EXPERIMENT

Compounds and their structure

Goal This experiment will go over the ideas of molecular geometry and bond-hybridization. On one hand, you will learn how to predict the geometry of a molecule and how to differentiate, for example, a linear molecule from a bent molecule. Also you will learn to predict the hybridization of atomic orbitals involved in a chemical bond.

Background Molecules result from the combination of atoms. For example, a H_2O molecule results of the combination of one oxygen atom with two hydrogen atoms. The atoms of a molecule combine by exchanging or sharing electrons, depending on the type of bond. Water is a covalent molecule and the oxygen and hydrogen atoms share the electrons in the bond. Only electrons in the outermost electron shell participate in chemical bonds. Those electrons are called valence electrons. Core electrons, electrons in inner shells of the atom, do not participate in chemical bonds. The electron configuration of oxygen is $1s^2 2s^2 2p^4$. Valence electrons are highlighted with bold letters and are those in the energy level $n = 2$. Chemists use several theories to describe the formation of a bond, and here we will cover three of these theories: the valence-shell electron-pair repulsion model (VSEPR), the valence bond theory, and the molecular orbital theory. These theories describe different aspects of the formation of a bond, sometimes complementing each other.

Valence Electrons

The valence electrons of an atom are those located in the electronic valence shell. For example, the electron configuration of lithium is $1s^2 2s^1$. This atom has two electrons in the $1s$ atomic orbital and one electron in the $2s$ higher-energy atomic orbital. The first two electrons belongs to the core, as the level $1s$ is completely filled with electrons. Differently, the second energy level is not completely filled and hence the single electron in this level is a valence electron. Another example would be oxygen,$1s^2 2s^2 2p^4$, which contains two core electrons–located in the $1s$ level–and six valence electrons. The number of valence electrons of an atom can be easily determine by looking at the group number. For example, oxygen belongs to the group 16(6A) and has six valence electrons. Similarly, nitrogen belongs to group 15(5A) and hence will have five valence electrons.

The Octet rule

Atoms gain or loose electrons when they combine to form molecules. The octet rule says that each atom in a molecule is surrounded by eight electrons. There are two important exceptions to this rule: hydrogen (H) will only surrounded by two electrons, and boron (B) by six.

Lewis dot symbol of an atom

The Lewis dot symbol of an atom is a representation of the element symbol surrounded by the valence electrons in the form of dots. For example, Li has one valence electron and hence its Lewis dot symbol will be $\cdot\mathrm{Li}$. The Lewis dot symbol for O, with six valence electrons, will be $\cdot\ddot{\underset{\cdot\cdot}{\mathrm{O}}}\cdot$. At this point is not that important how do you distribute the dots, and in case of doubt a wise choice is to pair the dots.

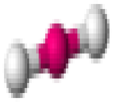
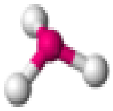
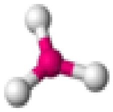
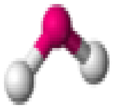
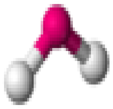
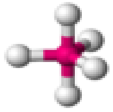
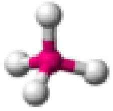
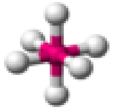
Lewis structure of diatomic molecules

In order to build up Lewis structures or electron-dot structures for diatomic molecules,

1. set up the element symbols next to each other.
2. count the total number of valence electrons in the molecule, by adding the valence electrons of each atom.
3. Add as many electrons (dots) as necessary to complete the octets (or duets) for each element. Make sure that there are at least two electrons shared (a single bond) between the two elements.

4. Count how many electrons are used in the resulting structure
    (a) If the structure uses as many electrons as valence electrons are available, this is the final structure.
    (b) If the structure uses more electrons than valence electrons are available, double bonds (four electrons shared) or triple bonds (six electrons shared) need to be used. Each double bound will save two electrons with respect to a single bond. Each triple bound will save two electrons with respect to a double bound.

Table 1: Molecular Geometries

ABE Code	Molecular shape	Bond Angle	3D model
AB_2	Linear	180°	
AB_3E	Trigonal pyramidal	109°	
AB_3	Trigonal Planar	120°	
AB_2E_2	Bent	109°	
AB_2E	Bent	120°	
AB_5	Trigonal bipyramidal	90°, 120°,180°	
AB_4	Tetrahedral	109°	
AB_6	Octahedral	90°, 180°,180°	

Lewis structures of polyatomic molecules

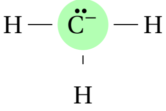
For polyatomic molecules the procedure is exactly the same. The only difference is to arrange the elements correctly. Typically, finding the central atom is the key. Two tricks to find the central atom.

1. the central atom is the one with a lower index in the molecule (e.g. in H_2O is O or in NH_3 is N)
2. the central atom is that with the lowest electronegativity.

The pairs of electrons that connect two atoms are called *bonds*. In Lewis structures these two electrons can be replaced by lines joining the elements. The pairs not involved in a bond are called *lone pairs*. Notice that the atoms arrangement (if the structure looks like a line, a triangle or so) is not necessary representative of the real, three-dimensional molecular geometry.

Atomic charges in a molecule and polyatomic ions

In order to build up the electron-dot structures of a molecule you need to count the number of valence electrons of the whole molecule. Each atom contributes with a different number of valence electrons to the molecule. For example, H contributes with one electron whereas O contributes with two. When you arrange the electron pairs in the molecule, each atom should have no less than the number of electrons that they bring. For example in the electron-dot structure of HCl, $\mathrm{H}\!:\!\ddot{\underset{\cdot\cdot}{\mathrm{Cl}}}\!:$ the hydrogen atom contributes with one electron to the molecule, and in the molecule the H atom owns one electron, as in $\mathrm{H}\!:$ one of the dots belongs to H and the other belongs to the Cl–the electrons are shared in a covalent bond. In the same way, the Cl atom contributes with seven electrons and in the molecule it owns seven electrons, as in $:\!\ddot{\underset{\cdot\cdot}{\mathrm{Cl}}}\!:$ one of the dots belongs to H and the other seven belong to Cl. In another words, the $\mathrm{H}\!:\!\ddot{\underset{\cdot\cdot}{\mathrm{Cl}}}\!:$ electron-dot structure is the combination of $\mathrm{H}\cdot$ and $\cdot\ddot{\underset{\cdot\cdot}{\mathrm{Cl}}}\!:$. We say that the charges on each atom are zero, as each atom in the molecule owns the same number of electrons that it originally brings. The lewis structure should also display the electron distribution in polyatomic ions. Look for example at $CH_3{}^-$ ions. Comparing the valence electrons of each atom and the number of electrons surrounding each atom in this structure, one can see that the C atom has an extra electron, and hence it is responsible of the negative charge:



$$\begin{array}{ccccc} \mathrm{H} & — & \ddot{\mathrm{C}}^{-} & — & \mathrm{H} \\ & & | & & \\ & & \mathrm{H} & & \end{array}$$

Example

Construct the electron-dot structure of H_2O indicating the number of bonds and lone pairs.

Answer: we first arrange the atoms in the molecule as H O H. The central atom is O, as oxygen has the lower index in the H_2O molecule–the index for O is one and the index for H is two. Now we count the total number of valence electrons, including all atoms: 2xH($1e^-$) and O($6e^-$) that gives a total of eight electrons. Now we distribute the pair on each atoms knowing that each atom has to have 8 electrons with the exception of hydrogen that can only be surrounded by two.

$$\mathrm{H}\!:\!\ddot{\underset{\cdot\cdot}{\mathrm{O}}}\!:\!\mathrm{H}$$

and using lines instead of pairs (this is not necessary but makes the electron-dot structure look better) we obtain

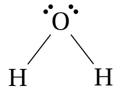
$$\mathrm{H} — \ddot{\underset{\cdot\cdot}{\mathrm{O}}} — \mathrm{H}$$

The molecule has two bonds, each one connecting a H to the oxygen atom, and two lone pairs located on the oxygen atom.

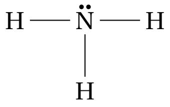
VSEPR theory and molecular geometry

Molecules are arrangements of atoms, and these arrangements can have different forms. Think about a H_2O molecule, which contains two hydrogen atoms and one oxygen. Knowing that both hydrogens are connected to oxygen by means of a covalent bond, one can envision several molecular geometries such as

$\mathrm{H} — \ddot{\underset{\cdot\cdot}{\mathrm{O}}} — \mathrm{H}$ or maybe



The goal of this section is to identify the geometry of a given molecule. In order to do this, the electron-dot structure of the molecule is the key. If the molecule contains two atoms, there is only a possible geometry these two atoms can exhibit, and this is a linear arrangement. For the case of more complex molecules, in order to identify the geometry you need to figure out the ABE code of the molecule. In this code B refers to the number of atoms connected to the central atom in a molecule, and E is the number of lone pairs on the central atom. For example, the electron-dot $\mathrm{H}-\underset{\cdot\cdot}{\ddot{\mathrm{O}}}-\mathrm{H}$ structure has two bonds with the central atom B_2 and two lone pairs on top of the central atom E_2 and hence the ABE code of the molecule would be AB_2E_2. Another example, the ABE code for ammonia



$$\begin{array}{c}\mathrm{H}-\ddot{\mathrm{N}}-\mathrm{H}\\ | \\ \mathrm{H}\end{array}$$

would be AB_3E, as the molecule has three atoms connected to the central nitrogen and and N has a single lone pair. You can find a list of the equivalence between ABE codes and the molecular geometry in Table 1. In order to predict the geometry of a molecule, once you have the ABE code, Table 1 will give you the geometry. For example, an AB_2 molecule will be linear, whereas an AB_2E_2 is a bent. The bond angles are also indicated in the table, and for example a CO_2 molecule, which will be linear, will have 180° angles. This means both C-O bonds will form a line.

STUDENT INFO

Name: ______________________ Date: ________
Pre-lab Done: ☐

Pre-lab Questions

Compounds and their structure

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1. Calculate the number of valence electrons for the following atoms and molecules:

$BeCl_2$ ____________________ CFH_3 ____________________
NF_3 ____________________ SH_2 ____________________

2. Draw the lewis structure of the following compounds: NF_3, CFH_3, $BeCl_2$.

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Name: ______________________ Date: ________
Pre-lab Done: ☐

Experiment

Compounds and their structure

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1. Lewis structure of molecules

1. Calculate the number of valence electrons for the following atoms and molecules:

N	____________	CO_3^{2-}	____________
O	____________	SO_4^{2-}	____________
P	____________	ICl_4^{-}	____________
Br	____________	CH_2Cl_2	____________

2. Draw the lewis structure of the following compounds: H_2O, HF, HCl.

3. Draw the lewis structure of the following compounds and indicate their polarities: CH_4, CH_2Cl_2, $CHCl_3$.

Formula	Lewis Structure	# valence e^-	# e^- pairs	Geometry	Angles	Polar?
NH_3						
H_2O						
CH_4						
CH_2Cl_2						

Formula	Lewis Structure	# valence e^-	# e^- pairs	Geometry	Angles	Polar?
PCl_3						
ClO_2^-						
BrO_2^-						
CCl_3^-						