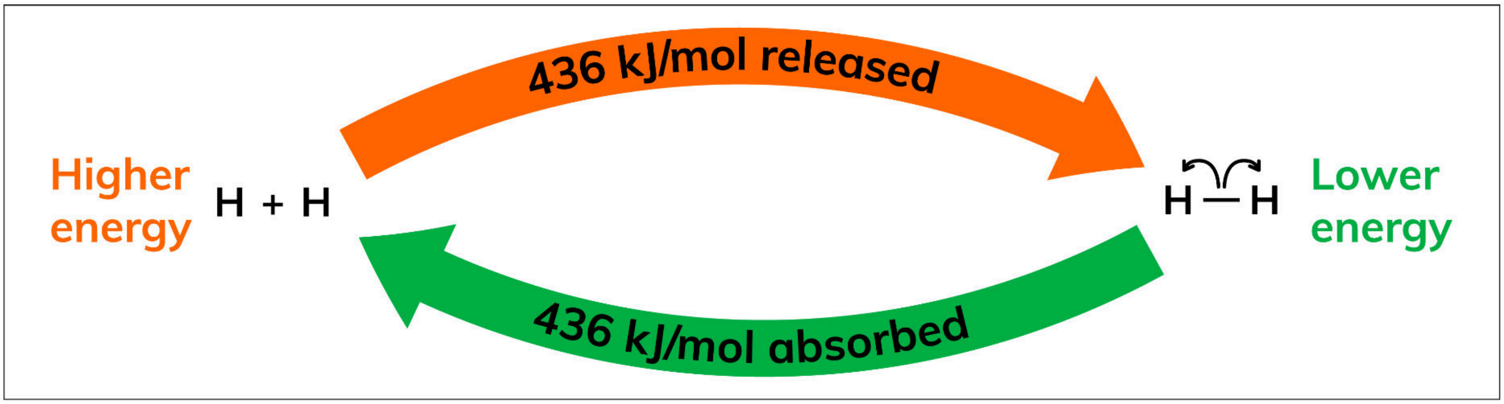
- When 2 atoms get bound together, there are repulsion forces and attractive forces
  - The electrons from one atom are attracted to the other atom's nucleus (attraction)
  - But the nuclei from both atoms can't get too close (repulsion because of + charges)
  - When the forces balance out we form a bond!

Circle the most stable bond in the diagram above (this is how the bond will exist).

Bond length: this is the **distance between two nuclei** that are bound together when they are at their **lowest possible energy state**

- **Note:** In the graph, energy rises when atoms have a shorter or longer bond length than what is optimal
- When atoms with larger atomic radii bind together, the bond length (distance between their nuclei) is (shorter/longer) ________

Bond Dissociation Energy (BDE)



Bond dissociation energy: is the **amount of energy needed to break a bond** homolytically

In the diagram, this is represented by the blue arrow. Indicate where the BDE can be found on the graph above.

WIZE CONCEPT

Breaking bonds will always **require energy!**
Forming bonds on the other hand will **release energy** since bonds are stable and lower in energy!

The higher the BDE the stronger/weaker the bond: ____________

Bond Order

Bond order: the number of bonds between adjacent atoms

Examples:

The bond order of H-F is _____

The bond order of C=O is _____

The bond order of $C{\equiv}C$ is _____

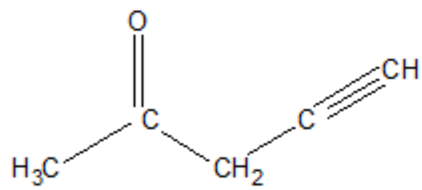
How are Bond Order, Bond Length, and Bond Energy Related?

- For bonds between the same elements, the **higher the bond order, the shorter the bond length and the stronger the bond (higher BDE)**
- Bond length is given in units angstroms (Å) where 1 Å=10^{-10}m

Average Bond Lengths and Bond Energies for Some Common Bonds		
Bond	**Bond Length (Å)**	**Bond Energy (kJ/mol)**
C–C	1.54	345
$C=C$	1.34	611
$C\equiv C$	1.20	837
C–N	1.43	290
$C=N$	1.38	615
$C\equiv N$	1.16	891
C–O	1.43	350
$C=O$	1.23	741
$C\equiv O$	1.13	1080

Example: Bond Order

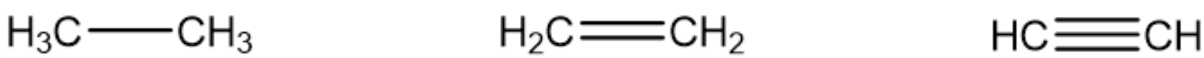
What is the bond order of each bond in this molecule?

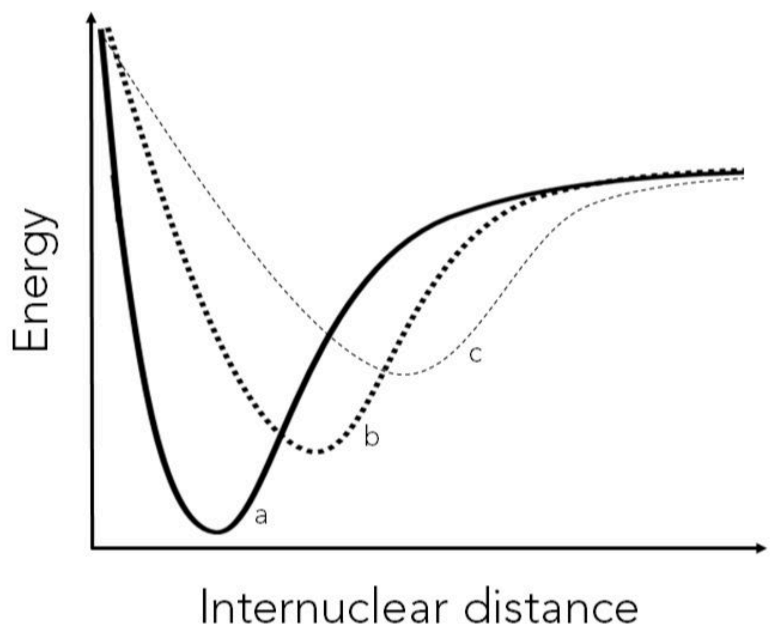


Practice: Potential Energy Diagrams

The following figure shows the potential energy diagrams for the carbon-carbon bond in ethane, ethene, and ethyne. Structures of these molecules are shown below. Identify which molecule corresponds to each potential energy curve.

ethane ethene ethyne





A. ethyne

B. ethene

C. ethane

- [ ] potential energy diagram a
- [ ] potential energy diagram b
- [ ] potential energy diagram c

4.3 How to Draw Lewis Structures

4.3.1

Drawing Lewis Structures

Drawing the "best" Lewis structure for a molecule is a great skill to have for your chemistry class! This concept will come in handy in the upcoming chapters as well. We will follow the steps below each time.

WIZE TIP

Steps for Drawing Lewis Structures:

1) Calculate the total number of **valence electrons** for the molecule.

2) Write out all atoms, with the **least electronegative atom in the middle (but H is never in the middle)**

3) Connect all atoms with **single bonds.**

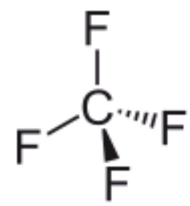
4) Put **lone pairs** on atoms, except H, until you run out of electrons. Put extra lone pairs on the central atom.

5) **Shift lone pairs to make double or triple bonds** to satisfy the **Octet Rule** and get the best **formal charges.**

Octet Rule: atoms need to have 8 electrons in the valence shell

Examples: C, N, O, F all need 8 electrons in their valence shell to have the "best" Lewis structure

Example: $CF_4 \rightarrow$ the C atom has 8 valence electrons and each F atom has 8 valence electrons in the Lewis Structure

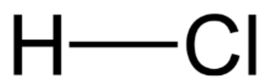


Exceptions to the Octet Rule

Some elements are **octet deficient** (require less than 8 electrons in their valence shell)

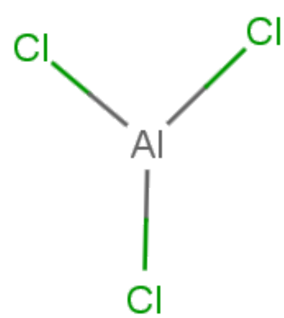
Examples:

H and **He** can only have **2 electrons**



Be can only have **4 electrons**

In group 13, **Al and B** can only have **6 electrons**

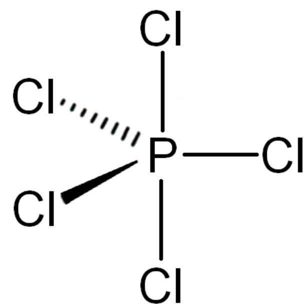


Some elements have an **expanded octet** (can have more than 8 electrons in their valence shell)

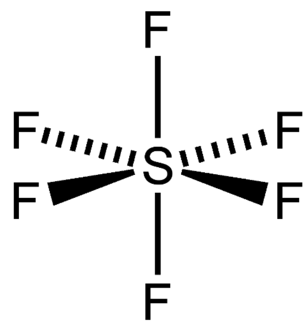
Examples:

Non-metals in period 3 and onwards can have expanded octet.

P can have **10 electrons**



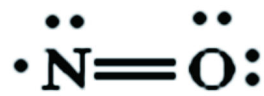
S can have **12 electrons**



Some molecules like **radicals** have an **odd number of electrons** (these are rare!)

Example: NO
First let's count the number of valence electrons (VE) in both atoms.

- N →5 VEs
- O → 6 VEs
    - So in total there are 11 VEs which is an odd number. We would be left with a molecule that looks like this:



Note: There is an **unpaired electron on the N**. This is called a **radical** molecule and is highly reactive so it is very short-lived.

Formal Charges

The last thing we need to check to ensure we have the **BEST Lewis Structure** is to count formal charges.

WIZE CONCEPT

The best formal charge for an atom is zero.
If the formal charges for a molecule can't be 0 the **best Lewis Structure for that molecule will have the lowest possible formal charges.**

If formal charge is not zero, consider assigning **negative formal charge to more electronegative elements** and positive formal charges to less electronegative elements, if possible.

$$\boxed{FC = VE - \text{bonds connected to the atom - lone pair electrons on the atom}}$$

FC *is the* ***formal charge*** *of an atom*
VE *are the* ***valence electrons*** *the atom has*

Example:
OF_2

4.3.2

Example: Lewis Structures

Draw Lewis structures of the following molecules.

a) PCl_3

b) NH_4^+

c) SeF_4

Example: Lewis Structure

Draw the Lewis Structure for SO_4^{2-}

Practice: Formal Charges and Lewis Structures

Draw the Lewis structure of SO_2Cl_2 to answer the following questions.

What is the formal charge on sulfur?

What is the formal charge on each chlorine?

What is the formal charge on each oxygen?

How many double bonds are there in the molecule?

How many single bonds are there in the molecule?

4.3.5

Practice: Drawing Best Lewis Structures

Complete the “best” Lewis diagrams for the following species and use them to answer the next three questions

$SeCl_2$

PO_2^+

AlI_3

Part 1

Which Lewis diagram has double bond(s)?

- AlI_3
- PO_2^+
- $SeCl_2$
- all of the above
- none of the above

Practice: Drawing Best Lewis Structures

Complete the “best” Lewis diagrams for the following species and use them to answer the next three questions

$SeCl_2$

PO_2^+

AlI_3

Part 2

Which Lewis diagram has an atom that exceeds the octet rule?

- AlI_3
- PO_2+
- $SeCl_2$
- all of the above
- none of the above

Practice: Drawing Best Lewis Structures

Complete the “best” Lewis diagrams for the following species and use them to answer the next three questions

$SeCl_2$

PO_2^+

AlI_3

Part 3

Which Lewis diagram has lone pair(s) on the central atom?

- AlI_3
- PO_2+
- $SeCl_2$
- all of the above
- none of the above

4.4 Resonance

4.4.1

Resonance Structures

Resonance structures: are used to describe molecules with **delocalized electrons** which cannot be described by a single Lewis structure.

Resonance structures follow the same rules as Lewis structures and the same features that make a good Lewis structure also make good resonance structures.

WIZE CONCEPT

The atoms will be connected in the exact same way for each resonance structure (no single bonds can change).

The **only thing that moves are the multiple bonds and lone pairs!**

WIZE TIP

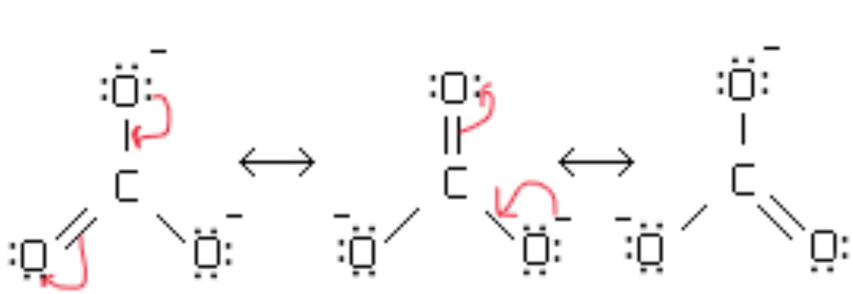
How to Draw Resonance Structures:

1. If it is not provided, **draw a Lewis structure.**

2. **Move lone pairs and double bond** around to spread out charge.

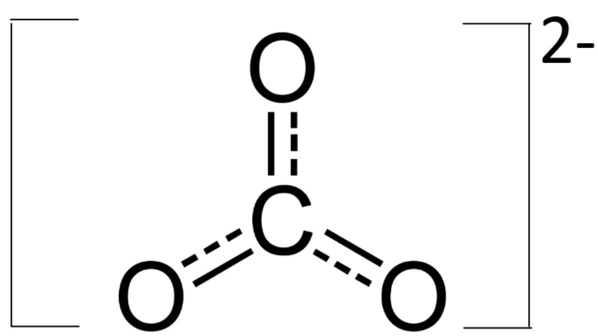
3. If you move a lone pair into a multiple bond, **make sure your new structure doesn't break the octet rule.**

Example: Resonance structures for CO_3^{2-}



Resonance structures are not discrete molecules which exist individually, but rather the molecule exists as an average of all of its resonance structures.

Resonance hybrid: The "average" of all of a molecule's resonance structures (see below)



Average C-O bond order: 1 1/3
Average Charge on oxygen: -2/3

4.4.2

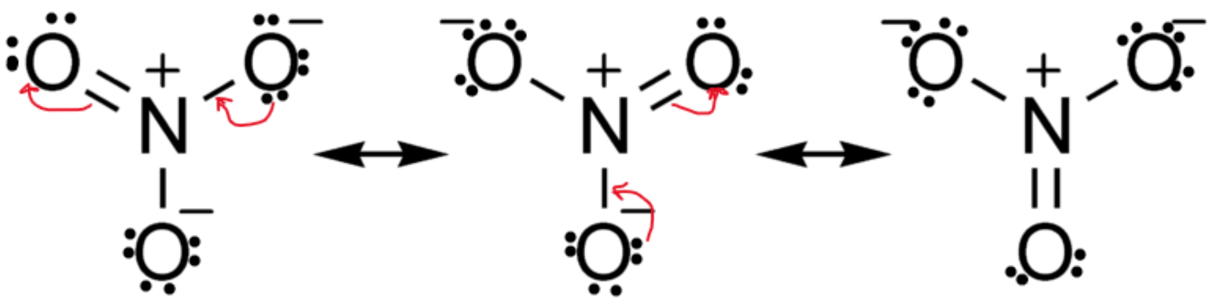
Equivalent Vs Non-Equivalent Resonance Structures

If there is more than one relatively good Lewis structure for a molecule, the molecule exhibits **resonance**.

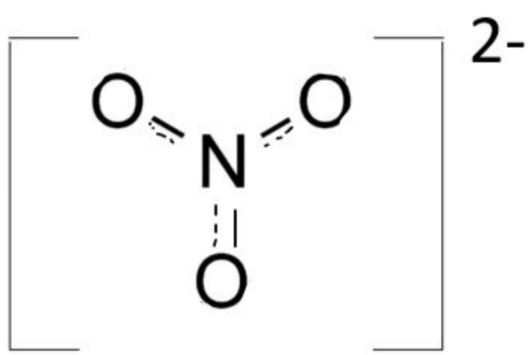
Equivalent Resonance Structures

All resonance structures are **equally stable.**

Example:



In reality, the molecular structure will be the average (hybrid) of each resonance form:

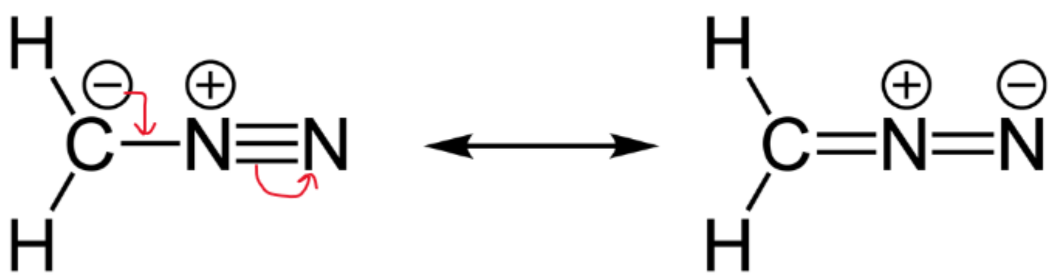


Non-Equivalent Resonance Structures

One resonance structure is better than the other.

> **WIZE TIP**
>
> The **major contributor (aka the more stable resonance structure)** is the one where the **negative charge** resides on the **most electronegative atom!**
> The major contributor will also have the **smallest charges (charges more spread out).**
>
> You could be asked to identify the most stable resonance structure on an exam.

Example:



Out of these two non-equivalent resonance structures, which is the more stable one? The one on the left or right? ________

Example: Draw the Resonance Structures

Draw all the reasonable resonance structures for SO_3F^- . Are these equivalent or non-equivalent resonance structures?

Example: Resonance Structures and Stability

Draw all reasonable resonance structures for the following compounds.
Are they equivalent or non-equivalent resonance structures?
If one resonance structure is more stable than the other(s), indicate which one is most stable.

a) N_3^-

b) PO_4^{3-}

4.4.5

MARK YOURSELF QUESTION

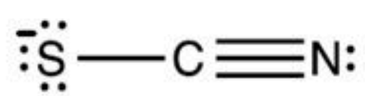
1. Grab a piece of paper and try this problem yourself.
2. When you're done, check the "I have answered this question" box below.
3. View the solution and report whether you got it right or wrong.

Practice: Drawing Arrows for Resonance Structures and Stability

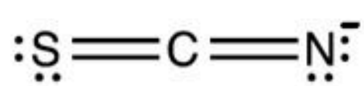
There are three resonance structures one can draw where the octet rule is satisfied for all the atoms of the polyatomic ions SCN^{-}. These three resonance structures are shown below.

a) On the Resonance Structures draw curved arrows that show how one could go from Resonance Structure 1 to 2 and Resonance Structure 2 to 3.

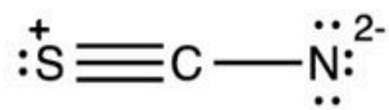
Resonance Structure 1



Resonance Structure 2



Resonance Structure 3



b) Which of the structure(s) would you identify to be the best Lewis structure(s)? Explain your reasoning.

4.4.6

Practice: Invoking Resonance Structures

For which of the following molecules do we need to invoke resonance to effectively describing the bonding?

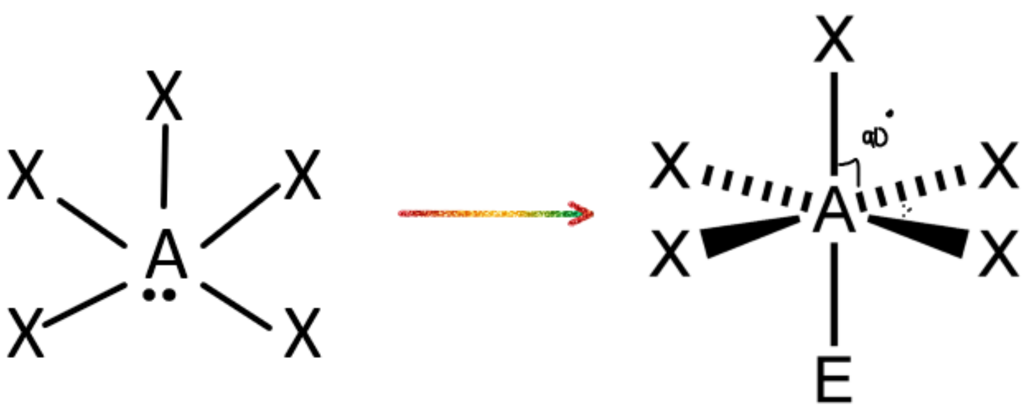
- SO_3^{2-}
- CCl_4
- N_2
- PF_6^-
- NH_4^+

4.5 VSEPR (Molecular Shapes)

4.5.1

VSEPR Theory

VSEPR aka Valence Shell Electron Pair Repulsion theory: states that repulsion of electron pairs (both bonds and lone pairs) in the valence shell will dictate the molecular geometry of a compound.



Lewis Structure

VSEPR tells us the molecular shape: Square Based Pyramid

WIZE CONCEPT

To predict a molecular shape using VSEPR we need the **BEST Lewis Structure!**

Drawing the best Lewis Structure will provide us with two key pieces of information:

- The number of **lone pairs** on the central atom
- The number of **bound atoms** to the central atom

Once we have this information we can determine the **electron geometry** and the **molecular shape** as well as the **bond angles** of the molecule in question! These are all very common exam questions :)

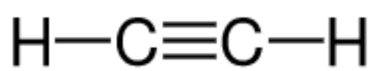
Electron Geometry (aka Orbital Geometry or Parent Shape)

Electron geometry is based on the number of **electron groups** around the central atom

$$\boxed{EGs = \text{number of lone pairs of electrons} + \text{number of bound atoms}}$$

EGs are **electron groups**

Example:
How many electron groups does the C atom on the left have?



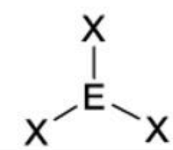
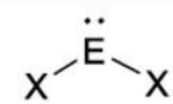
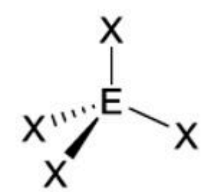
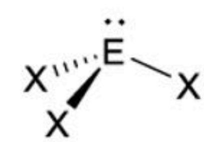
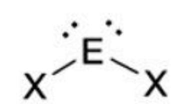
! WATCH OUT!

The **triple bond has no effect on EGs** because we are counting the number of bound atoms, so whether there is a **C bound to another C with a single bond, double bond, or triple bond, those will all just count as 1 EG!**

Molecular Shape

The shape of a molecule is determined by where the atoms are located.

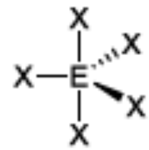
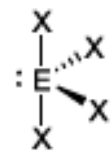
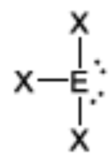
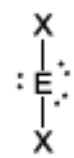
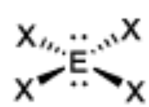
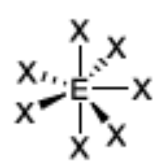
Write the number of electron groups on the left side of the table.

l.p.	b.a.	Parent Shape	Molecular Shape	Picture	Angles
0	2	Linear	Linear	X—E—X	180°
0	3	Trigonal Planar	Trigonal Planar		120°
1	2		Bent		< 120°
0	4	Tetrahedral	Tetrahedral		109.5°
1	3		Trigonal Pyramidal		107°
2	2		Bent		104°

WIZE TIP

The tables in this lesson are very commonly tested on!
Take a few minutes to memorize these tables as you will likely see many questions relating to VSEPR theory on your exams!

Write the number of electron groups on the left side of the table.

l.p.	b.a.	Parent Shape	Molecular Shape	Picture	Angles
0	5	Trigonal Bipyriamidal	Trigonal Bipyriamidal		120^{o}_{eq} 90^{o}_{ax}
1	4		See Saw		120^{o}_{eq} 90^{o}_{ax}
2	3		T-shaped		90^{o}
3	2		Linear		180^{o}
0	6	Octahedral	Octahedral		90^{o}
1	5		Square Based Pyramid		90^{o}
2	4		Square Planar		90^{o}
0	7	Pentagonal Byprimdal	Pentagonal Byprimdal		72^{o}_{eq} 90^{o}_{ax}

Note:

- Wedges mean the bond is coming out of the page and dashes mean the bond is going back into the page.
- LP=lone pairs of electrons
- BA=bound atoms
- **Lone pairs give more push** (are even more repelled by other electrons), which is why wee see the bond angles change slightly.

4.5.2

Example: Parent and Molecular Shape

Determine the parent shape and molecular shape for the following.

a) NH_3

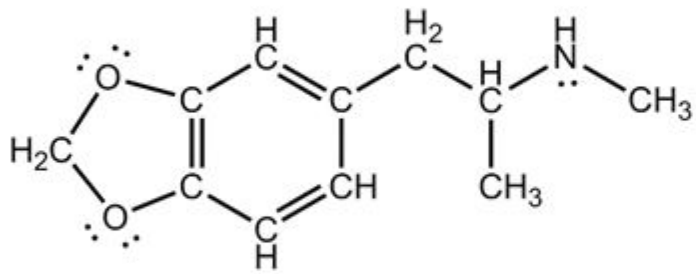
b) SCl_2

c) IF_7

d) SF_4

Example: VSEPR and Molly

MDMA (3,4-methylenedioxy-methamphetamine) or “Molly” is a psychoactive drug commonly used for recreational purposes, which has been investigated as a treatment for PTSD. It functions by triggering serotonin release and inhibiting serotonin reuptake in the human brain, causing euphoric and empathogenic effects on the user. The structure of MDMA is shown below.



a) What is the molecular shape of the nitrogen atom in MDMA?

b) Approximate the O-C-O bond angle in MDMA?

c) How many atoms with a trigonal planar electron geometry are there in MDMA?

4.5.4

Practice: VSEPR Shapes

Consider the VSEPR for the “best” Lewis diagrams for the following species and use them to answer the next three questions

1. PH_3

2. AlH_4^-

3. IO_3^-

Part 1

Which of the following has a central atom with a tetrahedral electron-pair geometry?

- PH_3 and AlH_4^-
- AlH_4^-
- IO_3^-
- AlH_4^- and IO_3^-
- All of the chemical species have a central atom with a tetrahedral electron pair geometry

Practice: VSEPR Shapes

Consider the VSEPR for the “best” Lewis diagrams for the following species and use them to answer the next three questions

1. PH_3

2. AlH_4^-

3. IO_3^-

Part 2

Which of the following has a trigonal planar molecular shape around the central atom?

- PH_3
- AlH_4^-
- IO_3^-
- None of the above
- All of the above

Practice: VSEPR Shapes

Consider the VSEPR for the "best" Lewis diagrams for the following species and use them to answer the next three questions

1. PH_3

2. AlH_4^-

3. IO_3^-

Part 3

Which of the following displays resonance?

- PH_3
- AlH_4^-
- IO_3^-
- None of the above
- All of the above

4.5.5

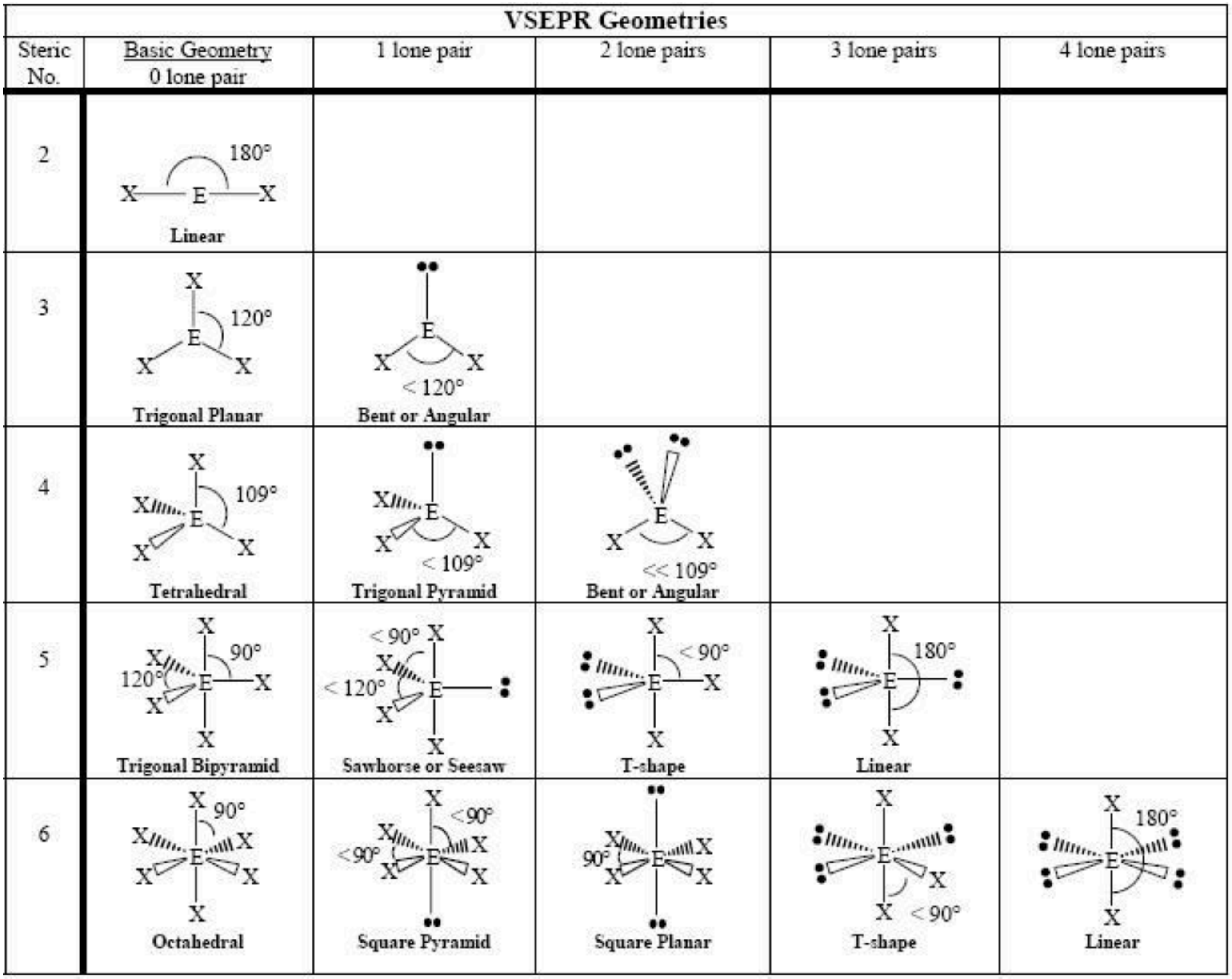
Practice: Bond Angle Identification

Which of the following compounds has a 120^{o} bond angle?

- NH_3
- H_2O
- BF_3
- BrF_5
- SF_6

4.5.6

VSEPR and Molecular Shapes - Cheatsheet



The last shape when 7 atoms are bound to the central atom: pentagonal bipyramidal

4.6 BDE Calculation

4.6.1

Bond Energies

Enthalpy (H) is the energy stored in bonds.

Bond dissociation energy (BDE) is the energy needed to break a chemical bond.

$$\Delta H_{rxn} = \left[\left(\sum nH_{bonds\ broken}\right) - \left(\sum nH_{bonds\ formed}\right)\right]$$

Or (an easier way to think about it):

$$\boxed{\Delta Hrxn = [(\sum nBDE_{reactants}) - [(\sum nBDE_{products})]}$$

$\Delta H_{rxn} =$ enthalpy change for the reaction (kJ/mol)
BDE = bond energy per mole of bonds (kJ/mol), always positive

$$\boxed{\Delta Hrxn = [(\sum nBDE_{reactants}) - [(\sum nBDE_{products})]}$$

Bond Energies (kJ/mol)							
Bond	Bond Energy		Bond	Bond Energy		Bond	Bond Energy
H–H	436		C–S	260		F–Cl	255
H–C	415		C–Cl	330		F–Br	235
H–N	390		C–Br	275		Si–Si	230
H–O	464		C–I	240		Si–P	215
H–F	569		N–N	160		Si–S	225
H–Si	395		$\mathbf{N=N}$	418		Si–Cl	359
H–P	320		$\mathbf{N\equiv N}$	946		Si–Br	290
H–S	340		N–O	200		Si–I	215
H–Cl	432		N–F	270		P–P	215
H–Br	370		N–P	210		P–S	230
H–I	295		N–Cl	200		P–Cl	330
C–C	345		N–Br	245		P–Br	270
$\mathbf{C=C}$	611		O–O	140		P–I	215
$\mathbf{C\equiv C}$	837		$\mathbf{O=O}$	498		S–S	215

4.6.2

Predict the overall change in enthalpy (i.e. change in enthalpy, change in heat, ΔHrxn in kJ/mol) for the reaction:

N_2 (g) + 3 H_2 (g) → 2 NH_3 (g).

BDE:
NN = 945 kJ/mol
H-H = 436 kJ/mol
N-H = 391 kJ/mol

- -93
- 87
- 1077
- 1209
- -869

4.6.3

Properties of Covalent Bonds

Bonds can have various bond lengths and bond energies. There can also be a different number of bonds between different atoms. We will take a look at some of these terms and properties of bonds now.

Bond Length

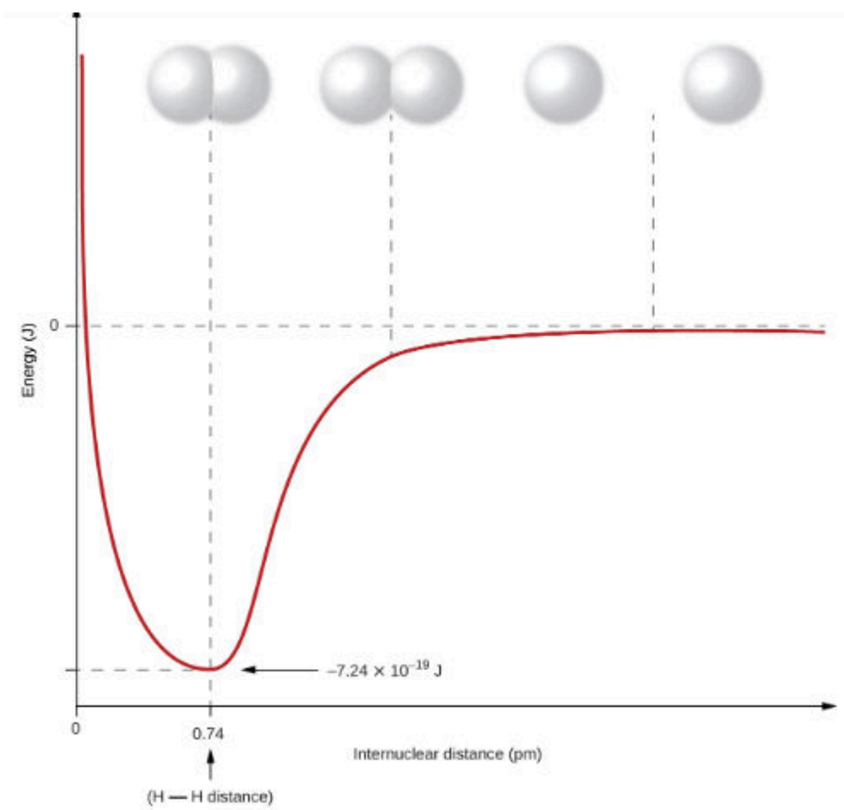


Photo by Rice University / CC BY

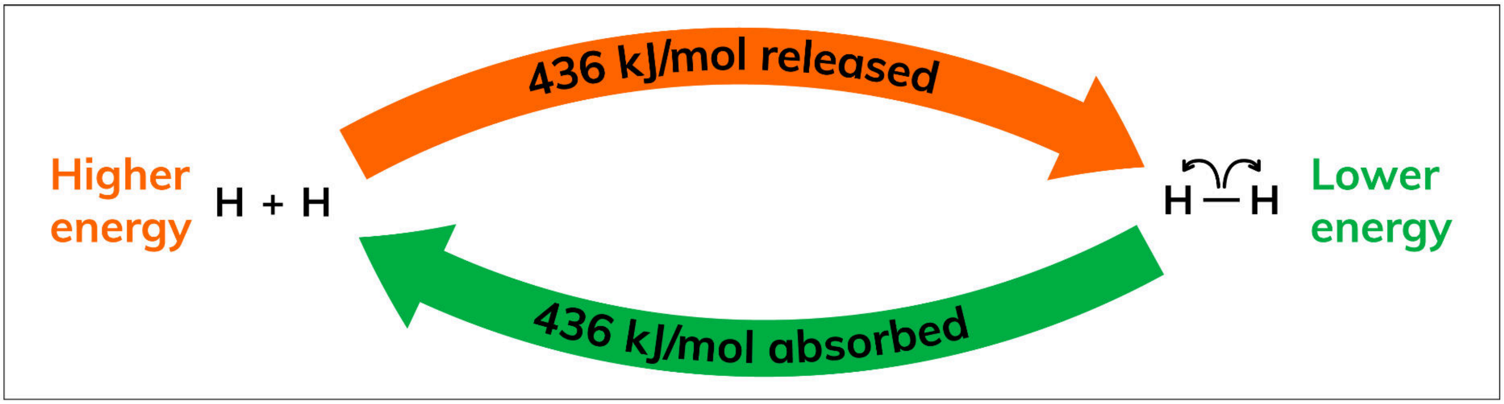
- When 2 atoms get bound together, there are repulsion forces and attractive forces
  - The electrons from one atom are attracted to the other atom's nucleus (attraction)
  - But the nuclei from both atoms can't get too close (repulsion because of + charges)
  - When the forces balance out we form a bond!

Circle the most stable bond in the diagram above (this is how the bond will exist).

Bond length: this is the **distance between two nuclei** that are bound together when they are at their **lowest possible energy state**

- **Note:** In the graph, energy rises when atoms have a shorter or longer bond length than what is optimal
- When atoms with larger atomic radii bind together, the bond length (distance between their nuclei) is (shorter/longer) ________

Bond Dissociation Energy (BDE)



Bond dissociation energy: is the **amount of energy needed to break a bond** homolytically

In the diagram, this is represented by the blue arrow. Indicate where the BDE can be found on the graph above.

> **WIZE CONCEPT**
> **Breaking bonds** will always **require energy!**
> **Forming bonds** on the other hand will **release energy** since bonds are stable and lower in energy!

The higher the BDE the stronger/weaker the bond: ____________

Bond Order

Bond order: the number of bonds between adjacent atoms

Examples:

The bond order of H-F is ____

The bond order of C=O is ____

The bond order of $C\equiv C$ is ____

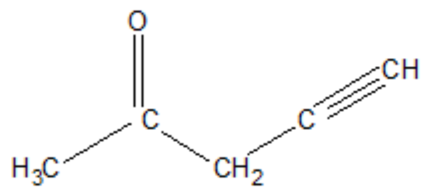
How are Bond Order, Bond Length, and Bond Energy Related?

- For bonds between the same elements, the **higher the bond order, the shorter the bond length and the stronger the bond (higher BDE)**
- Bond length is given in units angstroms (Å) where 1 Å=10^{-10}m

Average Bond Lengths and Bond Energies for Some Common Bonds		
Bond	**Bond Length (Å)**	**Bond Energy (kJ/mol)**
C–C	1.54	345
$C=C$	1.34	611
$C\equiv C$	1.20	837
C–N	1.43	290
$C=N$	1.38	615
$C\equiv N$	1.16	891
C–O	1.43	350
$C=O$	1.23	741
$C\equiv O$	1.13	1080

Example: Bond Order

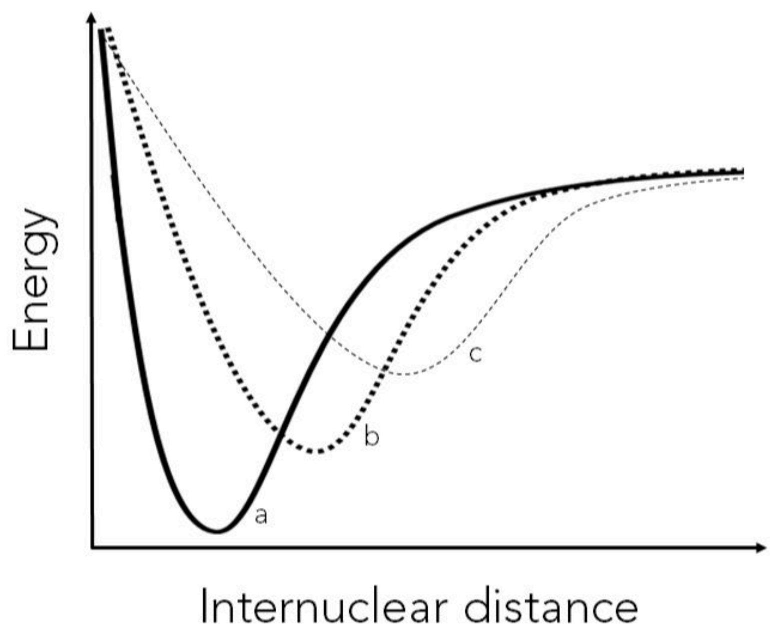
What is the bond order of each bond in this molecule?



Practice: Potential Energy Diagrams

The following figure shows the potential energy diagrams for the carbon-carbon bond in ethane, ethene, and ethyne. Structures of these molecules are shown below. Identify which molecule corresponds to each potential energy curve.

ethane	ethene	ethyne
$H_3C{-}CH_3$	$H_2C{=}CH_2$	$HC{\equiv}CH$



A. ethane

B. ethene

C. ethyne

☐ potential energy diagram a

☐ potential energy diagram b

☐ potential energy diagram c