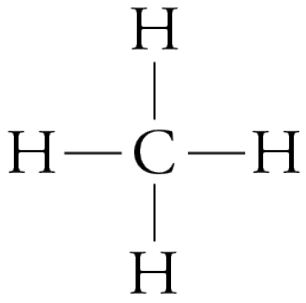
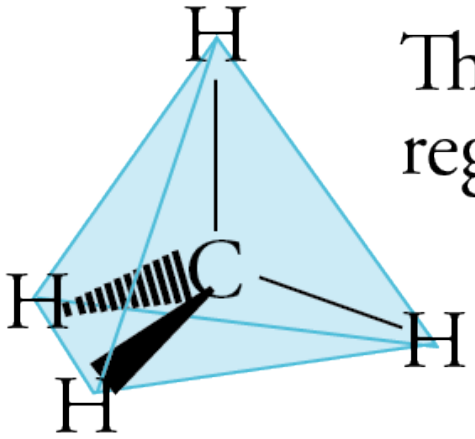
Molecular Shape and Function

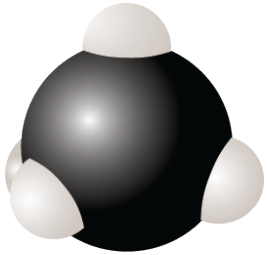
- The shapes of molecules play a major role in determining their function.
- The shape of ethanol molecules allows them to fit into specific sites on nerve cell membranes and slow the transfer of information from one neuron to another.
- There are enzymes in your body that can speed necessary chemical reactions up to millions of times faster than they would go without the enzymes, and for the enzymes to do their job, the reactants must have the correct shape to fit into a portion of the enzyme called the active site.

Methane, CH_4

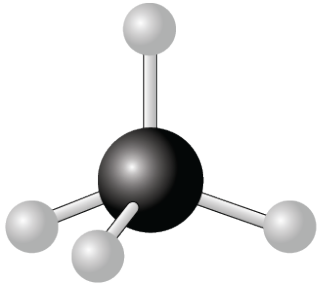




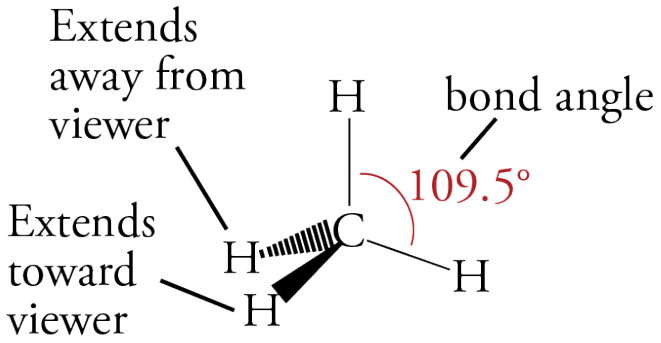
The shaded shape is a regular tetrahedron.



Space-filling model

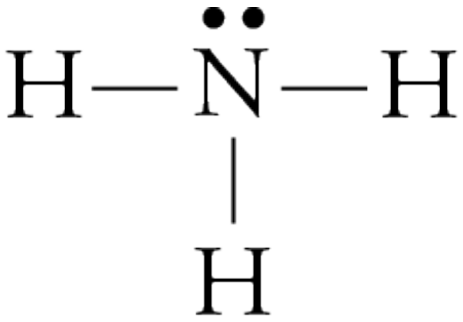


Ball-and-stick model



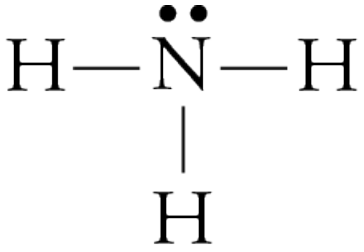
Geometric Sketch

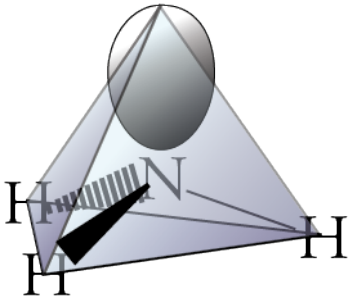
Ammonia, NH_3



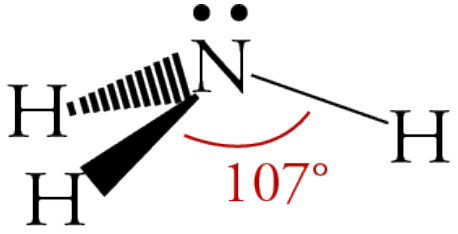
- The ammonia molecule has four electron groups around the central nitrogen atom: three single bonds and one lone pair.
- Each of the following is considered an electron group.
  - Single bond
  - Multiple bond (double or triple bond)
  - Lone pair

Ammonia, NH_3





Electron group geometry
(tetrahedral)

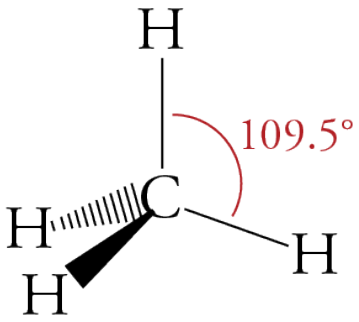


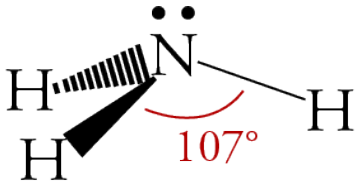
Molecular geometry
(trigonal pyramid)

- **Electron group geometry** describes the arrangement of all of the electron groups, including lone pairs.
- **Molecular geometry** just describes the arrangement of the atoms.

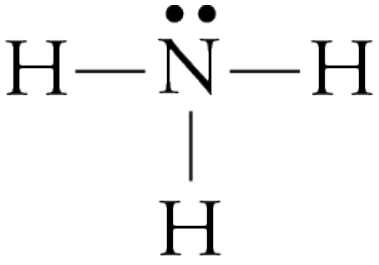
Molecular Geometry

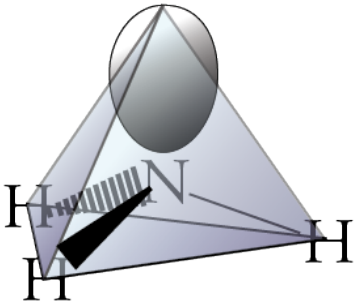
- Being able to predict the ***electron group geometry*** around an atom is useful because it allows us to predict the approximate bond angles and guides us in drawing the geometric sketch.
- Sometimes it's useful to describe the arrangement of atoms in terms of the ***molecular geometry***, which disregards the lone pairs on central atoms.



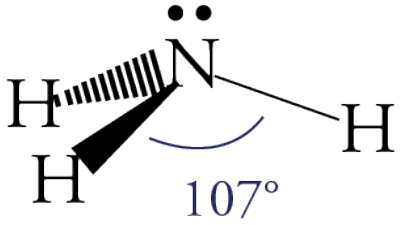


Ammonia, NH_3

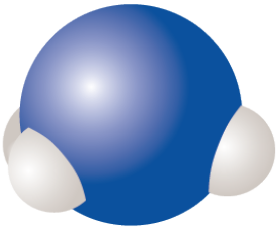




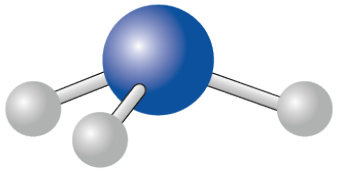
Electron group geometry
(tetrahedral)



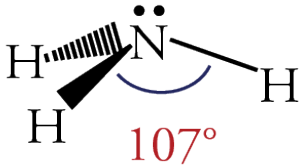
Molecular geometry
(trigonal pyramid)



Space-filling model



Ball-and-stick model

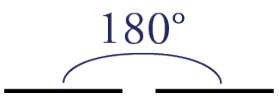
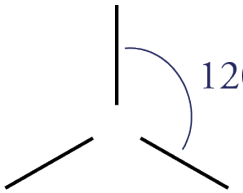
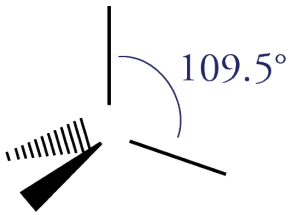


Geometric sketch

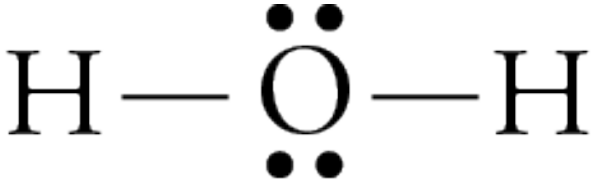
Steps for Molecular Geometry

- **Step 1:** Count the number of electron groups around each central atom.
- **Step 2:** Apply the guidelines found on Table 5.2 of the atoms-first version of my text or Table 12.3 of the chemistry-first version.
- The following are electron groups.
  - A single bond
  - A multiple bond (double or triple) counts as one group.
  - A lone pair

Predicting Molecular Geometry

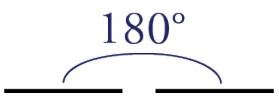
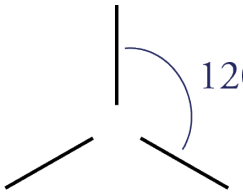
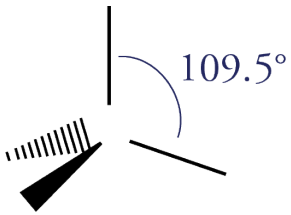
e- groups	e- group geometry	General geometric sketch	Bond angles	Bond groups	Lone pairs	molecular geometry
2	linear		180°	2	0	linear
3	trigonal planar		120°	3	0	trigonal planar
				2	1	bent
4	tetrahedral		109.5°	4	0	tetrahedral
				3	1	trigonal pyramid
				2	2	bent

Water, H_2O

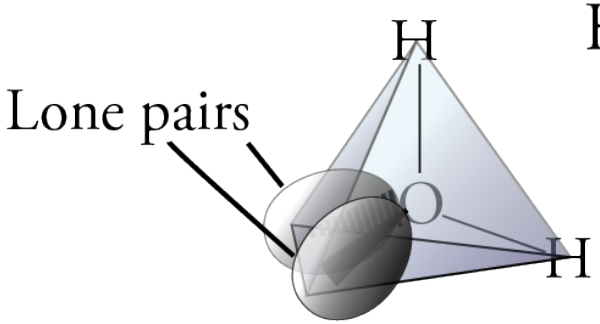


- The water molecule has four electron groups around the central oxygen atom: two single bonds and two lone pairs.

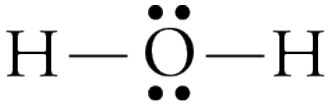
Predicting Molecular Geometry

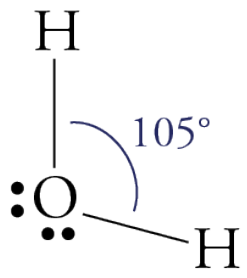
e- groups	e- group geometry	General geometric sketch	Bond angles	Bond groups	Lone pairs	molecular geometry
2	linear		180°	2	0	linear
3	trigonal planar		120°	3	0	trigonal planar
				2	1	bent
4	tetrahedral		109.5°	4	0	tetrahedral
				3	1	trigonal pyramid
				2	2	bent

Water, H_2O

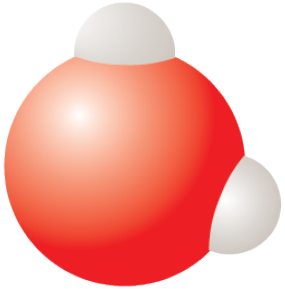


Electron group geometry
(tetrahedral)

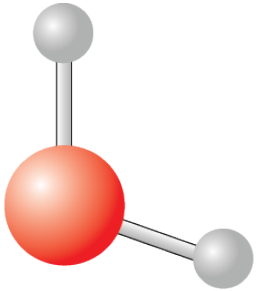




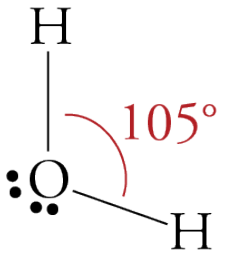
Molecular geometry
(bent)



Space-filling model

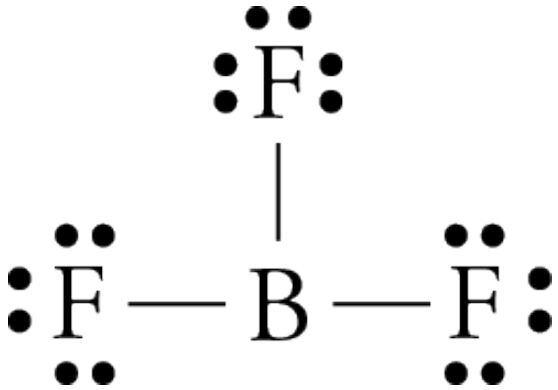


Ball-and-stick model



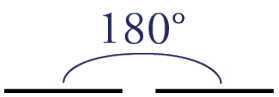
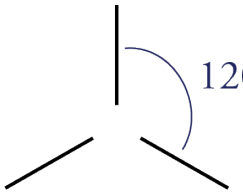
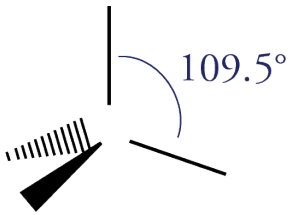
Geometric Sketch

Boron Trifluoride, BF_3

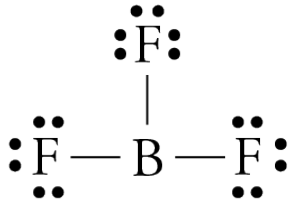


- The boron trifluoride molecule has three electron groups around the central boron atom: three single bonds.

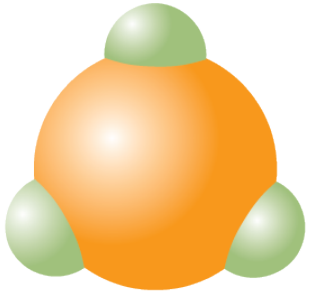
Predicting Molecular Geometry

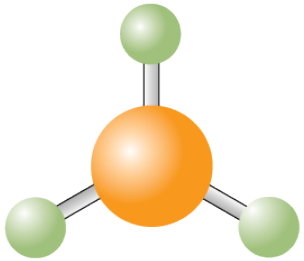
e- groups	e- group geometry	General geometric sketch	Bond angles	Bond groups	Lone pairs	molecular geometry
2	linear		180°	2	0	linear
3	trigonal planar		120°	3	0	trigonal planar
				2	1	bent
4	tetrahedral		109.5°	4	0	tetrahedral
				3	1	trigonal pyramid
				2	2	bent

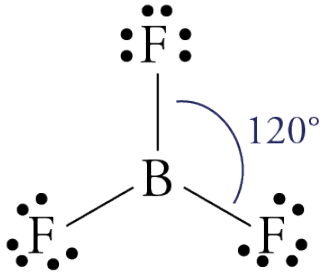
Trigonal Planar Geometry – BF_3



Lewis structure

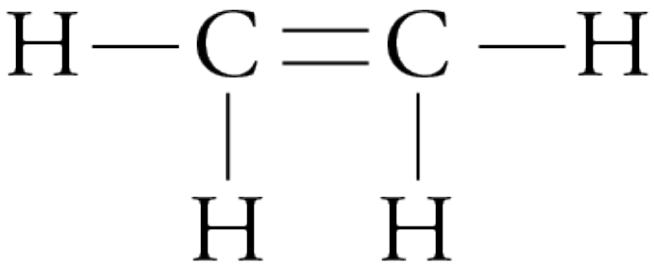

Space-filling model


Ball-and-stick model



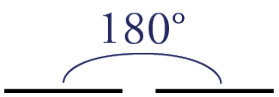
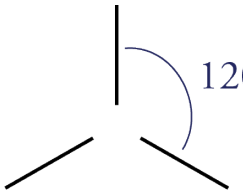
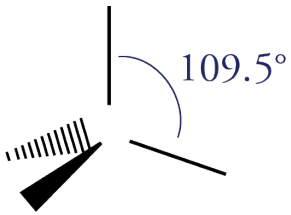
Geometric Sketch

Ethene, C_2H_4

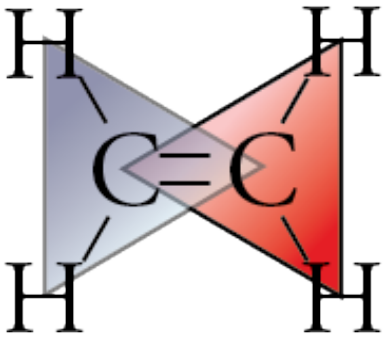


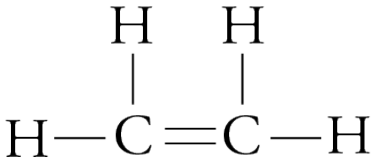
- Ethene (often called ethylene) has two central atoms, so we consider them separately.
- They each have three electron groups around them: two single bonds and a double bond.

Predicting Molecular Geometry

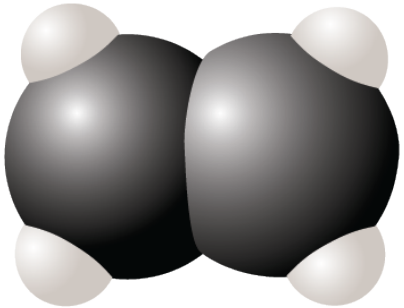
e- groups	e- group geometry	General geometric sketch	Bond angles	Bond groups	Lone pairs	molecular geometry
2	linear		180°	2	0	linear
3	trigonal planar		120°	3	0	trigonal planar
				2	1	bent
4	tetrahedral		109.5°	4	0	tetrahedral
				3	1	trigonal pyramid
				2	2	bent

Ethene (ethylene)

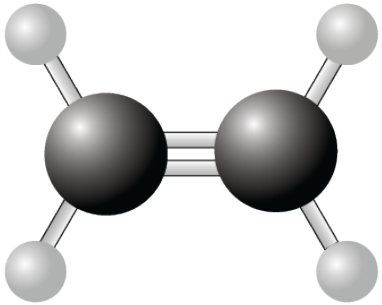




Lewis structure

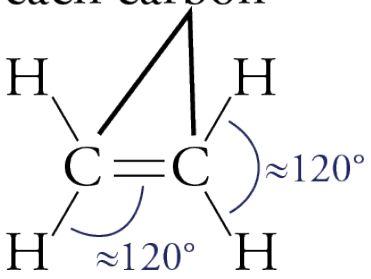


Space-filling model



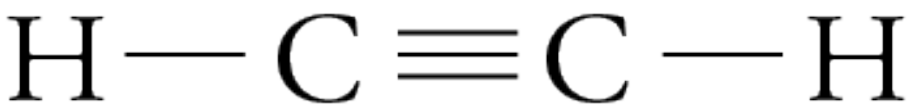
Ball-and-stick model

Trigonal planar geometry around each carbon



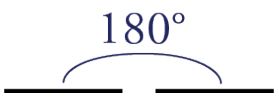
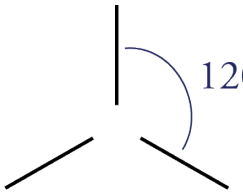
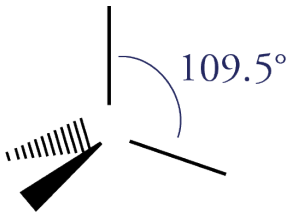
Geometric Sketch

Ethyne, C_2H_2



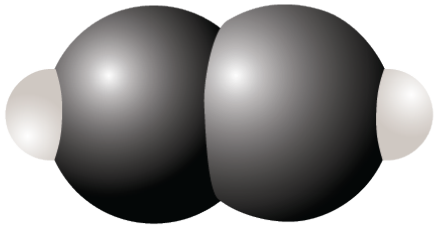
- Ethyne (often called acetylene) has two central atoms, so we consider them separately.
- They each have two electron groups around them: one single bond and one triple bond.

Predicting Molecular Geometry

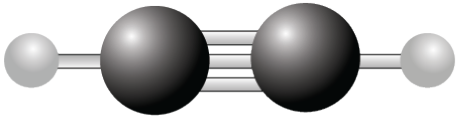
e- groups	e- group geometry	General geometric sketch	Bond angles	Bond groups	Lone pairs	molecular geometry
2	linear		180°	2	0	linear
3	trigonal planar		120°	3	0	trigonal planar
				2	1	bent
4	tetrahedral		109.5°	4	0	tetrahedral
				3	1	trigonal pyramid
				2	2	bent

Ethyne (acetylene) , C_2H_2

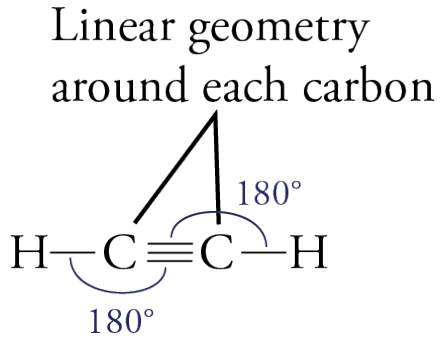
Lewis structure



Space-filling model



Ball-and-stick model



Geometric Sketch

Practice

- You can see more examples of this task by looking at Examples 5.9 and 5.10 in the atoms-first version of my text or Examples 12.6 and 12.7 of the chemistry-first version.
- You can get practice with this task by working Exercise 5.6 and the end-of-chapter problems in the atoms-first version or Exercise 12.3 and the end-of-chapter problems in the chemistry-first version.

https://preparatorychemistry.com/Bishop_Book_atoms_5.pdf

https://preparatorychemistry.com/Bishop_Book_12_eBook.pdf