

1.2: Background

Atoms within an organic molecule can adopt a variety of differing geometries based upon the number and type of bonds that they contain as well as the number of non-bonding electrons that they have. One of the methods that organic chemists use to determine the geometry of atoms in a molecule is Valence Shell Electron Pair Repulsion (VSEPR). This method puts the bonding and non-bonding electrons in a molecule into groups.

Because the negative charges in each electron group repel each other, the atom is most stable when the electron groups are positioned as far apart from each other as possible. As shown in Figure 1, atoms with 2 VSEPR groups will put these groups in a linear arrangement. Atoms with 3 VSEPR groups will place these groups in a trigonal plane, while atoms with 4 VSEPR groups will place these groups at the corners of a regular tetrahedron. These three electronic geometries, linear, trigonal planar, and tetrahedral, compose most electronic geometries in organic chemistry.

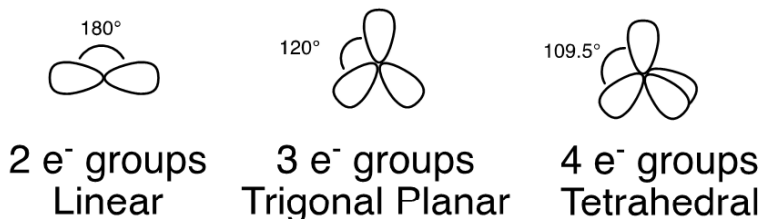


Figure 1. Electronic geometries for 2, 3, and 4 VSEPR electron groups.

In VSEPR theory a group of electrons is composed of either a σ (sigma or single) bond or a pair of non-bonding electrons. For example, as shown in Figure 2A, the nitrogen atom in trimethylamine has 4 groups, 3 σ bonds and one non-bonding pair of electrons.

This means that the nitrogen in this compound has a tetrahedral electronic geometry. The carbon atom in tetrachloroethene, however, only has 3 electron groups because it has 3 σ bonds and it doesn't have any lone pairs (Figure 2B). Remember that a double bond is made up of 1 σ bond and 1 π or pi bond; π bonds exist in the same area as the σ bond and so the electrons together only form one group. Therefore, the carbon in tetrachloroethene has a trigonal planar electronic geometry. Finally, the indicated carbon in 2-butyne (Figure 1C.) has a linear electronic geometry because it has two σ bonds and no pairs of non-bonding electrons. Similar to the double bond, a triple bond is made up of 1 σ bond and 2 π bonds and therefore only counts as one group.

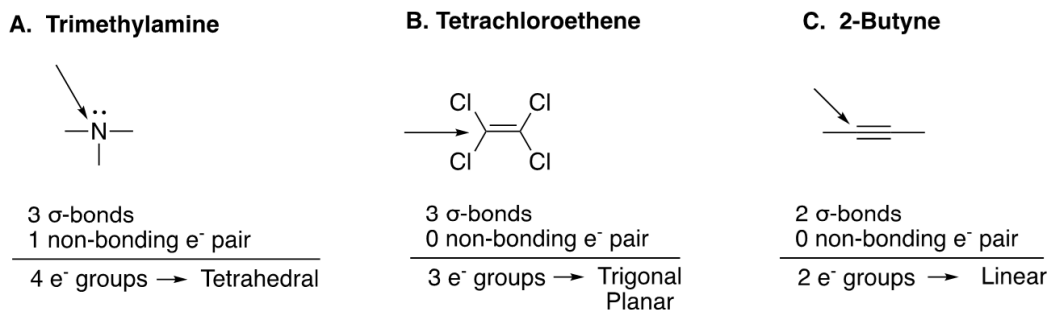


Figure 2. Determining the number of VSEPR groups for indicated atoms.

Electronic geometry reflects the position of electrons around each atom, but many molecular properties are only dependent on the position of the atoms, not those of the electrons. We define the molecular geometry based solely upon the position of atoms around a central nucleus, and not upon electron groups. The molecular geometry is however directly influenced by electronic geometry. For example, the electronic geometry of the oxygen in water (H_2O) is tetrahedral because it has four groups (2 σ bonds and 2 non-bonding electron pairs). However, when only the atoms in the water molecule are considered, water will appear bent rather than tetrahedral. The relationship between electronic geometry and molecular geometry is described in Figure 3.

Electronic Geometry	Molecular Geometry			
	0 lone pairs	1 lone pair	2 lone pairs	3 lone pairs
109.5° 4 e ⁻ groups Tetrahedral	 Tetrahedral	 Trigonal Pyramidal	 Bent	 Undefined
120° 3 e ⁻ groups Trigonal Planar	 Trigonal Planar	 Bent	 Undefined	
180° 2 e ⁻ groups Linear	 Linear	 Undefined		

Figure 3. The relationship between the number of electron lone pairs and the molecular geometry of an atom.

An important point to note about VSEPR theory is that it provides idealized bond angles and geometries for atoms in molecules. The experimental or computed bond angles may be slightly different. For instance, the $\text{H}-\text{O}-\text{H}$ bond angle in water would be predicted to be 109.5° because of its tetrahedral electronic geometry. The experimental value of this angle is slightly smaller at 104.45° . One reason for this is that the non-bonding electron pairs are better at repelling other groups than sigma bonds because they don't have any positively charged atomic nuclei to draw in the electrons. This has the effect of "squishing" the two $\text{O}-\text{H}$ sigma bonds closer together than the ideal bond angle predicted by VSEPR (Figure 4).

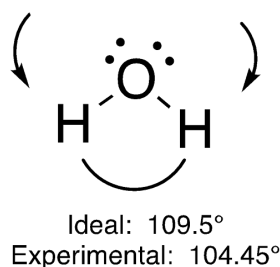


Figure 4. Efficient repulsion by the non-bonding electron pairs of water "squishes" the $\text{O}-\text{H}$ bonds closer together than the idealized bond angle.

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