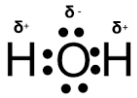
Geometry of Molecules in Chemistry

While atomic bonding of covalent compounds is largely dependent upon the availability of valence electrons that can be shared, the structure of the resulting compound can be influenced by a variety of factors. The **Valence Shell Electron-Pair Repulsion Theory (VSEPR)** examines how electrons, as negatively charged subatomic particles, interact and repel each other.

As Lewis Structures show, compounds can have both bonded (shared) and non-bonded (lone-Pair) electrons. Therefore, the first step requires the production of a Lewis diagram for each atom. We will use the common example of water, H_2O. Using oxygen as the central atom, the electron dot diagram is as follows:

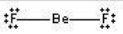
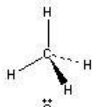
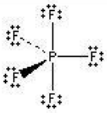
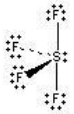
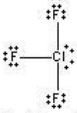
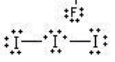
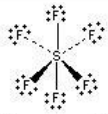


Oxygen, as shown, has two lone pairs of unbonded electrons.

Using the chart on the right, we can determine that with two bonding groups and two lone pairs, water is a "bent" molecule.

It is important, when considering the polarity of the molecule, to understand both the geometry and the electronegativity difference between the individual atoms.

Electron and Molecular Geometry On Central Atom.

Electron Regions & hybridization	Bonding Regions	Lone Pairs	Electron Region Geometry	Molecular Geometry	Examples	
2	2	0	linear	linear	BeF_2, CO_2	
sp	1	1		linear	CO, N_2	
3	3	0	trigonal planar	trigonal planar	BF_3, CO_3^{2-}	
sp^2	2	1		bent	O_3, SO_2	
	1	2		linear	O_2	
4	4	0	tetrahedral	tetrahedral	CH_4, SO_4^{2-}	
sp^3	3	1		trigonal pyramidal	NH_3, H_3O^+	
	2	2		bent	H_2O, ICl_2^+	
	1	3		linear	HF, OH^-	
5	5	0	trigonal bipyramidal	trigonal bipyramidal	PF_5	
sp^3d	4	1		seesaw	SF_4, $TeCl_4$, IF_4^+	
	3	2		T-shaped	ClF_3	
	2	3		linear	I_3^-, XeF_2	
6	6	0	octahedral	octahedral	SF_6, PF_6^-, SiF_6^{2-}	
sp^3d^2	5	1		square pyramidal	BrF_5, $SbCl_5^{2-}$	
	4	2		square planar	XeF_4, ICl_4^-	

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Again considering the example of water, one might assume that the equal pull toward the more electronegative oxygen would result in a net nonpolar structure. This is complicated by the bend in the molecule, however, which is caused by the repulsion of the lone pairs and allows for a partial negative region at the central oxygen. Thus, each hydrogen atom carries a partial positive charge, and the water is ultimately polar. This quality is the basis for many of water's life-sustaining properties.