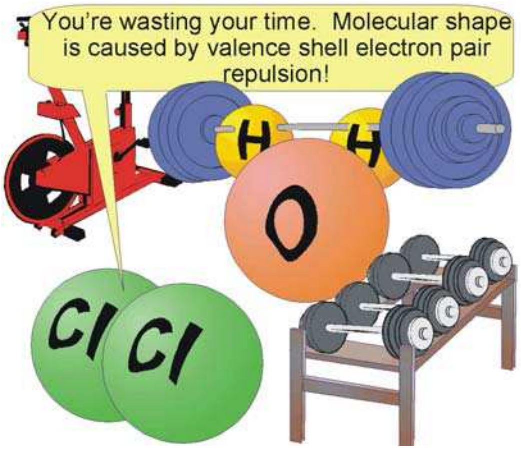
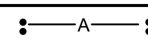
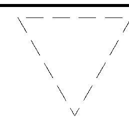
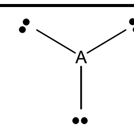
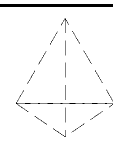
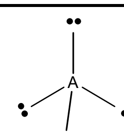
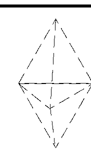
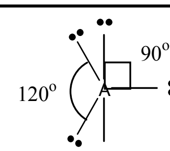
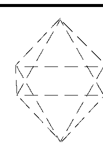
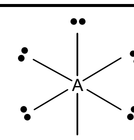
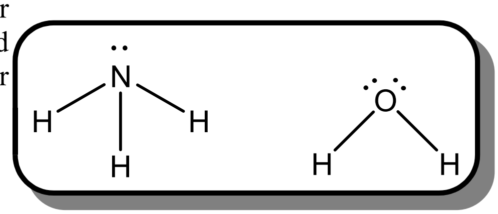
Predicting Molecular Shapes



One approach to predicting molecular shape is the valence shell electron repulsion model (VSEPR). According to VSEPR theory, repulsion between sets of valence shell electrons causes them to be as far apart as possible. Taking this repulsion into account, the shape of a molecule depends upon how many pairs of valence electrons surround the central atom, the number of lone pairs of electrons, and the presence of multiple bonds (double bonds or tripe bonds). Two pairs of valence electrons will be at 180° to each other producing a linear molecule, three pairs will be at 120° to each other in a single plane producing a trigonal planar molecule, and four pairs will be at 109.5° to each other producing a tetrahedral molecule, a three sided pyramid with a triangular base. The cental atom is in the center of the pyramid and the attached atoms are at the four apices. Five pairs of valence electrons around the central atom produces a trigonal bipyramid, a molecule with a trigonal planar portion having bond angles of 120° and two bonding sites above and below the plane at 90° to it. Six pairs of valence electrons around the central atom produces an octahedral molecule with 90°angles in all six directions. See below.

Number of Electron Pairs	Shape	Arrangement of Electron Pairs	
2	Linear	— — — — —	
3	Trigonal planar		
4	Tetrahedral		
5	Trigonal bipyramidal		
6	Octahedral		

If the central atom and has a full octet of valence electrons, but some of them are lone pairs, the bond angle changes from the standard 109.5° tetrahedral angle. Lone pairs of electrons increase the repulsion reducing the angle between bonded pairs. The shape of the molecule includes only the bonded atoms and not the lone pair electrons. As a result, ammonia (NH_3) is pyramidal with a bond angle of 107°, and water (H_2O) is bent with a bond angle of 105°. The bond angle is smaller in water than in ammonia because it has two lone pairs of electrons instead of one.



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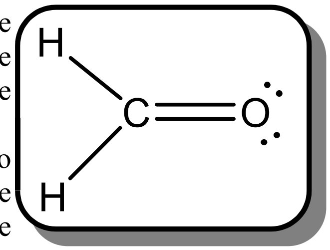
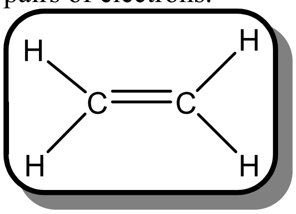
Double and triple bonds are treated like single bonds. As a result, CH_2O is trigonal planar. See the diagram to the right. The double bond between the oxygen and the carbon behaves like a single bond with one pair of electrons in the VSEPR model. This means that carbon has only three effective pairs of electrons.



For molecules in which there is no central atom, it is possible to predict the shape of sections of the molecule. In the molecule ethene (C_2H_4), for example, each of the carbons behaves like a central atom. The shape around each is trigonal planar. See the diagram to the left.



Draw the Lewis structures for each of the molecules below, and predict whether each is _Linear_, _Trigonal planar_, _Tetrahedral_, _Trigonal bipyramidal_, _Octahedral_, _Pyramidal_, or _Bent_.

1. C_2Cl_2
2. SO_3
3. CS_2
4. CF_4
5. AsF_5
6. SeI_6
7. H_2Te
8. AsF_3
9. SiO_2
10. NH_4^+
11. NO_3^-
12. PCl_5