



AP Exam Prep AP Chemistry Exam Prep Course

Fall 2024, Chapter 2 Notes

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2. Molecular and Ionic Compound Structure & Properties

2.1 Types of Bonds

2.1.1

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

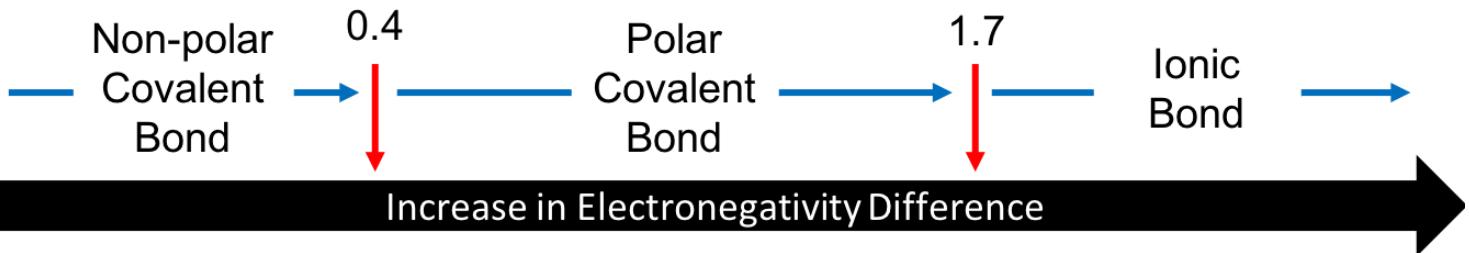
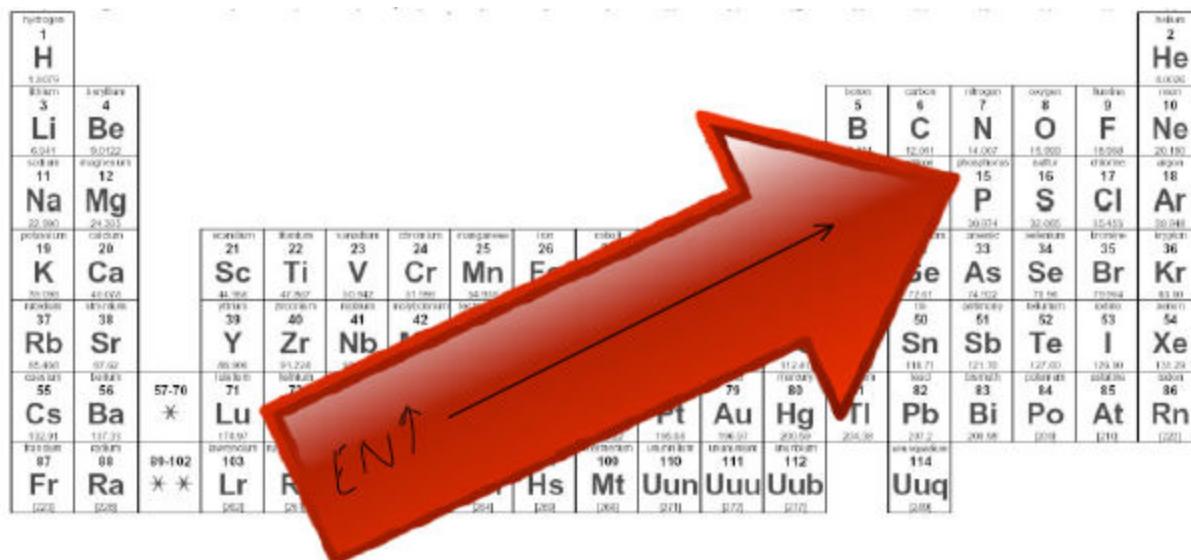
Electronegativity: is the tendency of an atom to pull bonding electrons towards itself

- 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.**



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** ($\Delta\text{EN} > 1.7$) in these bonds
- The **metal gives electrons to the non-metal** (no sharing of electrons)

Example:

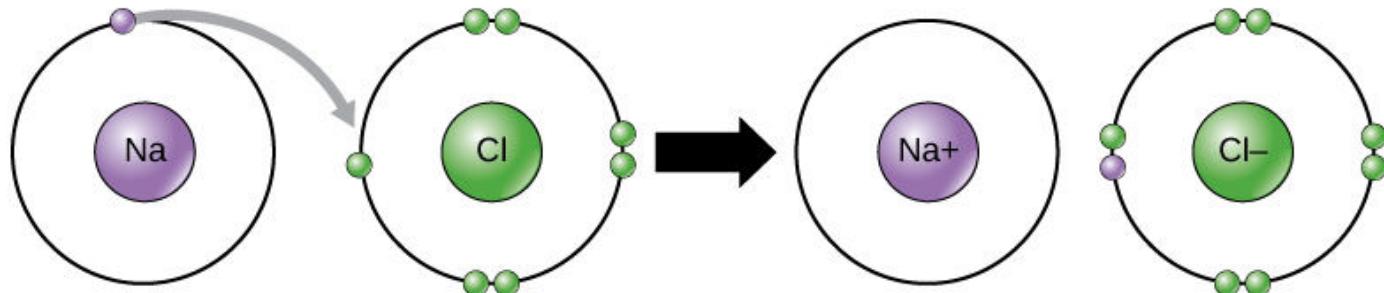


Photo by CNS Openstax/ CC BY

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, $0 < \Delta\text{EN} < 0.4$

Examples: H₂, O₂, N₂, Cl₂, *S₈, *P₄

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!

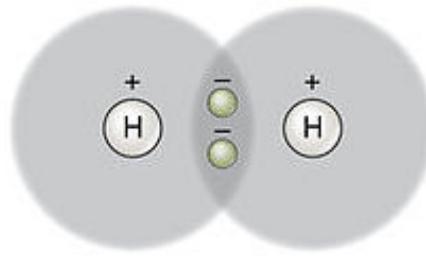


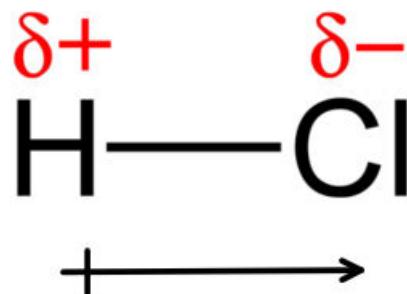
Photo by OpenStax College / CC BY

Polar Covalent Bonds:

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

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!**



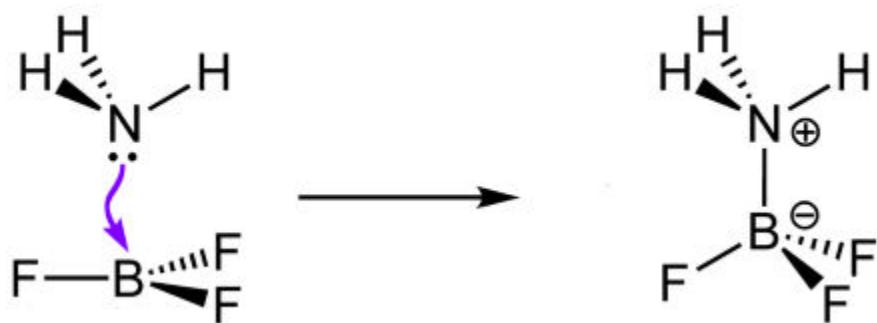
i WIZE TIP

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: NH₃ reacting with BF₃



- 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

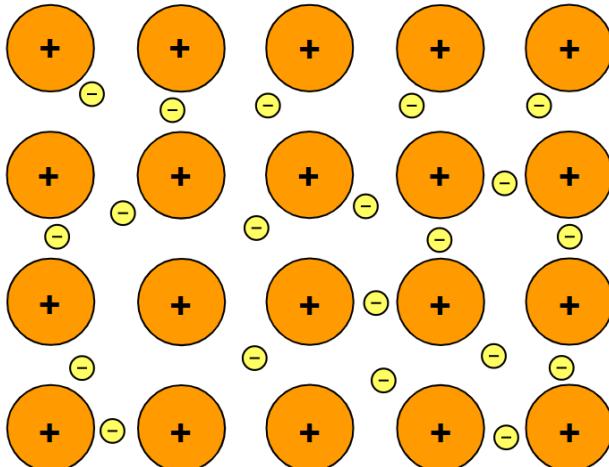


Photo by Muskid / CC BY

- 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.

2.1.3

Example: Ionic vs Covalent Bonding

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



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

2.1.5

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

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.** non-polar covalent bond(s)
- C.** polar covalent bond(s)

H_2

CCl_4

MgF_2

2.2

Properties of Covalent Bonds

2.2.1

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

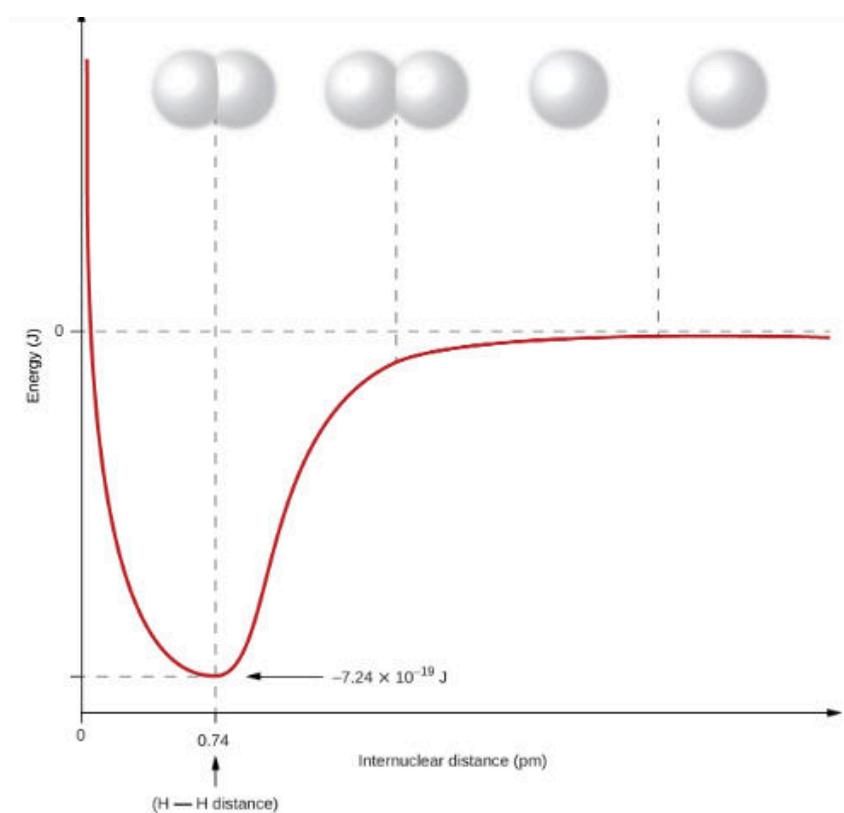


Photo by Rice University / CC BY

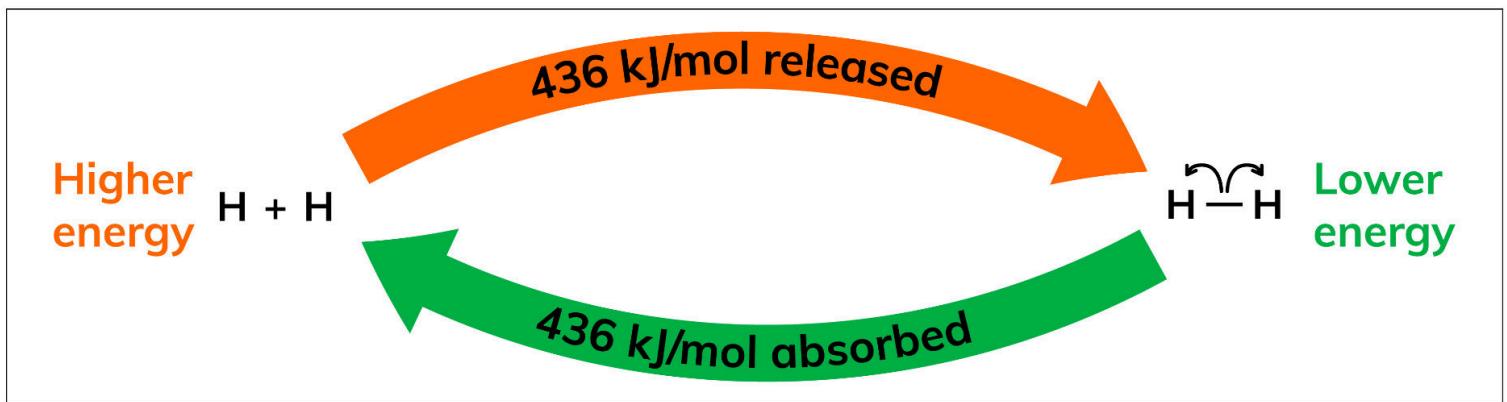
- When 2 atoms get bound together, there are repulsion forces and attractive forces
 - The electrons from one atom are attracted to the other atom's nucleus (attraction)
 - But the nuclei from both atoms can't get too close (repulsion because of + charges)
 - When the forces balance out we form a bond!

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 $\text{C}\equiv\text{C}$ is _____

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

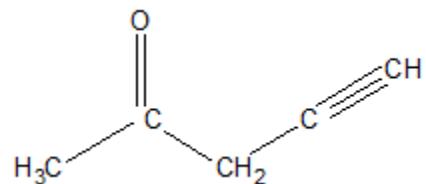
- For bonds between the same elements, the **higher the bond order, the shorter the bond length and the stronger the bond (higher BDE)**
- Bond length is given in units angstroms (\AA) where $1 \text{\AA} = 10^{-10} \text{m}$

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

2.2.2

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.

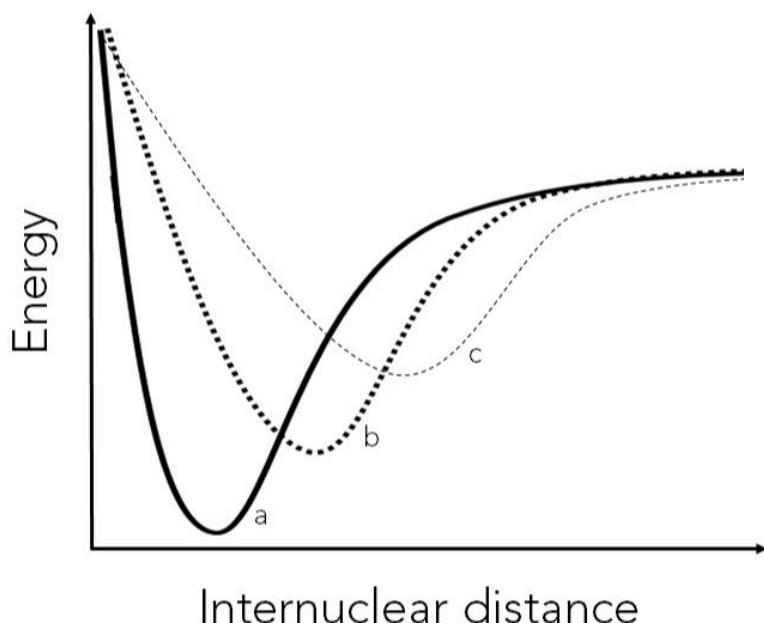
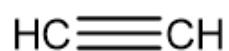
ethane



ethene



ethyne



A. ethyne

B. ethene

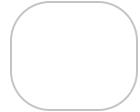
C. ethane



potential energy diagram a



potential energy diagram b



potential energy diagram c

2.3

Lattice Energy of Ionic Bonds

2.3.1

Lattice Energy

Lattice energy: is the **energy required to break ionic bonds into cation anion pairs**, or the amount of energy released by forming the ionic compound from the constituent ions.



The lattice energy for an ionic compound depends on the strength of the electrostatic interactions between the cation and anion which can be calculated using the equation below.

$$E_{lattice} = k \frac{Q_1 Q_2}{d}$$

$E_{lattice}$ is the **lattice energy**

k is a constant $8.99 \times 10^9 \text{ J m/C}^2$

Q_1 is the **charge of ion 1**

Q_2 is the **charge of ion 2**

d is the **bond length**

i WIZE TIP

On an exam, it is very unlikely that you would see a question that asks you to calculate the lattice energy.

A more typical exam question will ask you to compare the lattice energies between two different ionic compounds and **determine which of the ionic compounds has the higher lattice energy**.

If an ionic bond has a higher lattice energy, it means that ionic bond is (stronger/weaker) _____

$$E_{lattice} = k \frac{Q_1 Q_2}{d}$$

According to the equation for lattice energy, answer the following questions.

1. If the **ions** that are forming the ionic bond have **greater charges**, will the lattice energy be higher or lower? _____
2. If the atomic radii of the atoms forming the ionic bond is larger, the **bond length will be larger** and the lattice energy will be larger or smaller? _____

 **WIZE TIP**

Charge is more important than size when ranking compounds based on their lattice energy.

2.3.2

Example: Lattice Energy

Which of the following pairs of ionic compounds will have stronger ionic bonding (*i.e. higher lattice energy*)

Group →	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
↓ Period																		
1	1 H																2 He	
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Ms	116 Lv	117 Ts	118 Og
Lanthanides		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu		
Actinides		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr		

a) LiF vs BeO

b) LiF vs CsF

c) LiF vs MgS

Example: Ranking Lattice Energy

Rank the following compounds in order of increasing lattice energy, RbCl, CaI₂, BaSe.

Practice: Ionic Bond Strength

Consider two compounds: CaS and NaCl. Which ionic compound would have a larger Lattice Energy released upon forming their respective ionic compounds. Why?

CaS, because the two ions are larger than the ions in LiCl.

CaS, because the two ions have double the charge compared to the ions in LiCl.

CaS, because the two ions are smaller than the ions in LiCl.

LiCl, because the two ions are larger than the ions in CaS.

LiCl, because the two ions have smaller charges than the two ions in CaS.

LiCl, because the two ions are smaller than the ions in CaS.

2.3.5

Practice: Highest Lattice Energy

Choose the option below with the highest lattice energy.

LiCl

CO₂

MgO

CaS

MgI₂

2.4

How to Draw Lewis Structures

2.4.1

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

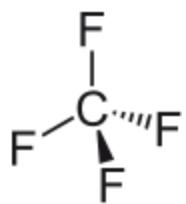
Steps for Drawing Lewis Structures:

- 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: $\text{CF}_4 \rightarrow$ 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:

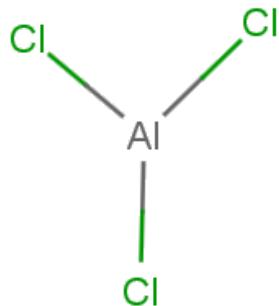
H and He can only have **2 electrons**



Be can only have **4 electrons**



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

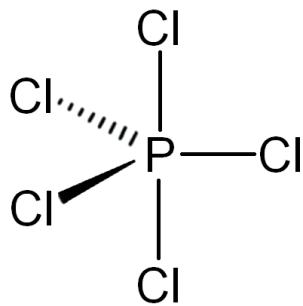


Some elements have an **expanded octet** (can have more than 8 electrons in their valence shell)

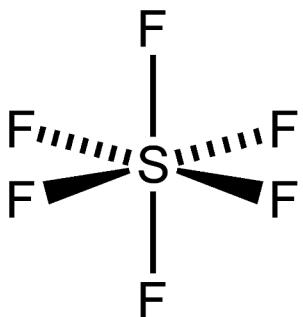
Examples:

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.

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

FC is the **formal charge** of an atom

VE are the **valence electrons** the atom has

Example:



2.4.2

Example: Lewis Structures

Draw Lewis structures of the following molecules.

a) PCl_3

b) NH_4^+

c) SeF_4

2.4.3

Example: Lewis Structure

Draw the Lewis Structure for SO_4^{2-}

2.4.4

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?

Practice: Drawing Best Lewis Structures

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



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



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



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

2.5 Resonance Structures

2.5.1

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).

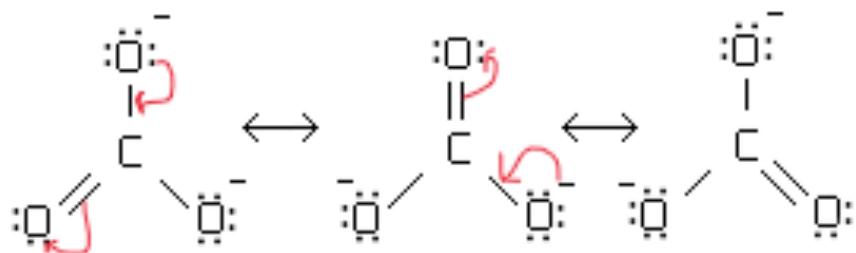
The **only thing that moves are the multiple bonds and lone pairs!**

WIZE TIP

How to Draw Resonance Structures:

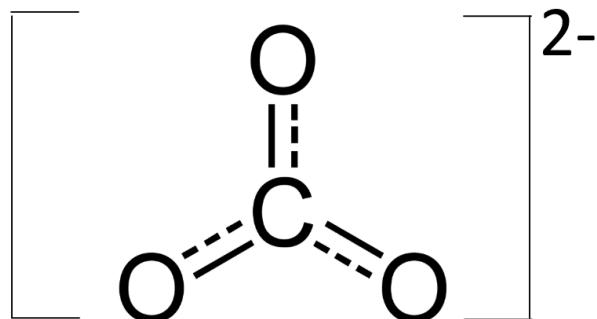
1. If it is not provided, **draw a Lewis structure**.
2. **Move lone pairs and double bond** around to spread out charge.
3. If you move a lone pair into a multiple bond, **make sure your new structure doesn't break the octet rule**.

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: $1 \frac{1}{3}$
Average Charge on oxygen: $-\frac{2}{3}$

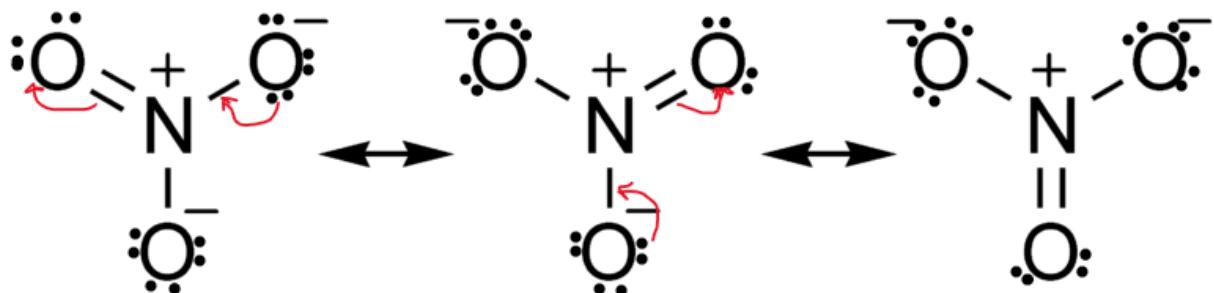
Equivalent Vs Non-Equivalent Resonance Structures

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

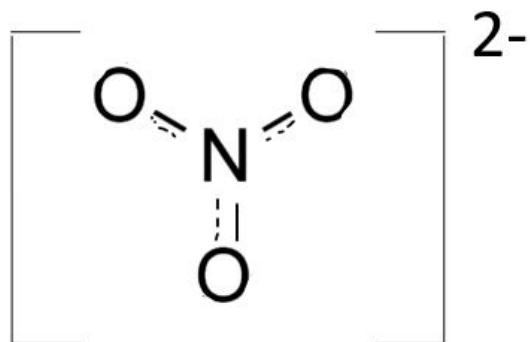
Equivalent Resonance Structures

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.

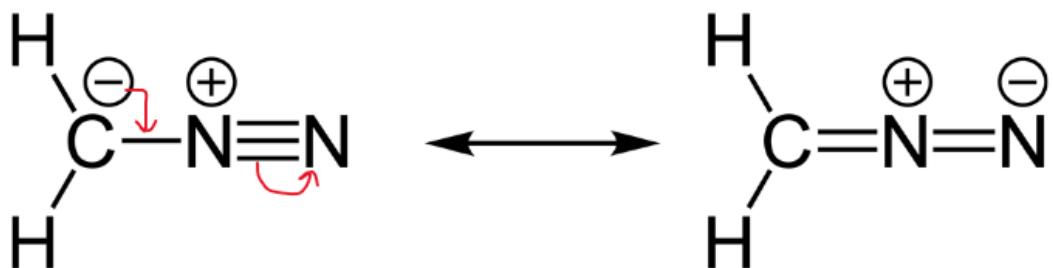
i WIZE TIP

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? _____

2.5.3

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-}

Practice: Invoking Resonance Structures

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



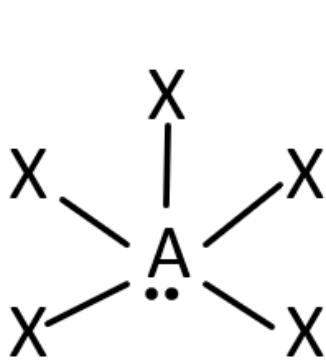
2.6

VSEPR (Molecular Shapes)

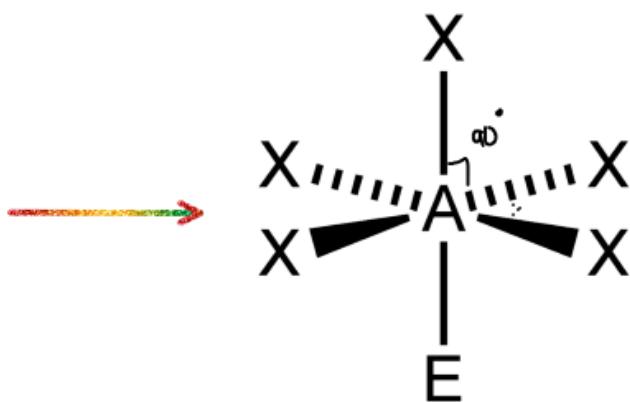
2.6.1

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

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

EGs are **electron groups**

Example:

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



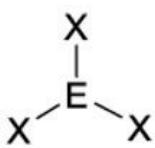
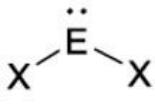
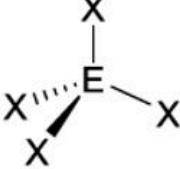
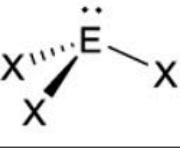
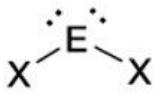
! WATCH OUT!

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.

I.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.

I.p.	b.a.	Parent Shape	Molecular Shape	Picture	Angles
0	5	Trigonal Bipyramidal	Trigonal Bipyramidal		120°_{eq} 90°_{ax}
1	4		See Saw		120°_{eq} 90°_{ax}
2	3		T-shaped		90°
3	2	Octahedral	Linear		180°
0	6		Octahedral		90°
1	5		Square Based Pyramid		90°
2	4		Square Planar		90°
0	7	Pentagonal Bypyrimdal	Pentagonal Bypyrimdal		72°_{eq} 90°_{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 we see the bond angles change slightly.

2.6.2

Example: Parent and Molecular Shape

Determine the parent shape and molecular shape for the following.

a) NH_3

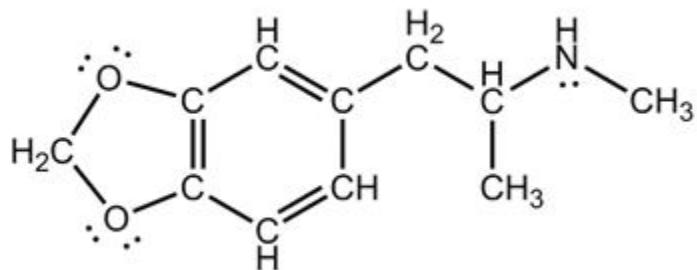
b) SCI_2

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?

Practice: VSEPR Shapes

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



Part 1

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

PH₃ and AlH₄⁻

AlH₄⁻

IO₃⁻

AlH₄⁻ and IO₃⁻

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



Part 2

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



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



Part 3

Which of the following displays resonance?



None of the above

All of the above

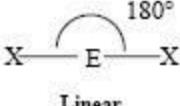
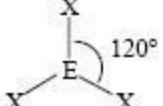
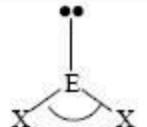
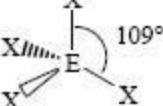
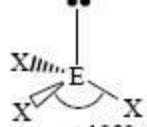
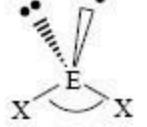
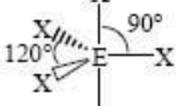
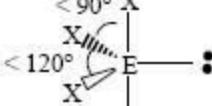
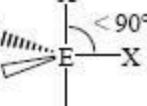
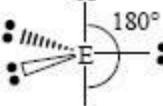
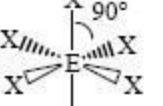
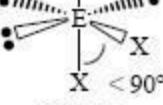
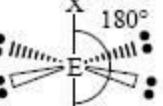
2.6.5

Practice: Bond Angle Identification

Which of the following compounds has a 120° bond angle?



VSEPR and Molecular Shapes - Cheatsheet

VSEPR Geometries					
Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 Linear				
3	 Trigonal Planar	 Bent or Angular			
4	 Tetrahedral	 Trigonal Pyramid	 Bent or Angular		
5	 Trigonal Bipyramidal	 Sawhorse or Seesaw	 T-shape	 Linear	
6	 Octahedral	 Square Pyramid	 Square Planar	 T-shape	 Linear

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

2.7 Molecular Polarity

2.7.1

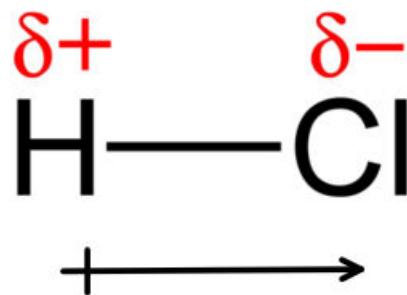
Polar Covalent Bonds

Polar Covalent Bonds:

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

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!**



i 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!).

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.

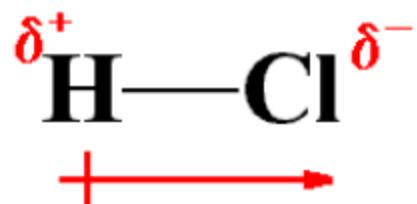
 **WIZE CONCEPT**

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

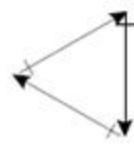
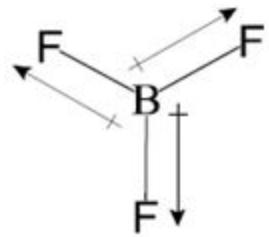
If they are **polar bonds but they are symmetrical**, their dipole moments will cancel each other out-> molecule is **non-polar!**

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: AlCl₃

Are there polar bonds? _____

Is there an overall dipole moment? _____

Therefore, AlCl₃ is (polar/non-polar): _____

WIZE TIP

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

Example #2: Is H₂O a polar molecule?

Are there polar bonds? _____

Is there an overall dipole moment? _____

Therefore, H₂O is (polar/nonpolar): _____

Example #3: Is NH₃ polar or non-polar?

Are there polar bonds? _____

Is there an overall dipole moment? _____

Therefore, NH₃ 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

2.7.4

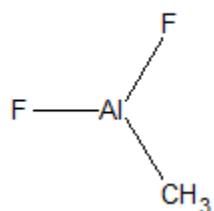
Practice: Polar Molecules

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



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



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

2.8 Hybridization

2.8.1

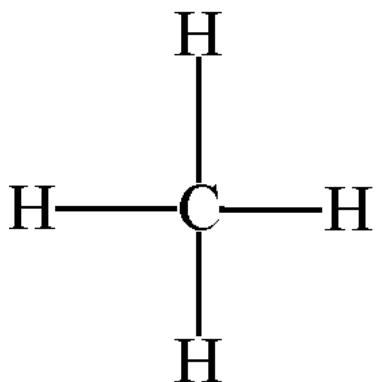
Determining Hybridization

To determine the hybridization of an atom in a molecule, we need to first determine the number of **electron groups** that molecule has.

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

EGs are **electron groups**

Example: CH₄



- C has _____ EGs
- We saw that C in CH₄ was sp³ hybridized.
- If we add up the exponents in sp³ (s¹p³ → 1+3) = 4 (which is the number of electron groups!)

i WIZE TIP

How to Determine the Hybridization of an Atom:

Step 1: Draw the Lewis Structure

Step 2: Count the number of electron groups (electron groups are bound atoms + lone pairs)

Step 3: Determine hybridization of the central atom → **exponents of hybrid orbitals add up to the number of electron groups** around the central atom

Step 4: Once you know the hybridization, you can predict the **geometry** (as shown below)

To determine a molecule's hybridization we can use the following table:

Regions of Electron Density	Arrangement	Hybridization
2	linear	sp
3	trigonal planar	sp^2
4	tetrahedral	sp^3
5	trigonal bipyramidal	sp^3d
6	octahedral	sp^3d^2

The shapes listed above are "**parent shapes**" (aka electron geometries) that we get from knowing the number of electron groups.

What is the Hybridization of C in CO₂?

1) Draw the BEST Lewis Structure

2) Find the Number of EGs that C has

EGs= # of lone pairs of electrons + # of bound atoms

$$= \underline{\hspace{2cm}}$$

$$= \underline{\hspace{2cm}}$$

3) Determine the Hybdridization Based on the Number of EGs

Since there were EGs, that means the hybridization must be .

What is the Hybridization for Se in SeBr_2 ?

1) Draw the BEST Lewis Structure

2) Find the Number of EGs that Se has

EGs= # of lone pairs of electrons + # of bound atoms

$$\begin{aligned} &= \underline{\hspace{2cm}} \\ &= \underline{\hspace{2cm}} \end{aligned}$$

3) Determine the Hybridization Based on the Number of EGs

Since there were EGs, that means the hybridization must be .

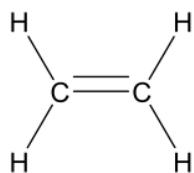
Example: Hybridization

Identify the hybridization of each non-hydrogen atom in the following compounds:

a) POCl_3

Identify the hybridization of each non-hydrogen atom in the following compounds:

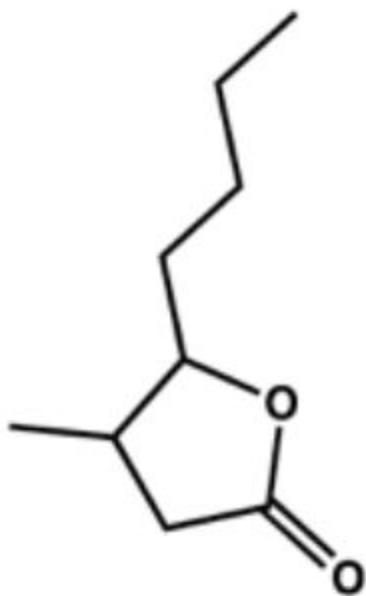
b)



Example: Hybridization of Atoms in a Line Diagram

Whiskey lactone is an important ingredient in the aroma of whiskey. Its structure is shown below.

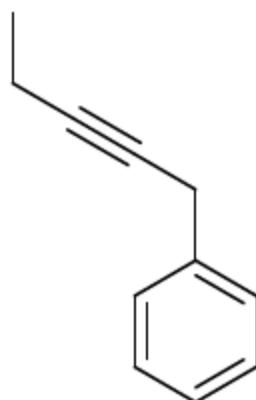
On the structure, there are _____ sp^3 hybridized carbons, _____ sp^2 hybridized carbons and _____ sp hybridized carbons.



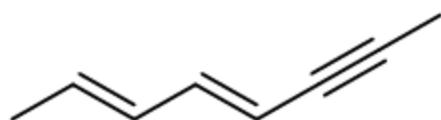
2.8.4

Label each carbon atom with its hybridization

a)



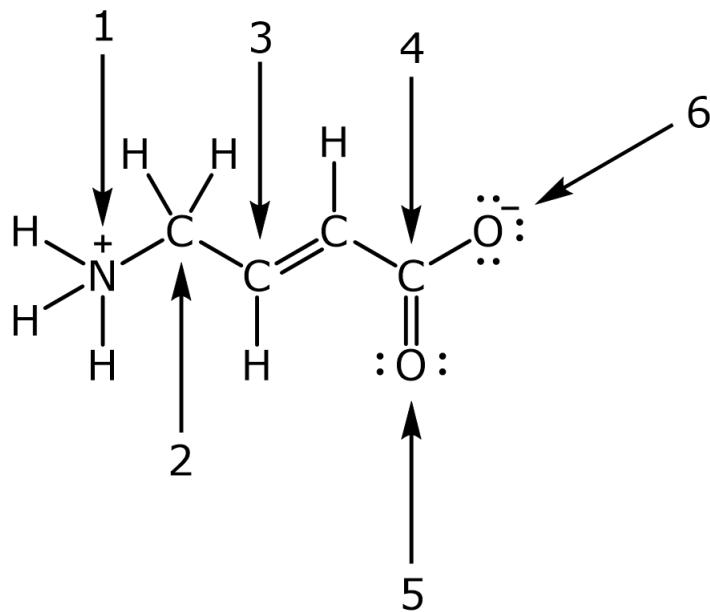
b)



2.8.5

Practice: Hybridization in Organic Compounds

Answer the following questions for the compound shown below.



What is the hybridization for atom 1?

What is the hybridization for atom 2?

What is the hybridization for atom 3?

What is the hybridization for atom 4?

What is the hybridization for atom 5?

What is the hybridization for atom 6?

What is the electron geometry for atom 2?

2.9

Practice with Sigma and Pi Bonds

2.9.1

Sigma (σ) and Pi (π) Bonds

There are two ways orbitals can overlap:

- Sigma (σ) type overlap, and pi (π) type overlap.
 - **Sigma overlap** is when 2 electrons in a bond are localized between 2 nuclei (along the internuclear axis)
 - Formed from the end-to-end overlap of hybridized orbitals (or orbital s orbital for H)
 - **Pi overlap** is when 2 electrons are localized in the region above and below the plane formed by 2 bonded nuclei (occurs above and below the internuclear axis)
 - Formed from side to side alignment of unhybridized p orbitals in adjacent atoms to form a bond

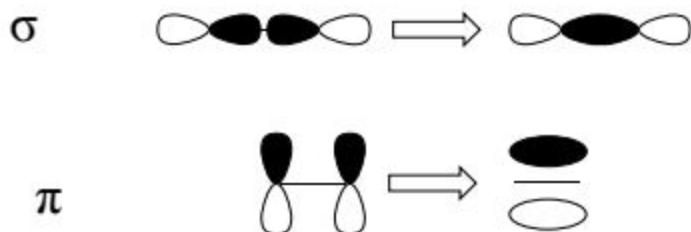


Figure 14.2 Sigma and Pi type Overlap.

If asked how many sigma and pi bonds there are in a molecule, it's very simple to count!

i WIZE TIP

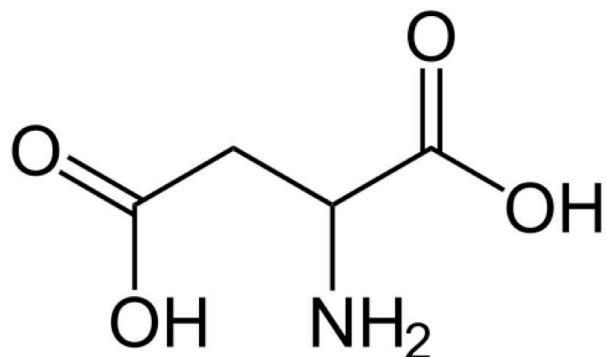
For every single bond you see = 1 sigma bond

For every double bond you see= 1 sigma bond AND 1 pi bond

For every triple bond you see= 1 sigma bond AND 2 pi bonds

2.9.2

Ex. In this molecule of aspartic acid, how many sigma and pi bonds are there?



Aspartic Acid

8 sigma bonds; 0 pi bonds

8 sigma bonds; 2 pi bonds

12 sigma bonds; 2 pi bonds

15 sigma bonds; 2 pi bonds

2.9.3

Propyne, H₃CCCH, has how many sigma (σ) and pi (π) bonds, respectively?

5,3



5,1



6,2



3,2



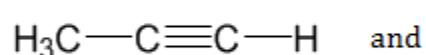
8,0



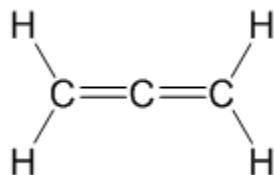
2.10 Orbital Overlap Diagrams

2.10.1

Use Valence Bond Theory to draw an orbital overlap diagram for:



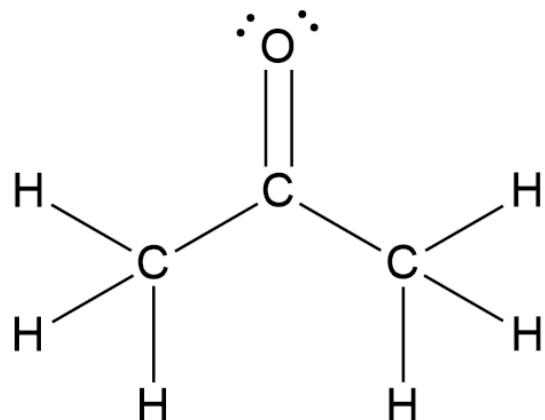
and



Make sure to label all orbitals and list the bonds between each atom.

2.10.2

Acetone C_3H_6O is shown below



- a) What is the hybridization of each non-hydrogen atom?
- b) What type of bond is formed between the carbon atoms of acetone? Use valence bond theory nomenclature.

c) Draw a valence bond diagram and an orbital overlap diagram for the C=O bond in acetone.