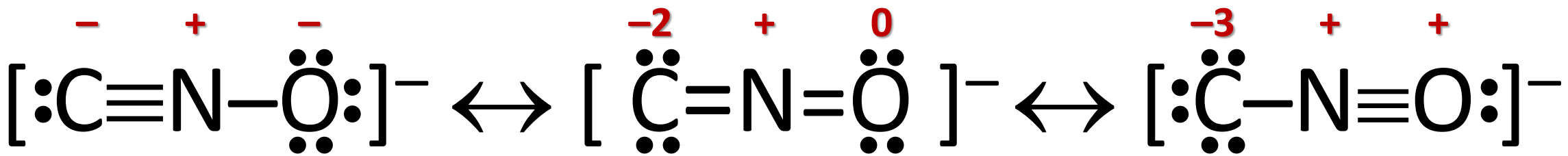
Announcements for Wednesday, 16OCT2024

- **Exam 2 Location Requests** **due by Friday, 18OCT2024, 11:59 PM (EDT)**
  - for students having a class ending at 7:00 PM or later on exam day
- Exam 1 is now available for reviewing through ***Gradescope***
- Requests for Exam Question Regrades Now Open
  - Monday, 14OCT2024, 12:01 AM (EDT) – **Wednesday, 16OCT2024, 11:59 PM (EDT)**
  - MUST be submitted through ***Gradescope*** (do not email instructors)
  - see Canvas announcement from Oct 11 for regrading policies and procedure
  - after the deadline, Exam 1 grades will not be changed

ANY GENERAL QUESTIONS? Feel free to see me after class!

Try This On Your Own

Draw the different Lewis structures for the fulminate ion (CNO^-) (nitrogen is central atom) and determine the BEST structure based on formal charges.



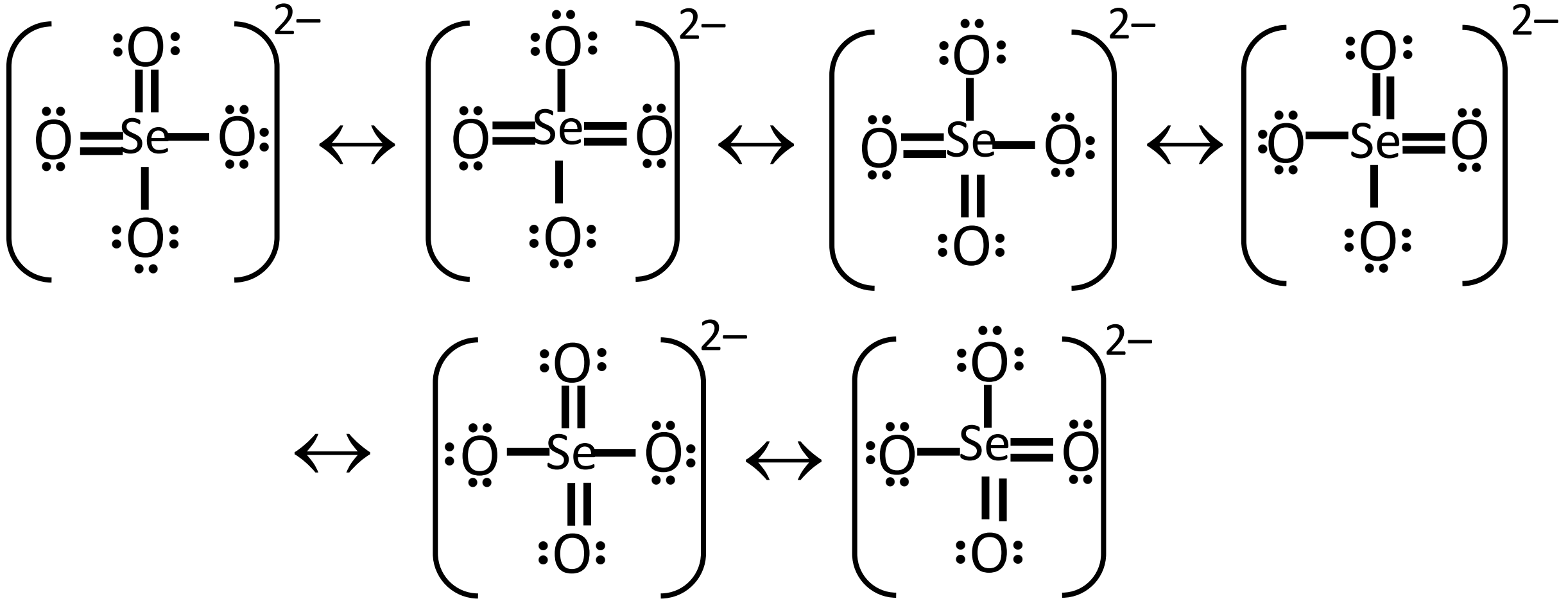
- BEST Resonance structure
  - minimized formal charges
- the true structure has negative charge on **both ends** of the ion

- Bad Resonance structure
  - excessive formal charge on carbon
- this structure has negative charge localized only on carbon

- WORST Resonance structure
  - excessive formal charges
  - (+!) on oxygen and (3!!) on carbon
- this structure has negative charge localized only on carbon

Try This On Your Own

How many resonance structures can be drawn for the selenate ion (SeO_4^{2-}) in which the central atom has zero formal charge?



Average Bond Length

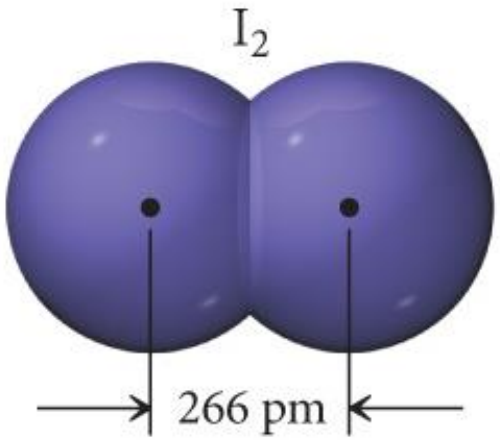


TABLE 5.4 Average Bond Lengths

Bond	Bond Length (pm)	Bond	Bond Length (pm)	Bond	Bond Length (pm)
H—H	74	C—C	154	N≡N	110
H—C	110	C=C	134	O—O	145
H—N	100	C≡C	120	O=O	121
H—O	97	C—O	143	F—F	143
H—F	92	C=O	120	Cl—Cl	199
H—Cl	127	C—Cl	178	Br—Br	228
H—Br	141	N—N	145	I—I	266
H—I	161	N=N	123		

- **bond length =** distance between the nuclei of the two atoms taking part in the covalent bond
  - an average of the bond length from several different compounds containing a particular bond
- closely (though not perfectly) related to atomic radius
  - **F_2 vs. Cl_2 vs. Br_2 vs. I_2** and **HF vs. HCl vs. HBr vs. HI**
- in general when comparing the same two atoms, bond length decreases as the number of bonds increase
  - **C–C vs. C=C vs. C≡C** and **C–O vs. C=O**

Try This On Your Own

Rank the following species in order of increasing N-O bond length:

NO_2^-, NO^+, NO_2^+

Hint: Start by drawing the Lewis structures

Shapes of Molecules

- shape is responsible for many properties of a molecule
  - shape impacts polarity which impacts intermolecular forces which impacts physical properties
  - the shape of drug molecules and enzymes are responsible for their bioactivity
  - the shapes of large, complex molecules can be understood by focusing on the shape around each central atom

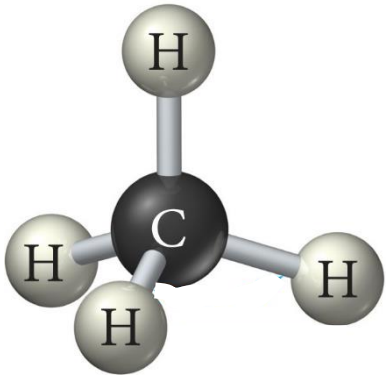
valence shell electron pair repulsion (VSEPR) theory

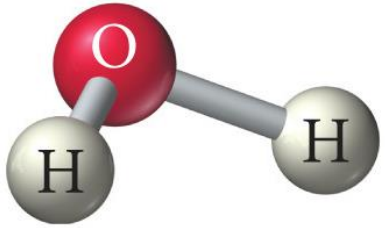
- **electron groups (?!?)** around an atom want to get as far away from one another to minimize repulsion
  - a **single bond** is one electron group
  - a **double bond** is one electron group
  - a **triple bond** is one electron group
  - a **lone pair** is one electron group
  - a **single electron** (in a radical species) is an electron group
- the maximum separation of electron groups around an interior/central atom leads to the shape of a molecule

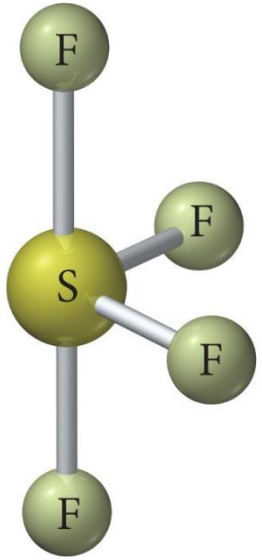
Electron Group Geometry vs. Molecular Geometry

- **electron group geometry (e.g.g.) =** the spatial arrangement taken by the **electron groups** around a central atom
- **molecular geometry (m.g.) =** the spatial arrangement of **ONLY the BONDS** around a central atom

- sometimes the e.g.g. and the m.g. can be the same
  - CO_2 and CH_4
- sometimes they can be different
  - H_2O and SF_4
- electron groups repel one another and try to get as far away from one another to minimize repulsions
  - the ideal geometry of electron groups depends on the total number of them around the central atom

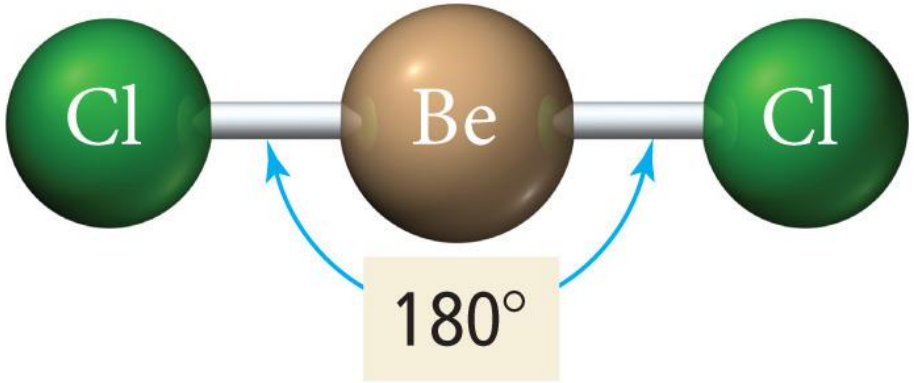






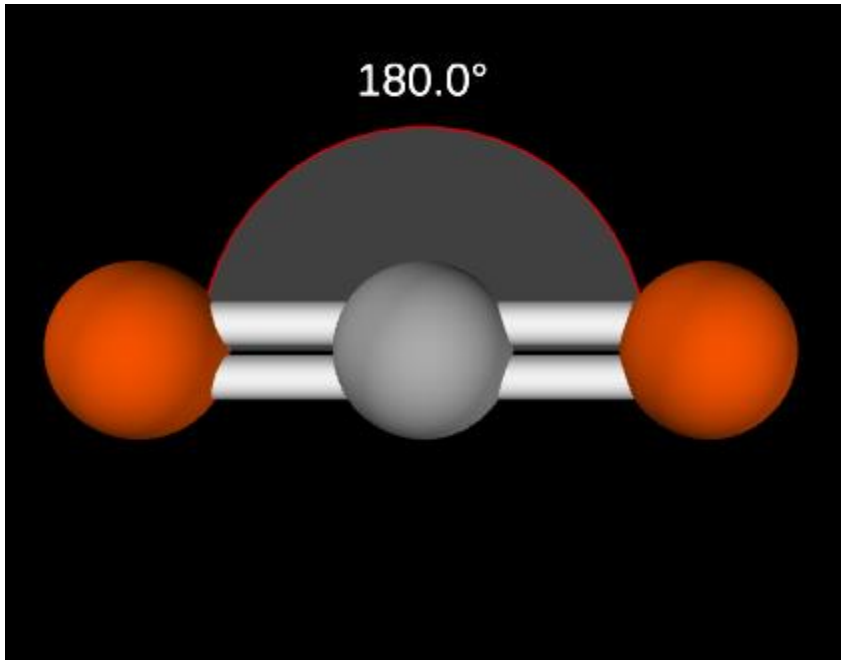
Two Electron Groups – Linear

- all of the atoms and bonds lie along the same line
- bond angles of 180°



Two Electron Groups

2 bonds, 0 lone pairs

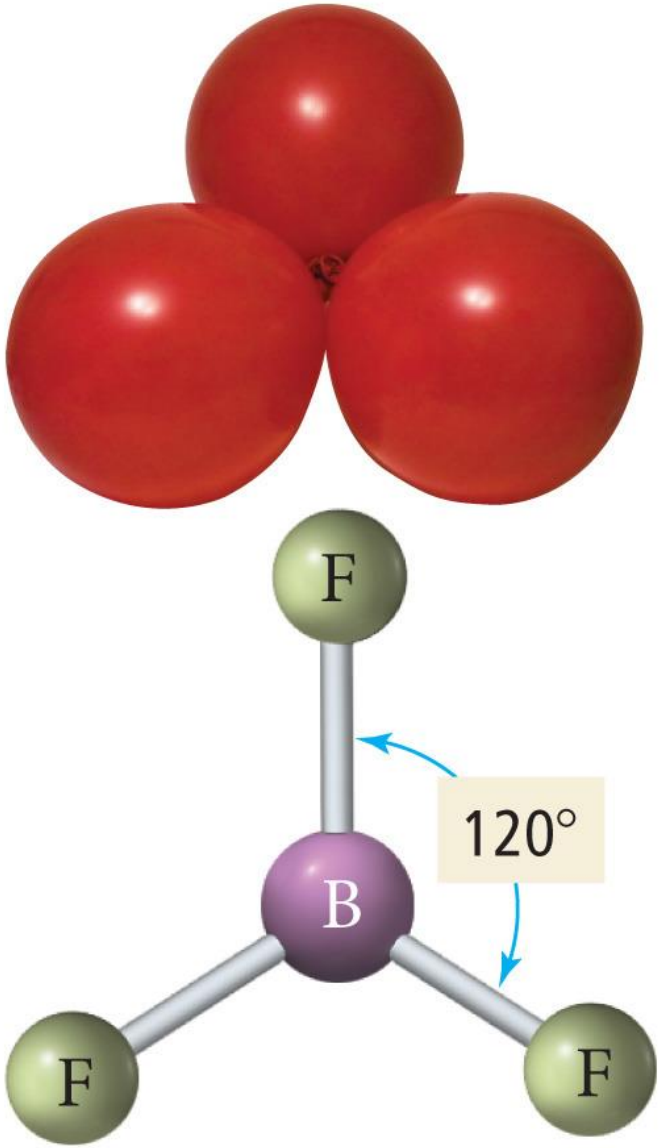


electron group geometry:
linear

molecular geometry:
linear

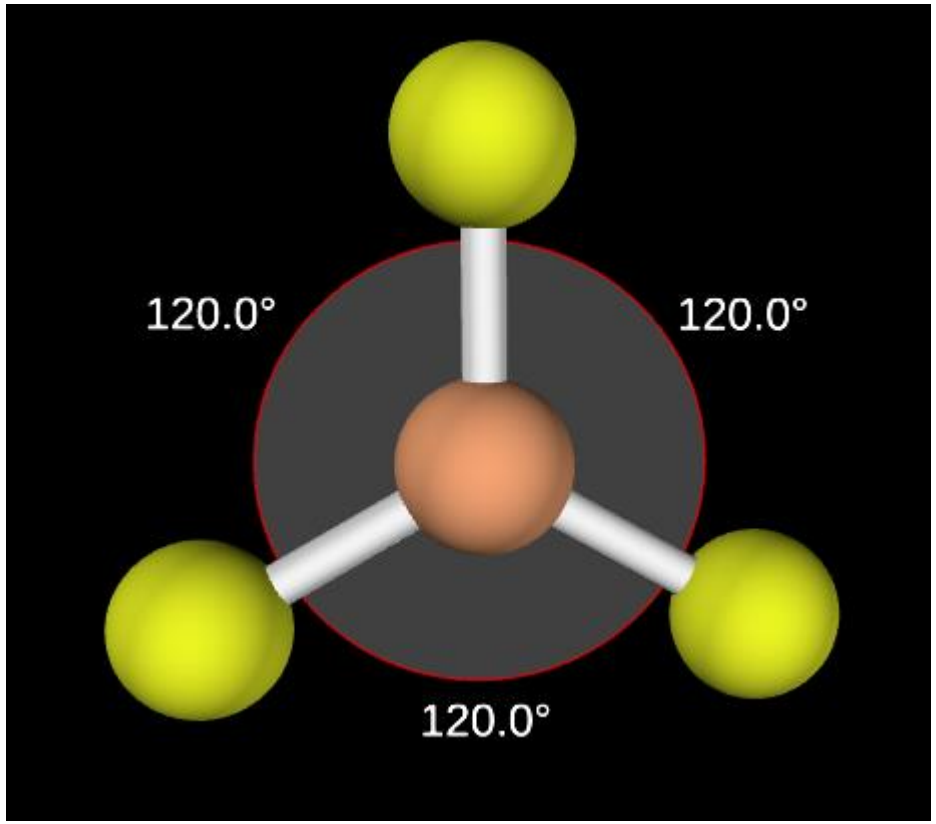
Three Electron Groups – Trigonal Planar

- trigonal = “triangle” and planar = “flat”
- all of the atoms/bonds lie in the same plane
  - a flat molecule
- bond angles of 120°



Three Electron Groups

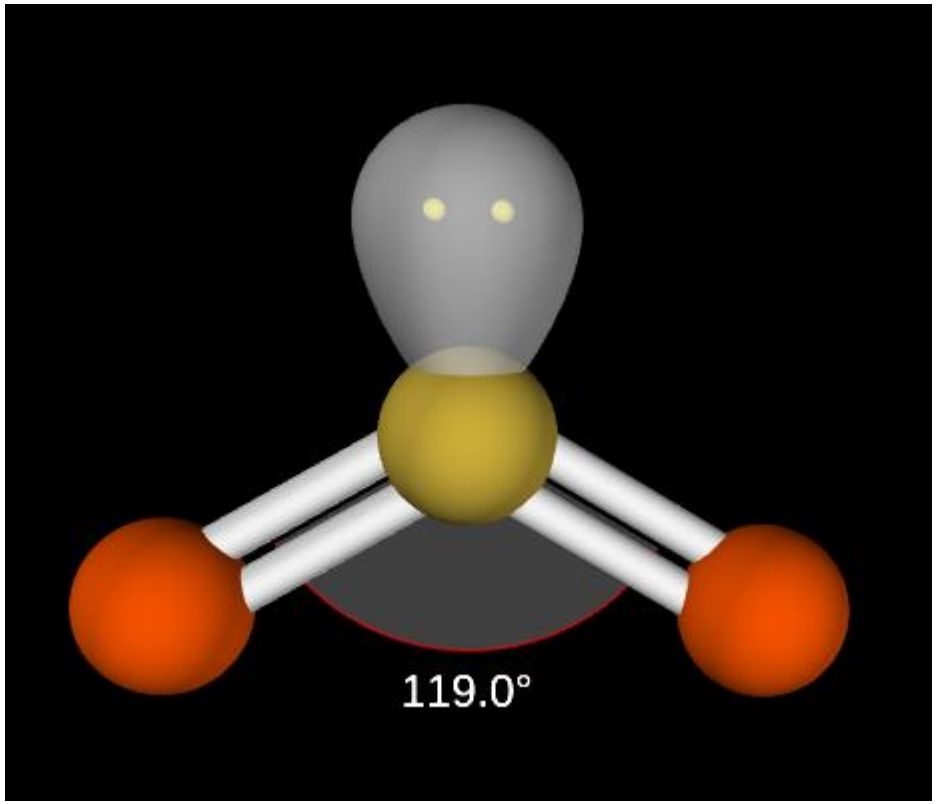
3 bonds, 0 lone pairs



electron group geometry:
trigonal planar

molecular geometry:
trigonal planar

2 bonds, 1 lone pair

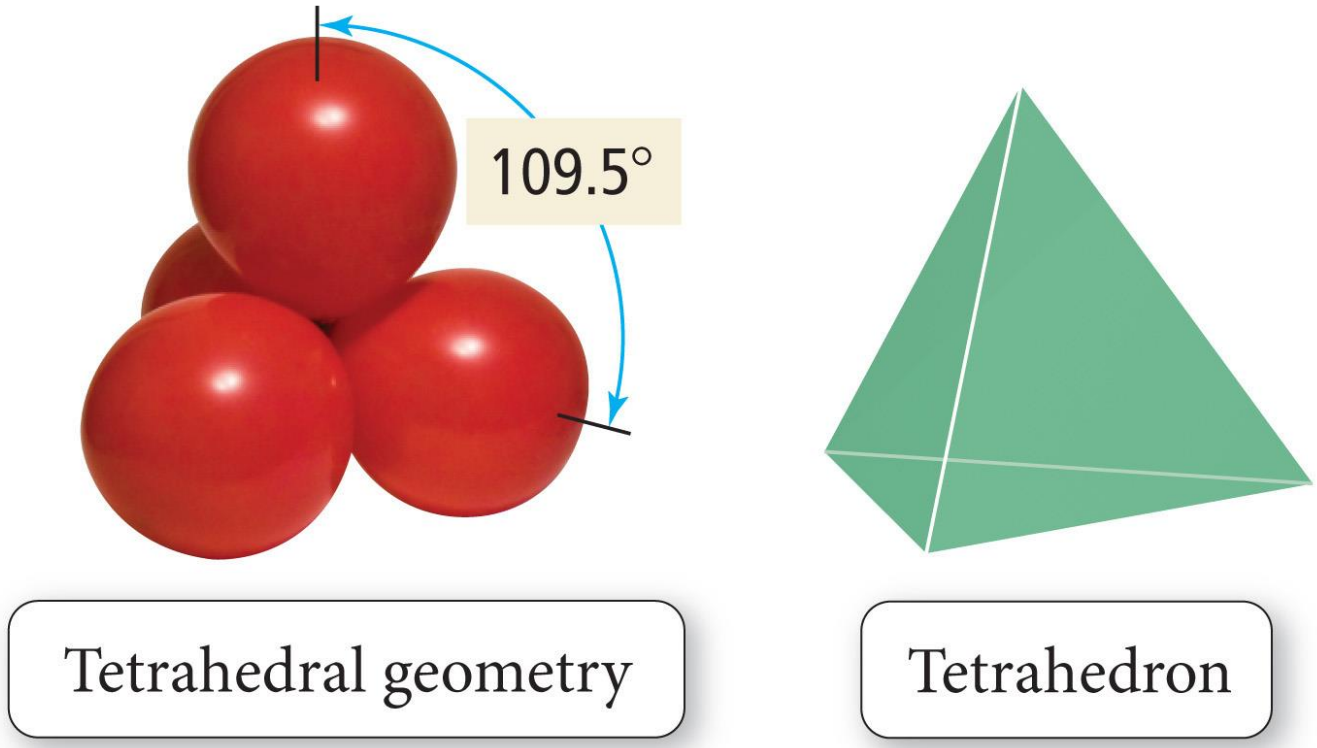


electron group geometry:
trigonal planar

molecular geometry:
bent

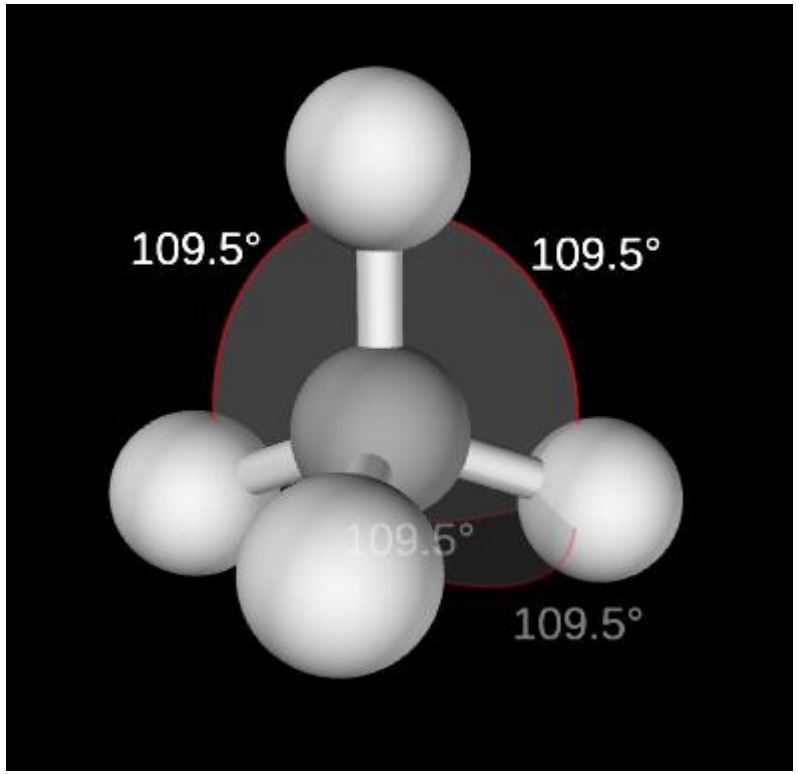
Four Electron Groups – Tetrahedral

- three-dimensional shape
- bond angles of 109.5°



Four Electron Groups

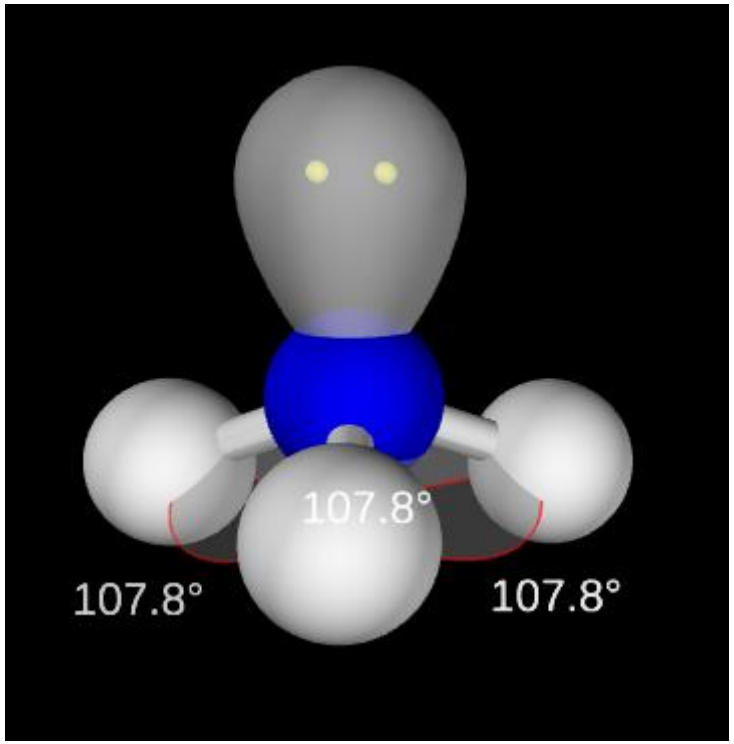
4 bonds, 0 lone pairs



electron group geometry:
tetrahedral

molecular geometry:
tetrahedral

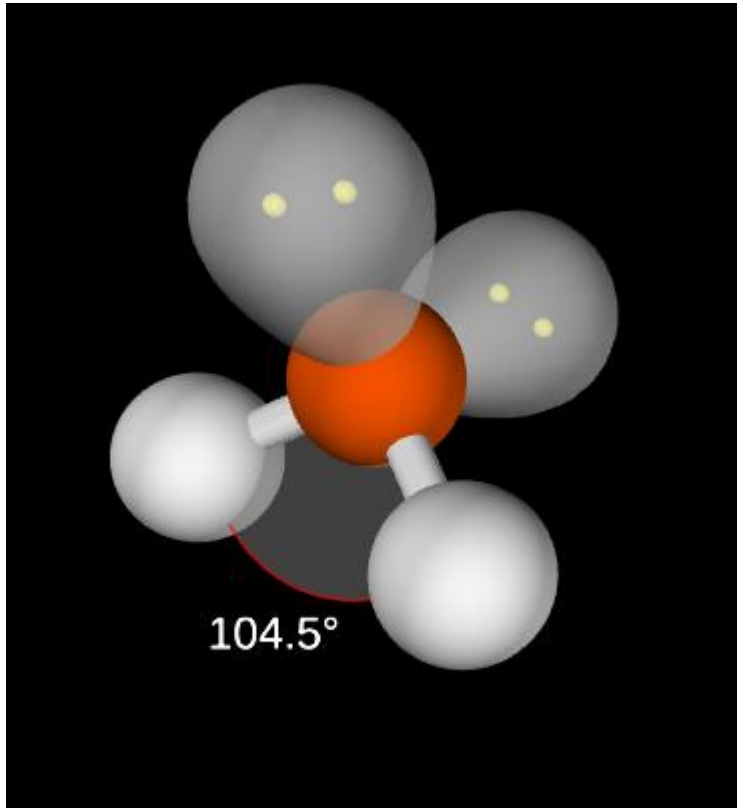
3 bonds, 1 lone pair



electron group geometry:
tetrahedral

molecular geometry:
trigonal pyramidal

2 bonds, 2 lone pairs

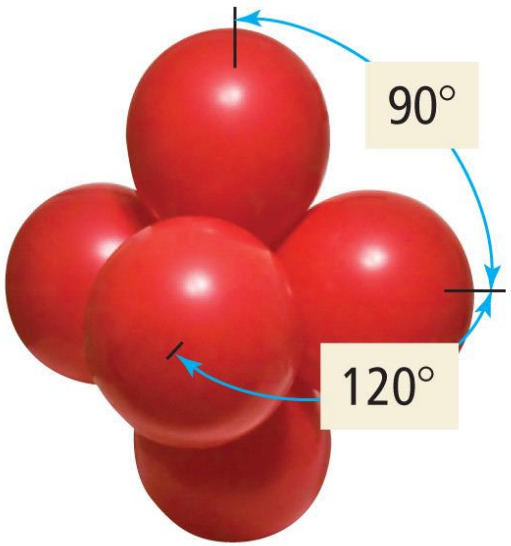


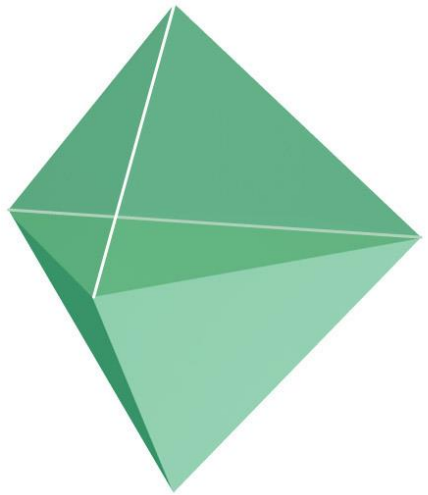
electron group geometry:
tetrahedral

molecular geometry:
bent

Five Electron Groups – Trigonal Bipyramidal

- trigonal = “triangle” and bipyramidal = “two pyramids”
- axial positions vs. equatorial positions
- bond angles of 90°, 120°, and 180°



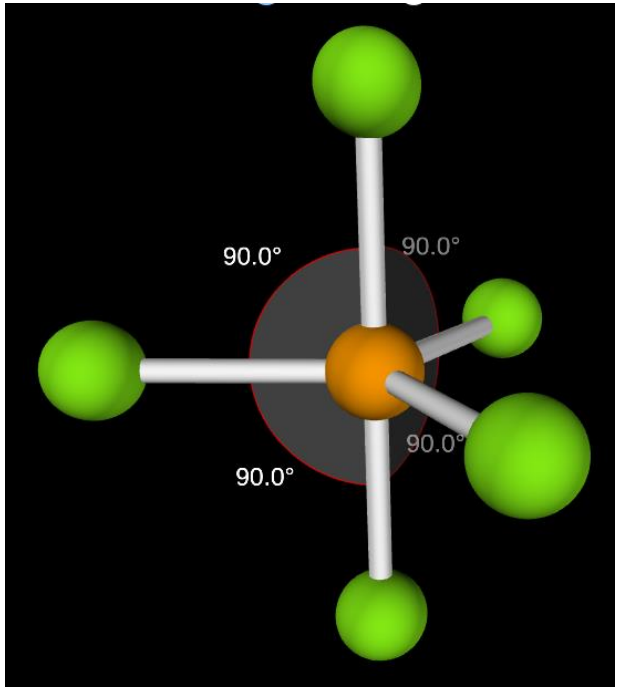


Trigonal bipyramidal geometry

Trigonal bipyramid

Five Electron Groups

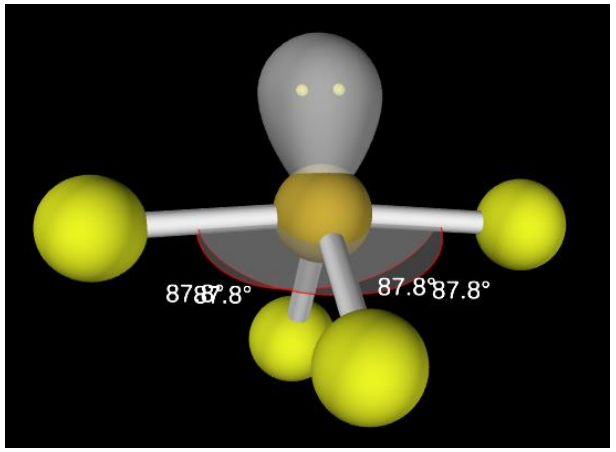
5 bonds, 0 lone pairs



electron group geometry:
trigonal bipyramidal

molecular geometry:
trigonal bipyramidal

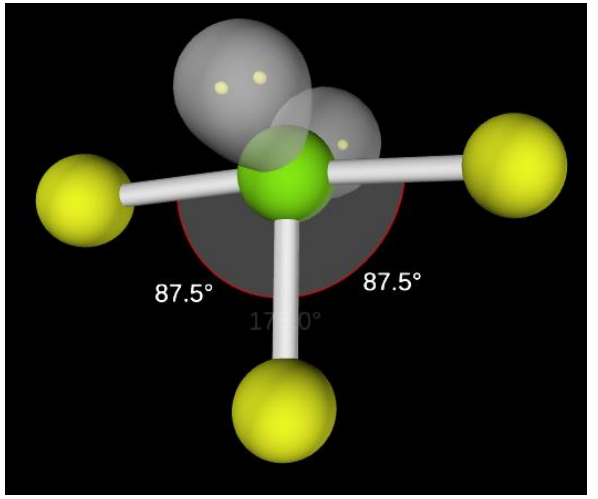
4 bonds, 1 lone pair



electron group geometry:
trigonal bipyramidal

molecular geometry:
seesaw

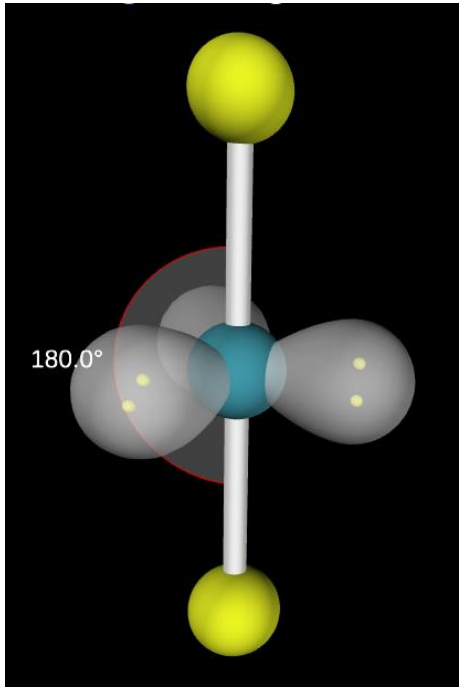
3 bonds, 2 lone pairs



electron group geometry:
trigonal bipyramidal

molecular geometry:
T-shape

2 bonds, 3 lone pairs

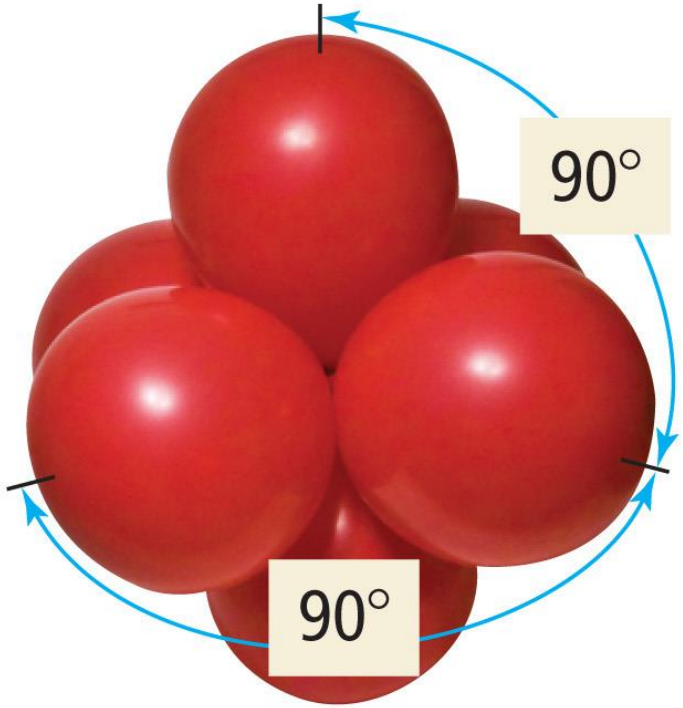


electron group geometry:
trigonal bipyramidal

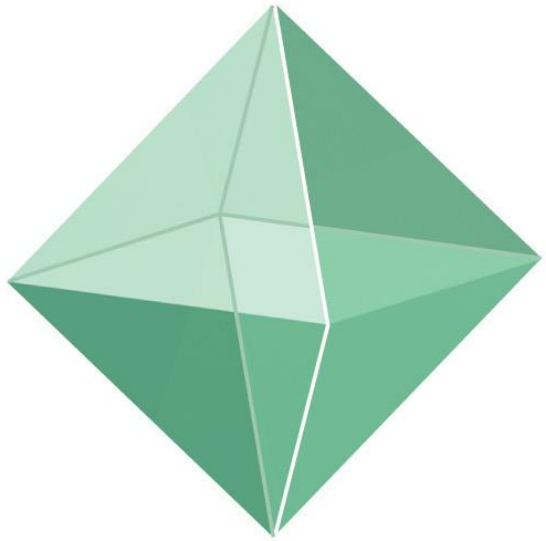
molecular geometry:
linear

Six Electron Groups – Octahedral

- all positions are equivalent
- bond angles of 90° and 180 °



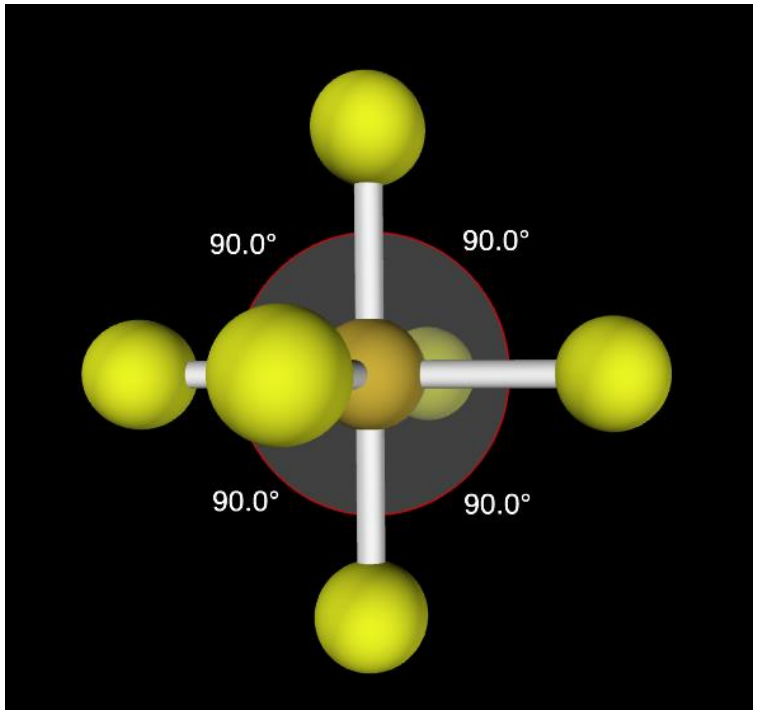
Octahedral geometry



Octahedron

Six Electron Groups

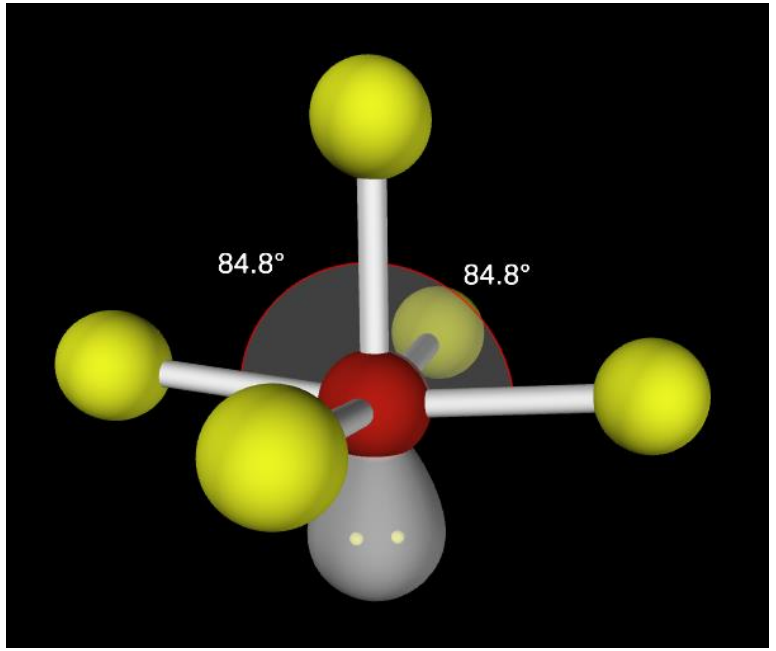
6 bonds, 0 lone pairs



electron group geometry:
octahedral

molecular geometry:
octahedral

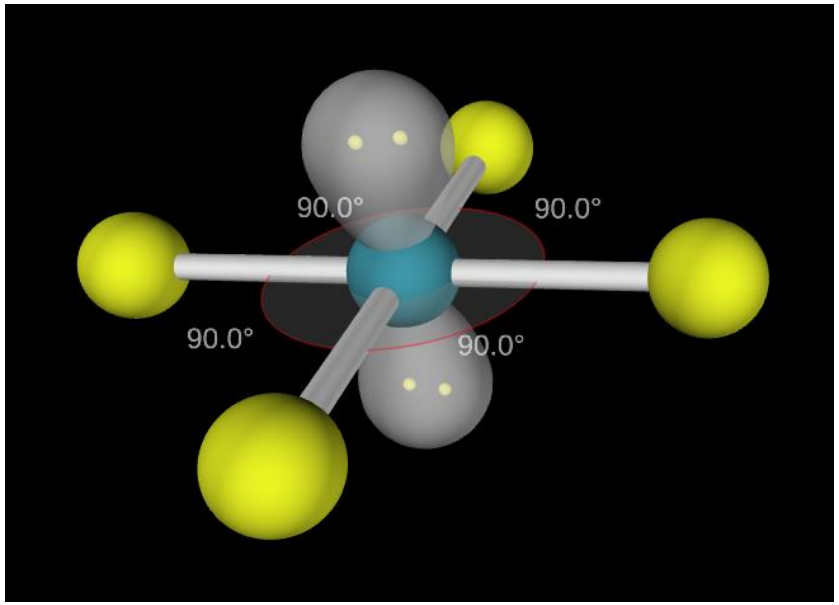
5 bonds, 1 lone pair



electron group geometry:
octahedral

molecular geometry:
square pyramidal

4 bonds, 2 lone pairs



electron group geometry:
octahedral

molecular geometry:
square planar

Electron Group Geometry

MEMORIZE THESE		
number of electron groups	**electron group geometry**	**ideal bond angles**
2	linear	180°
3	trigonal planar	120°
4	tetrahedral	109.5°
5	trigonal bipyramidal	90°, 120°, and 180°
6	octahedral	90° and 180°

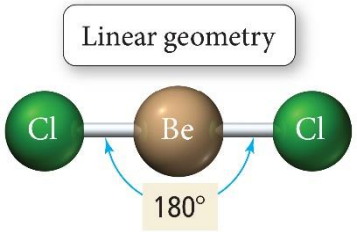
Molecular Geometry

DON'T MEMORIZE THESE **– DERIVE THEM** from the e^- group geometries		
number of electron groups	**possible molecular geometries**	**bond angles**
2	linear	180°
3	trigonal planar	120°
	bent	**< 120°**
4	tetrahedral	109.5°
	trigonal pyramidal	< 109.5°
	bent	**< 109.5°**
5	trigonal bipyramidal	90° (axial/equatorial), 120°(equatorial/equatorial), and 180°(axial/axial)
	seesaw	< 90°(axial/equatorial), < 120°(equatorial/equatorial), and < 180° (axial/axial)
	T-shaped	< 90°(axial/equatorial) and < 180° (axial/axial)
	linear	180°(axial/axial)
6	octahedral	90° and 180°
	square pyramidal	< 90° and < 180°
	square planar	90° and 180°

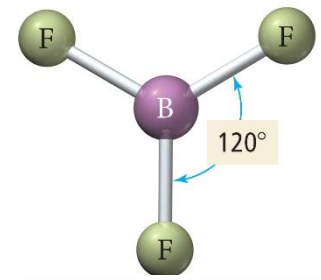
Molecular Geometries

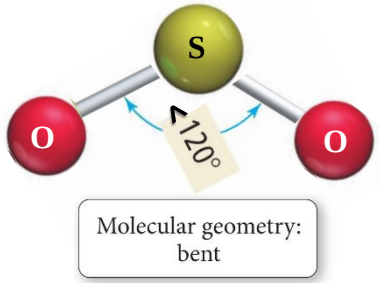
- **know 'em…**

2 e⁻ groups

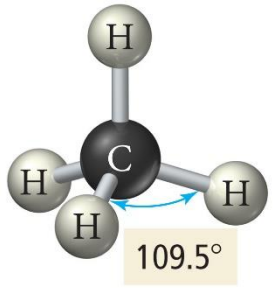


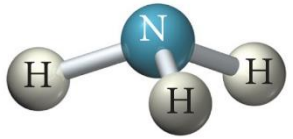
3 e⁻ groups

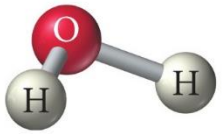




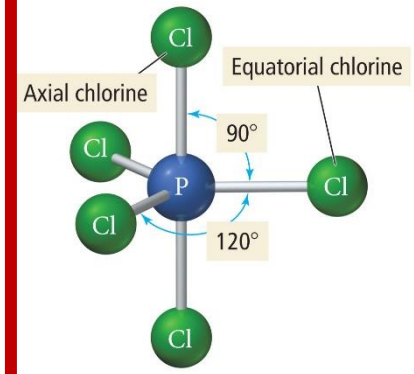
4 e⁻ groups

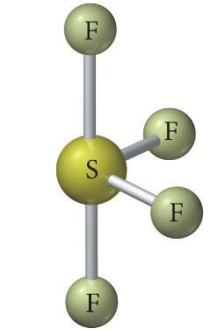


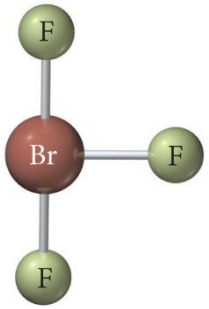




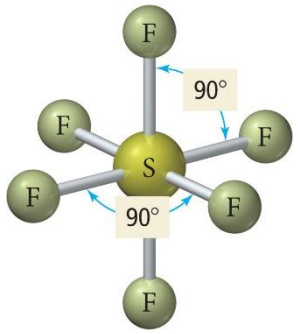
5 e⁻ groups

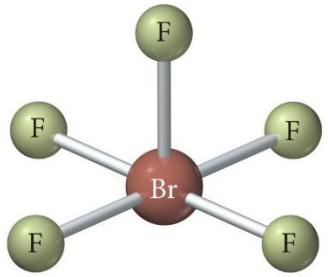


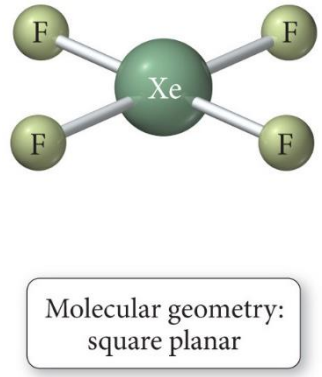




6 e⁻ groups







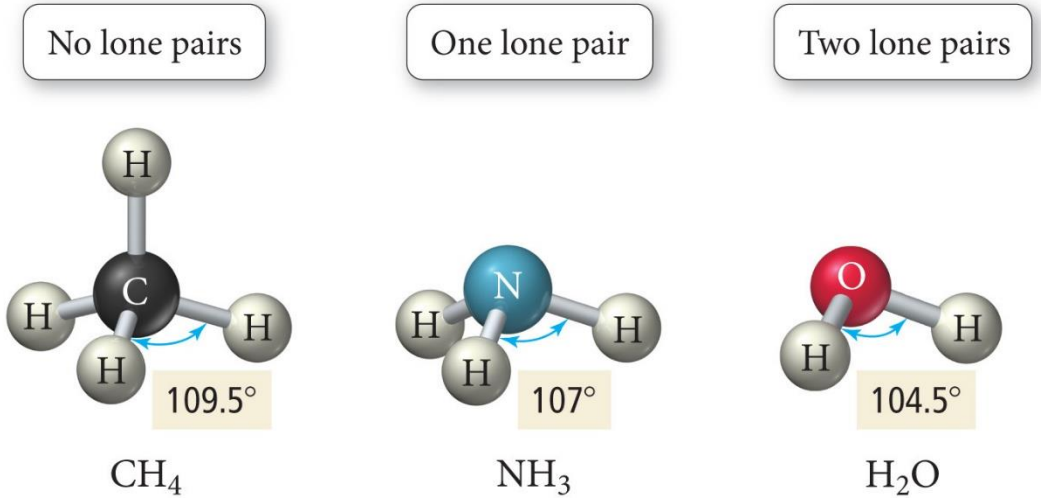
Deviation from Ideal Bond Angles

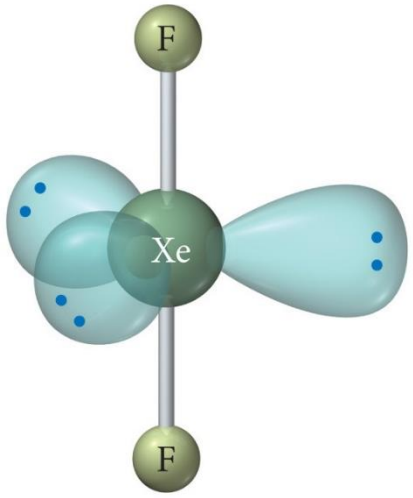
- the presence of lone pairs *unsymmetrically* around the central atom will cause the bond geometries to deviate from their ideal values
  - the H–O–H bond angle of water is 104.5° (5° less than what it is predicted to be)
- lone pairs repel bonding electrons, causing compression of bond angles

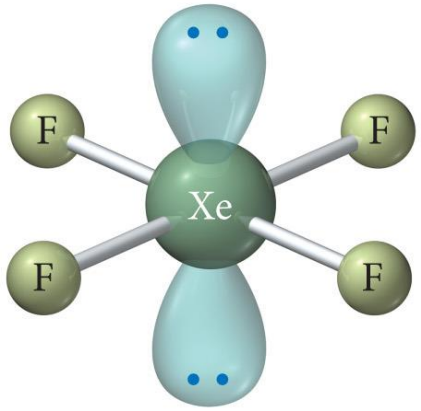
lp/lp repulsion > lp/bp repulsion > bp/bp repulsion

lp = lone pair and bp = bonding pair

- in general, more lone pairs around the central atom = more angle compression
  - CH_4 vs. NH_3 vs. H_2O
- if lone pairs are ***symmetrically*** distributed, then bond angles won't deviate
  - XeF_2 (180°) and XeF_4 (90°)





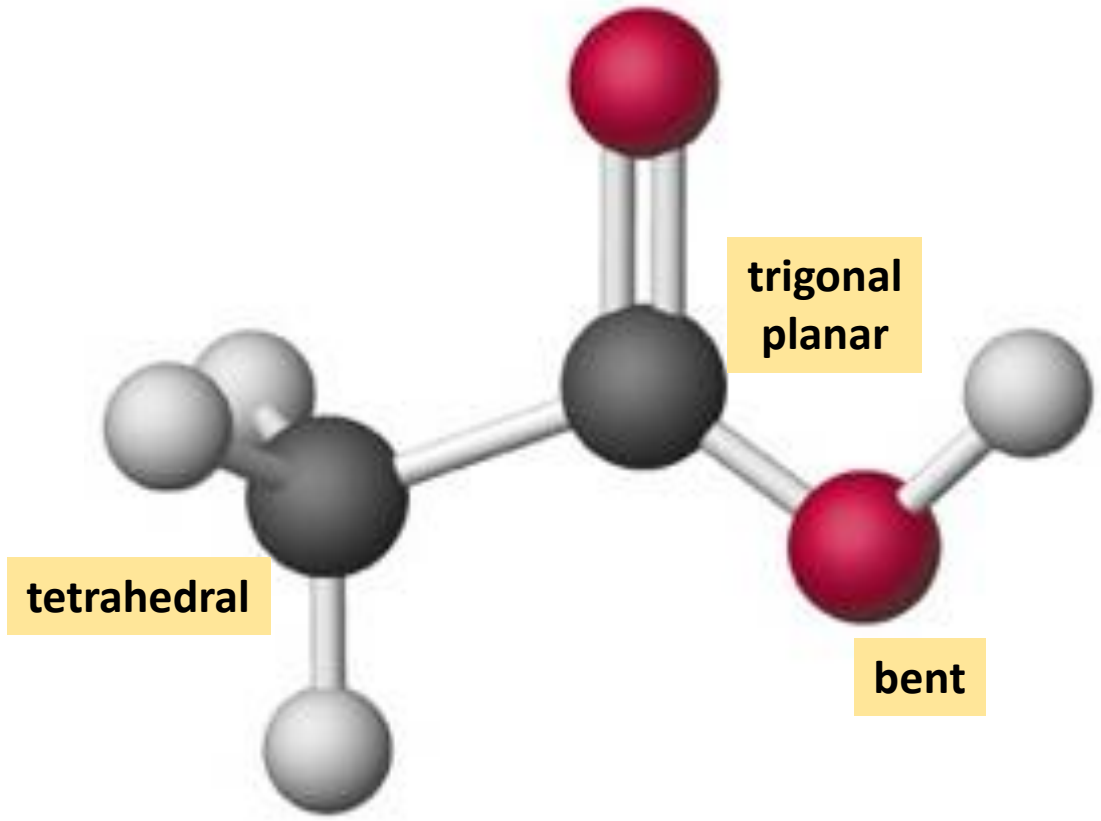


Deriving Molecular Geometry from Electron Group Geometry

1. establish the number of electron groups around the central atom
2. establish the electron group geometry and ideal bond angles
3. mentally replace the necessary bonds around the central atom with lone pairs according to the Lewis structure of the molecule
   a. in trigonal bipyramidal, only replace equatorial bonds with lone pairs, not axial bonds
   b. in octahedral, maximize distance between lone pairs by replacing bonds that are 180° apart from each other
4. adjust bond angles due to the presence of lone pairs around central atom
5. see what geometry the molecule has by focusing only on the arrangement of bonds (not lone pairs)

Shapes of Larger Molecules

- molecules with two or more interior/central atoms
- the overall shape of the molecule will be determined by the shape around each interior atom
  - example: acetic acid (CH_3COOH)



Try This On Your Own

Predict the electron geometry, molecular geometry, and approximate bond angle(s) for the following species: