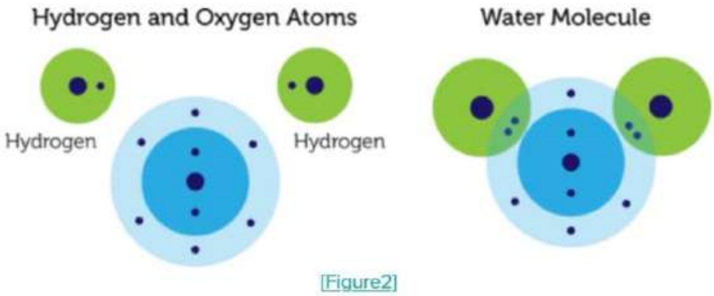
Chemical bonding

What Is a Chemical Bond?

A **chemical bond** is a force of attraction between atoms or ions. Bonds form when atoms share or transfer valence electrons. Valence electrons are the electrons in the outer energy level of an atom that may be involved in chemical interactions. Valence electrons are the basis of all chemical bonds.

Why Bonds Form

To understand why chemical bonds form, consider the common compound known as water, or H_2O. It consists of two hydrogen (H) atoms and one oxygen (O) atom. As you can see in the on the left side of the **Figure** below, each hydrogen atom has just one electron, which is also its sole valence electron. The oxygen atom has six valence electrons. These are the electrons in the outer energy level of the oxygen atom.



Left: Hydrogen and oxygen atoms unbonded to show valence electrons in each atom.
Right: Water molecule showing shared valence electrons between hydrogen and oxygen atoms.

In the water molecule, each hydrogen atom shares a pair of electrons with the oxygen atom. By sharing electrons, each atom has electrons available to fill its sole or outer energy level. The hydrogen atoms each have a pair of shared electrons, so their first and only energy level is full. The oxygen atom has a total of eight valence electrons, so its outer energy level is full. A full outer energy level is the most stable possible arrangement of electrons. It explains why elements form chemical bonds with each other.

Types of Chemical Bonds

Not all chemical bonds form in the same way as the bonds in water. There are actually three different types of chemical bonds, called covalent, ionic, and metallic bonds. Each type of bond is described below.

- A covalent bond is the force of attraction that holds together two nonmetal atoms that share a pair of electrons. One electron is provided by each atom, and the pair of electrons is attracted to the positive nuclei of both atoms. The water molecule contains covalent bonds.
- An ionic bond is the force of attraction that holds together oppositely charged ions. Ionic bonds form crystals instead of molecules. Table salt contains ionic bonds.

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-A metallic bond is the force of attraction between a positive metal ion and the valence electrons that surround it—both its own valence electrons and those of other ions of the same metal. The ions and electrons form a lattice-like structure.

Electron Dot Diagrams

Recall that the valence electrons of an atom are the electrons located in the highest occupied principal energy level. Valence electrons are primarily responsible for the chemical properties of elements. The number of valence electrons can be easily determined from the electron configuration. Several examples from the second period elements are shown in the **Table** below.

lithium	$1s^2 2s^1$	1 valence electron
beryllium	$1s^2 2s^2$	2 valence electrons
nitrogen	$1s^2 2s^2 2p^3$	5 valence electrons
neon	$1s^2 2s^2 2p^6$	8 valence electrons

In each case, valence electrons are those in the second principal energy level. As one proceeds left to right across a period, the number of valence electrons increases by one. In the *s* block, Group 1 elements have one valence electron, while Group 2 elements have two valence electrons. In the *p* block, the number of valence electrons is equal to the group number minus ten. Group 13 has three valence electrons, Group 14 has four, up through Group 18 with eight. The eight valence electrons, a full outer *s* and *p* sublevel, give the noble gases their special stability.

When examining chemical bonding, it is necessary to keep track of the valence electrons of each atom. **Electron dot diagrams** are diagrams in which the valence electrons of an atom are shown as dots distributed around the element's symbol. A beryllium atom, with two valence electrons, would have the electron dot diagram below.

• Be •

Since electrons repel each other, the dots for a given atom are distributed evenly around the symbol before they are paired.

Octet Rule

The noble gases are unreactive because of their electron configurations. The noble gas neon has the electron configuration of $1s^2 2s^2 2p^6$. It has a full outer shell and cannot incorporate any more electrons into the valence shell. The other noble gases have the same outer shell electron configuration even though they have different numbers of inner-shell electrons.

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Electron configuration of neon atom.

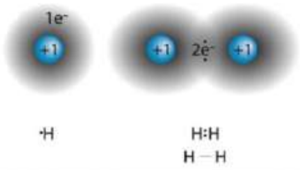
American chemist Gilbert Lewis (1875-1946) used this observation to explain the types of ions and molecules that are formed by other elements. He called his explanation the **octet rule.** The octet rule states that atoms tend to form compounds in ways that give them eight valence electrons and thus the electron configuration of a noble gas. An exception to an octet of electrons is in the case of the first noble gas, helium, which only has two valence electrons. This primarily affects the element hydrogen, which forms stable compounds by achieving two valence electrons. Lithium, an alkali metal with three electrons, is also an exception to the octet rule. Lithium tends to lose one electron to take on the electron configuration of the nearest noble gas, helium, leaving it with two valence electrons.

There are two ways in which atoms can satisfy the octet rule. One way is by sharing their valence electrons with other atoms. The second way is by transferring valence electrons from one atom to another. Atoms of metals tend to lose all of their valence electrons, which leaves them with an octet from the next lowest principal energy level. Atoms of nonmetals tend to gain electrons in order to fill their outermost principal energy level with an octet.

Lewis Electron-Dot Structures

In a previous chapter, you learned that the valence electrons of an atom can be shown in a simple way with an electron dot diagram. A hydrogen atom is shown as H• because of its one valence electron. The structures of molecules that are held together by covalent bonds can be diagrammed by **Lewis electron-dot structures**. The hydrogen molecule is shown in **Figure** below.

The shared pair of electrons is shown as two dots in between the two H symbols (H:H). This is called a **single covalent bond**, when two atoms are joined by the sharing of one pair of electrons. The single covalent bond can also be shown by a dash in between the two symbols (H–H). A **structural formula** is a formula that shows the arrangement of atoms in a molecule and represents covalent bonds between atoms by dashes.



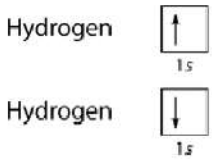
On the left is a single hydrogen atom with one electron. On the right is an H_2 molecule showing the electron cloud overlap.

The Octet Rule and Covalent Bonds

When ions form, they conform to the **octet rule** by either losing or gaining electrons in order to achieve the electron configuration of the nearest noble gas. In a similar way, nonmetal atoms share electrons in the formation of a covalent in bond such a way that each of the atoms involved in the bond can attain a noble-gas electron configuration. The shared electrons are "counted" for each of the atoms involved in the sharing. For hydrogen (H_2), the shared pair of electrons means that each of the atoms is able to attain the electron configuration of helium, the noble gas with two electrons. For atoms other than hydrogen, the sharing of electrons will usually provide each of the atoms with eight valence electrons.

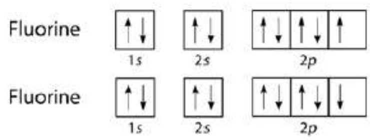
Single Covalent Bonds

A covalent bond forms when two orbitals with one electron each overlap each other. For the hydrogen molecule, this can be shown as:

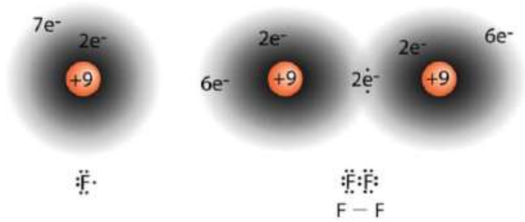


Upon formation of the H_2 molecule, the shared electrons must have opposite spin, so they are shown with opposite spin in the atomic 1*s* orbital.

The halogens also form single covalent bonds in their diatomic molecules. An atom of any halogen, such as fluorine, has seven valence electrons. Its unpaired electron is located in the 2*p* orbital.



The single electrons in the third 2*p* orbital combine to form the covalent bond:



On the left is a fluorine atom with seven valence electrons. On the right is the F_2 molecule.

The diatomic fluorine molecule (F_2) contains a single shared pair of electrons. Each F atom also has three pair of electrons that are not shared with the other atom. A **lone pair** is a pair of electrons in a Lewis electron-dot structure that is not shared between atoms. The oxygen atom in the water molecule shown below has two lone pair sets of electrons. Each F atom has three lone pairs. Combined with the two electrons in the covalent bond, each F atom follows the octet rule.

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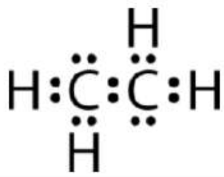
Multiple Covalent Bonds

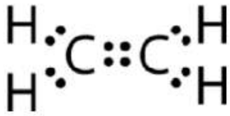
Some molecules are not able to satisfy the octet rule by making only single covalent bonds between the atoms. Consider the compound ethene, which has a molecular formula of C_2H_4. The carbon atoms are bonded together, with each carbon also being bonded to two hydrogen atoms.

If the Lewis electron dot structure was drawn with a single bond between the carbon atoms and with the octet rule followed, it would look like this:



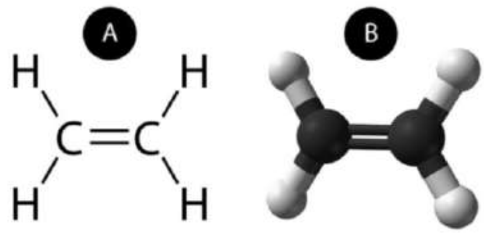
Incorrect dot structure of ethene.

This Lewis structure is incorrect because it contains a total of 14 electrons. However, the Lewis structure can be changed by eliminating the lone pairs on the carbon atoms and having the share two pairs instead of only one pair.



Correct dot structure for ethene.

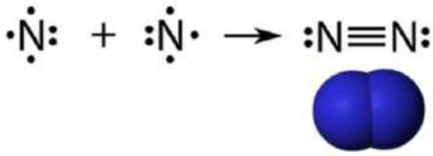
A **double covalent bond** is a covalent bond formed by atoms that share two pairs of electrons. The double covalent bond that occurs between the two carbon atoms in ethane can also be represented by a structural formula and with a molecular model as shown in **Figure** below.



(A) The structural model for C2H4 consists of a double covalent bond between the two carbon atoms and single bonds to the hydrogen atoms. (B) Molecular model of C2H4.

A **triple covalent bond** is a covalent bond formed by atoms that share three pairs of electrons. The element nitrogen is a gas that composes the majority of Earth's atmosphere. A nitrogen atom has five valence electrons, which can be shown as one pair and three single electrons. When combining with another nitrogen atom to form a diatomic molecule, the three single electrons on each atom combine to form three shared pairs of electrons.

Chemical bonding

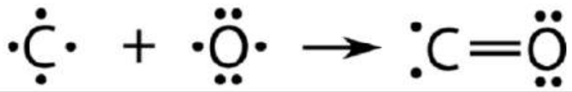


Triple bond in N2.

Each nitrogen atom follows the octet rule with one lone pair of electrons and six electrons that are shared between the atoms.

Coordinate Covalent Bonds

Each of the covalent bonds that we have looked at so far has involved each of the atoms that are bonding contributing one of the electrons to the shared pair. There is an alternate type of covalent bond in which one of the atoms provided both of the electrons in a shared pair. Carbon monoxide, CO, is a toxic gas that is released as a by-product during the burning of fossil fuels. The bonding between the C atom and the O atom can be thought of as proceeding in this way.



Formation of a CO double bond (incorrect structure).

At this point, a double bond has formed between the two atoms, with each atom providing one of the electrons to each bond. The oxygen atom now has a stable octet of electrons, but the carbon atom only has six electrons and is unstable. This situation is resolved if the oxygen atom contributes one of its lone pairs in order to make a third bond with the carbon atom.

Correct CO structure.

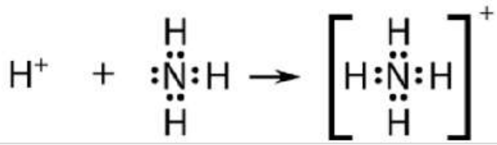
The carbon monoxide molecule is correctly represented by a triple covalent bond between the carbon and oxygen atoms. One of the bonds is a **coordinate covalent bond**, a covalent bond in which one of the atoms contributes both of the electrons in the shared pair.

Once formed, a coordinate covalent bond is the same as any other covalent bond. It is not as if the two conventional bonds in the CO molecule are stronger or different in any other way than the coordinate covalent bond.

Chemical bonding

Polyatomic Ions

Recall that a **polyatomic ion** is a group of atoms that are covalently bonded together and which carry an overall electrical charge. The ammonium ion, NH_4^+, is formed when a hydrogen ion (H^+) attaches to the lone pair of an ammonia (NH_3) molecule in a coordinate covalent bond.



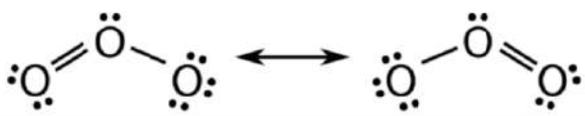
The ammonium ion.

When drawing the Lewis structure of a polyatomic ion, the charge of the ion is reflected in the number of total valence electrons in the structure. In the case of the ammonium ion:

It is customary to put the Lewis structure of a polyatomic ion into a large set of brackets, with the charge of the ion as a superscript outside the brackets.

Resonance

There are some cases in which more than one viable Lewis structure can be drawn for a molecule. An example is the ozone (O_3) molecule in **Figure**. There are a total of 18 electrons in the structure and so the following two structures are possible.

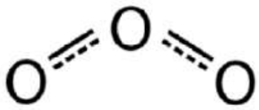


Resonance forms of ozone.

The structure on the left (see **Figure**) can be converted to the structure on the right by a shifting of electrons without altering the positions of the atoms.

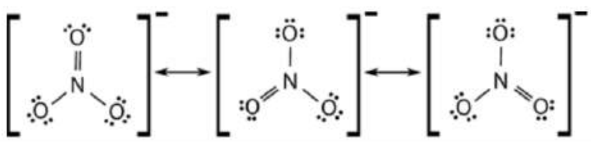
It was once thought that the structure of a molecule such as O_3 consisted of one single bond and one double bond which then shifted back and forth as shown above. However, further studies showed that the two bonds are identical. Any double covalent bond between two given atoms is typically shorter than a single covalent bond. Studies of the O_3 and other similar molecules showed that the bonds were identical in length. Interestingly, the length of the bond is in between the lengths expected for an O-O single bond and a double bond.

Resonance is the use of two or more Lewis structures to represent the covalent bonding in a molecule. One of the valid structures is referred to as a resonance structure. It is now understood that the true structure of a molecule which displays resonance is that of an average or a hybrid of all the resonance structures. In the case of the O_3 molecule, each of the covalent bonds between O atoms is best thought of as being "one and a half" bonds, as opposed to either a pure single bond or a pure double bond. This "half-bond" can be shown as a dotted line in both the Lewis structure and the molecular model (see **Figure**).



"Half-bond" model of ozone molecule.

Many polyatomic ions also display resonance. In some cases, the true structure may be an average of three valid resonance structures, as in the case of the nitrate ion, NO_3^- (see **Figure**).



Resonance structure of nitrate anion.

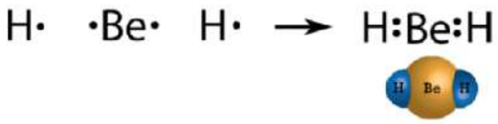
The bond lengths between the central N atom and each O atom are identical and the bonds can be approximated as being equal to one and one-third bonds.

Exceptions to the Octet Rule

As the saying goes, all rules are made to be broken. When it comes to the octet rule, that is true. Exceptions to the octet rule fall into one of three categories: (1) an **incomplete octet**, (2) **odd-electron molecules**, and (3) an **expanded octet.**

Incomplete Octet

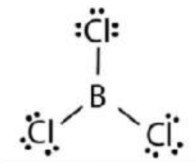
In some compounds, the number of electrons surrounding the central atom in a stable molecule is fewer than eight. Beryllium is an alkaline earth metal and so may be expected to form ionic bonds. However, its very small size and somewhat higher ionization energy compared to other metals actually lead to beryllium forming primarily molecular compounds. Since beryllium only has two valence electrons, it does not typically attain an octet through sharing of electrons. The Lewis structure of gaseous beryllium hydride (BeH_2) consists of two single covalent bonds between Be and H (see **Figure**).



Beryllium hydride.

Chemical bonding

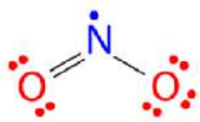
Boron and aluminum, with three valence electrons, also tend to form covalent compounds with an incomplete octet. The central boron atom in boron trichloride (BCl_3) has six valence electrons as shown in **Figure**



Boron trichloride.

Odd-Electron Molecules

There are a number of molecules whose total number of valence electrons is an odd number. It is not possible for all of the atoms in such a molecule to satisfy the octet rule. An example is nitrogen dioxide (NO_2). Each oxygen atom contributes six valence electrons and the nitrogen atom contributes five for a total of seventeen. The lewis structure for NO_2 appears in **Figure**.

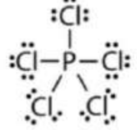


The Lewis structure for nitrogen dioxide, an odd electron molecule.

Expanded Octets

Atoms of the second period cannot have more than eight valence electrons around the central atom. However, atoms of the third period and beyond are capable of exceeding the octet rule by having more than eight electrons around the central atom. Starting with the third period, the *d* sublevel becomes available, so it is possible to use these orbitals in bonding, resulting in an expanded octet.

Phosphorus and sulfur are two elements that react with halogen elements and make stable compounds with expanded octets. In phosphorus pentachloride, the central phosphorus atom makes five single bonds to chlorine atoms and as a result has ten electrons surrounding it. In sulfur hexafluoride, the central sulfur atom has twelve electrons from its six bonds to fluorine atoms.



Phosphorus pentachloride. Lewis structure

Chemical bonding

Bond Energy

The formation of a chemical bond results in a decrease in potential energy. Consequently, breaking a chemical bond requires an input of energy. **Bond energy** is the energy required to break a covalent bond between two atoms. A high bond energy means that a bond is strong and the molecule that contains that bond is likely to be stable and less reactive. More reactive compounds will contain bonds that have generally lower bond energies. Some bond energies are listed in **Table** below.

Bond Energies

Bond	Bond Energy (kJ/mol)
H–H	436
C–H	414
C–C	347
C=C	620
C≡C	812
F–F	157
Cl–Cl	243
Br–Br	193
I–I	151
N≡N	941

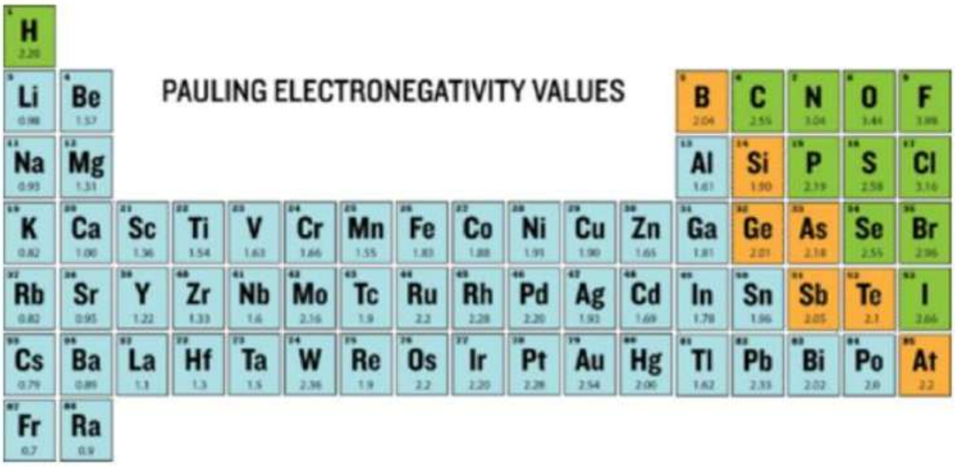
The halogen elements all exist naturally as diatomic molecules (F_2, Cl_2, Br_2, and I_2). They are generally very reactive and thus have relatively low bond energies.

As can be seen by a comparison of the bond energies for the various carbon-carbon bonds, double bonds are substantially stronger than single bonds. Likewise, triple bonds are even stronger. The triple bond that exists between the nitrogen atoms in nitrogen gas (N_2) makes it very unreactive. All plants and animals require the element nitrogen, but it cannot be obtained from the direct absorption of nitrogen gas from the atmosphere because of its strong, unreactive triple bond. Instead, bacteria convert the nitrogen to a more usable form such as ammonium and nitrate ions, which is then absorbed by plants from the soil. Animals only obtain nitrogen by eating those plants.

Bond Polarity

Chemical bonding

Electronegativity is defined as the ability of an atom to attract electrons when the atoms are in a compound. Electronegativities of elements are shown in the periodic table below.

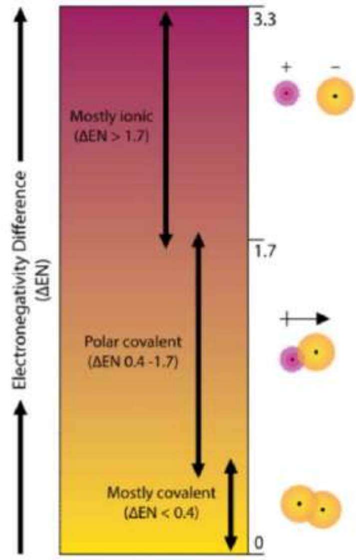


Electronegativities of elements.

The degree to which a given bond is ionic or covalent is determined by calculating the difference in electronegativity between the two atoms involved in the bond.

As an example, consider the bond that occurs between an atom of potassium and an atom of fluorine. Using the table, the difference in electronegativity is equal to 4.0 - 0.8 = 3.2. Since the difference in electronegativity is relatively large, the bond between the two atoms is ionic. Since the fluorine atom has a much larger attraction for electrons than the potassium atom does, the valence electron from the potassium atom is completely transferred to the fluorine atom. The diagram below shows how difference in electronegativity relates to the ionic or covalent character of a chemical bond.

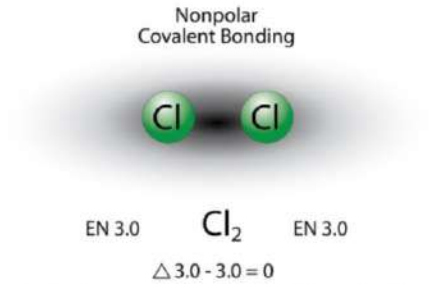
Chemical bonding



Bond type is predicated on the difference in electronegativity of the two elements involved in the bond.

Non-polar Covalent Bonds

A bond in which the electronegativity difference is less than 1.7 is considered to be mostly covalent in character. However, at this point we need to distinguish between two general types of covalent bonds. A **non-polar covalent bond** is a covalent bond in which the bonding electrons are shared equally between the two atoms. In a non-polar covalent bond, the distribution of electrical charge is balanced between the two atoms.



A nonpolar covalent bond is one in which the distribution of electron density between the two atoms is equal.

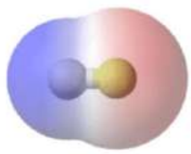
The two chlorine atoms share the pair of electrons in the single covalent bond equally, and the electron density surrounding the Cl_2 molecule is symmetrical. Also note that molecules in which the electronegativity difference is very small (<0.4) are also considered non-polar covalent. An example would be a bond between chlorine and bromine

$(\Delta EN = 3.0 - 2.8 = 0.2)$.

Chemical bonding

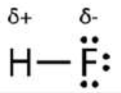
Polar Covalent Bonds

A bond in which the electronegativity difference between the atoms is between 0.4 and 1.7 is called a polar covalent bond. A **polar covalent bond** is a covalent bond in which the atoms have an unequal attraction for electrons and so the sharing is unequal. In a polar covalent bond, sometimes simply called a polar bond, the distribution of electrons around the molecule is no longer symmetrical.



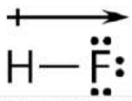
In the polar covalent bond of HF, the electron density is unevenly distributed. There is a higher density (red) near the fluorine atom, and a lower density (blue) near the hydrogen atom.

An easy way to illustrate the uneven electron distribution in a polar covalent bond is to use the Greek letter delta δ .



Use of δ to indicate partial charge.

The atom with the greater electronegativity acquires a partial negative charge, while the atom with the lesser electronegativity acquires a partial positive charge. The delta symbol is used to indicate that the quantity of charge is less than one. A crossed arrow can also be used to indicate the direction of greater electron density.

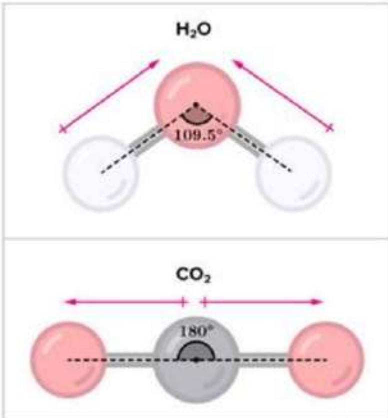


Use of crossed arrow to indicate polarity.

Chemical bonding

Molecular Geometry

VSEPR Theory



Why is the water molecule bent like that?

The characteristic bent shape of the water molecule shown above was a puzzling discovery for scientists at first. The shape allows the molecule to be polar, increasing its boiling point and making it possible for life on earth to exist as we know it. But what makes it bend? The structure is almost the same as carbon dioxide which is known to be a gas at room temperature, why not water too?

Putting atoms together to form compounds can be done on paper or in the lab. However, when the shape of the molecule made in the lab is different from the shape of the molecule drawn on paper, then we need to rethink our ideas and find better explanations.

VSEPR Theory

In 1956, British scientists R.J. Gillespie and R.S. Nyholm recognized that the current model for explaining bond angles did not work well. The theory at that time relied on hybrid orbitals to explain all aspects of bonding. The problem was that the theory gave incorrect prediction of bond angles for many compounds. They developed a new approach based on earlier work by other scientists that incorporated a consideration of electron pairs in predicting three-dimensional structure.

The **valence shell** is the outermost electron-occupied shell of an atom. The valence shell holds the electrons that are involved in bonding and are the electrons shown in a Lewis structure. The acronym VSEPR stands for the **valence-shell electron pair repulsion** model. The model states that electron pairs will repel each other such that the shape of the molecule will adjust so that the valence electron-pairs stay as far apart from each other as possible. Molecules can be systematically classified according to the number of bonding pairs of electrons as well as the number of nonbonding or lone pairs around the central atom. For the purposes of the VSEPR model, a double or triple bond is no different in terms of repulsion than a single bond.

Chemical bonding

Central Atom with No Lone Pairs

In order to easily understand the types of molecules possible, we will use a simple system to identify the parts of any molecule.

A = **central atom** in a molecule

B = atoms surrounding the central atom

Subscripts after the B will denote the number of B atoms that are bonded to the central A atom. For example, AB_4 is a molecule with a central atom surrounded by four covalently bonded atoms. Again, it does not matter if those bonds are single, double, or triple bonds.

AB_2: Beryllium hydride (BeH_2)

Beryllium hydride consists of a central beryllium atom with two single bonds to hydrogen atoms. Recall that it violates the octet rule.

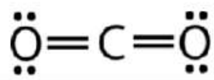
H-Be-H

According to the requirement that electron pairs maximize their distance from one another, the two bonding pairs in the BeH_2 molecules will arrange themselves on directly opposite sides of the central Be atom. The resulting geometry is a linear molecule, shown in the **Figure** below in a "ball and stick" model.

Beryllium hydride model.

The bond angle from H-Be-H is 180° because of its linear geometry.

Carbon dioxide is another example of a molecule which falls under the AB_2 category. Its Lewis structure consists of double bonds between the central carbon and the oxygen atoms (see **Figure** below).



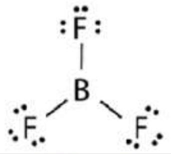
Carbon dioxide bonding.

The repulsion between the two groups of four electrons (two pairs) is no different than the repulsion of the two groups of two electrons (one pair) in the BeH_2 molecule. Carbon dioxide is also linear (see **Figure** below).

Chemical bonding

AB_3: Boron Trifluoride (BF_3)

Boron trifluoride consists of a central boron atom with three single bonds to fluorine atoms(see **Figure** below). The boron atom also has an incomplete octet.

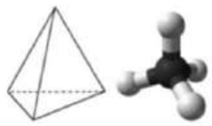


Boron trifluoride bonding.

The geometry of the BF_3 molecule is called trigonal planar (see **Figure** below). The fluorine atoms are positioned at the vertices of an equilateral triangle. The F-B-F angle is 120° and all four atoms lie in the same plane.

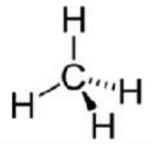
AB_4: Methane (CH_4)

Methane is an organic compound that is the primary component of natural gas. Its structure consists of a central carbon atom with four single bonds to hydrogen atoms (see **Figure** below). In order to maximize their distance from one another, the four groups of bonding electrons do not lie in the same plane. Instead, each of the hydrogen atoms lies at the corners of a geometrical shape called a tetrahedron. The carbon atom is at the center of the tetrahedron. Each face of a tetrahedron is an equilateral triangle.



Tetrahedral structure of methane

The molecular geometry of the methane molecule is tetrahedral (see **Figure** below). The H-C-H bond angles are 109.5°, which is larger than the 90° that they would be if the molecule was planar. When drawing a structural formula for a molecule such as methane, it is advantageous to be able to indicate the three-dimensional character of its shape. The structural formula below is called a perspective drawing. The dotted line bond is to be visualized as receding into the page, while the solid triangle bond is to be visualized as coming out of the page.



Methane perspective model.

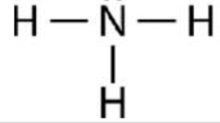
Central Atom with One or More Lone Pairs

Chemical bonding

The molecular geometries of molecules change when the central atom has one or more lone pairs of electrons. The total number of electron pairs, both bonding pairs and lone pairs, leads to what is called the **electron domain geometry.** When one or more of the bonding pairs of electrons is replaced with a lone pair, the molecular geometry (actual shape) of the molecule is altered. In keeping with the A and B symbols established in the previous section, we will use E to represent a lone pair on the central atom (A). A subscript will be used when there is more than one lone pair. Lone pairs on the surrounding atoms (B) do not affect the geometry.

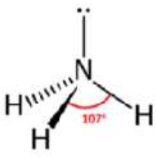
AB_3E: Ammonia, NH_3

The ammonia molecule contains three single bonds and one lone pair on the central nitrogen atom (see **Figure** below).



Lone pair electrons in ammonia.

The domain geometry for a molecule with four electron pairs is tetrahedral, as was seen with CH_4. In the ammonia molecule, one of the electron pairs is a lone pair rather than a bonding pair. The molecular geometry of NH_3 is called trigonal pyramidal (see **Figure** below).

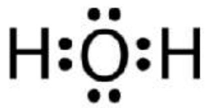


Ammonia molecule.

Recall that the bond angle in the tetrahedral CH_4 molecule is 109.5°. Again, the replacement of one of the bonded electron pairs with a lone pair compresses the angle slightly. The H-N-H angle is approximately 107°.

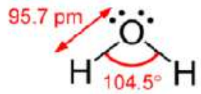
AB_2E_2: Water, H_2O

A water molecule consists of two bonding pairs and two lone pairs (see **Figure** below).



Lone pair electrons on water.

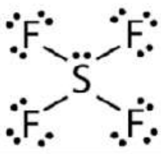
As for methane and ammonia, the domain geometry for a molecule with four electron pairs is tetrahedral. In the water molecule, two of the electron pairs are lone pairs rather than bonding pairs. The molecular geometry of the water molecule is bent. The H-O-H bond angle is 104.5°, which is smaller than the bond angle in NH_3 (see **Figure** below).



Water molecule.

AB_4E: Sulfur Tetrafluoride, SF_4

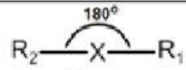
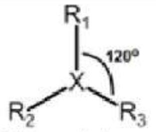
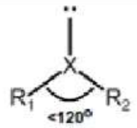
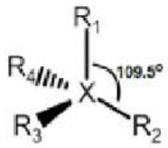
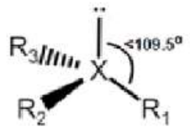
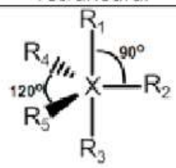
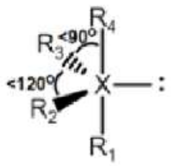
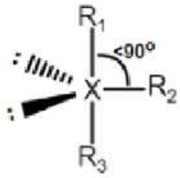
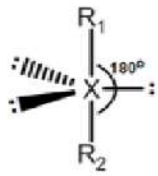
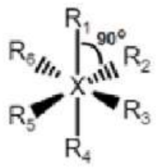
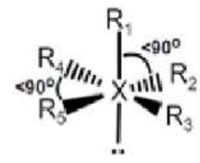
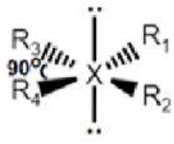
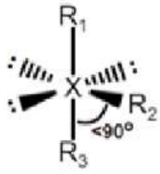
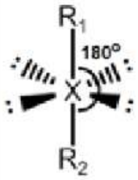
The Lewis structure for SF_4 contains four single bonds and a lone pair on the sulfur atom (see **Figure** below).



Lone pair electrons in SF_4

The sulfur atom has five electron groups around it, which corresponds to the trigonal bipyramidal domain geometry, as in PCl_5 (see **Figure** below). Recall that the trigonal bipyramidal geometry has three equatorial atoms and two axial atoms attached to the central atom. Because of the greater repulsion of a lone pair, it is one of the equatorial atoms that are replaced by a lone pair. The geometry of the molecule is called a distorted tetrahedron or seesaw.

Chemical bonding

Steric No.	Electron Domain Geometry	Molecular Geometry				
		No Lone Pairs	1 Lone Pair	2 Lone Pair	3 Lone Pair	4 Lone pair
2	Linear	 Linear				
3	Trigonal Planar	 Trigonal planar	 Bent			
4	Tetrahedral	 Tetrahedral	 Trigonal pyramidal	 Bent		
5	Trigonal Bipyramidal	 Trigonal Bipyramidal	 Sawhorse	 T-shaped	 Linear	
6	Octahedral	 Octahedral	 Square pyramidal	 Square planar	 T-shaped	 Linear