Molecular Shapes and Structures

Lewis Structures:

Describe the distribution of electrons in covalently bonded molecules and ions

Can give clues about stability or reactivity

Do ***not*** show 3 dimensional structure

Often don’t work well for transition metal complexes

Drawing Lewis Structures:

1. Add up all valence electrons
2. Draw a skeleton structure using single bonds, usually the least electronegative atom is in the center
3. Fill octets (or duets) of all peripheral atoms, place extra electrons on the central atom
4. Minimize formal charge distribution with multiple bonds if possible

Drawing Lewis Structures:

1. Add up all valence electrons

SO_2

Sulfur has 6 valence electrons, each oxygen has 6 valence electrons

6 + 2(6) = 18 valence electrons

Drawing Lewis Structures:

2. Draw a skeleton structure using single bonds, usually the least electronegative atom is in the center

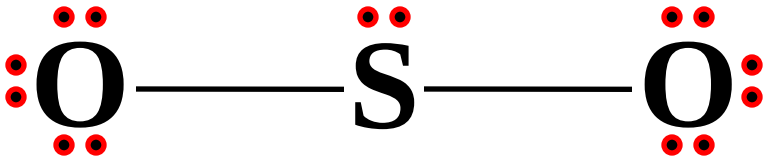
SO_2

O—S—O

Drawing Lewis Structures:

3. Fill octets (or duets) of all peripheral atoms, place extra electrons on the central atom

SO_2



Formal Charge:

Assumes perfect/pure covalent bonds

1. Assign all lone pair electrons and half of each bonding pair of electrons to each atom.

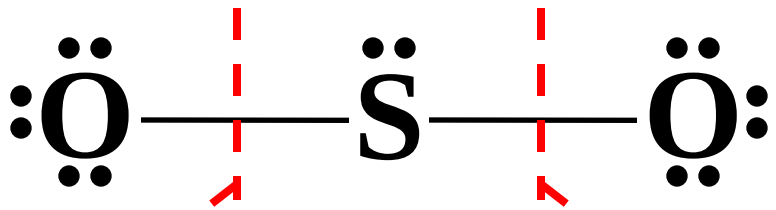
2. Compare assigned electrons to the number of electrons in the neutral atom

The sum of all formal charges is equal to the charge of the ion or molecule

Drawing Lewis Structures:

4. Minimize formal charge distribution with multiple bonds if possible

SO_2

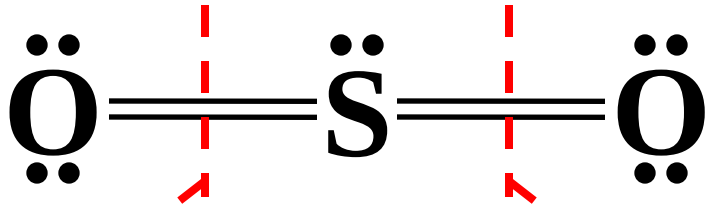


Assigned = 7	Assigned = 4	Assigned = 7
Neutral = 6	Neutral = 6	Neutral = 6
FC = -1	FC = +2	FC = -1

Drawing Lewis Structures:

4. Minimize formal charge distribution with multiple bonds if possible

SO_2



Assigned = 6
Neutral = 6
FC = 0

Assigned = 6
Neutral = 6
FC = 0

Assigned = 6
Neutral = 6
FC = 0

Valence Shell Electron Pair Repulsion Theory (VSEPR)

Regions of electron density around an atom will repel each other and arrange themselves to minimize that repulsion.

A “region of electron density” is a bond or a lone pair, and the number of regions of electron density (R.E.D.) determines the electronic shape of a molecule or ion.

2 Regions of Electron Density

Electronic geometry:	Linear
Bond angles:	180°
Possible molecular shapes:	Linear (3-atom)
	Linear (2-atom)

3 Regions of Electron Density

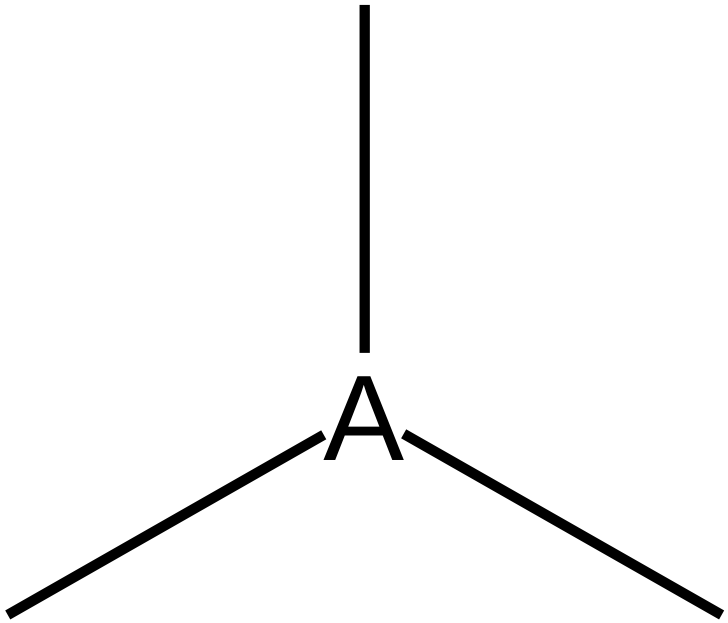
Electronic geometry: Trigonal planar

Bond angles: 120°

Possible molecular shapes: Trigonal Planar

Bent

Linear (2-atom)



4 Regions of Electron Density

Electronic geometry: Tetrahedral

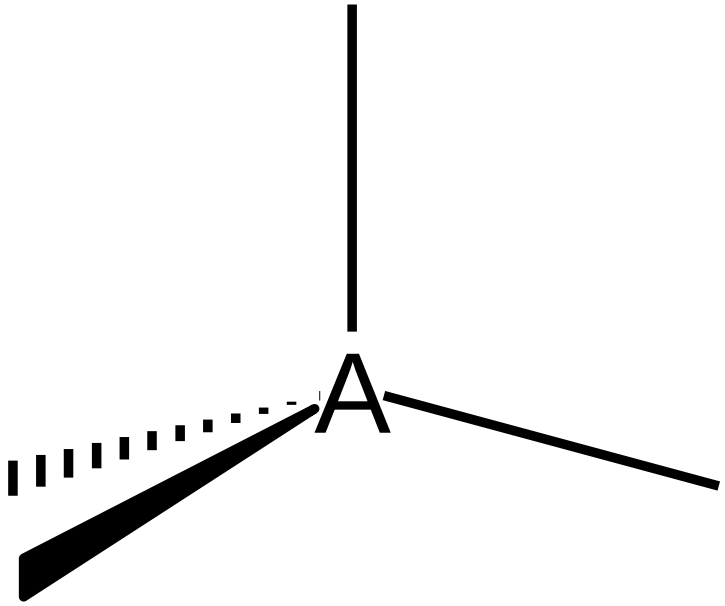
Bond angles: 109.5°

Possible molecular shapes: Tetrahedral

Trigonal pyramidal

Bent

Linear (2-atom)



5 Regions of Electron Density

Electronic geometry: Trigonal bipyramidal

Bond angles: 120° and 90°

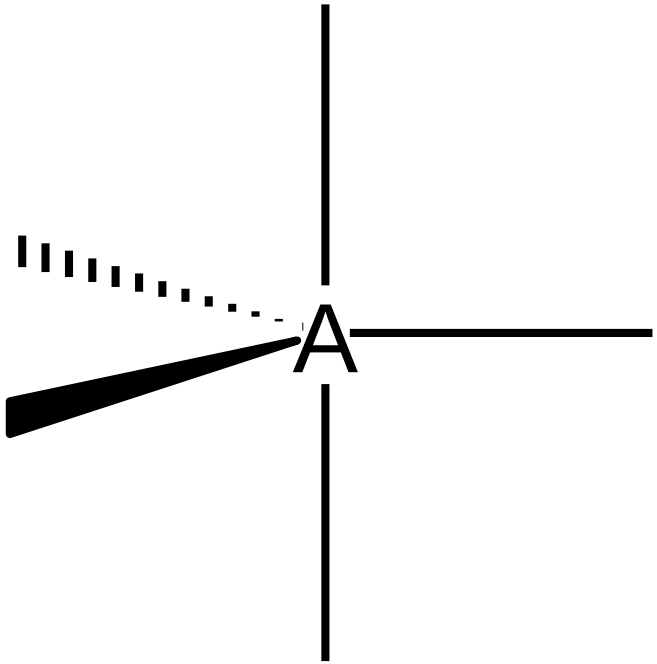
Possible molecular shapes: Trig. bipyramidal

See-saw shaped

T-shaped

Linear (3-atom)

Linear (2-atom)



6 Regions of Electron Density

Electronic geometry: Octahedral

Bond angles: 90°

Possible molecular shapes: Octahedral

Square pyramidal

Square planar

T-shaped

Linear (3-atom)

Linear (2-atom)