Chem With Com

Molecular Structure and Polarity

- Chapter 4.6 (Molecular Structure and Polarity)
- Chapter 4.2 (Covalent Bonding)

Adapted From: Paul Flowers, Edward J. Neth, William R. Robinson, PhD, Klaus Theopold, Richard Langley; Chemistry: Atoms First 2e; OpenStax; Feb 14, 2019; Houston Texas; https://openstax.org/books/chemistry-atoms-first-2e/pages/1-introduction

Molecular Structure

- Chapter 4.6 (Molecular Structure and Polarity)

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Shapes of Molecules and Compounds

Compounds
(two or more different atoms)

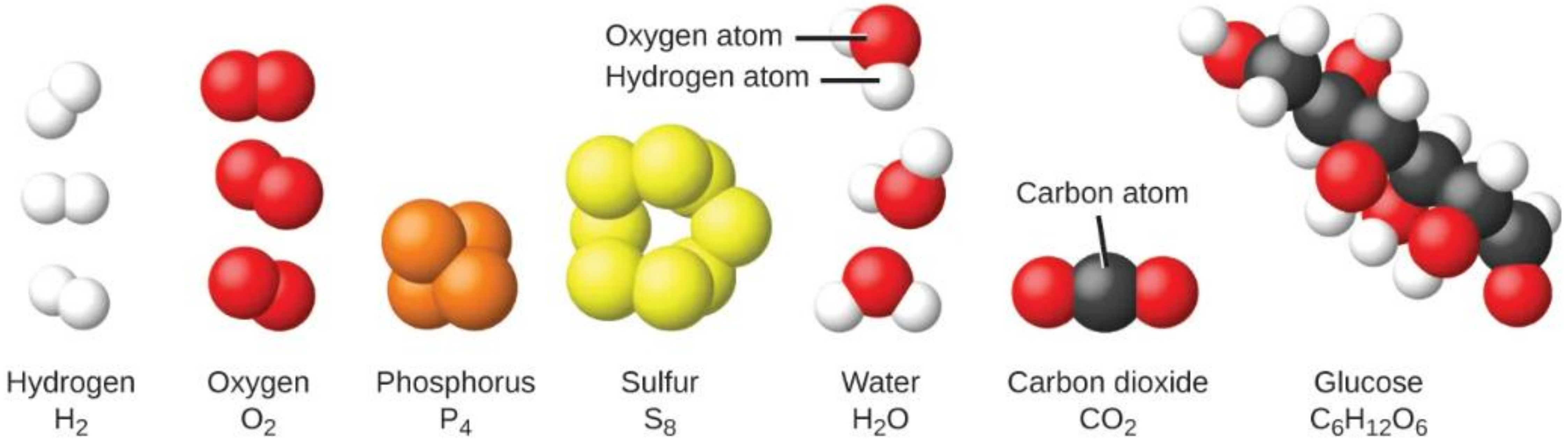


Figure 1.14 The elements hydrogen, oxygen, phosphorus, and sulfur form molecules consisting of two or more atoms of the same element. The compounds water, carbon dioxide, and glucose consist of combinations of atoms of different elements.

molecules
(more than one atom)

Very Science Version

VSEPR Theory

Valence shell electron-pair repulsion theory (VSEPR theory) enables us to predict the molecular structure, including approximate bond angles around a central atom, of a molecule from an examination of the number of bonds and lone electron pairs in its Lewis structure. The VSEPR model assumes that electron pairs in the valence shell of a central atom will adopt an arrangement that minimizes repulsions between these electron pairs by maximizing the distance between them. The electrons in the valence shell of a central atom form either bonding pairs of electrons, located primarily between bonded atoms, or lone pairs. The electrostatic repulsion of these electrons is reduced when the various regions of high electron density assume positions as far from each other as possible.

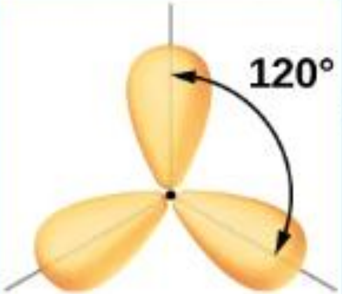
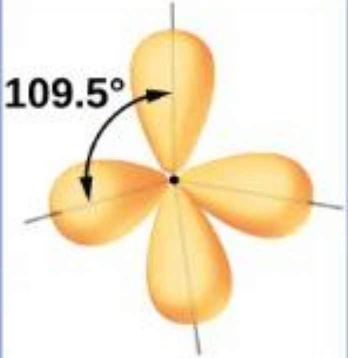
Com's Version

- When atoms start covalently bonding (sharing of valence electrons) to form molecules, the atoms that are bonding to the "central" atom stay as far apart as possible.
  - imagine getting on a bus and there is 1 stranger sitting, would you sit next to them or give them space?
- This is because the outsides of atoms have exterior unbonded electrons and they are negatively charged. And same charges repel each other just like magnets with the same magnetic poles.
- When molecules start forming, they take on 2 and 3 dimensional shapes around the "central" atom and this is called the electron geometry

3D Simulation

- https://phet.colorado.edu/en/simulations/molecule-shapes

Electron-Pair Geometry (Electron Geometry)

Connections to center atom	**1 or 2**	**3**	**4**
Number of regions	Two regions of high electron density (bonds and/or unshared pairs)	Three regions of high electron density (bonds and/or unshared pairs)	Four regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement			
Electron Geometry	**Linear**	**Trigonal planar**	**tetrahedral**

*Connections (regions of high electron density) =

- Atoms
- Lone pairs

Atoms
+ Lone Pairs
Connections

Covalent Bonds and Lewis Structures (com's way)

- Count total valence electrons of all atoms
  - Negative charges mean add electrons, positive charges mean subtract electrons
- Draw the skeletal structure with these tips
  - symmetrical
  - H, F, Cl, Br, I on the outsides
- Place bonding electrons in pairs to connect atoms
- Put rest of electrons on the outsides in pairs following the "octet" rule
  - If an atom doesn't have all it's electrons, share your neighbor's electron pairs
- Other common things (usual but not always):
  - C = 4 bonds, 0 lone pair
  - N = 3 bonds, 1 lone pair
  - O = 2 bonds, 2 lone pairs
  - halogens = 1 bond, 3 lone pairs

Lewis Structures to Electron Geometry

CO

\+ **Atoms**
Lone Pairs
Connections

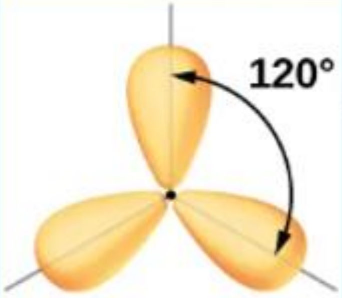
CO_2

\+ **Atoms**
Lone Pairs
Connections

Connections to center atom	**1 or 2**
Number of regions	Two regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement	
Electron Geometry	**Linear**

Lewis Structures to Electron Geometry

CH_2O

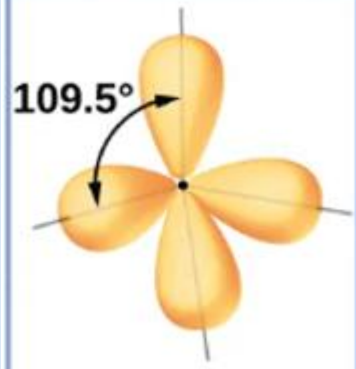
Connections to center atom	**3**
Number of regions	Three regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement	
Electron Geometry	**Trigonal planar**

\+ Atoms
Lone Pairs

Connections

Lewis Structures to Electron Geometry

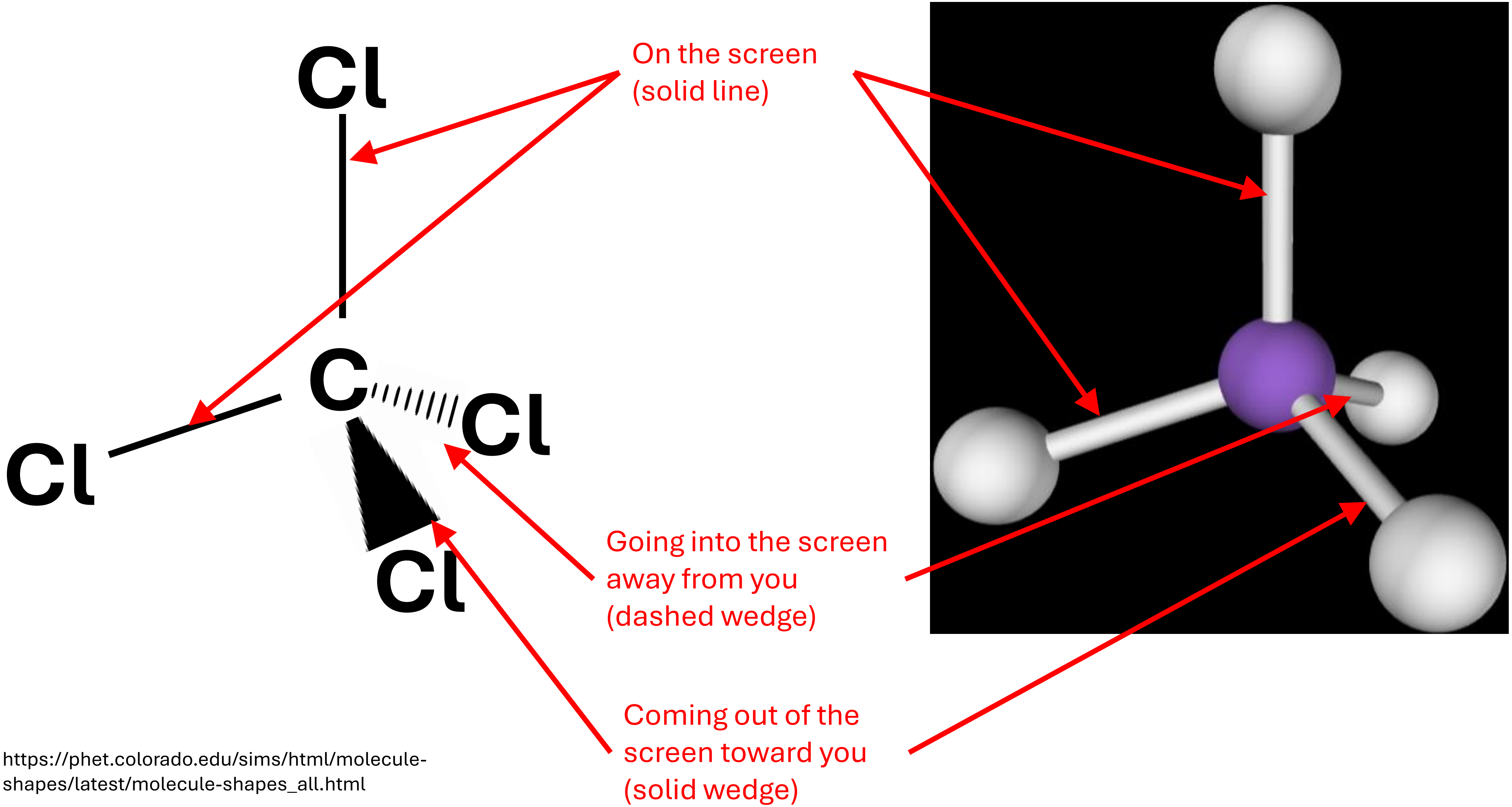
CCl_4

Connections to center atom	**4**
Number of regions	Four regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement	
Electron Geometry	**tetrahedral**

\+ Atoms
Lone Pairs

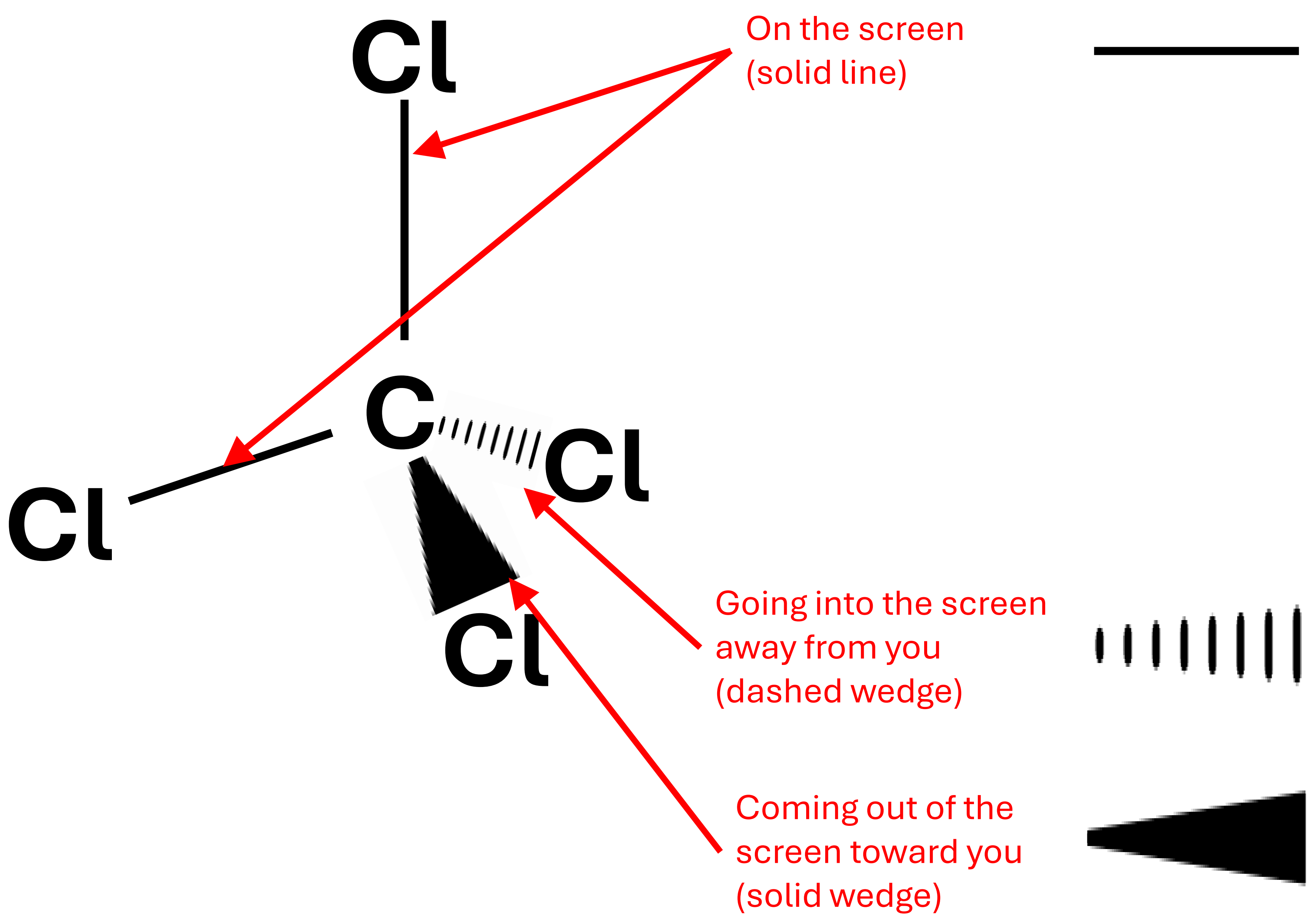
Connections

Drawing 3D Molecules



https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_all.html

Drawing 3D Molecules

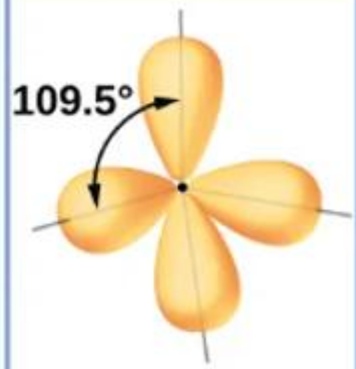


Electron Geometry and Molecular Structure

H_2O

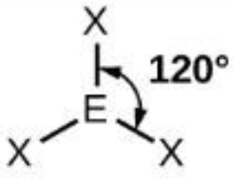
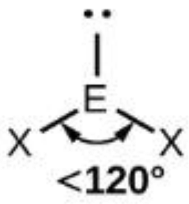
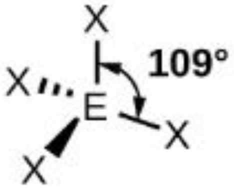
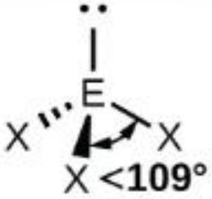
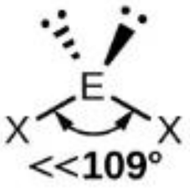
+ Atoms
Lone Pairs

Connections

Connections to center atom	4
Number of regions	Four regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement	
Electron Geometry	tetrahedral
Molecular Structure (no lone pairs)	bent

Electron Geometry and Molecular Structure

If there are lone pairs on the center atom, the molecular structure is different than the electron geometry

Number of electron regions	Electron region geometries: 0 lone pair	1 lone pair	2 lone pairs
2	 Linear		
3	 Trigonal planar	 Bent or angular	
4	 Tetrahedral	 Trigonal pyramid	 Bent or angular

Com's Way

Electron Geometry - draw the 3D molecule with all the atoms and lone pairs and that's the electron geometry

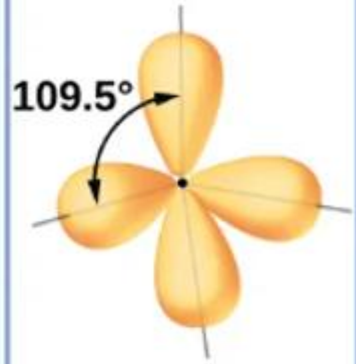
Molecular Structure – put out your thumb like you're giving me a thumbs up, close one eye, and cover up the lone pairs with your thumb and that's the molecular shape

Electron Geometry and Molecular Structure

NH_3

+ Atoms
Lone Pairs

Connections

Connections to center atom	4
Number of regions	Four regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement	
Electron Geometry	tetrahedral
Molecular Structure (no lone pairs)	Trigonal pyramidal

Check Your Learning

Carbonate, $CO_3{}^{2-}$, is a common polyatomic ion found in various materials from eggshells to antacids. What are the electron-pair geometry and molecular structure of this polyatomic ion?

Check Your Learning

The hydronium ion, H_3O^+, forms when acids are dissolved in water. Predict the electron-pair geometry and molecular structure of this cation.

Electronegativity and Polar Covalent Bonds

- Chapter 4.2 (Covalent Bonding)

Adapted From: Paul Flowers, Edward J. Neth, William R. Robinson, PhD, Klaus Theopold, Richard Langley; Chemistry: Atoms First 2e; OpenStax; Feb 14, 2019; Houston Texas; https://openstax.org/books/chemistry-atoms-first-2e/pages/1-introduction

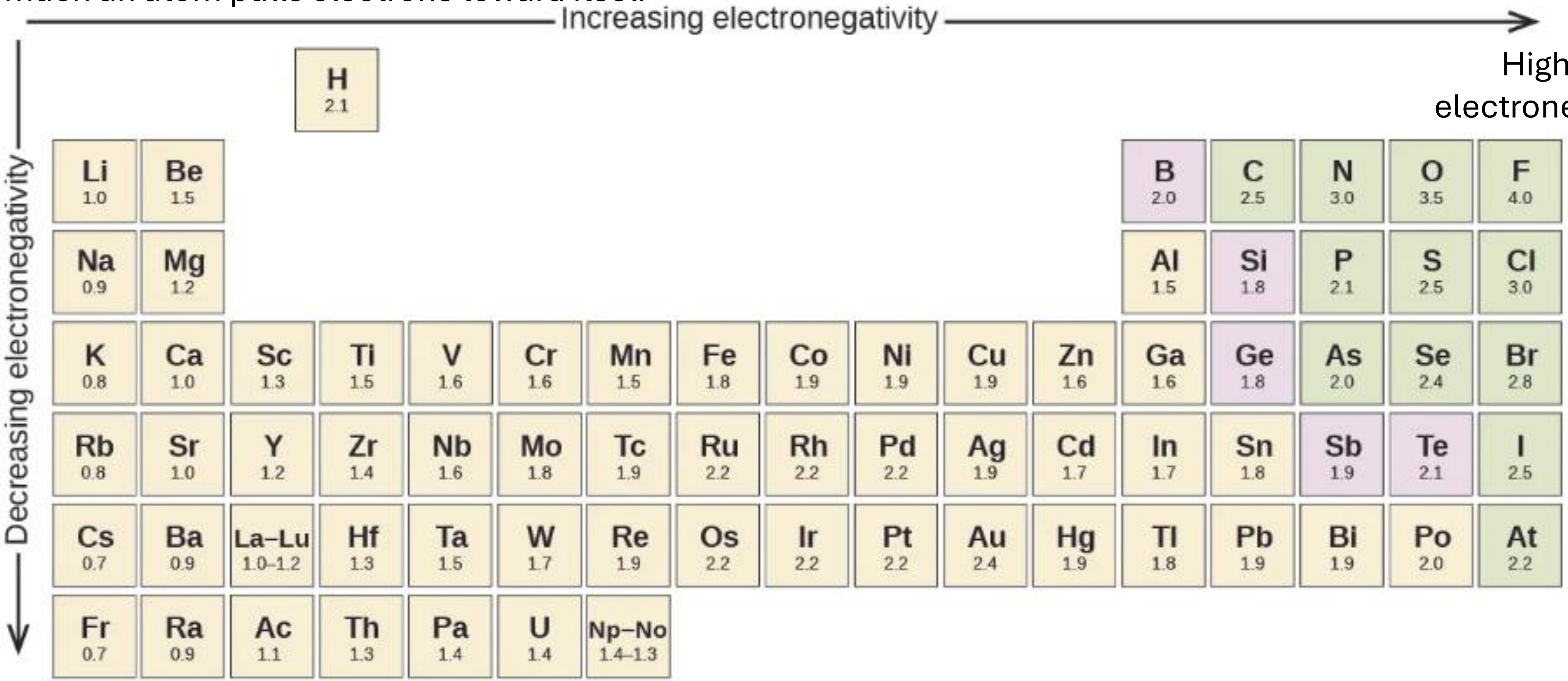
Pure Covalent VS Polar Covalent Bonds (Polar Bonds)

- Pure Covalent Bonds
  - Nonmetal + nonmetal
  - Held together by covalent bonds
  - Covalent bonds are formed by atoms sharing electrons

- Polar Covalent Bonds (Polar Bonds)
  - Nonmetal + nonmetal
  - Held together by covalent bonds
  - Covalent bonds are formed by atoms sharing electrons ***<u>unequally</u>***

Electronegativity

How much an atom pulls electrons toward itself



Highest electronegativity

Figure 4.6 The electronegativity values derived by Pauling follow predictable periodic trends, with the higher electronegativities toward the upper right of the periodic table.

Lowest electronegativity

Lewis Structures and Sharing of Electrons

H_2 Cl_2 HCl

Lewis Structures and Sharing of Electrons

HCl

Symbol for partial positive (delta)

Symbol for partial negative (delta)

Polarity vector, with arrow showing which side of the molecule the electrons are. The small plus sign is where there is less electron density

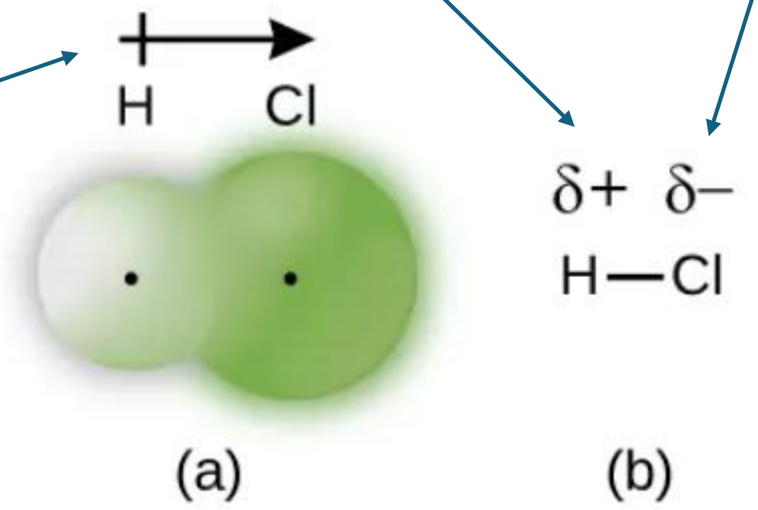
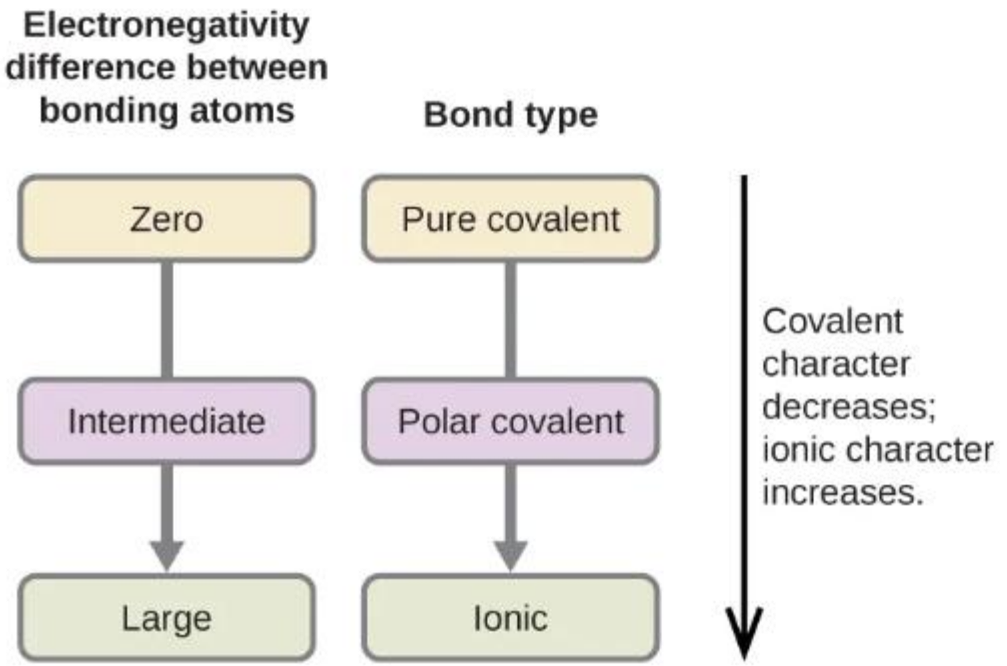


Figure 4.5 (a) The distribution of electron density in the HCl molecule is uneven. The electron density is greater around the chlorine nucleus. The small, black dots indicate the location of the hydrogen and chlorine nuclei in the molecule. (b) Symbols δ+ and δ– indicate the polarity of the H–Cl bond.

Lewis Structures and Sharing of Electrons

HCl



Bond Type	Electronegativity Difference
pure covalent	< 0.4
polar covalent	between 0.4 and 1.8
ionic	> 1.8

Figure 4.8 As the electronegativity difference increases between two atoms, the bond becomes more ionic.

Check Your Learning

Silicones are polymeric compounds containing, among others, the following types of covalent bonds: Si–O, Si–C, C–H, and C–C. Using the electronegativity values in Figure 4.6, arrange the bonds in order of increasing polarity and designate the positive and negative atoms using the symbols δ+ and δ–.

H 2.1	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0

Molecular Polarity

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Polar Bonds

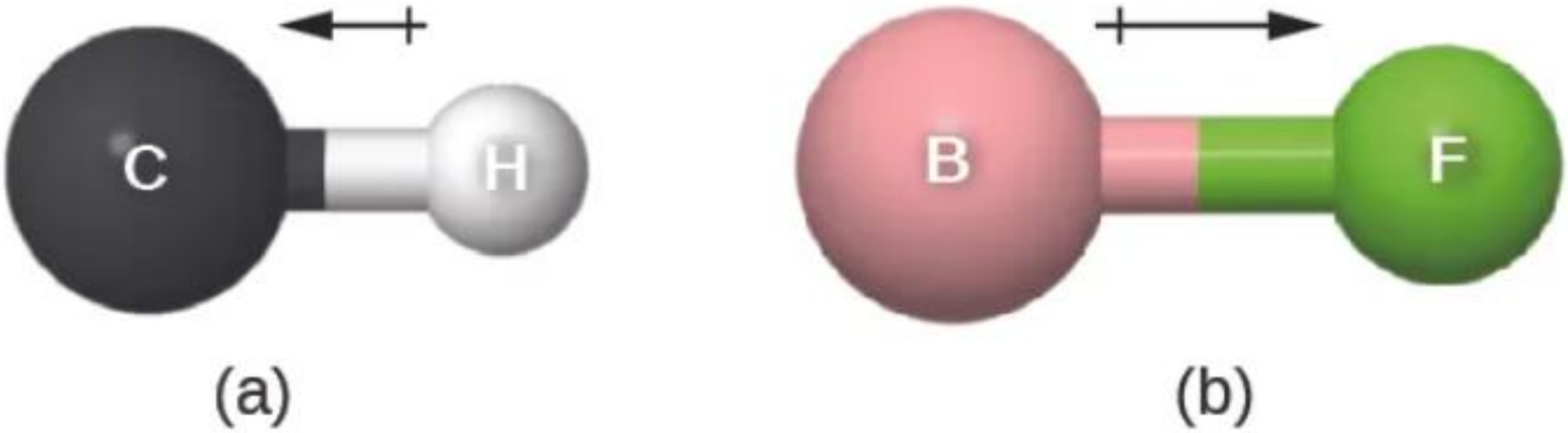


Figure 4.26 (a) There is a small difference in electronegativity between C and H, represented as a short vector. (b) The electronegativity difference between B and F is much larger, so the vector representing the bond moment is much longer.

H 2.1	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0

Polar Molecules?

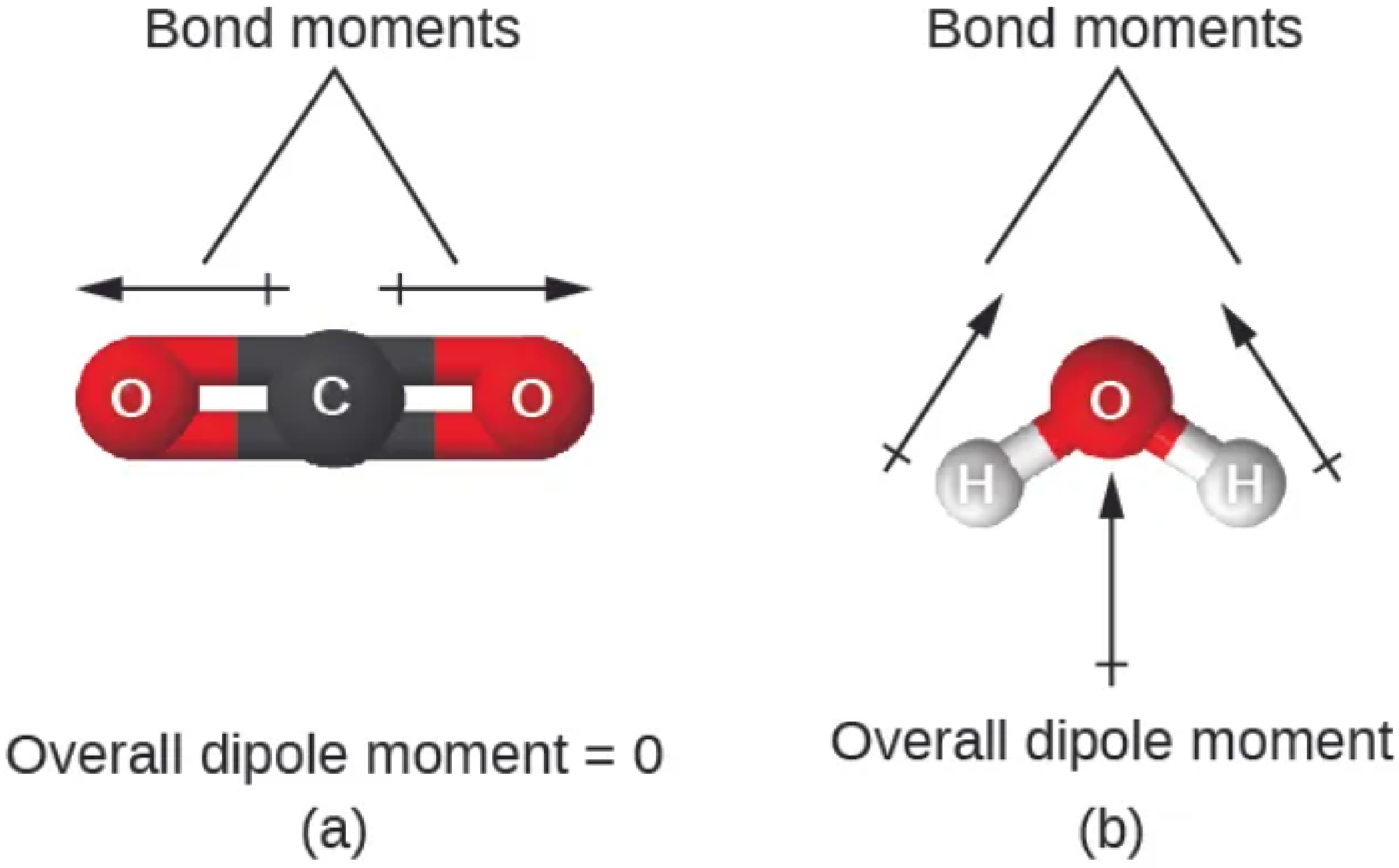
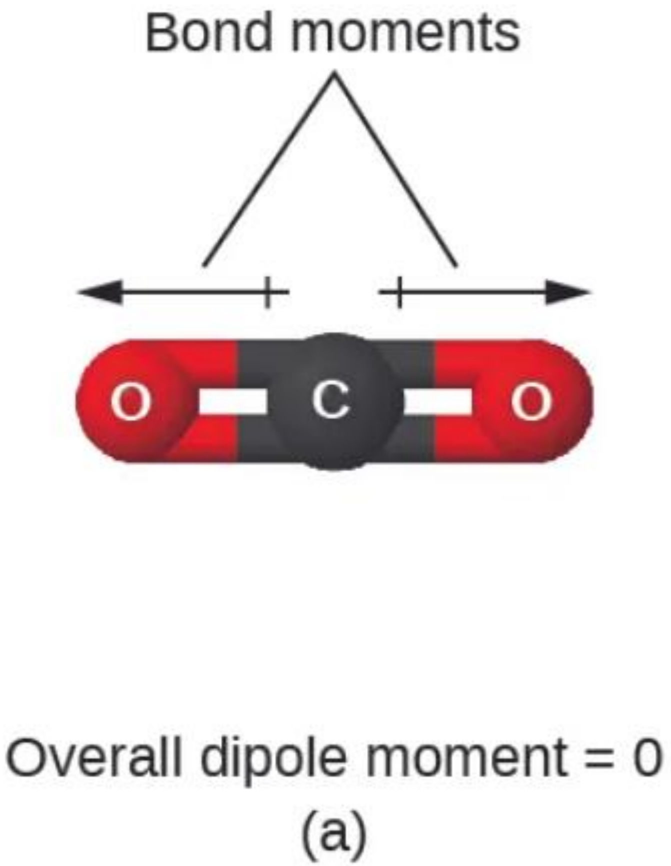
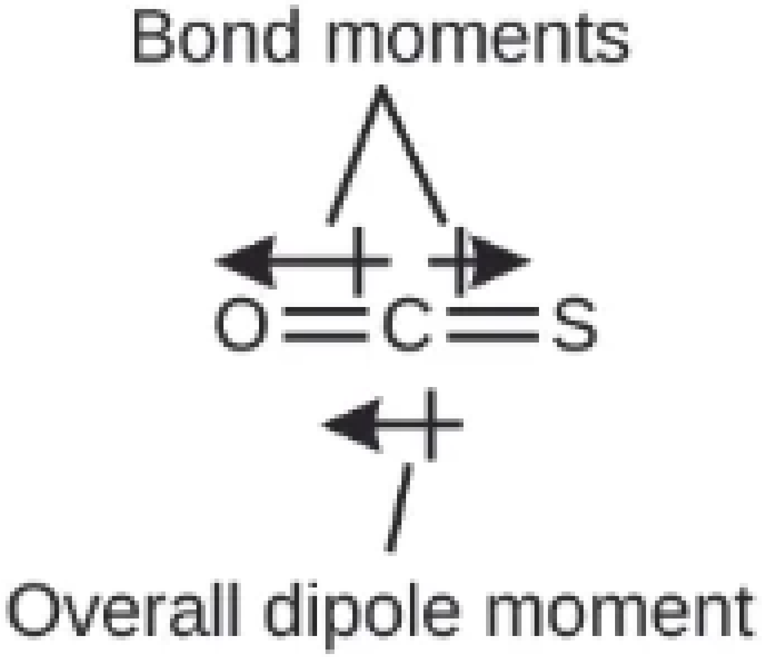


Figure 4.27 The overall dipole moment of a molecule depends on the individual bond dipole moments and how they are arranged. (a) Each CO bond has a bond dipole moment, but they point in opposite directions so that the net CO_2 molecule is nonpolar. (b) In contrast, water is polar because the OH bond moments do not cancel out.

Polar Molecules?





B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0

Is something polar?

Book Version

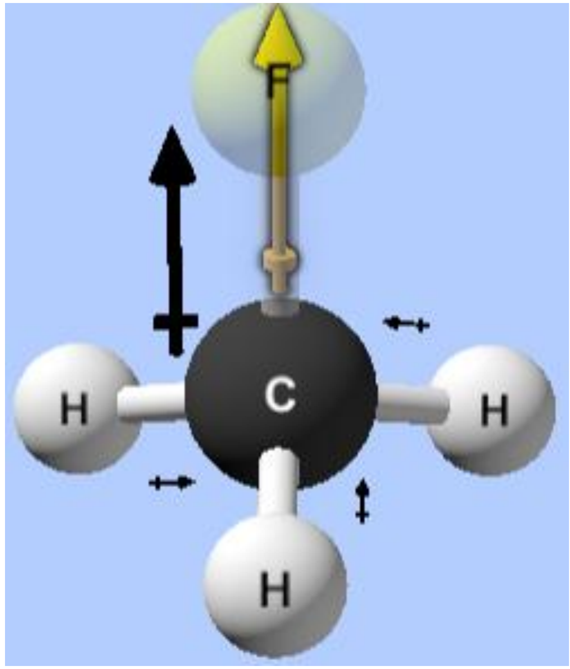
To summarize, to be polar, a molecule must:

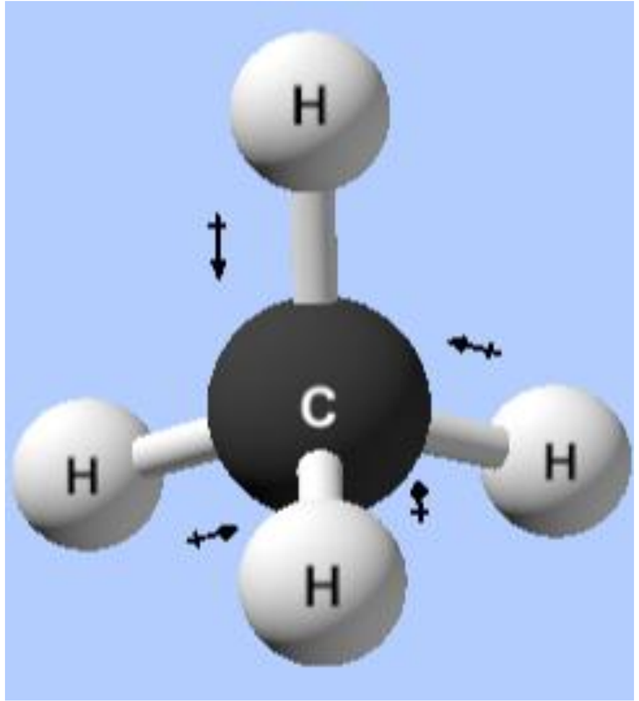
1. Contain at least one polar covalent bond.
2. Have a molecular structure such that the sum of the vectors of each bond dipole moment does not cancel.

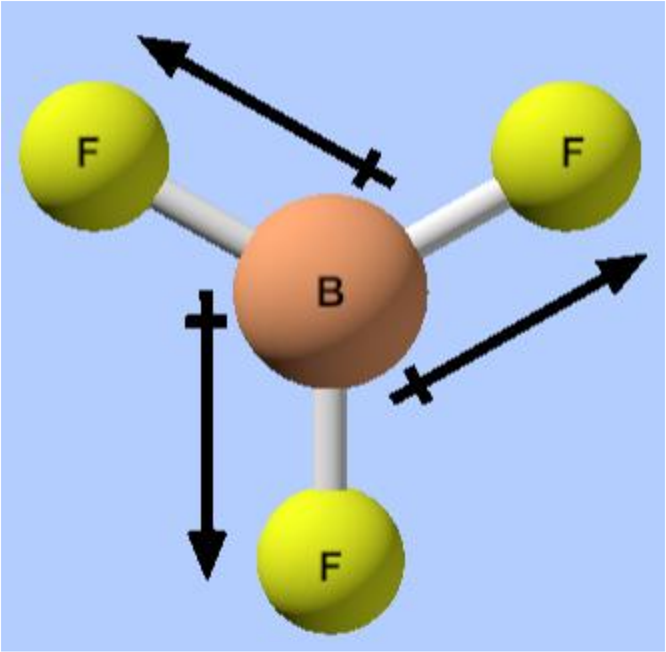
Com's Way (works most of the time)

1. Draw the 3D structure of the molecule (most of the time the Lewis structure works).
2. Label all exterior atoms with their electronegativities (δ- and δ+) based on periodic table trends. (up and to the right are most electronegative)
3. Try to draw a straight line that separates the δ- and δ+ atoms. If you can, it's polar, if you can't it's nonpolar.

Polar and Nonpolar







https://phet.colorado.edu/sims/html/molecule-polarity/latest/molecule-polarity_all.html

Practice Problems

- Draw the 3D structures for the following molecules, label each exterior atom with their partial charges (δ- and δ+): H_2, Cl_2, HCl, CO, CO_2, CH_2O, CCl_4, CH_4, CH_3F, H_2O, NH_3.
- Indicate if they are polar or not and if so, draw the dipole moment.
- Do not use the periodic table for electronegativity values, just use the trend of atoms higher and to the right on the periodic table are more electronegative.

H_2

Cl_2

HCl

CO

CO_2

CH_2O

CCl_4

CH_4

CH_3F

H_2O

NH_3

Polarity Simulation

- https://phet.colorado.edu/en/simulations/molecule-polarity

Chem With Com