CHAPTER 3

Atomic Combinations

CONTENTS

LIST OF TABLES

LIST OF FIGURES

We live in a world that is made up of many complex compounds. All around us we see evidence of chemical bonding from the chair you are sitting on, to the book you are holding, to the air you are breathing. Imagine if all the elements on the periodic table did not form bonds but rather remained on their own. Our world would be pretty boring with only 100 or so elements to use.

Imagine you were painting a picture and wanted to show the colours around you. The only paints you have are red, green, yellow, blue, white and black. Yet you are able to make pink, purple, orange and many other colours by mixing these paints. In the same way, the elements can be thought of as natures paint box. The elements can be joined together in many different ways to make new compounds and so create the world around you.

In Grade 10 we started exploring chemical bonding. In this chapter we will go on to explain more about chemical bonding and why chemical bonding occurs. We looked at the three types of bonding: covalent, ionic and metallic. In this chapter we will focus mainly on covalent bonding and on the molecules that form as a result of covalent bonding.

TIP

In this chapter we will use the term molecule to mean a covalent molecular structure. This is a covalent compound that interacts and exists as a single entity.

1 CHEMICAL BONDS

1.1 Why do atoms bond?

As we begin this section, it's important to remember that what we will go on to discuss is a *model* of bonding, that is based on a particular *model* of the atom. You will remember from the discussion on atoms (in Grade 10) that a model is a *representation* of what is happening in reality. In the model of the atom that you are learnt in Grade 10, the atom is made up of a central nucleus, surrounded by electrons that are arranged in fixed energy levels (sometimes called *shells*). Within each energy level, electrons move in *orbitals* of different shapes. The electrons in the outermost energy level of an atom are called the **valence electrons**. This model of the atom is useful in trying to understand how different types of bonding take place between atoms.

TIP

A model takes what we see in the world around us and uses that to make certain predictions about what we cannot see.

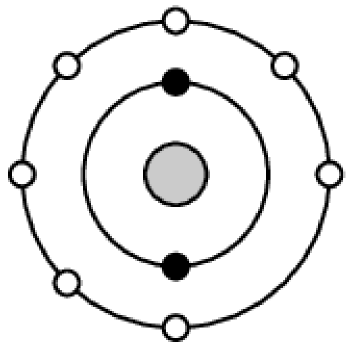


Figure 1: Electron arrangement of a fluorine atom. The black electrons (small circles on the inner ring) are the core electrons and the white electrons (small circles on the outer ring) are the valence electrons

The following points were made in these earlier discussions on electrons and energy levels:

- Electrons always try to occupy the lowest possible energy level.
- The noble gases have a full valence electron orbital. For example neon has the following electronic configuration: $1\text{s}^2 2\text{s}^2 2\text{p}^6$. The second energy level is the outermost (valence) shell and is full.
- Atoms form bonds to try to achieve the same electron configuration as the noble gases.
- Atoms with a full valence electron orbital are less reactive.

1.2 Energy and bonding

There are two cases that we need to consider when two atoms come close together. The first case is where the two atoms come close together and form a bond. The second case is where the two atoms come close together but do not form a bond. We will use hydrogen as an example of the first case and helium as an example of the second case.

Case 1: A bond forms

Let's start by imagining that there are two hydrogen atoms approaching one another. As they move closer together, there are three forces that act on the atoms at the same time. These forces are described below:

1. **repulsive force** between the electrons of the atoms, since like charges repel

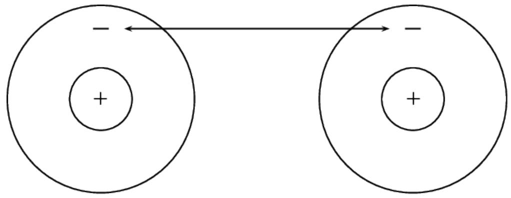


Figure 2: Repulsion between electrons

2. **attractive force** between the nucleus of one atom and the electrons of another

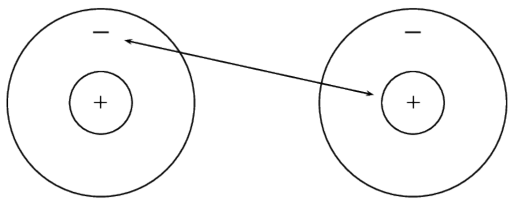


Figure 3: Attraction between electrons and protons

3. **repulsive force** between the two positively-charged nuclei

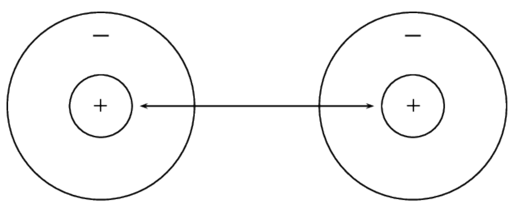


Figure 4: Repulsion between protons

These three forces work together when two atoms come close together. As the total force experienced by the atoms changes, the amount of energy in the system also changes.
Now look at Figure 5 to understand the energy changes that take place when the two atoms move towards each other.

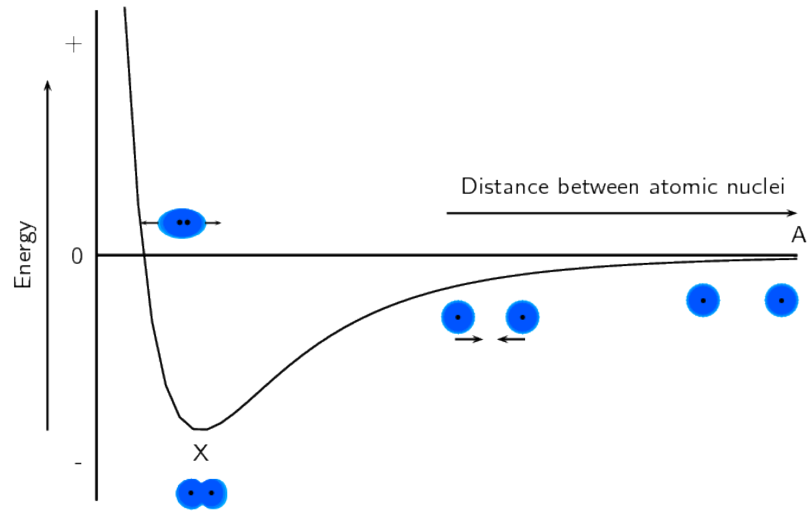


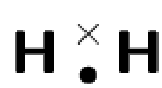
Figure 5: Graph showing the change in energy that takes place as two hydrogen atoms move closer together

Let us imagine that we have fixed the one atom and we will move the other atom closer to the first atom. As we move the second hydrogen atom closer to the first (from point A to point X) the energy of the system decreases. Attractive forces dominate this part of the interaction. As the second atom approaches the first one and gets closer to point X, more energy is needed to pull the atoms apart. This gives a negative potential energy.

At point X, the attractive and repulsive forces acting on the two hydrogen atoms are balanced. The energy of the system is at a minimum.

Further to the left of point X, the repulsive forces are stronger than the attractive forces and the energy of the system increases.

For hydrogen the energy at point X is low enough that the two atoms stay together and do not break apart again. This is why when we draw the Lewis diagram for a hydrogen molecule we draw two hydrogen atoms next to each other with an electron pair between them.



We also note that this arrangement gives both hydrogen atoms a full outermost energy level (through the sharing of electrons or covalent bonding).

Case 2: A bond does not form

Now if we look at helium we see that each helium atom has a filled outer energy level. Looking at Figure 6 we find that the energy minimum for two helium atoms is very close to zero. This means that the two atoms can come together and move apart very easily and never actually stick together.

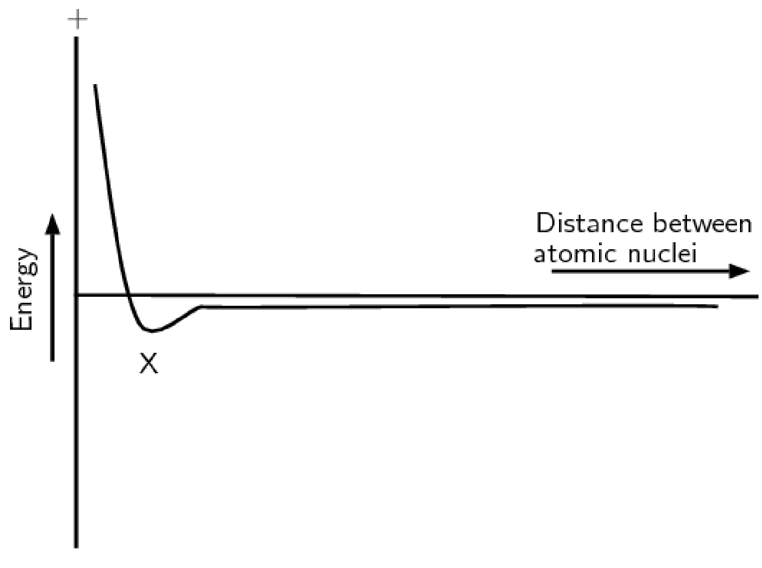


Figure 6: Graph showing the change in energy that takes place as two helium atoms move closer together

For helium the energy minimum at point X is not low enough that the two atoms stay together and so they move apart again. This is why when we draw the Lewis diagram for helium we draw one helium atom on its own. There is no bond.

We also see that helium already has a full outermost energy level and so no compound forms.

1.3 Valence electrons and Lewis diagrams

Now that we understand a bit more about bonding we need to refresh the concept of Lewis diagrams that you learnt about in Grade 10. With the knowledge of why atoms bond and the knowledge of how to draw Lewis diagrams we will have all the tools that we need to try to predict which atoms will bond and what shape the molecule will be.

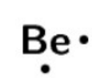
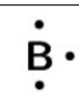
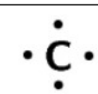
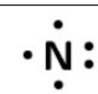
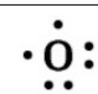
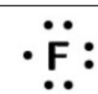
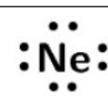
In Grade 10 we learnt how to write the electronic structure for any element. For drawing Lewis diagrams the one that you should be familiar with is the spectroscopic notation. For example the electron configuration of chlorine in spectroscopic notation is: $1s^2 2s^2 2p^5$. Or if we use the condensed form: $[He]2s^2 2p^5$. The condensed spectroscopic notation quickly shows you the valence electrons for the element.

Using the number of valence electrons we can easily draw Lewis diagrams for any element. In Grade 10 you learnt how to draw Lewis diagrams. We will refresh the concepts here as they will aid us in our discussion of bonding.

TIP

*A **Lewis diagram** uses dots or crosses to represent the electrons on different atoms. The chemical symbol of the element is used to represent the nucleus and the core electrons of the atom.*

Lewis diagrams for the elements in period 2 are shown below:

Element	Group number	Valence electrons	Spectroscopic notation	Lewis diagram
Lithium	1	1	$[He]2s^1$	
Beryllium	2	2	$[He]2s^2$	
Boron	13	3	$[He]2s^2 2p^1$	
Carbon	14	4	$[He]2s^2 2p^2$	
Nitrogen	15	5	$[He]2s^2 2p^3$	
Oxygen	16	6	$[He]2s^2 2p^4$	
Fluorine	17	7	$[He]2s^2 2p^5$	
Neon	18	8	$[He]2s^2 2p^6$	

TIP

You can place the unpaired electrons anywhere (top, bottom, left or right). The exact ordering in a Lewis diagram does not matter.

1.4 Covalent bonds and bond formation

Covalent bonding involves the sharing of electrons to form a chemical bond. The outermost orbitals of the atoms overlap so that unpaired electrons in each of the bonding atoms can be shared. By overlapping orbitals, the outer energy shells of all the bonding atoms are filled. The shared electrons move in the orbitals around *both* atoms. As they move, there is an attraction between these negatively charged electrons and the positively charged nuclei. This attractive force holds the atoms together in a covalent bond.

Definition : Covalent bond

A form of chemical bond where pairs of electrons are shared between atoms.

TIP

Covalent bonds are examples of interatomic forces.

We will look at a few simple cases to deduce some rules about covalent bonds.

TIP

Remember that it is only the valence electrons that are involved in bonding, and so when diagrams are drawn to show what is happening during bonding, it is only these electrons that are shown. Dots or crosses represent electrons in different atoms.

Case 1: Two atoms that each have an unpaired electron

For this case we will look at hydrogen chloride and methane.

WORKED EXAMPLE 1: LEWIS DIAGRAMS: SIMPLE MOLECULES

QUESTION

Represent hydrogen chloride *(HCl)* using a Lewis diagram

SOLUTION

Step 1: For each atom, determine the number of valence electrons in the atom, and represent these using dots and crosses.

The electron configuration of hydrogen is $1\,s^1$ and the electron configuration for chlorine is $[He]2\,s^2 2p^5$. The hydrogen atom has 1 valence electron and the chlorine atom has 7 valence electrons.

The Lewis diagrams for hydrogen and chlorine are:.

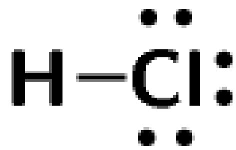
Notice the single unpaired electron (highlighted in blue) on each atom. This does not mean this electron is different, we use highlighting here to help you see the unpaired electron.

Step 2: Arrange the electrons so that the outermost energy level of each atom is full.

Hydrogen chloride is represented below.

Notice how the two unpaired electrons (one from each atom) form the covalent bond.

The dot and cross in between the two atoms, represent the pair of electrons that are shared in the covalent bond. We can also show this bond using a single line:



Note how we still show the other electron pairs around chlorine.

From this we can conclude that any electron on its own will try to pair up with another electron. So in practise atoms that have at least one unpaired electron can form bonds with any other atom that also has an unpaired electron. This is not restricted to just two atoms.

WORKED EXAMPLE 2: LEWIS DIAGRAMS: SIMPLE MOLECULES

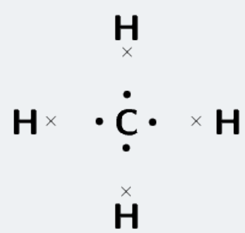
QUESTION

Represent methane (CH_4) using a Lewis diagram

SOLUTION

Step 1: For each atom, determine the number of valence electrons in the atom, and represent these using dots and crosses.

The electron configuration of hydrogen is $1\,s^1$ and the electron configuration for carbon is $[He]2\,s^22p^2$. Each hydrogen atom has 1 valence electron and the carbon atom has 4 valence electrons.

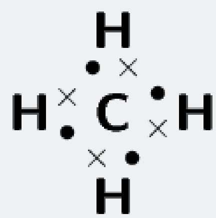


Remember that we said we can place unpaired electrons at any position (top, bottom, left, right) around the elements symbol.

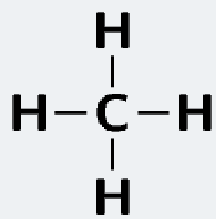
WORKED EXAMPLE 2: LEWIS DIAGRAMS: SIMPLE MOLECULES (continued)

Step 2: Arrange the electrons so that the outermost energy level of each atom is full.

The methane molecule is represented below.



Or:



Case 2: Atoms with lone pairs

We will use water as an example. Water is made up of one oxygen and two hydrogen atoms. Hydrogen has one unpaired electron. Oxygen has two unpaired electrons and two electron pairs. From what we learnt in the first examples we see that the unpaired electrons can pair up. But what happens to the two pairs? Can these form bonds?

WORKED EXAMPLE 3: LEWIS DIAGRAMS: SIMPLE MOLECULES

QUESTION

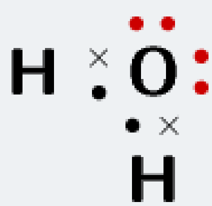
Represent water (H_2O) using a Lewis diagram

SOLUTION

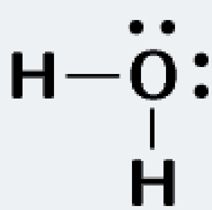
Step 1: For each atom, determine the number of valence electrons in the atom, and represent these using dots and crosses.

The electron configuration of hydrogen is $1\,s^1$ and the electron configuration for oxygen is $[He]2\,s^2 2p^4$. Each hydrogen atom has 1 valence electron and the oxygen atom has 6 valence electrons.

Step 2: Arrange the electrons so that the outermost energy level of each atom is full.



Or:



TIP

Notice how in this example we wrote a 2 in front of the hydrogen? Instead of writing the Lewis diagram for hydrogen twice, we simply write it once and use the 2 in front of it to indicate that two hydrogens are needed for each oxygen.

And now we can answer the questions that we asked before the worked example. We see that oxygen forms two bonds, one with each hydrogen atom. Oxygen however keeps its electron pairs and does not share them. We can generalise this to any atom. If an atom has an electron pair it will normally not share that electron pair.

A **lone pair** is an unshared electron pair. A lone pair stays on the atom that it belongs to.

TIP

A lone pair can be used to form a dative covalent bond.

In the example above the lone pairs on oxygen are highlighted in red. When we draw the bonding pairs using lines it is much easier to see the lone pairs on oxygen.

Case 3: Atoms with multiple bonds

We will use oxygen and hydrogen cyanide as examples.

WORKED EXAMPLE 4: LEWIS DIAGRAMS: MOLECULES WITH MULTIPLE BONDS

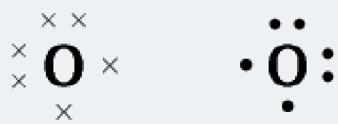
QUESTION

Represent oxygen (O_2) using a Lewis diagram

SOLUTION

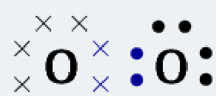
Step 1: For each atom, determine the number of valence electrons that the atom has from its electron configuration.

The electron configuration of oxygen is $[\text{He}]2s^2 2p^4$. Oxygen has 6 valence electrons.

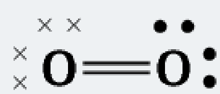


Step 2: Arrange the electrons in the O_2 molecule so that the outermost energy level in each atom is full.

The (O_2) molecule is represented below. Notice the two electron pairs between the two oxygen atoms (highlighted in blue). Because these two covalent bonds are between the same two atoms, this is a double bond.



Or:



Each oxygen atom uses its two unpaired electrons to form two bonds. This forms a double covalent bond (which is shown by a double line between the two oxygen atoms).

WORKED EXAMPLE 5: LEWIS DIAGRAMS: MOLECULES WITH MULTIPLE BONDS

QUESTION

Represent hydrogen cyanide *(HCN)* using a Lewis diagram

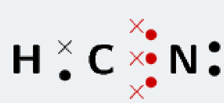
SOLUTION

Step 1: For each atom, determine the number of valence electrons that the atom has from its electron configuration.

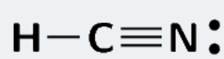
The electron configuration of hydrogen is $1\,s^1$, the electron configuration of nitrogen is $[He]2\,s^2 2p^3$ and for carbon is $[He]2\,s^2 2p^2$. Hydrogen has 1 valence electron, carbon has 4 valence electrons and nitrogen has 5 valence electrons.

Step 2: Arrange the electrons in the *HCN* molecule so that the outermost energy level in each atom is full.

The *HCN* molecule is represented below. Notice the three electron pairs (highlighted in red) between the nitrogen and carbon atom. Because these three covalent bonds are between the same two atoms, this is a triple bond.



Or:



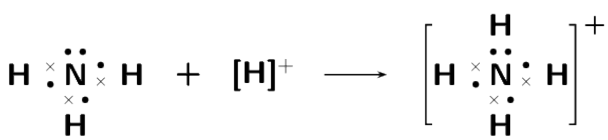
As we have just seen carbon shares one electron with hydrogen and three with nitrogen. Nitrogen keeps its electron pair and shares its three unpaired electrons with carbon.

Case 4: Co-ordinate or dative covalent bonds

> **Definition : Dative covalent bond**
>
> *This type of bond is a description of covalent bonding that occurs between two atoms in which both electrons shared in the bond come from the same atom.*

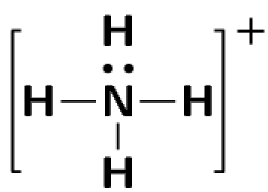
A dative covalent bond is also known as a coordinate covalent bond. Earlier we said that atoms with a pair of electrons will normally not share that pair to form a bond. But now we will see how an electron pair can be used by atoms to form a covalent bond.

One example of a molecule that contains a dative covalent bond is the ammonium ion $\left(NH_4^+\right)$ shown in the figure below. The hydrogen ion H^+ does not contain any electrons, and therefore the electrons that are in the bond that forms between this ion and the nitrogen atom, come only from the nitrogen.



Notice that the hydrogen ion is charged and that this charge is shown on the ammonium ion using square brackets and a plus sign outside the square brackets.

We can also show this as:



Note that we do not use a line for the dative covalent bond.

Another example of this is the hydronium ion (H_3O^+).

To summarise what we have learnt:

- Any electron on its own will try to pair up with another electron. So in theory atoms that have at least one unpaired electron can form bonds with any other atom that also has an unpaired electron. This is not restricted to just two atoms.

- If an atom has an electron pair it will normally not share that pair to form a bond. This electron pair is known as a lone pair.
- If an atom has more than one unpaired electron it can form multiple bonds to another atom. In this way double and triple bonds are formed.
- A dative covalent bond can be formed between an atom with no electrons and an atom with a lone pair.

2 MOLECULAR SHAPE

Molecular shape (the shape that a single molecule has) is important in determining how the molecule interacts and reacts with other molecules. Molecular shape also influences the boiling point and melting point of molecules. If all molecules were linear then life as we know it would not exist. Many of the properties of molecules come from the particular shape that a molecule has. For example if the water molecule was linear, it would be non-polar and so would not have all the special properties it has.

2.1 Valence shell electron pair repulsion (VSEPR) theory

The shape of a covalent molecule can be predicted using the Valence Shell Electron Pair Repulsion (VSEPR) theory. Very simply, VSEPR theory says that the valence electron pairs in a molecule will arrange themselves around the central atom(s) of the molecule so that the repulsion between their negative charges is as small as possible.

In other words, the valence electron pairs arrange themselves so that they are as **far apart** as they can be.

Definition : Valence Shell Electron Pair Repulsion Theory

Valence shell electron pair repulsion (VSEPR) theory is a model in chemistry, which is used to predict the shape of individual molecules. VSEPR is based upon minimising the extent of the electron-pair repulsion around the central atom being considered.

VSEPR theory is based on the idea that the geometry (shape) of a molecule is mostly determined by repulsion among the pairs of electrons around a central atom. The pairs of electrons may be bonding or non-bonding (also called lone pairs). Only valence electrons of the central atom influence the molecular shape in a meaningful way.

2.2 Determining molecular shape

To predict the shape of a covalent molecule, follow these steps:

1. Draw the molecule using a Lewis diagram. Make sure that you draw all the valence electrons around the molecule's central atom.
2. Count the number of electron pairs around the central atom.
3. Determine the basic geometry of the molecule using the table below. For example, a molecule with two electron pairs (and no lone pairs) around the central atom has a *linear* shape, and one with four electron pairs (and no lone pairs) around the central atom would have a *tetrahedral* shape.

TIP

The central atom is the atom around which the other atoms are arranged. So in a molecule of water, the central atom is oxygen. In a molecule of ammonia, the central atom is nitrogen.

The table below gives the common molecular shapes. In this table we use **A** to represent the central atom, **X** to represent the terminal atoms (i.e. the atoms around the central atom) and **E** to represent any lone pairs.

Table 1: The effect of electron pairs in determining the shape of molecules. Note that in the general example A is the central atom and X represents the terminal atoms.

Number of bonding electron pairs	Number of lone pairs	Geometry	General formula
1 or 2	0	linear	AX or AX_2
2	2	bent or angular	AX_2E_2
3	0	trigonal planar	AX_3
3	1	trigonal pyramidal	AX_3E
4	0	tetrahedral	AX_4
5	0	trigonal bipyramidal	AX_5
6	0	octahedral	AX_6

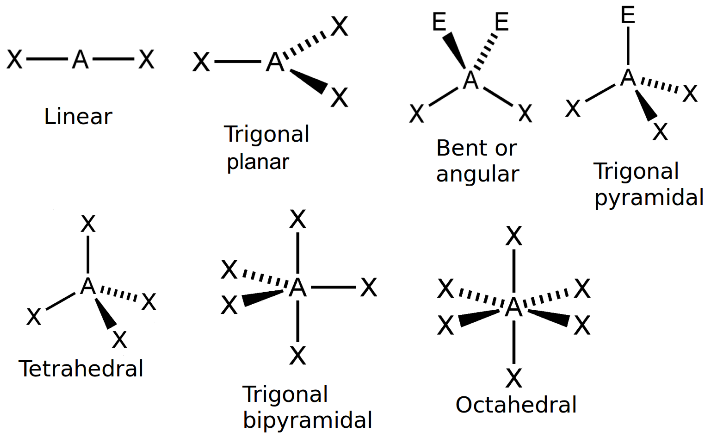


Figure 7: The common molecular shapes

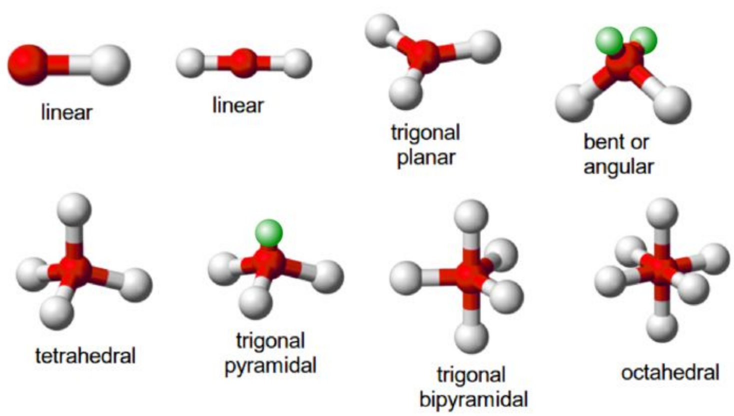


Figure 8: The common molecular shapes in 3-D

In Figure 8 the green balls represent the lone pairs (E), the white balls (X) are the terminal atoms and the red balls (A) are the center atoms.

Of these shapes, the ones with no lone pairs are called the **ideal shapes**. The five ideal shapes are: linear, trigonal planar, tetrahedral, trigonal bypramidal and octahedral.
One important point to note about molecular shape is that all diatomic (compounds with two atoms) compounds are **linear**. So H_2, HCl and Cl_2 are all linear.

WORKED EXAMPLE 6: MOLECULAR SHAPE

QUESTION

Determine the shape of a molecule of $BeCl_2$

SOLUTION

Step 1: Draw the molecule using a Lewis diagram

The central atom is beryllium.

Step 2: Count the number of electron pairs around the central atom

There are two electron pairs.

Step 3: Determine the basic geometry of the molecule

There are two electron pairs and no lone pairs around the central atom. $BeCl_2$ has the general formula: AX_2. Using this information and Table 1, we find that the molecular shape is linear.

Step 4: Write the final answer

The molecular shape of $BeCl_2$ is linear.

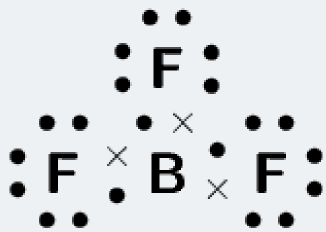
WORKED EXAMPLE 7: MOLECULAR SHAPE

QUESTION

Determine the shape of a molecule of BF_3

SOLUTION

Step 1: Draw the molecule using a Lewis diagram



The central atom is boron.

Step 2: Count the number of electron pairs around the central atom

There are three electron pairs.

Step 3: Determine the basic geometry of the molecule

There are three electron pairs and no lone pairs around the central atom. The molecule has the general formula AX_3. Using this information and Table 1, we find that the molecular shape is trigonal planar.

Step 4: Write the final answer

The molecular shape of BF_3 is trigonal planar.

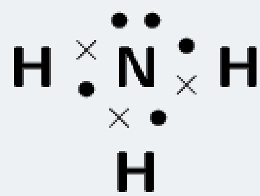
WORKED EXAMPLE 8: MOLECULAR SHAPE

<u>QUESTION</u>

Determine the shape of a molecule of NH_3

<u>SOLUTION</u>

Step 1: Draw the molecule using a Lewis diagram



The central atom is nitrogen.

Step 2: Count the number of electron pairs around the central atom

There are four electron pairs.

Step 3: Determine the basic geometry of the molecule

here are three bonding electron pairs and one lone pair. The molecule has the general formula AX_3E. Using this information and Table 1, we find that the molecular shape is trigonal pyramidal.

Step 4: Write the final answer

The molecular shape of NH_3 is trigonal pyramidal.

TIP

We can also work out the shape of a molecule with double or triple bonds. To do this, we count the double or triple bond as one pair of electrons.

DISCUSSION

Building molecular models

In groups, you are going to build a number of molecules using jellytots to represent the atoms in the molecule, and toothpicks to represent the bonds between the atoms. In other words, the toothpicks will hold the atoms (jellytots) in the molecule together. Try to use different coloured jellytots to represent different elements.

You will need jellytots, toothpicks, labels or pieces of paper.

On each piece of paper, write the words: "lone pair".

You will build models of the following molecules:

HCl_4CH_4, H_2O, BF_3, PCl_5, SF_6 and NH_3

For each molecule, you need to:

- Determine the molecular geometry of the molecule
- Build your model so that the atoms are as far apart from each other as possible (remember that the electrons around the central atom will try to avoid the repulsions between them).
- Decide whether this shape is accurate for that molecule or whether there are any lone pairs that may influence it. If there are lone pairs then add a toothpick to the central jellytot. Stick a label (i.e. the piece of paper with "lone pair" on it) onto this toothpick.
- Adjust the position of the atoms so that the bonding pairs are further away from the lone pairs.
- How has the shape of the molecule changed?
- Draw a simple diagram to show the shape of the molecule. It doesn't matter if it is not 100% accurate. This exercise is only to help you to visualise the 3-dimensional shapes of molecules. (See Figure 7 to help you).

Do the models help you to have a clearer picture of what the molecules look like? Try to build some more models for other molecules you can think of.

3 ELECTRONEGATIVITY

So far we have looked at covalent molecules. But how do we know that they are covalent? The answer comes from electronegativity. Each element (except for the noble gases) has an electronegativity value.

Electronegativity is a measure of how strongly an atom pulls a shared electron pair towards it. The table below shows the electronegativities of the some of the elements.

For a full list of electronegativities see the periodic table at the front of the book. On this periodic table the electronegativity values are given in the top right corner. Do not confuse these values with the other numbers shown for the elements. Electronegativities will always be between 0 and 4 for any element. If you use a number greater than 4 then you are not using the electronegativity.

TIP

Depending on which source you use for electronegativities you may see slightly different values.

Table 2: Table of electronegativities for selected elements.

Element	**Electronegativity**	**Element**	**Electronegativity**
Hydrogen *(H)*	$2,1$	Lithium *(Li)*	$1,0$
Beryllium *(Be)*	$1,5$	Boron *(B)*	$2,0$
Carbon *(C)*	$2,5$	Nitrogen *(N)*	$3,0$
Oxygen *(O)*	$3,5$	Fluorine *(F)*	$4,0$
Sodium *(Na)*	$0,9$	Magnesium *(Mg)*	$1,2$
Aluminium *(Al)*	$1,5$	Silicon *(Si)*	$1,8$
Phosphorous *(P)*	$2,1$	Sulfur *(S)*	$2,5$
Chlorine *(Cl)*	$3,0$	Potassium *(K)*	$0,8$
Calcium *(Ca)*	$1,0$	Bromine *(Br)*	$2,8$

Definition : Electronegativity

Electronegativity is a chemical property which describes the power of an atom to attract electrons towards itself.

FACT

The concept of electronegativity was introduced by Linus Pauling in 1932, and this became very useful in explaining the nature of bonds between atoms in molecules. For this work, Pauling was awarded the Nobel Prize in Chemistry in 1954. He also received the Nobel Peace Prize in 1962 for his campaign against above-ground nuclear testing.

The greater the electronegativity of an atom of an element, the stronger its attractive pull on electrons. For example, in a molecule of hydrogen bromide *(HBr)*, the electronegativity of bromine $(2,8)$ is higher than that of hydrogen $(2,1)$, and so the shared electrons will spend more of their time closer to the bromine atom. Bromine will have a slightly negative charge, and hydrogen will have a slightly positive charge. In a molecule like hydrogen (H_2) where the electronegativities of the atoms in the molecule are the same, both atoms have a neutral charge.

WORKED EXAMPLE 9: CALCULATING ELECTRONEGATIVITY DIFFERENCES

QUESTION

Calculate the electronegativity difference between hydrogen and oxygen.

SOLUTION

Step 1: Read the electronegativity of each element off the periodic table.

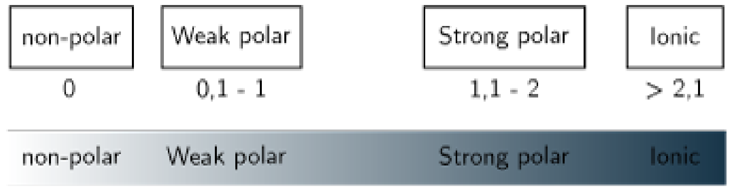
From the periodic table we find that hydrogen has an electronegativity of $2,1$ and oxygen has an electronegativity of $3,5$.

Step 2: Calculate the electronegativity difference

$3,5 - 2,1 = 1,4$

3.1 Electronegativity and bonding

The electronegativity difference between two atoms can be used to determine what type of bonding exists between the atoms. The table below lists the approximate values. Although we have given ranges here bonding is more like a spectrum than a set of boxes.



Electronegativity difference	Type of bond
0	Non-polar covalent
$0 - 1$	Weak polar covalent
$1,1 - 2$	Strong polar covalent
$> 2,1$	Ionic

TIP

Note that metallic bonding is not given here. Metals have low electronegativities and so the valence electrons are not drawn strongly to any one atom. Instead, the valence electrons are loosely shared by all the atoms in the metallic network.

3.2 Non-polar and polar covalent bonds

It is important to be able to determine if a molecule is polar or non-polar since the *polarity* of molecules affects properties such as *solubility, melting points* and *boiling points*.

Electronegativity can be used to explain the difference between two types of covalent bonds. **Non-polar covalent bonds** occur between two identical non-metal atoms, e.g. H_2, Cl_2 and O_2. Because the two atoms have the same electronegativity, the electron pair in the covalent bond is shared equally between them. However, if two different non-metal atoms bond then the shared electron pair will be pulled more strongly by the atom with the higher electronegativity. As a result, a **polar covalent bond** is formed where one atom will have a slightly negative charge and the other a slightly positive charge.

This slightly positive or slightly negative charge is known as a partial charge. These partial charges are represented using the symbols δ^{+} (slightly positive) and δ^{-} (slightly negative). So, in a molecule such as hydrogen chloride *(HCl)*, hydrogen is $H^{\delta^{+}}$ and chlorine is $Cl^{\delta^{+}}$.

TIP

The symbol δ is read as delta.

3.3 Polar molecules

Some molecules with polar covalent bonds are **polar molecules**, e.g. H_2O. But not *all* molecules with polar covalent bonds are polar. An example is CO_2. Although CO_2 has two polar covalent bonds (between $C^{\delta+}$ atom and the two $O^{\delta+}$ atoms), the molecule itself is not polar. The reason is that CO_2 is a linear molecule, with both terminal atoms the same, and is therefore symmetrical. So there is no difference in charge between the two ends of the molecule.

Definition : Polar molecules

A ***polar molecule*** *is one that has one end with a slightly positive charge, and one end with a slightly negative charge. Examples include water, ammonia and hydrogen chloride.*

Definition : Non-polar molecules

A ***Non polar molecule*** *is one where the charge is equally spread across the molecule or a symmetrical molecule with polar bonds. Examples include carbon dioxide and oxygen.*

TIP

To determine if a molecule is symmetrical look first at the atoms around the central atom. If they are different then the molecule is not symmetrical. If they are the same then the molecule may be symmetrical and we need to look at the shape of the molecule.

We can easily predict which molecules are likely to be polar and which are likely to be non-polar by looking at the molecular shape. The following activity will help you determine this and will help you understand more about symmetry.

ACTIVITY

Polar and non-polar molecules

The following table lists the molecular shapes. Build the molecule given for each case using jellytots and toothpicks. Determine if the shape is symmetrical. (Does it look the same whichever way you look at it?) Now decide if the molecule is polar or non-polar.

Geometry	**Molecule**	**Symmetrical**	**Polar or non-polar**
Linear	HCl		
Linear	CO_2		
Linear	HCN		
Bent or angular	H_2O		
Trigonal planar	BF_3		
Trigonal planar	BF_2Cl		
Trigonal pyramidal	NH_3		
Tetrahedral	CH_4		
Tetrahedral	CH_3Cl		
Trigonal bipyramidal	PCl_5		
Trigonal bipyramidal	PCl_4F		
Octahedral	SF_6		
Octahedral	SF_5Cl		

WORKED EXAMPLE 10: POLAR AND NON-POLAR MOLECULES

QUESTION

State whether hydrogen (H_2) is polar or non-polar.

SOLUTION

Step 1: Determine the shape of the molecule

The molecule is linear. There is one bonding pair of electrons and no lone pairs.

Step 2: Write down the electronegativities of each atom

Hydrogen: $2,1$

Step 3: Determine the electronegativity difference for each bond

There is only one bond and the difference is 0.

Step 4: Determine the polarity of each bond

The bond is non-polar.

Step 5: Determine the polarity of the molecule

The molecule is non-polar.

WORKED EXAMPLE 11: POLAR AND NON-POLAR MOLECULES

QUESTION

State whether methane (CH_4) is polar or non-polar.

SOLUTION

Step 1:Determine the shape of each molecule

The molecule is tetrahedral. There are four bonding pairs of electrons and no lone pairs.

Step 2: Determine the electronegativity difference for each bond

There are four bonds. Since each bond is between carbon and hydrogen, we only need to calculate one electronegativity difference. This is: $2,5 – 2,1 = 0,4$

Step 3: Determine the polarity of each bond

Each bond is polar.

Step 4: Determine the polarity of the molecule

The molecule is symmetrical and so is non-polar.

WORKED EXAMPLE 12: POLAR AND NON-POLAR MOLECULES

QUESTION

State whether hydrogen cyanide *(HCN)* is polar or non-polar.

SOLUTION

Step 1:Determine the shape of the molecule

The molecule is linear. There are four bonding pairs, three of which form a triple bond and so are counted as 1. There is one lone pair on the nitrogen atom.

Step 2: Determine the electronegativity difference and polarity for each bond

There are two bonds. One between hydrogen and carbon and the other between carbon and nitrogen. The electronegativity difference between carbon and hydrogen is $0,4$ and the electronegativity difference between carbon and nitrogen is $0,5$. Both of the bonds are polar.

Step 3: Determine the polarity of the molecule

The molecule is not symmetrical and so is polar.

4 ENERGY AND BONDING

As we saw earlier in the chapter we can show the energy changes that occur as atoms come together (Figure 9). Shown below is the same image but this time with two extra pieces of information: the bond energy and the bond length.

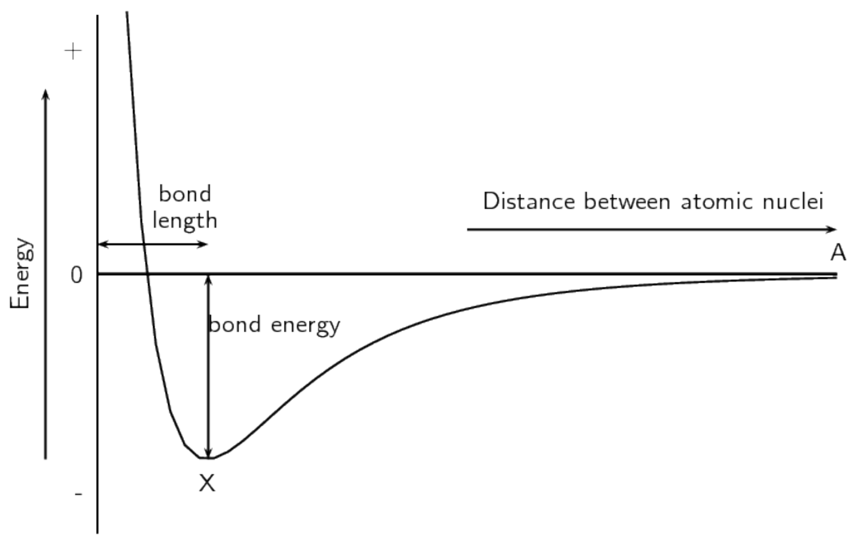


Figure 9: Graph showing the change in energy that takes place as atoms move closer together

Definition : Bond length

The distance between the nuclei of two adjacent atoms when they bond.

Definition : Bond energy

The amount of energy that must be added to the system to break the bond that has formed.

It is important to remember that bond length is measured between two atoms that are bonded to each other. The following diagrams show the bond length for CO and for CO_2. The grey circle represents carbon and the white circle represents oxygen.

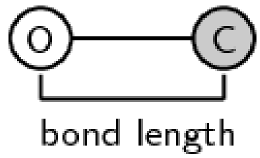


Figure 10: The bond length for carbon monoxide (CO)

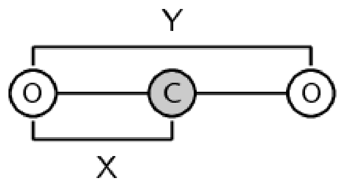


Figure 11: The bond length for each C–O bond in carbon dioxide CO_2 is indicated by X. Y is not the bond length

A third property of bonds is the bond strength. **Bond strength** means how strongly one atom attracts and is held to another. The strength of a bond is related to the bond length, the size of the bonded atoms and the number of bonds between the atoms. In general:

- the shorter the bond length, the stronger the bond between the atoms.
- the smaller the atoms involved, the stronger the bond.
- the more bonds that exist between the same atoms, the stronger the bond.

5 CHAPTER SUMMARY

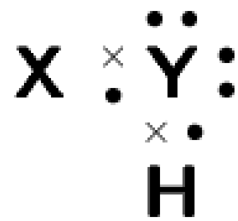
- A **chemical bond** is the physical process that causes atoms to be attracted together and to be bound in new compounds.
- The noble gases have a full valence shell. Atoms bond to try fill their outer valence shell.
- There are three **forces** that act between atoms: attractive forces between the positive nucleus of one atom and the negative electrons of another; repulsive forces between like-charged electrons, and repulsion between like-charged nuclei.
- The **energy** of a system of two atoms is at a minimum when the attractive and repulsive forces are balanced.
- **Lewis** diagrams are one way of representing molecular structure. In a Lewis diagram, dots or crosses are used to represent the valence electrons around the central atom.

- A **covalent bond** is a form of chemical bond where pairs of electrons are shared between two atoms.
- A **single** bond occurs if there is one electron pair that is shared between the same two atoms.
- A **double** bond occurs if there are two electron pairs that are shared between the same two atoms.
- A **triple** bond occurs if there are three electron pairs that are shared between the same two atoms.
- A **dative covalent bond** is a description of covalent bonding that occurs between two atoms in which both electrons shared in the bond come from the same atom.
- Dative covalent bonds occur between atoms of elements with a lone pair and atoms of elements with no electrons. Examples include the hydronium ion (H_3O^+) and the ammonium ion $\left(NH_4^+\right)$.
- The **shape of molecules** can be predicted using the VSEPR theory.
- Valence shell electron pair repulsion (VSEPR) theory is a model in chemistry, which is used to predict the shape of individual molecules. VSEPR is based upon minimising the extent of the electron-pair repulsion around the central atom being considered.
- **Electronegativity** is a chemical property which describes the power of an atom to attract electrons towards itself in a chemical.
- Electronegativity can be used to explain the difference between two types of covalent bonds: **polar covalent bonds** (between non-identical atoms) and **non-polar covalent bonds** (between identical atoms or atoms with the same electronegativity).
- A **polar** molecule is one that has one end with a slightly positive charge, and one end with a slightly negative charge. Examples include water, ammonia and hydrogen chloride.
- A **non-polar** molecule is one where the charge is equally spread across the molecule or a symmetrical molecule with polar bonds.
- **Bond length** is the distance between the nuclei of two atoms when they bond.
- **Bond energy** is the amount of energy that must be added to the system to break the bond that has formed.
- **Bond strength** means how strongly one atom attracts and is held to another atom. Bond strength depends on the length of the bond, the size of the atoms and the number of bonds between the two atoms.

6 EXERCISES

6.1 Exercise 1

1. Give the shorthand spectroscopic notation and draw the Lewis diagram for each of the following elements
   1.1 Magnesium
   1.2 Sodium
   1.3 Chlorine
   1.4 Aluminium
   1.5 Argon
2. Draw the Lewis structure and show all lone pairs for the following molecules
   2.1 Chlorine (Cl_2)
   2.2 Boron trifluoride (BF_3)
   2.3 Ammonia (NH_3)
   2.4 Oxygen difluoride (OF_2)
3. Draw the following Lewis dot structures for the coordinate/dative covalent or normal covalent bonds
   3.1 Acetylene (C_2H_2)
   3.2 Formaldehyde (CH_2O)
4. Nitrogen and hydrogen react to form (NH_3); answer the following questions about the reaction
   4.1 How many valence electrons does N have?
   4.2 How many valence electrons does H have?
   4.3 Draw the Lewis dot diagram of the product that forms.
   4.4 What is the name of the product?
5. Carbon and hydrogen react to form (CH_4); answer the following questions about the reaction
   5.1 How many valence electrons does C have?
   5.2 How many valence electrons does H have?
   5.3 Draw the Lewis dot diagram of the product that forms.
   5.4 What is the name of the product?
6. A chemical compound has the following Lewis diagram:



6.1 How many valence electrons does element Y have?

6.2 How many valence electrons does element X have?

6.3 How many covalent bonds are in the molecule?

6.4 Suggest a name for the elements X and Y.

7. Answer the following questions for CO_2

   7.1 Draw its Lewis dot structure

   7.2 How many bonding pairs does it have?

   7.3 How many non-bonding pairs does it have?

   7.4 How many and what type bonds does it have?

8. Answer the following questions for SO_2

   (a) Draw its Lewis dot structure

   (b) How many bonding pairs does it have?

   (c) How many non-bonding pairs does it have?

   (d) How many and what type bonds does it have?

9. Give one word/term for each of the following descriptions.

   9.1 The distance between two adjacent atoms in a molecule.

   9.2 A type of chemical bond that involves the sharing of electrons between two atoms.

   9.3 A measure of an atom's ability to attract electrons to itself in a chemical bond.

10. Which ONE of the following best describes the bond formed between an H^+ ion and the NH_3 molecule?

11. Explain the meaning of each of the following terms:

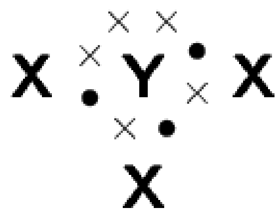
   11.1 valence electrons

   11.2 bond energy

   11.3 covalent bond

12. Which of the following reactions will *not* take place? Explain your answer.
    a. $H + H \rightarrow H_2$
    b. $Ne + Ne \rightarrow Ne_2$
    c. $Cl + Cl \rightarrow Cl_2$

13. Given the following Lewis diagram, where X and Y each represent a different element:



    13.1 How many valence electrons does element Y have?
    13.2 How many valence electrons does element X have?
    13.3 How many covalent bonds are in the molecule?
    13.4 Suggest a name for the elements X and Y.

6.2 Exercise 2

1. Determine the shape of the following molecules.
    1.1 $BeCl_2$
    1.2 F_2
    1.3 PCl_5
    1.4 SF_6
    1.5 CO_2

6.3 Exercise 3

1. Are the following molecules polar or non-polar?

    1.1 O_2

    1.2 $MgBr_2$

    1.3 BF_3

    1.4 CH_2O

2. In a molecule of beryllium chloride ($BeCl_2$)

    2.1 Is the bond a non-polar or polar covalent bond?

    2.2 Is the molecule polar or non-polar?

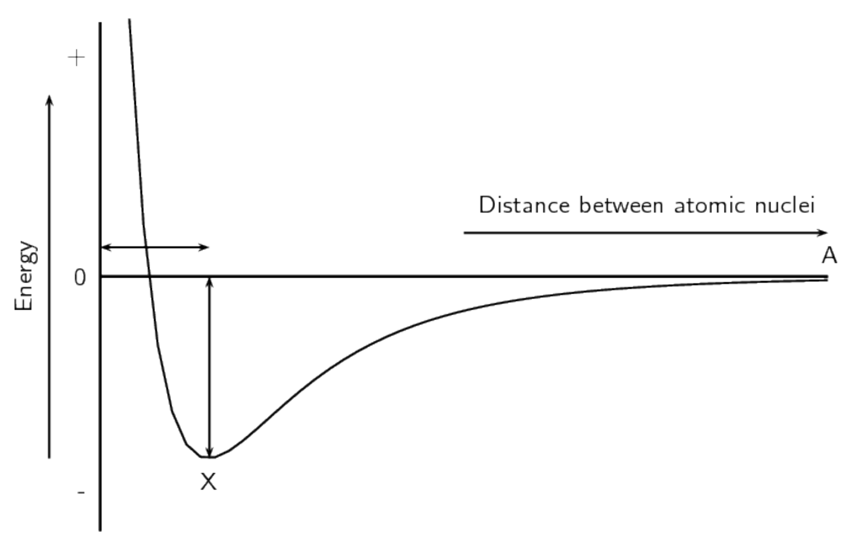
3. Consider the following molecule: H_2O

    3.1 What is difference in electronegativity between the atoms?

    3.2 Is the bond a non-polar/polar covalent bond?

    3.3 Is it a polar/non-polar molecule?

4. Given the following graph for hydrogen:



Indicate a bond length of 74 pm and a bond energy of 436 kJ · mol^{-1} on the blank graph

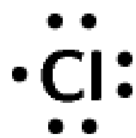
7 ANSWERS FOR EXERCISES

7.1 Exercise 1

1.1 $[Ne]3s^2$

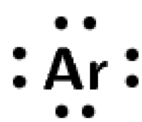
1.2 $[Ne]3s^1$

1.3 $[Ne]3s^2 3p^5$

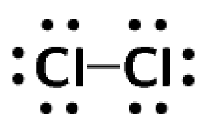


1.4 $[Ne]3s^2 3p^1$

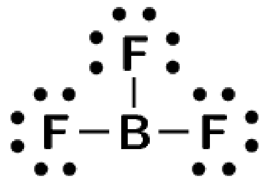
1.5 $[Ne]3s^2 3p^6$



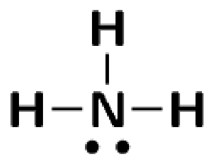
2.1



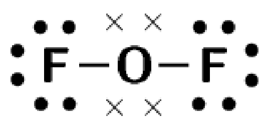
2.2



2.3

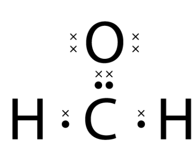


2.4



3.1

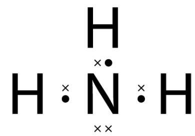
3.2



4.1 5

4.2 1

4.3

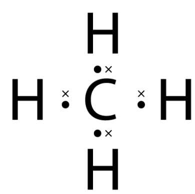


4.4 Ammonia

5.1 4

5.2 1

5.3



5.4 Methane

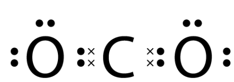
6.1 6

6.2 1

6.3 2

6.4 **X**: Hydrogen
Y: Oxygen

7.1

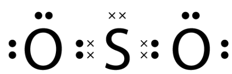


7.2 4

7.3 4

7.4 2 normal double covalent bonds

8.1



8.2 5

8.3 0

8.4 1 triple and 2 single normal covalent bonds

9.1 Bond length

9.2 Covalent bond

9.3 Electronegativity

10. Dative covalent bond

11.1 The number of electrons in the outermost shell of an atom that are available for use in bonding either by sharing, donating or accepting.

11.2 The amount of energy needed for a bond to break.

11.3 A type of bond that occurs between two atoms with a difference in electronegativity between 0 and $2,1$.

12. **Ne** $+$ **Ne** $\rightarrow$ **Ne**$_2$ will not take place as neon does not have electrons available for bonding. Neon is a noble gas and has a full outer shell of electrons.

13.1 5

13.2 1

13.3 3

13.4 **X**: Hydrogen
Y: Nitrogen

7.2 Exercise 2

1.1 Linear

1.2 Linear

1.3 Trigonal bipyramidal

1.4 Octahedral

1.5 Linear

7.3 Exercise 3

1.1 Non-polar

1.2 Non-polar

1.3 Non-polar

1.4 Polar

2.1 Weak polar covalent

2.2 Non-polar

3.1 1.4

3.2 Polar covalent bond

3.3 Polar

4.