19.8: Molecular Shapes - Lone Pair(s) on Central Atom


Figure 19.8.1(Used under license from Shutterstock.com; Image copyright Jandrie Lombard, 2014 via http://www.shutterstock.com)

How can all these clothes fit into such a small space?

When we travel, we often take a lot more stuff than we need. Trying to fit it all into a suitcase can be a real challenge. We may have to repack or just squeeze it all in. Atoms often have to rearrange where the electrons are in order to create a more stable structure.

Central Atom with One or More Lone Pairs

The molecular geometries of molecules change when the central atom has one or more lone pairs of electrons. The total number of electron pairs, both bonding pairs and lone pairs, leads to what is called the **electron domain geometry**. When one or more of the bonding pairs of electrons is replaced with a lone pair, the molecular geometry (actual shape) of the molecule is altered. In keeping with the A and B symbols established in the previous section, we will use E to represent a lone pair on the central atom (A). A subscript will be used when there is more than one lone pair. Lone pairs on the surrounding atoms (B) do not affect the geometry.

AB_3E: Ammonia, NH_3

The ammonia molecule contains three single bonds and one lone pair on the central nitrogen atom (see figure below).

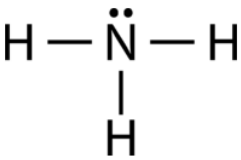
Figure 19.8.2 Lone pair electrons in ammonia. (CC BY-NC 3.0; Joy Sheng via CK-12 Foundation)

The domain geometry for a molecule with four electron pairs is tetrahedral, as was seen with CH_4. In the ammonia molecule, one of the electron pairs is a lone pair rather than a bonding pair. The molecular geometry of NH_3 is called trigonal pyramidal (see figure below).

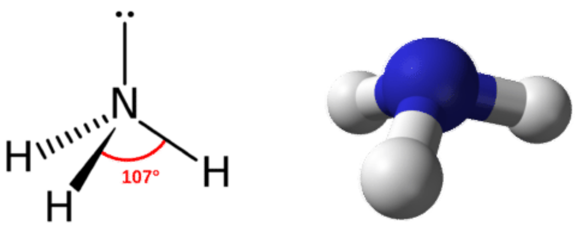

Figure 19.8.3Ammonia molecule. (Public Domain; (Left) User: Booyabazooka/ Wikimedia Commons; (Right) Ben Mills (Wikimedia: Benjah-bmm27) via (Left) http://commons.wikimedia.org/wiki/File:Ammonia_lone_electron_pair.svg; (Right) http://commons.wikimedia.org/wiki/File:Ammonia-3D-balls-A.png)

Recall that the bond angle in the tetrahedral CH_4 molecule is 109.5^o. Again, the replacement of one of the bonded electron pairs with a lone pair compresses the angle slightly. The $H-N-H$ angle is approximately 107^o.

AB_2E_2: Water, H_2O

A water molecule consists of two bonding pairs and two lone pairs (see figure below).

Figure 19.8.4 Lone pair electrons on water. (CC BY-NC 3.0; Joy Sheng via CK-12 Foundation)

As for methane and ammonia, the domain geometry for a molecule with four electron pairs is tetrahedral. In the water molecule, two of the electron pairs are lone pairs rather than bonding pairs. The molecular geometry of the water molecule is bent. The $H-O-H$ bond angle is 104.5^{o}, which is smaller than the bond angle in NH_3 (see figure below).

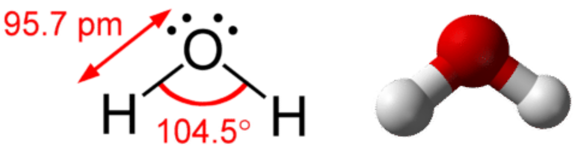

Figure 19.8.5 Water molecule. (Public Domain; Ben Mills (Wikimedia: Benjah-bmm27) via (Left) http://commons.wikimedia.org/wiki/File:Water-dimensions-from-Greenwood%2526Earnshaw-2D.png; (Right) http://commons.wikimedia.org/wiki/File:Water-3D-balls-A.png; http://commons.wikimedia.org/wiki/File:Zeepzieden.jpg)

AB_4E: Sulfur Tetrafluoride, SF_4

The Lewis structure for SF_4 contains four single bonds and a lone pair on the sulfur atom (see figure below).

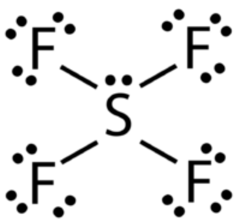

Figure 19.8.6 Lone pair electrons in SF_4. (CC BY-NC 3.0; Joy Sheng via CK-12 Foundation)

The sulfur atom has five electron groups around it, which corresponds to the trigonal bipyramidal domain geometry, as in PCl_5 (see figure below). Recall that the trigonal bipyramidal geometry has three equatorial atoms and two axial atoms attached to the central atom. Because of the greater repulsion of a lone pair, it is one of the equatorial atoms that are replaced by a lone pair. The geometry of the molecule is called a distorted tetrahedron, or seesaw.

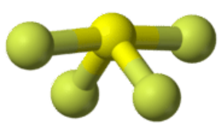

Figure 19.8.7 Ball and stick model for SF_4. (Public Domain; Ben Mills (Wikimedia: Benjah-bmm27) via Wikipedia)

Table 19.8.1: Geometries in Which the Central Atom Has One or More Lone Pairs

Total Number of Electron Pairs	Number of Bonding Pairs	Number of Lone Pairs	Electron Domain Geometry	Molecular Geometry	Examples
3	2	1	Trigonal Planar	Bent	O_3
4	3	1	Tetrahedral	Trigonal Pyramidal	NH_3
4	2	2	Tetrahedral	Bent	H_2O
5	4	1	Trigonal Bipyramidal	Distorted Tetrahedron (Seesaw)	SF_4
5	3	2	Trigonal Bipyramidal	T-shaped	ClF_3
5	2	3	Trigonal Bipyramidal	Linear	I_3^-
6	5	1	Octahedral	Square Pyramidal	BrF_5

Total Number of Electron Pairs	Number of Bonding Pairs	Number of Lone Pairs	Electron Domain Geometry	Molecular Geometry	Examples
6	4	2	Octahedral	Square Planar	XeF_4

Summary

- The presence of lone pair electrons influences the three-dimensional shape of the molecule.

Review

1. Why does water have a bent geometry?
2. Why is ammonia not a planar molecule?
3. How would we write the configuration for xenon tetrafluoride using the ABE system?

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