Molecular Properties

Objective

Models will be built according to the VSEPR theory to illustrate the regular patterns that occur in the shapes of molecules.

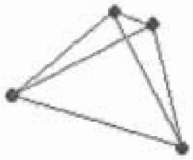
Introduction – (more information on ~~pg. 380-400~~ in textbook)

The basic explanation of molecular shapes arises from the shell electron-pair repulsion theory, usually known by its abbreviation, **VSEPR.** This theory considers the environment of the most central atom in a molecule and imagines first how the valence electron pairs of that central atom must be arranged in three-dimensional space around the atom to minimize repulsion among the electron pairs. The general principle is: For a given number of pairs of electrons, the pairs will be oriented in three-dimensional space to be as *far away from each other as possible.* For example, if a central atom were to have only two pairs of valence electrons in it, the electron pairs would be expected to be 180° from each other.

The VSEPR theory then also considers which of the electron pairs around the central atom are **bonding pairs** (with atoms attached) and which are **nonbonding pairs** (lone pairs). The overall geometric shape of the molecule as a whole is determined by *how many* pairs of electrons are on the central atom and by which of those pairs are used for *bonding* to other atoms.

Consider the Lewis structures of the following four molecules: HCl, H_2O, NH_3, and CH_4.

The central atom in each of these molecules is surrounded by four pairs of valence electrons. According to the VSEPR theory, these four pairs of electrons will be oriented in three-dimensional space to be as far away from each other as possible. The four pairs of electrons point to the corners of the geometric figure known as a **tetrahedron.** The four pairs of electrons are said to be *tetrahedrally oriented* and are separated by angles of approximately 109.5°.

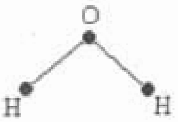


However, three of the molecules shown are *not* tetrahedral in *overall shape,* because some of the valence electron pairs in the HCl, H_2O, and NH_3 molecules are not *bonding* pairs. The shape of the molecule should describe the relative location of the molecule's nuclei (atoms). The angular position of the bonding pairs (and hence the overall shape of the molecule) is determined by the *total* number of valence electron pairs on the central atom, but the nonbonding electron pairs are *not* included in the description of the molecules' overall shape because they have no mass.

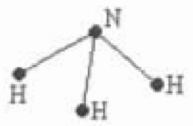
For example: (see pg. 392 F 8.17)

• The HCl molecule could hardly be said to be tetrahedral in shape, since there are only two atoms in the molecule. HCl is linear even though the valence electron pairs of the chlorine atom are tetrahedrally oriented.

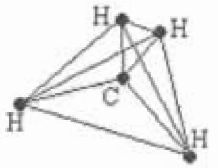
• Similarly, the H_2O molecule cannot be tetrahedral. Water is said to be V-shaped (bent, or nonlinear), the nonlinear shape being a result of the tetrahedral orientation of the valence electron pairs of oxygen.



• Ammonia's overall shape is said to be that of a trigonal (triangular) pyramid.



• Of the four molecules used as examples, only methane (CH_4) has both tetrahedrally oriented valence electron pairs and an overall geometric shape that can be described as tetrahedral (since all four pairs of electrons about the central atom are bonding pairs).



Thus the electron pairs help to determine how the atoms will be arranged. During this experiment, you will construct a small model of each structure and measure the bond angles with a protractor, sketch the structure and try to approximate what molecule has that structure. Remember, central atoms can have 2, 3, 4, 5, and 6 pairs of e^- around them.

Prelab

Draw Lewis electron dot structures for the following molecules. How many *bonding* and how many *nonbonding* electron pairs are located on the central atom in each molecule?

SiH_4, NBr_3, PF_3, $GeCl_4$, SF_6, ICl_5

Procedure

Use the table provided to help organize your investigation.

1.) For each structure you build and sketch, use the Lewis dot formula for each of the real molecules suggested.

2.) Construct models of the thirteen geometries for which the formulas are given. For the shapes more complex than tetrahedral, you may need to use the marshmallows and toothpicks.

3.) Sketch a representation of the models, and indicate the measured bond angles (use a protractor). Your sketch do not have to be fine artwork, but the overall shape of the molecule , as well as the position of all electron pairs on the central atom (both bonding and non bonding), must be clear.

Discussion Questions

1.) Explain how you would know if AB_2 is linear or bent.
2.) Explain how you would know if AB_3 is trigonal planar or trigonal pyramid.
3.) Draw Lewis dot structures and predict the bond angles in the following molecules.
PF_3 SF_6 ICl_5 HBr H_2Se
4.) The models you have built and sketched do not take into account the fact that bonding and nonbonding pairs of electrons do not repel each other to exactly the same extent; repulsion by nonbonding pairs is stronger than by bonding pairs. How will this affect the true geometric shape and bond angels of the molecules you have drawn? Check your ideas using text.
5.) The models you have built also do not consider those molecules having double or triple bonds predicted for their Lewis dot structures.
  a.) What effect might a second or third pair of electrons shared between two individual atoms have on the overall shape of a molecule?
  b.) Draw and give shape and show angle predictions for the following:
  1.) N_2 2.) O_2 3.) CO_2 4.) SO_3
6.) Draw and give shape and label angles of the ions: NO^+ CN^- NO_3^-

Table of Geometries

Type Formula	# valence pairs on central atom in molecule	# bonding pairs on central atom	Lewis Dot Formula	Arrangement of valence pairs	Model with angles	Example	Molecular shape
AB_2	2	2		Linear		BeH_2	Linear
AB_3	3	3		Trigonal planar		BCl_3	Trigonal planar
AB	4	1		Tetrahedral		HCl	Linear
AB_2	4	2		Tetrahedral		H_2O	Bent
AB_3	4	3		Tetrahedral		NH_3	Trigonal pyramid
AB_4	4	4		Tetrahedral		CH_4	Tetrahedral
AB_2	5	2		Trigonal bipyramid		I_3^-	Linear
AB_3	5	3		Trigonal bipyramid		BrF_3	T-shape
AB_4	5	4		Trigonal bipyramid		SF_4	See-saw
AB_5	5	5		Trigonal bipyramid		PCl_5	Trigonal bipyramid
AB_4	6	4		Octahedral		XeF_4	Square planar
AB_5	6	5		Octahedral		IF_5	Square pyramid
AB_6	6	6		Octahedral		SF_6	Octahedral