

## EXPERIMENT 0

# Compounds and their structure

### A. 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.

### B. Materials

- ☐ This is a theory-based experiment.

### C. Background

#### ***Electron-dot structures of atoms & molecules***

Protons, neutrons, and electrons make the atoms. Electrons—in particular valence electrons—are responsible for the main chemical properties of an atom. These electrons are loosely bound and can be exchanged easily with other atoms, in contrast to the strongly-tied core electrons. The electron-dot structure of an atom or a molecule—also called Lewis structures—is a visual representation of the electronic arrangement of the valence electrons. Atoms in a molecule will tend to be surrounded by eight electrons so that their electron configuration resembles a noble gas. This arrangement is known as the octet rule. This rule is responsible for the common negative charge of F:  $\text{F}^-$  ( $[\text{He}]2s^22p^6 = [\text{Ne}]$ ), and the positive charge of Na:  $\text{Na}^+$  ( $[\text{Ne}]3s^1$ ) can easily receive an extra electron producing ionic  $\text{F}^-$  ( $[\text{He}]2s^22p^6 = [\text{Ne}]$ ), and atomic Na ( $[\text{Ne}]3s^1$ ) can lose an electron producing ionic  $\text{Na}^+$  ( $[\text{He}]2s^22p^6 = [\text{Ne}]$ ). There are a few exceptions. A remarkable one is the case of the hydrogen atom that follows the duet rule.

#### ***Valence electrons of atoms, and molecules***

The electrons of an atom are divided into core electrons and valence electrons. The valence electrons of an atom are involved in chemical bonds as they are less bonded to the nucleus. *The number of valence electrons of an atom* corresponds to the group number. For example, hydrogen H belongs to the group IA, and hence it has one valence electron. Similarly, oxygen O belongs to the group VIA, having six valence electrons. Similarly, we can count the *number of valence electrons of a molecule* by adding the valence electrons of the atoms that make the molecule. For example, water ( $\text{H}_2\text{O}$ ) has eight valence electrons as each hydrogen has one valence electron and oxygen has six. The number of *pairs of electrons* is just the overall number of valence electrons divided by two. For example, water has eight valence electrons that correspond to 4 pairs of electrons.

#### Sample Problem 1

Indicate the number of valence electrons for the following atoms: N, O, C and S, and the number of pairs of electrons of the following molecules:  $\text{NH}_3$ , and  $\text{CO}_2$ .

#### **SOLUTION**

Nitrogen is in group VA and hence it has five valence electrons ( $5e^-$ ). Oxygen belongs to the group VIA and C belong to IVA, hence they have six and four valence electrons, respectively. For the molecules, we have that ammonia has 8 electrons (nitrogen has five valence electrons and each hydrogen has one electron) that correspond

to four pairs, whereas carbon dioxide has 16 electrons (carbon has four electrons and each oxygen has six) and eight pairs.

### STUDY CHECK

Indicate the number of valence electrons for the following atoms: Cl and B.

►Answer: Cl ( $7e^-$ ), B ( $3e^-$ ).

## The octet rule

Atoms exchange electrons when they combine to form molecules. This electron exchange is the driving force that drives the formation of molecules from single atoms. The octet rule states that each atom in a stable molecule should be surrounded by eight (octet) electrons achieving noble gas electron configurations. There are two important exceptions to this rule as H is surrounded only by two electrons (this is called the duet rule), and B by six. This rule comes from the experimental observation of numerous molecules.

## Electron-dot structure of an atom

The electron-dot structure of an atom is a visual representation of the arrangement of the valence electrons of the atom. To write the electron-dot structure of an atom, you just need to write down the symbol of the atom surrounded by the valence electrons located in the four directions of the space: top, bottom, right, and left. To place the electrons, you start in any of the directions and fill one electron at a time. For example, for the case of three electrons, we would have:  $\cdot\dot{\text{B}}\cdot$ . After all four directions have been filled, you need to start pairing the electrons. For example, for the case of five electrons, we would have:  $\cdot\dot{\text{P}}\cdot$ . Another example, oxygen has six valence electrons and hence, the electron-dot structure would be  $\cdot\ddot{\text{O}}\cdot$ . Similarly, the electron-dot structure of fluorine would be  $\cdot\ddot{\text{F}}\cdot$ . For ions, you need to add (if its an anion) or subtract (if its a cation) valence electrons, and for example the electron-dot structure of the oxide anion  $\text{O}^{2-}$  is  $:\ddot{\text{O}}:^{2-}$ . The electron-dot structure of atoms is useful to predict—or make sense—of the atomic valence. Mind that the number of valence electrons of an atom is not the same as the valence of the atom. The valence of an atom is a number used to combine with other atoms forming compounds. For example, the electron-dot structure of nitrogen is  $\cdot\ddot{\text{N}}\cdot$  and this atom needs to gain three electrons to reach the noble gas configuration with eight electrons:  $:\ddot{\text{N}}:^{3-}$  hence its valence is  $-3$ .

### Sample Problem 2

Write down the electron-dot structure for the following atoms: N, C and  $\text{Cl}^-$ .

### SOLUTION

N has five valence electrons, whereas C has four. Hence the electron-dot for both will be:  $\cdot\ddot{\text{N}}\cdot$  and  $\cdot\dot{\text{C}}\cdot$ .  $\text{Cl}^-$  has eight valence electrons, that is seven plus one, and hence its electron-dot structure will be  $:\ddot{\text{Cl}}:^-$ .

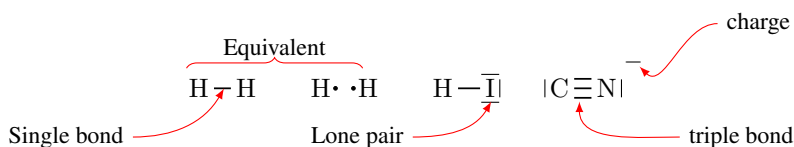
### STUDY CHECK

Write down the electron-dot structure for  $\text{N}^{3-}$

►Answer:  $:\ddot{\text{N}}:^{3-}$ .

## An introduction to electron-dot structures

Below, you will find some examples of electron-dot structures. Mind that the lines represent pairs of electrons hence below there are two equivalent representations for the hydrogen molecule. In these structures, you will find two different types of lines. Some pairs of electrons connect atoms. We call these types of pairs bonds. Other pairs lay on atoms. We call these lone pairs. Each atom can have a different number of lone pairs. For example, in the Lewis structures below carbon has one lone pair whereas iodide has three pairs. Bonds can be simple or multiple, double or triple. Finally, some molecules are charged and the charge is normally indicated on the top right side of the representation.



## Electron-dot structure of diatomic molecules

Electron-dot structures—or Lewis structures—of diatomic molecules are the most simple electron-dot structures of molecules that you will see. To obtain these structures, you need to follow the next steps. The first step is (1) to set up the atoms in the molecule in the form of a line. After that, (2) you need to count the total number of valence electrons in the molecule by adding the valence electrons of each atom (remember the number of valence electrons corresponds to the group number in the A notation). Then (3) compute the pairs of electrons represented by lines—the total number of valence electrons divided by two. Finally, (4) you need to start distributing the electron pairs in the molecule in a very specific way, first connecting the atoms among themselves, and then placing the remaining pairs surrounding the atoms. Following the octet rule, each atom except for H and B should be surrounded by four pairs, counting as pairs the bonds and lone pairs.

### Sample Problem 3

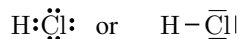
Construct the electron-dot structure of HCl.

#### SOLUTION

We first arrange the atoms in the molecule as indicated below and then we count the number of valence electrons: H(1) and Cl(7) that gives a total of eight electrons. We have four pairs of electrons.



Now we distribute the pair on each atoms knowing that each atom has to have four pairs with the exception of hydrogen that can only be surrounded by one pair. We can use lines instead of pairs



#### STUDY CHECK

Construct the electron-dot structure of HF.

►Answer:  $\text{H}-\overline{\text{F}}$ .

## Number of bonds and atomic nature

The number of covalent bonds that a nonmetal form is related to the number of electrons needed to complete the octet. For example, Hydrogen ( $1s^2$ ) tends to form one bond to make compounds, whereas Nitrogen ( $[\text{He}]2s^22p^3$ ) forms three bonds. For example, in the  $\text{NH}_3$  molecule, each H forms one bond whereas N forms three bonds. Table ?? gives the relation between the number of bonds formed by several elements.

## Electron-dot structure of general molecules

Now we will address how to build up electron-dot structures of more complex molecules given that one of the atoms is the central atom and the others are connected to this central atom. The first step is (1) to arrange the atoms in the molecule, in the form of a central atom and the remaining atoms around it; the central atom is the one with a lower index in the molecule (e.g. in  $\text{H}_2\text{O}$  is O or in  $\text{NH}_3$  is N). After that, (2) you need to count the total number of valence electrons in the molecule, dividing this number by two to obtain the number of pairs of electrons represented by lines. In the following (3) you need to connect the surrounding atoms to the central atom with electron pairs, and then (4) place electron pairs on top of the surrounding atoms, always placing a maximum of four atoms. Finally (5) place the remaining pairs in the central atom. Overall, each atom should be surrounded by four pairs (this is the octet rule) except H and B which should be surrounded by one and three pairs respectively. When drawing Lewis structures it is not important the atom

arrangement (if the molecule looks like a line, a triangle or so) as long as the connectivity (which atom goes in the center and the surroundings) is correct.

#### Sample Problem 4

Construct the electron-dot structure of  $\text{H}_2\text{O}$  indicating the number of bonds and lone pairs.

#### SOLUTION

- Step one:** 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  $\text{H}_2\text{O}$  molecule—the index for O is one and the index for H is two.
- Step two:** now we count the total number of valence electrons, including all atoms:  $2 \times \text{H}(1)$  and  $\text{O}(6)$  that gives a total of eight electrons.
- Step three:** let us count the pairs of electrons; we have eight electrons and that is four pairs.
- Step four:** now we distribute the pair on each atoms knowing that each atom has to have four pairs with the exception of hydrogen that can only be surrounded by one pair.  $\text{H}:\ddot{\text{O}}:\text{H}$  and using lines instead of pairs (this is not necessary but makes the electron-dot structure look better) we obtain  $\text{H}-\ddot{\text{O}}-\text{H}$ . The molecule has two bonds, each one connecting an H to the oxygen atom and two lone pairs located on the oxygen atom.

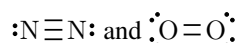
#### STUDY CHECK

Construct the electron-dot structure of  $\text{NH}_3$  indicating the number of bonds and lone pairs.

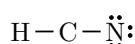
►Answer:  $\text{H}-\ddot{\text{N}}-\text{H}$ ; three bonds and one lone pair.

### Multiple bonds

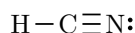
Often you are going to encounter electron-dot structures like the ones below



in which the atoms are connected through multiple bonds, double or triple bonds. Multiple bonds are formed while constructing electron-dot structures to impose the octet rule. Look for example the lewis structure for the HCN molecule below



In this structure, carbon does not follow the octet rule. We can enforce the octet rule by moving lone pairs from the atoms into the bond forming the structure below



In this structure both carbon and nitrogen follow the octet rule. Hence, we need to add one more step to the Lewis structure construction scheme: convert lone pairs of electrons into bonds to enforce the octet rule.

#### Sample Problem 5

Construct the electron-dot structure of  $\text{O}_2$ .

#### SOLUTION

- Step one:** We first arrange the atoms in the molecule as

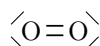


Now we count the total number of valence electrons, including all atoms:  $2 \times \text{O}(6)$  that gives a total of twelve

electrons. Let us count the pairs of electrons; we have twelve electrons and that is six pairs. Then we distribute the pairs, first connecting the atoms O—O (we have five extra pairs to distribute at this point), and we place the remaining pairs on top of the oxygen atoms



The right oxygen does not follow the octet rule. In order to enforce the octet rule we move lone pairs into the bond



### ◆ STUDY CHECK

Construct the electron-dot structure of CO<sub>2</sub>.

►Answer:  $\langle \text{O}=\text{C}=\text{O} \rangle$

## Atomic charges in a molecule

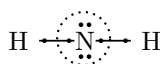
The electron-dot structure of a molecule results from counting the overall number of valence electrons of the molecule given that each atom brings a different number of valence electrons ( $n_e^{\text{free}}$ ). For example, two H atoms bring one electron each, whereas O brings two electrons, giving a total of six valence electrons. When arranging the electron pairs in the molecule, the number of electrons surrounding an atom is called the valence of this atom in the molecule ( $n_e^{\text{bonded}}$ ). We calculate the number of valence electrons of an atom in a molecule by accounting for the number of lone pairs on this atom and half the number of bonds:

$$n_e^{\text{bonded}} = \text{number of lone pairs} + 1/2 \text{number of bonds}$$

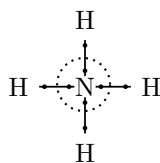
It is important to note that the valence of a free atom and the valence of this atom in a molecule is not necessarily the same. Indeed the difference between the valence electron of a free atom and the same atom in a molecule is the effective charge of that atom in the molecule,  $Q$ :

$$Q_{\text{eff}} = n_e^{\text{free}} - n_e^{\text{bonded}}$$

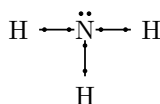
When the valence of an atom in a molecule is larger than the valence of the free atoms we have negative effective charges. In the example below



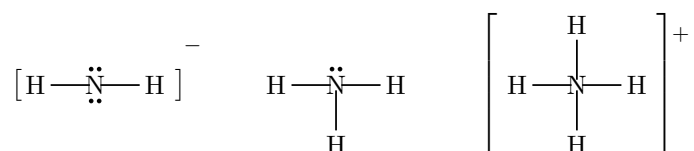
the number of electrons surrounding nitrogen is six electrons, more than the number of electrons originally brought to the molecule (five). We conclude that the atoms have a negative charge, and the effective atomic charge of nitrogen is  $Q=-1$ . In the next example,



the central atom, nitrogen, still has five valence electrons. After counting the electrons surrounding nitrogen, this time we find that this atom is surrounded by four electrons, less than the number of electrons originally brought to the molecule. We can conclude that nitrogen has a positive charge. In particular, the effective atomic charge of nitrogen in this molecule is the number of valence electrons minus the number of surrounding electrons. In this case, the atomic charge is  $Q=+1$ . When the valence of an atom in a molecule is the same as the valence of the free atoms we have zero effective charges. In this last example



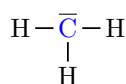
the central atom, nitrogen, has five valence electrons. After counting the electrons surrounding nitrogen—remember in a bond each atom shared an electron and hence each line around an atom counts as one electron—we find that this atom is surrounded by five electrons. As the number of valence electrons brought to the molecule is the same as the number of electrons surrounding the atom, we say the atomic charge of this atom is zero ( $Q=0$ ). Hence, the atom is neutral. In all the molecules above, hydrogen remains neutral and hence the atomic charge of nitrogen corresponds to the molecular charge of the molecule. We can hence summarize the three scenarios indicated, as we have a neutral molecule in the center, a positive molecule on the right, and a negative molecule on the left.



The atomic charge of an isolated atom can be well-defined. However, the atomic charge of an atom in a molecule is arbitrarily defined, and more than one definition exists. Formal charges are one of the possible definitions of atomic charges in a molecule, whereas redox numbers are an alternative definition of atomic charges in molecules. None of these definitions is exactly correct. For example, redox numbers tend to overestimate the atomic charges, as they assume that all shared electrons in a bond belong to the most electronegative atom. Normally, negative formal charges tend to reside on electronegative atoms and not on electropositive atoms. At the same time, the sum of all effective charges needs to give the overall charge of the species. Furthermore, atoms in molecules tend to achieve formal charges as close to zero as possible. One can use formal charges to assess the validity of a Lewis structure. When comparing a series of equivalent Lewis structures for a molecule, the structures that best describe the bonding in the molecule tend to be those with small effective charges located on electronegative atoms.

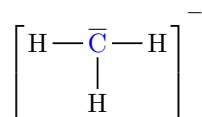
#### Sample Problem 6

Indicate the atomic charges of the blue highlighted atom



#### SOLUTION

The carbon atom brings four electrons and in the molecule it is surrounded by eight electrons, five of which belongs to it. Hence the charge of C is  $-1$ ; this means that carbon has one extra electron. Each hydrogen brings one electron and in the molecule each hydrogen has one electron (they share two electrons with C, one for C and one for H). The final Lewis structure with the local charge of carbon can be indicated as:












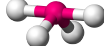



#### STUDY CHECK

Indicate the atomic charges of all atoms in the Lewis structure below



► Answer: left oxygen  $-1$ ; right oxygen  $+1$

Table 1 Molecular geometries							
Electron groups (AEs)	Electron-group geometry	Bonded atoms (Bs)	Lone pairs (Es)	ABE Code	Molecular shape	Bond Angle	3D model
2	Linear	2	0	AB <sub>2</sub>	Linear	180°	
3	Trigonal Planar	3	0	AB <sub>3</sub>	Trigonal Planar	120°	
3	Trigonal Planar	2	1	AB <sub>2</sub> E	Bent	120°	
4	Tetrahedral	4	0	AB <sub>4</sub>	Tetrahedral	109°	
4	Tetrahedral	3	1	AB <sub>3</sub> E	Trigonal pyramidal	109°	
4	Tetrahedral	2	2	AB <sub>2</sub> E <sub>2</sub>	Bent	109°	
5	trigonal bipyramidal	5	0	AB <sub>5</sub>	trigonal bipyramidal	90°, 120°, 180°	
6	octahedral	6	0	AB <sub>6</sub>	octahedral	90°, 180°, 180°	
5	trigonal bipyramidal	4	1	AB <sub>4</sub> E	see-saw	180°, 120°, 90°	
5	trigonal bipyramidal	3	2	AB <sub>3</sub> E <sub>2</sub>	T-shaped	90°, 180°	
5	trigonal bipyramidal	2	3	AB <sub>2</sub> E <sub>3</sub>	Linear	180°	
6	octahedral	5	1	AB <sub>5</sub> E	square pyramidal	90°	
6	octahedral	4	2	AB <sub>4</sub> E <sub>2</sub>	square planar	90°, 180°	

## Steps to obtain Lewis structures

The following steps can be used to obtain the Lewis structure of a general molecule:

- 1 **Step one:** Arrange the atoms in the molecule, in the form of a central atom and the surrounding atoms
- 2 **Step two:** Obtain the number of pairs of valence electrons by dividing the total number of valence electrons of the molecule by two
- 3 **Step three:** Connect the surrounding atoms to the central atom with electron pairs
- 4 **Step four:** Place electron pairs on top of the surrounding atoms, always placing a maximum of four atoms
- 5 **Step five:** Place the remaining pairs in the central atom.
- 6 **Step six:** Convert lone pairs of electrons into bonds to enforce the octet rule
- 7 **Step seven:** For extended octets place the extra electrons on the central atom
- 8 **Step eight:** When numerous equivalent Lewis structures exist, the best structures would have low formal charges, with negative charges located on electronegative atoms

## Atomic charges in a molecule

The electron-dot structure of a molecule results from counting the overall number of valence electrons of the molecule given that each atom brings a different number of valence electrons ( $n_e^{free}$ ). For example, two H atoms bring one electron each, whereas O brings two electrons, giving a total of six valence electrons. When arranging the electron pairs in the molecule, the number of electrons surrounding an atom is called the valence of this atom in the molecule ( $n_e^{bonded}$ ). We calculate the number of valence electrons of an atom in a molecule by accounting for the number of lone pairs on this atom and half the number of bonds:

$$n_e^{bonded} = \text{number of lone pairs} + 1/2 \text{number of bonds}$$

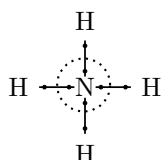
It is important to note that the valence of a free atom and the valence of this atom in a molecule is not necessarily the same. Indeed the difference between the valence electron of a free atom and the same atom in a molecule is the effective charge of that atom in the molecule,  $Q$ :

$$Q_{eff} = n_e^{free} - n_e^{bonded}$$

When the valence of an atom in a molecule is larger than the valence of the free atoms we have negative effective charges. In the example below

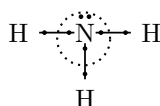


the number of electrons surrounding nitrogen is six electrons, more than the number of electrons originally brought to the molecule (five). We conclude that the atoms have a negative charge, and the effective atomic charge of nitrogen is  $Q=-1$ . In the next example,

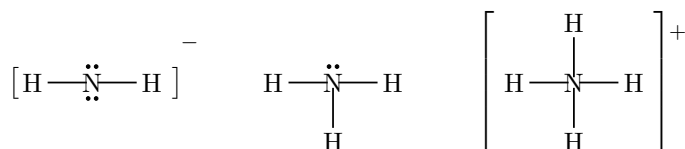


the central atom, nitrogen, still has five valence electrons. After counting the electrons surrounding nitrogen, this time we find that this atom is surrounded by four electrons, less than the number of electrons originally brought to the molecule. We can conclude that nitrogen has a positive charge. In particular, the effective atomic charge of nitrogen in this molecule is the number of valence electrons minus the number of surrounding electrons. In this case, the atomic charge is  $Q=+1$ . When the valence of an atom in a molecule is the same as the valence of the free atoms we have zero effective charges. In this last example





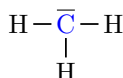
the central atom, nitrogen, has five valence electrons. After counting the electrons surrounding nitrogen—remember in a bond each atom shared an electron and hence each line around an atom counts as one electron—we find that this atom is surrounded by five electrons. As the number of valence electrons brought to the molecule is the same as the number of electrons surrounding the atom, we say the atomic charge of this atom is zero ( $Q=0$ ). Hence, the atom is neutral. In all the molecules above, hydrogen remains neutral and hence the atomic charge of nitrogen corresponds to the molecular charge of the molecule. We can hence summarize the three scenarios indicated, as we have a neutral molecule in the center, a positive molecule on the right, and a negative molecule on the left.



The atomic charge of an isolated atom can be well-defined. However, the atomic charge of an atom in a molecule is arbitrarily defined, and more than one definition exists. Formal charges are one of the possible definitions of atomic charges in a molecule, whereas redox numbers are an alternative definition of atomic charges in molecules. None of these definitions is exactly correct. For example, redox numbers tend to overestimate the atomic charges, as they assume that all shared electrons in a bond belong to the most electronegative atom. Normally, negative formal charges tend to reside on electronegative atoms and not on electropositive atoms. At the same time, the sum of all effective charges needs to give the overall charge of the species. Furthermore, atoms in molecules tend to achieve formal charges as close to zero as possible. One can use formal charges to assess the validity of a Lewis structure. When comparing a series of equivalent Lewis structures for a molecule, the structures that best describe the bonding in the molecule tend to be those with small effective charges located on electronegative atoms.

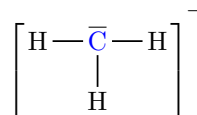
#### Sample Problem 7

Indicate the atomic charges of the blue highlighted atom



#### SOLUTION

The carbon atom brings four electrons and in the molecule it is surrounded by eight electrons, five of which belong to it. Hence the charge of C is  $-1$ ; this means that carbon has one extra electron. Each hydrogen brings one electron and in the molecule each hydrogen has one electron (they share two electrons with C, one for C and one for H). The final Lewis structure with the local charge of carbon can be indicated as:



#### STUDY CHECK

Indicate the atomic charges of all atoms in the Lewis structure below



►Answer: left oxygen  $-1$ ; right oxygen  $+1$

### Molecular shape

Molecules consist of arrangements of atoms presented in different forms. Let us use as an example the  $\text{H}_2\text{O}$  molecule, which contains two hydrogen atoms and one oxygen. Knowing that both hydrogens are connected to oxygen through a

covalent bond, one can envision several molecular geometries such as a linear geometry or maybe a v-shaped geometry with oxygen at the point. The geometry of a molecule determines its properties, and small geometrical changes can have severe consequences on the functioning of molecules. For example, at high temperatures, when proteins in the body denaturalize losing their unique structure they also lose their functionality. The goal of this section is to identify the approximate shape of a given molecule.

### ***The VSEPR model***

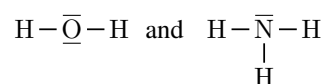
The VSEPR model, also known as the valence shell electron-pair repulsion model, is a model that predicts the geometries of molecules made of nonmetals. This model predicts the atomic arrangement of the molecules with an emphasis on the shape of the arrangement. However, it is not a very accurate model to predict geometries and there are better methods to obtain molecular geometries. The model predicts, for example, that water molecules have a v-shaped geometry and not a linear geometry while giving an estimate of the angle between the two O-H bonds. Still, VSEPR is not accurate enough to predict the O-H bond length and more advanced methods should be used for this purpose. The VSEPR model is based on the premise that the structure around a given atom results from minimizing the electron-pair repulsion. This way, the bonding and nonbonding pairs of electrons around a central atom are differently accounted for. Let us analyze a few cases in which the central atom only has bonding pairs of electrons. For example, the BeH<sub>2</sub> molecule has two bonding pairs around Be and the arrangement that maximizes the distance between both pairs hence minimizing repulsion is a linear arrangement. Hence, the BeH<sub>2</sub> molecule is linear with a 180° angle between both Be-H bonds. Another example would be the BH<sub>3</sub> molecules, a molecule with three bonding pairs. The geometry that maximizes the distance between the three pairs hence minimizing repulsion is a trigonal planar structure in which the three bonding pairs are in the same plane with an angle of 120° between the three bonds. A final example would be the methane molecule (CH<sub>4</sub>), a molecule with four bonding pairs. A tetrahedral arrangement with 109.5° between the C-H bonds is the most stable arrangement for this case.

### ***more***

For the case of five bonds, the geometrical arrangement that minimizes the electron-pair interaction is a trigonal bipyramidal arrangement consisting of two pyramidal arrangements sharing a common base. The PH<sub>5</sub> molecule presents this arrangement. In this arrangement, there are two different bond angles: 90° between the vertical and in-plane and 120° for the in-plane bonds. Finally, the octahedral structure minimizes the pair repulsion in the case of six bonds and for example, the SH<sub>6</sub> molecule has an octahedral arrangement. In this arrangement, all bonds have a 90° angle. All atomic arrangements discussed above are presented in the diagram below.

### ***ABE Molecular code***

We will use the ABE code to identify the molecular geometry of more complex molecules, with bonds and lone pairs. This code is based on the Lewis structure of the molecule, with B refers to the number of atoms connected to the central atom in the molecule (number of bonded atoms), and E is the number of lone pairs on the central atom. The overall number of bonded atoms and lone pairs is called the number of electron groups. Corresponding geometry for different ABE codes is tabulated. For example, an AB<sub>2</sub> molecule will be linear, whereas an AB<sub>2</sub>E<sub>2</sub> is bent. The electron-dot structure of water and ammonia are:



Water has two bonds with the central atom and hence two Bs and two lone pairs on top of the central atom and hence two Es. The ABE code of water is AB<sub>2</sub>E<sub>2</sub> and its geometry is bent. The ABE code of ammonia is AB<sub>3</sub>E, as the molecule has three atoms connected to the central nitrogen and N has a single lone pair. Its geometry would be trigonal pyramidal. Angles between the different bonds for the different atomic arrangements are also tabulated. For example, the angle between the two H-O bonds of water would be 104.5°, whereas the angle between two of the N-H bonds of ammonia would be 107°. The overall number of bonding and lone pairs is referred to as the number of electron regions and the

molecular geometry of the molecule is not necessarily the geometry of the electron regions. For example, the molecule methane has four bonds and a tetrahedral geometry. Ammonia has two bonds and two lone pairs. The geometry of the electron regions is also tetrahedral with three bonds pointing toward the lower part of the tetrahedron and the lone pair pointing toward the upper part. At the same time, the molecular geometry of ammonia is trigonal pyramidal. For the case of water, we have that again the geometry of the four electron regions is tetrahedral whereas the molecular geometry is bent. We can also conclude that lone pairs require more room than bonding pairs and this has an impact on the molecular angles. For example, the angle between two bonds in a tetrahedron is  $109.5^\circ$  being this value is the same as the molecule angles of methane. Differently, the molecular angles of ammonia—a molecule with one lone pair—are  $107^\circ$ , and the molecular angle of water—a molecule with two lone pairs—is  $104.5^\circ$ . These results indicate that as the number of lone pairs increases the bonding pairs are more squeezed together.

### ***Steps to use the VSEPR model***

The following steps can be used to obtain the molecular geometry using the VSEPR model:

- 1 **Step one:** Identify the central and the peripheral atoms.
- 2 **Step two:** Obtain the Lewis structure of the molecule
- 3 **Step three:** Obtain the ABE code with B being the number of peripheral atoms and E being the number of lone pairs. A represents the central atom. Multiple bonds (double, triple) count as a single B.
- 4 **Step four:** Use Table ?? to obtain the molecular geometry



**STUDENT INFO**

Name: \_\_\_\_\_ Date: \_\_\_\_\_

**Pre-lab Questions**

# Compounds and their structure

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

 $\text{BeCl}_2$ 

\_\_\_\_\_

 $\text{CFH}_3$ 

\_\_\_\_\_

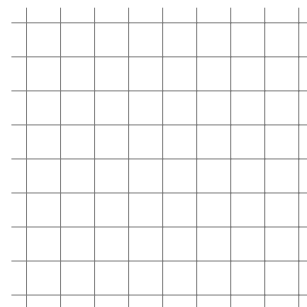
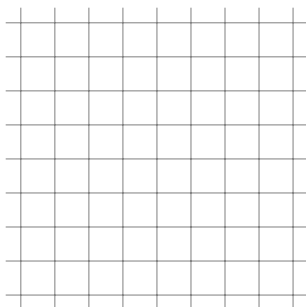
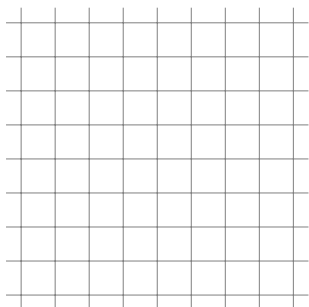
 $\text{NF}_3$ 

\_\_\_\_\_

 $\text{SH}_2$ 

\_\_\_\_\_

2. Draw the lewis structure of the following compounds:  $\text{NF}_3$ ,  $\text{CFH}_3$ ,  $\text{BeCl}_2$ .





**STUDENT INFO**

Name: \_\_\_\_\_ Date: \_\_\_\_\_

**Results  
EXPERIMENT**

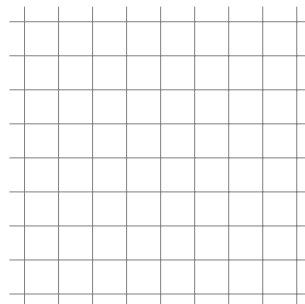
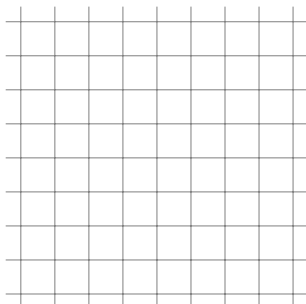
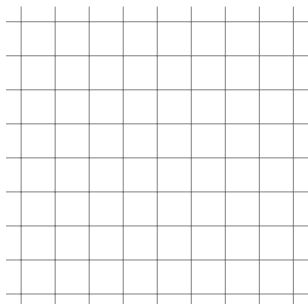
# Compounds and their structure

**1. Lewis structure of molecules**

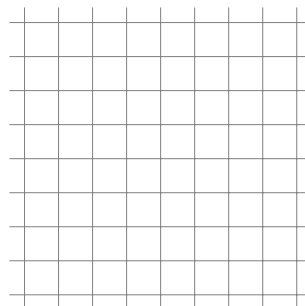
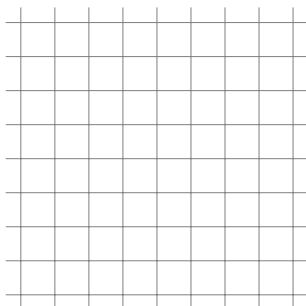
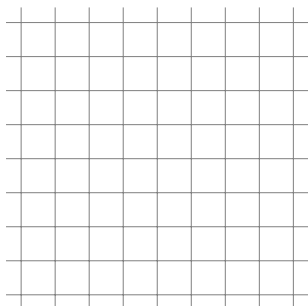
1. Calculate the number of valence electrons for the following atoms and molecules:

N	_____	$\text{CO}_3^{2-}$	_____
O	_____	$\text{SO}_4^{2-}$	_____
P	_____	$\text{ICl}_4^-$	_____
Br	_____	$\text{CH}_2\text{Cl}_2$	_____

2. Draw the lewis structure of the following compounds:  $\text{H}_2\text{O}$ , HF, HCl.



3. Draw the lewis structure of the following compounds and indicate their polarities:  $\text{CH}_4$ ,  $\text{CH}_2\text{Cl}_2$ ,  $\text{CHCl}_3$ .







Formula	Lewis Structure	# valence $e^-$	# $e^-$ pairs	Geometry	Angles	Polar?
$\text{NH}_3$						
$\text{H}_2\text{O}$						
$\text{CH}_4$						
$\text{CH}_2\text{Cl}_2$						



Formula	Lewis Structure	# valence $e^-$	# $e^-$ pairs	Geometry	Angles	Polar?
$\text{PCl}_3$						
$\text{ClO}_2^-$						
$\text{BrO}_2^-$						
$\text{CCl}_3^-$						