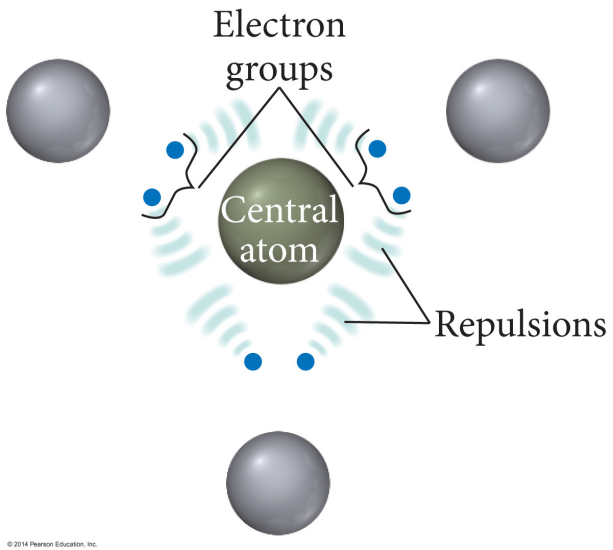
10.2: The Shapes of Molecules – VSEPR

The 3D Shape of a molecule can be predicted using **Valence Shell Electron Pair Repulsion (VSEPR)** theory.

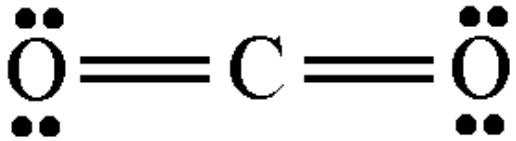
Basic idea: Because of repulsion between electrons, molecules will adopt a shape that allows the electrons in bonds and lone pairs to be located as far as possible from each other.

The shape of a molecule depends on the number of **electron groups** around the central atom.

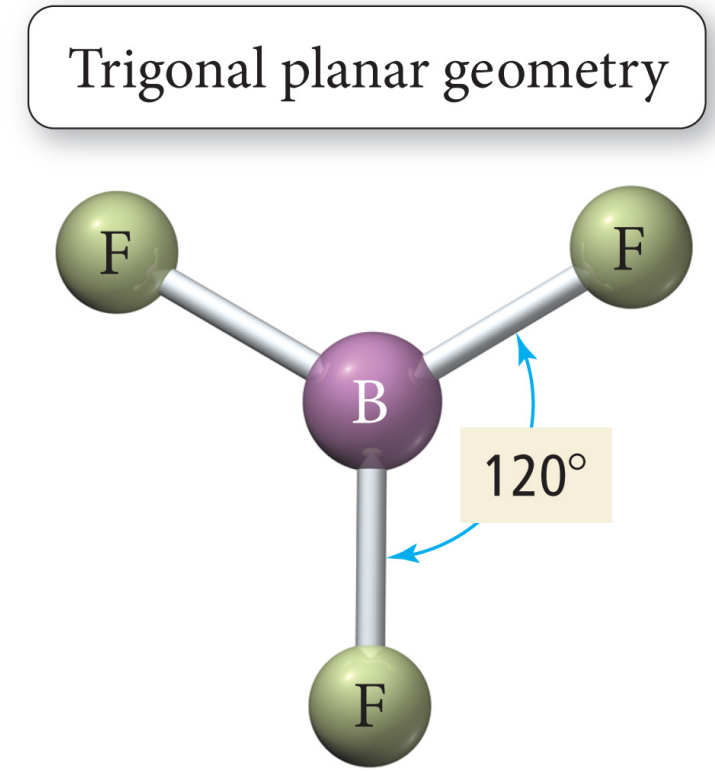
- Electron groups are other atoms bonded to the central atom, or lone pairs on the central atom.

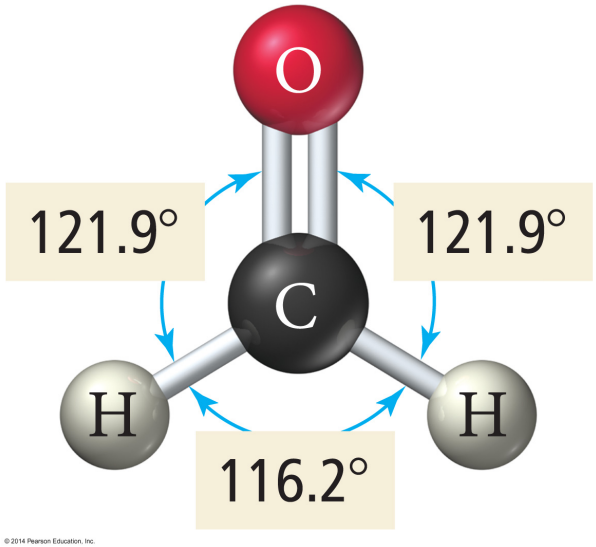


Two Electron Groups: Linear Geometry

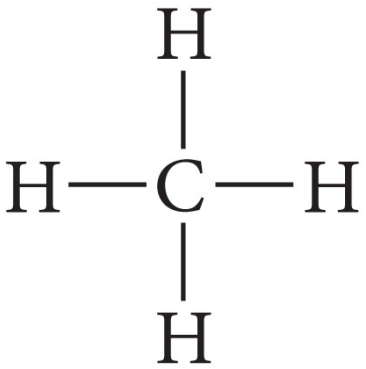


Three Electron Groups: Trigonal Planar Geometry





Four Electron Groups: Tetrahedral Geometry



10.3 VSEPR: The Effect of Lone Pairs

- Ozone has three electron groups around the central oxygen, so has the **trigonal planar electron geometry**.
- The **molecular geometry** is **bent**:

The Effect of Lone Pairs (contd.)

- With four electron groups (tetrahedral electron geometry), there can be one or two lone pairs around the central atom.
- Lone pairs repel more than bonds, so increasing the number of lone pairs **decreases** the bond angles.

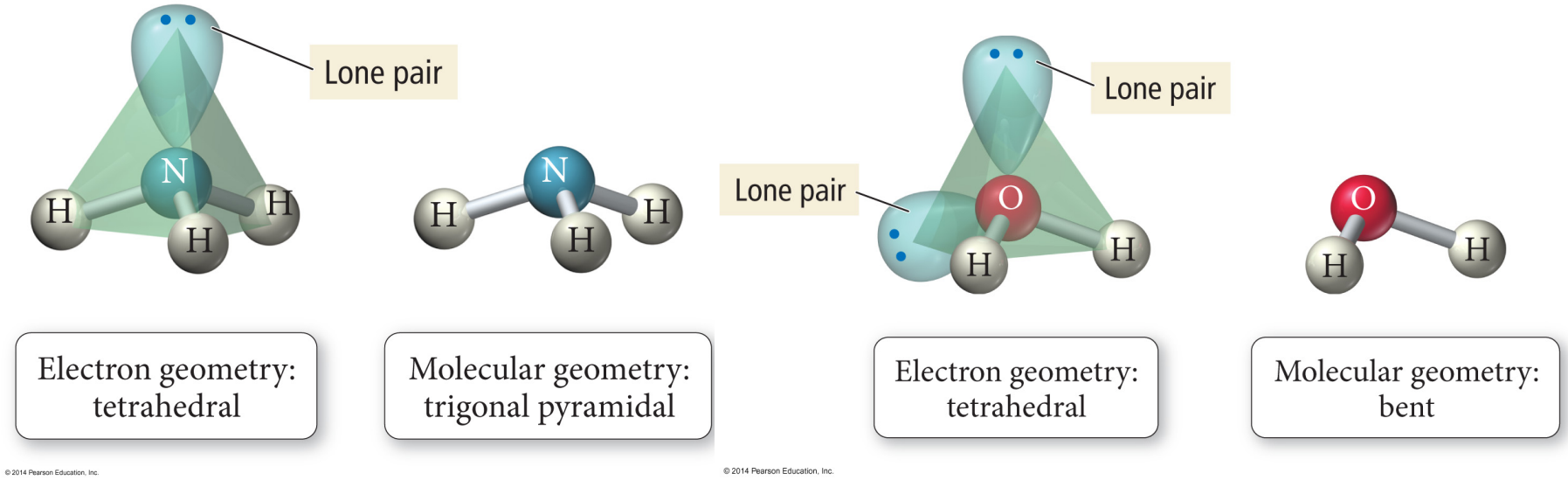
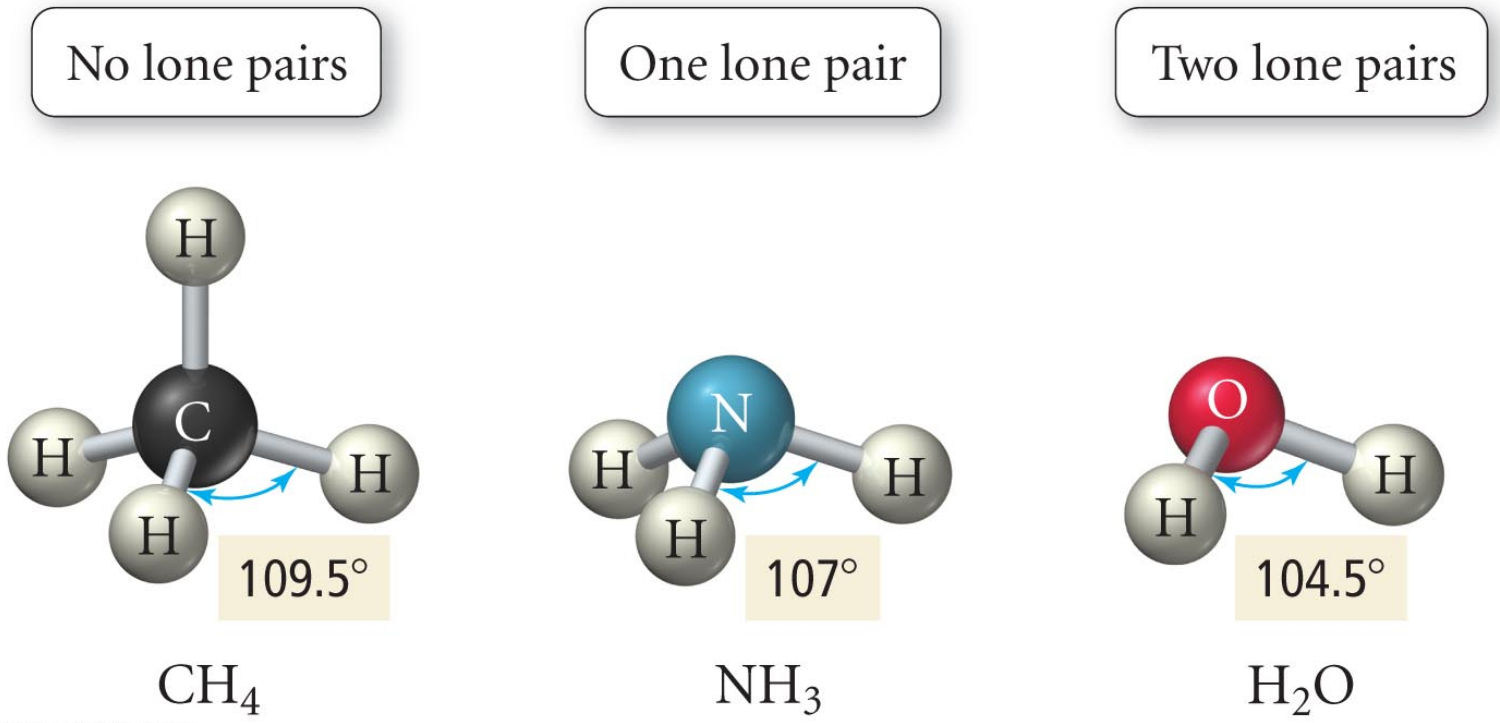
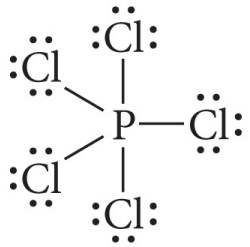
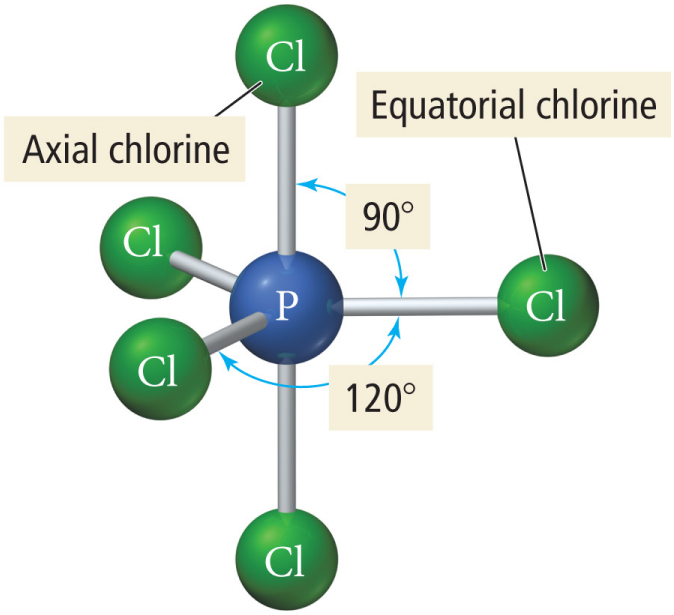


Figure 10.4 **Effect of Lone Pairs on Molecular Geometry**



Five Electron Groups: Trigonal Bipyramidal Geometry

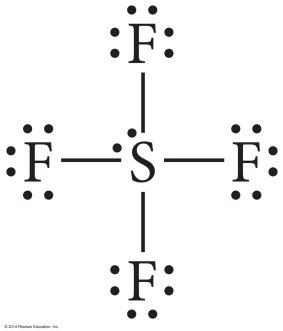


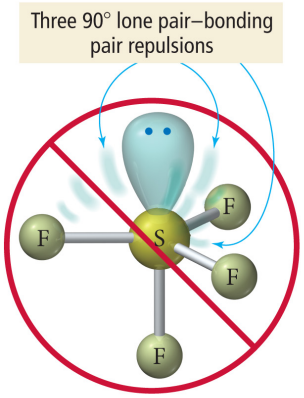


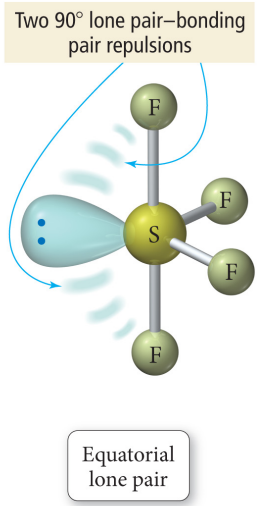
Trigonal bipyramidal geometry

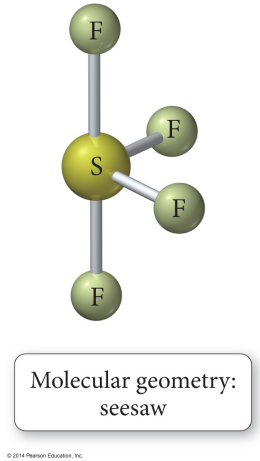
Trigonal Bipyramidal Geometry (contd.)

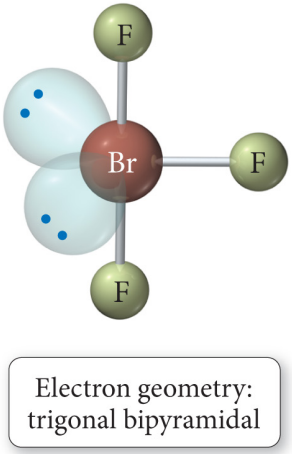
Lone pairs are **always equatorial** to minimize 90° interactions.

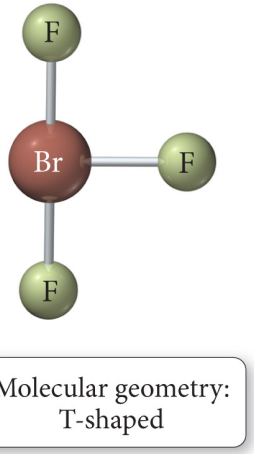


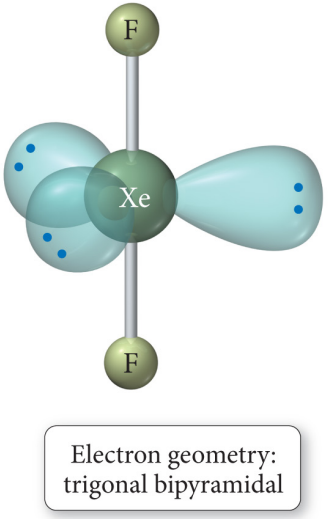


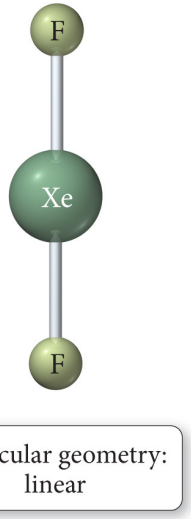




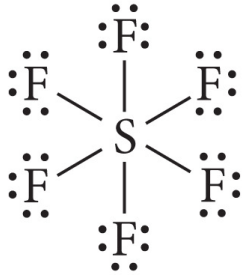


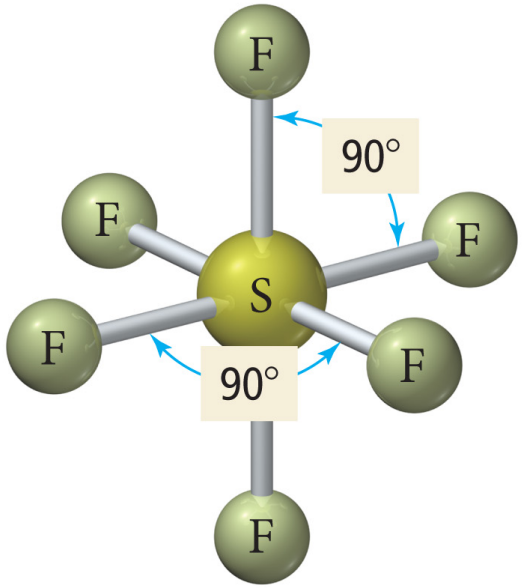






Six Electron Groups: Octahedral Geometry

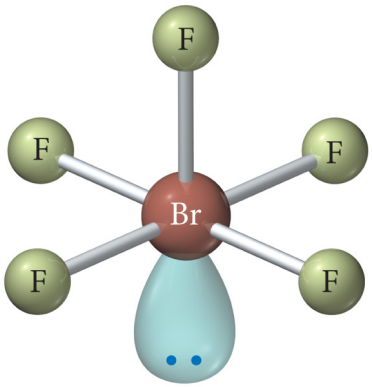




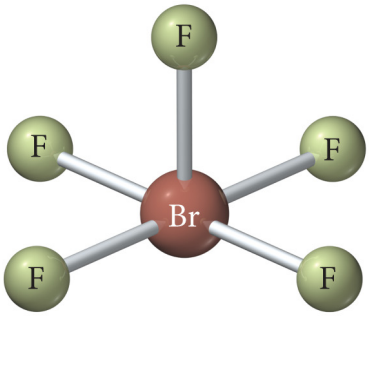
Octahedral geometry

Octahedral Geometry (contd.)

One lone pair:

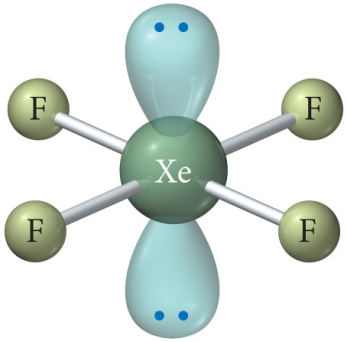


Electron geometry: octahedral

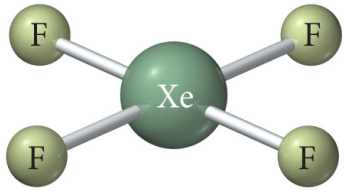


Molecular geometry: square pyramidal

Two lone pairs:
Lone pairs are 180° from each other



Electron geometry: octahedral



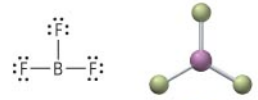
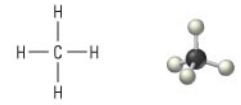
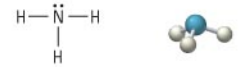
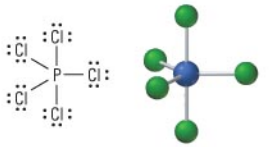
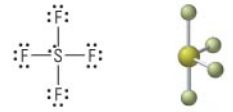
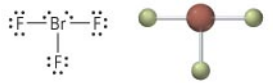
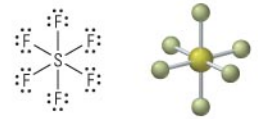
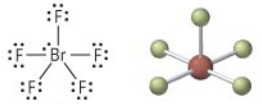
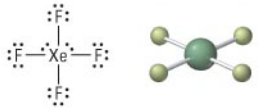
Molecular geometry: square planar

10.4: VSEPR Theory: Predicting Molecular Geometries

To determine the shape of a molecule, follow these steps:

1. Draw the molecule's Lewis structure.
2. Determine the total number of electron groups around the central atom.
3. The number of electron groups (2, 3, 4, 5 or 6) determines the "electron geometry," the basic shape and ideal angles.
4. If there are lone pair(s) on the central atom, the shape will be one of the variations of the basic geometries ("molecular geometry").

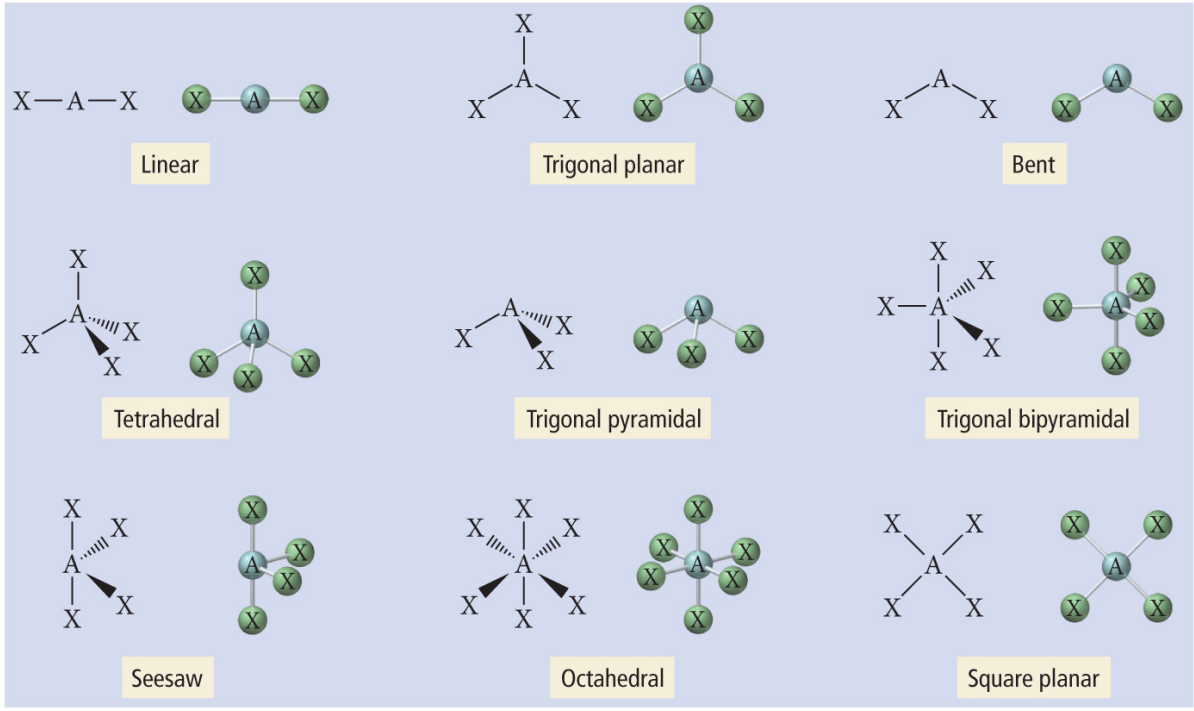
TABLE 10.1 Electron and Molecular Geometries

Electron Groups*	Bonding Groups	Lone Pairs	Electron Geometry	Molecular Geometry	Approximate Bond Angles	Example
2	2	0	Linear	Linear	180°	
3	3	0	Trigonal planar	Trigonal planar	120°	
3	2	1	Trigonal planar	Bent	<120°	
4	4	0	Tetrahedral	Tetrahedral	109.5°	
4	3	1	Tetrahedral	Trigonal pyramidal	<109.5°	
4	2	2	Tetrahedral	Bent	<109.5°	
5	5	0	Trigonal bipyramidal	Trigonal bipyramidal	120° (equatorial) 90° (axial)	
5	4	1	Trigonal bipyramidal	Seesaw	<120° (equatorial) <90° (axial)	
5	3	2	Trigonal bipyramidal	T-shaped	<90°	
5	2	3	Trigonal bipyramidal	Linear	180°	
6	6	0	Octahedral	Octahedral	90°	
6	5	1	Octahedral	Square pyramidal	<90°	
6	4	2	Octahedral	Square planar	90°	

*Count only electron groups around the central atom. Each of the following is considered one electron group: a lone pair, a single bond, a double bond, a triple bond, or a single electron.

Wedge-Dash Notation

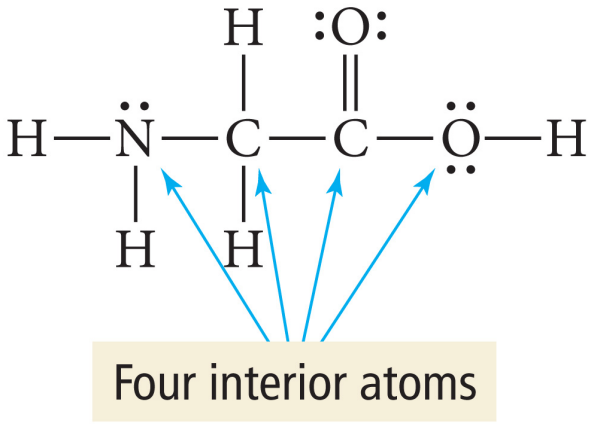
- A way to represent 3D molecular structures on paper (p. 437):

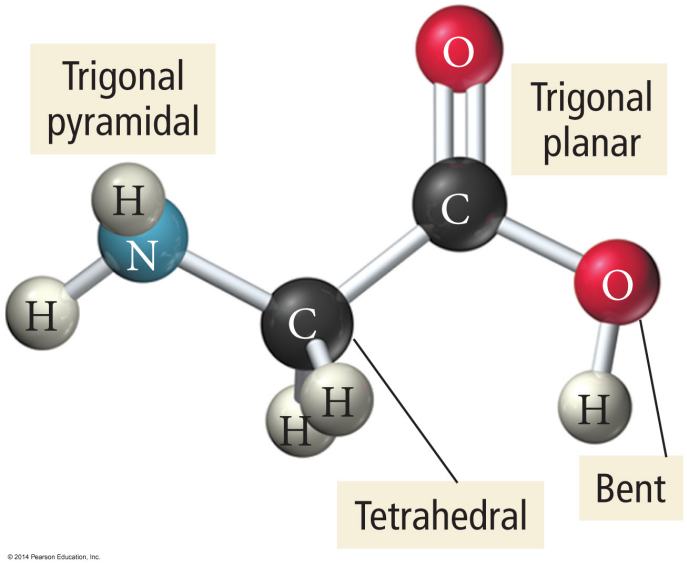


Molecules With More Than One Central Atom

Consider the geometry of each atom separately.

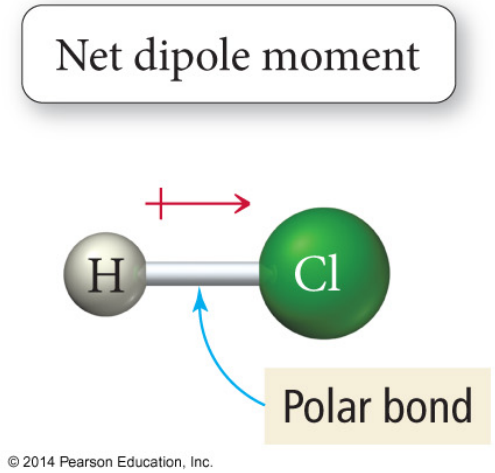
- See the example of glycine, p. 437.

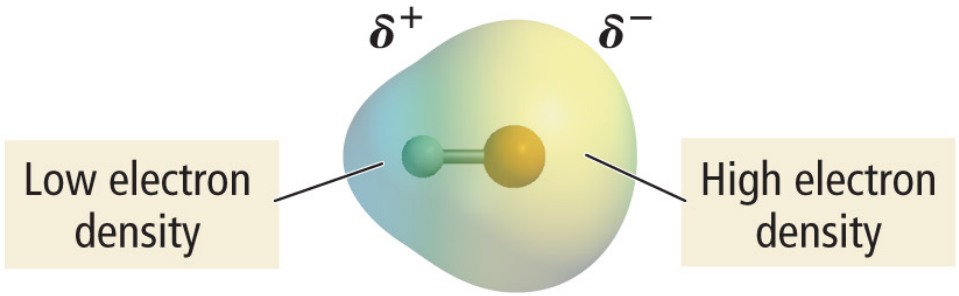




10.5: Molecular Shape and Polarity

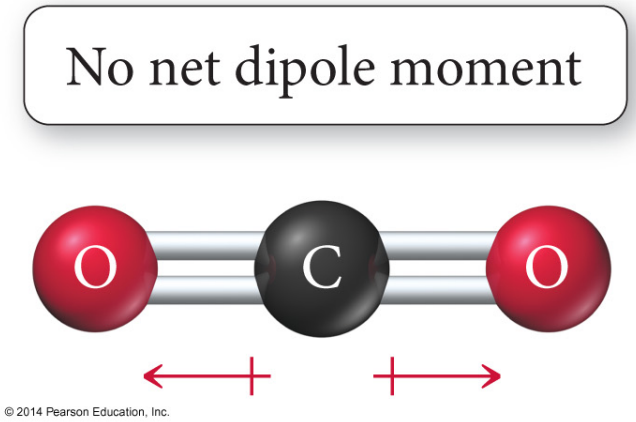
- Polar bonds have **dipole moments**:

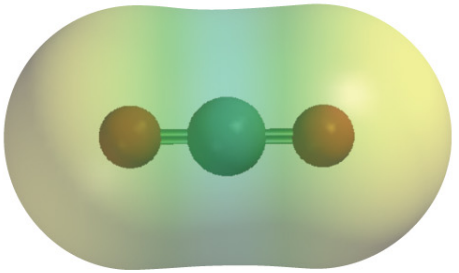




Molecular Shape and Polarity (contd.)

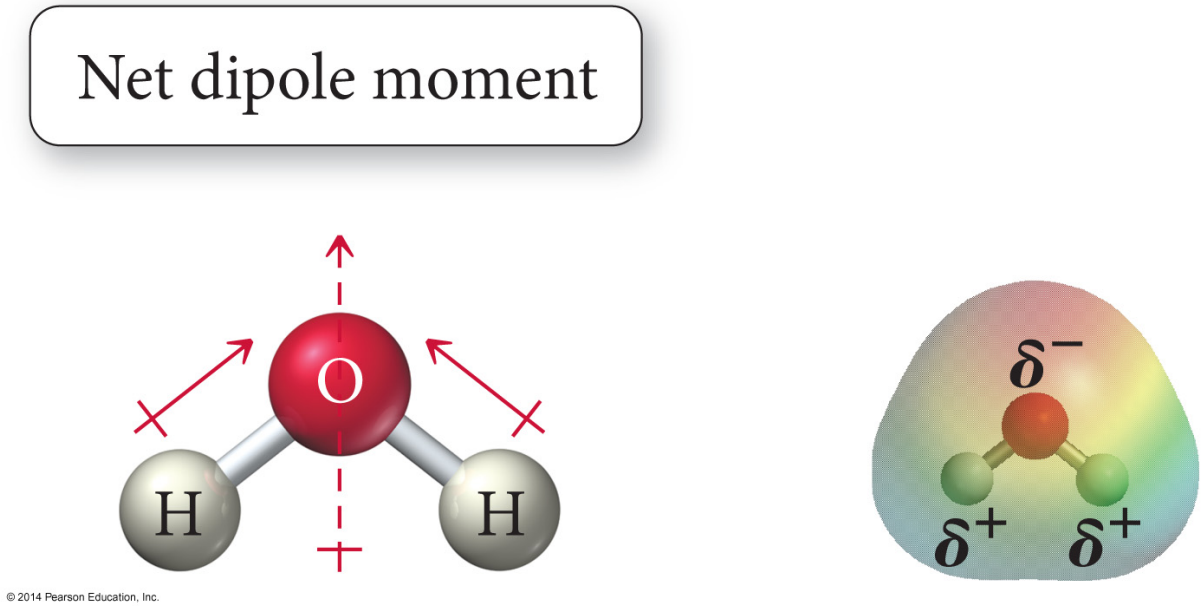
- For molecules with more than one bond, if the dipole moments combine to give a net dipole, the molecule is polar.
- In CO_2, the dipoles of the bonds cancel.
- So it is a **nonpolar molecule that has polar bonds**.





Molecular Shape and Polarity (contd.)

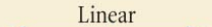
- In contrast, because water has a bent geometry the dipole moments combine to give a **net dipole**, so it is polar.



Molecular Shape and Polarity (contd.)

TABLE 10.2 Common Cases of Adding Dipole Moments to Determine whether a Molecule Is Polar

Linear



Nonpolar

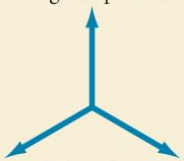
The dipole moments of two identical polar bonds pointing in opposite directions will cancel. The molecule is nonpolar.

Bent

Polar

The dipole moments of two polar bonds with an angle of less than 180° between them will not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.

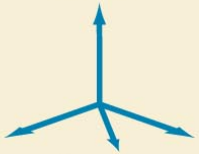
Trigonal planar



Nonpolar

The dipole moments of three identical polar bonds at 120° from each other will cancel. The molecule is nonpolar.

Tetrahedral



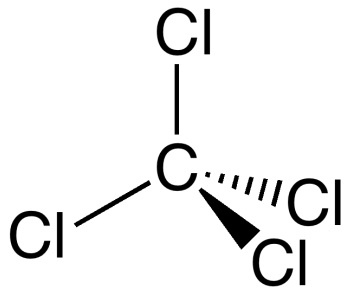
Nonpolar

The dipole moments of four identical polar bonds in a tetrahedral arrangement (109.5° from each other) will cancel. The molecule is nonpolar.

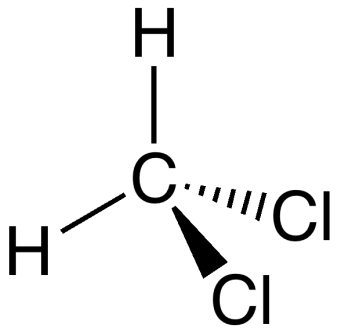
Trigonal pyramidal

Polar

The dipole moments of three polar bonds in a trigonal pyramidal arrangement (109.5° from each other) will not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.



Dipoles cancel – nonpolar (symmetric structure)



Polar (non-symmetric structure)

Note: In all cases where the dipoles of two or more polar bonds cancel, the bonds are assumed to be identical. If one or more of the bonds are different from the other(s), the dipoles will not cancel and the molecule will be polar.