

Compounds

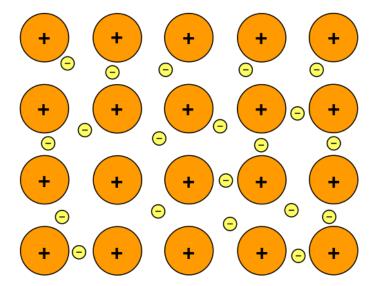
Have you heard of any advertisement claiming that their product is "chemical-free?" How did you react?

Well, for chemists, that is an example of a very bad and misleading advertisement. *Why*? It's because there's no such thing as "chemical-free." By definition, a chemical is a substance that can be represented using a fixed chemical formula and possess characteristic properties.

A compound is a type of chemical which is defined as a substance composed of atoms of two or more elements chemically united in fixed proportions. The water we drink and even the air we breathe are all considered "chemicals." Learn more about "chemicals" and compounds in this section!

Types of Chemical Bonds

1. Metallic Bond



This illustration of positive atomic nuclei (orange circles) surrounded by a sea of delocalized electrons (yellow circles), known as the Electron Sea Model, from LibreTexts is licensed under <u>CC BY-NC-SA 3.0 US</u>



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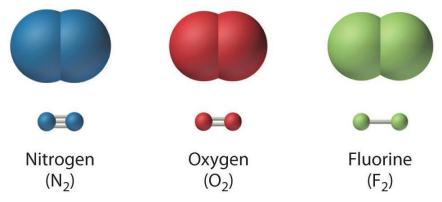


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This is a type of chemical bond that forms among metallic substances and is a direct consequence of attractive electrostatic forces between the negatively charged sea of delocalized electrons and the positively charged metal ions.

In solid metals, individual metal atoms are so close to one another that the electron cloud of one metal atom overlaps with its neighboring metal atom. This creates the "sea of delocalized electrons." In other words, the electrons are free to wander within the crystal structure.

2. Covalent Bond



This illustration of <u>elements with diatomic molecules</u> from <u>LibreTexts</u> is licensed under <u>CC BY-NC-SA 3.0 US</u>.

A covalent bond is a type of chemical bond wherein the electrons involved in bond formation are **shared** by the two atoms bonded with one another. As you know, a covalent bond is designated by a "dash" connecting one atom to another. Each covalent bond is composed of two electrons, and each atom being bonded covalently contributes one electron to that bond.

A covalent bond can be a single (ex: F_2), double (ex: O_2), or even triple (ex: N_2) bond.

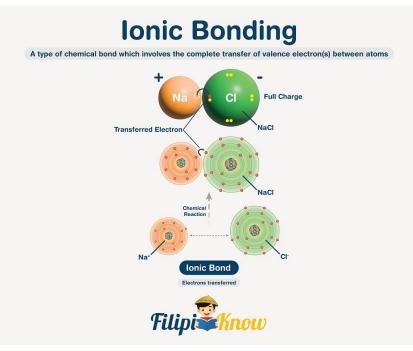


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3. Ionic Bond



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An ionic bond is a type of chemical bond which involves the complete transfer of valence electron(s) between atoms. This bond usually occurs between a metal and a nonmetal.

The transfer of electrons is made possible because metals tend to lose their valence electron(s) to become a positively-charged cation. In contrast, the nonmetals tend to gain the electron(s) lost by the cations to become a negatively-charged anion.

In writing ionic compounds, both ions are enclosed inside a square bracket, with their charge and numerical coefficient (if there is any) written outside the bracket. See the figure below.

4. Coordinate Covalent Bond

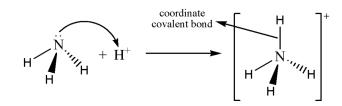


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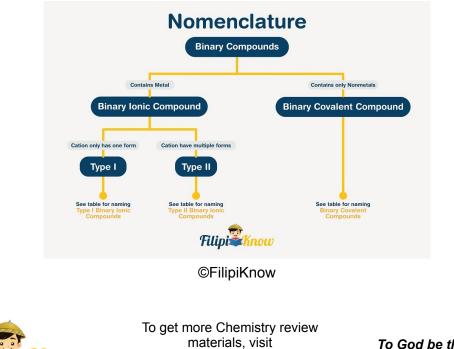


The coordinate covalent bond is also known as a *dative bond*. In this type of chemical bond, both electrons are supplied by one of the two bonded atoms. This is commonly observed among coordinate covalent compounds and inorganic complexes and is written just like a covalent bond.

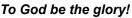
How To Name Compounds and Write Compound Formulas

There are different types of compounds, but in this part, we will only consider the nomenclature of binary covalent and ionic compounds, as well as some inorganic acids.

There are certain rules to follow in naming binary compounds, and the figure presented below is an excellent guide.



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1. Binary Covalent Compounds

A **binary covalent compound** is a covalent compound that is made up of exactly two elements only.

a. Naming Binary Covalent Compounds

Rule 1:	The first element in the chemical formula is named first using the name of that element.
Rule 2:	The second element in the chemical formula is named as if it is an anion.
Rule 3:	Indicate the number of that element using the appropriate prefix.
Rule 4:	The prefix <i>mono</i> - is never used in denoting the number of the first element.
Rule 5:	If the name of the element starts with a vowel, drop the "a" or "o" in the prefix.

The following prefixes must be used to denote the number of certain atoms in the compound's formula.

Number	Prefix	Number	Prefix
1	mono-	6	hexa-
2	di-	7	hepta-
3	tri-	8	octa-
4	tetra-	9	nona-
5	penta-	10	deca-



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Examples:

Chemical Formula	Chemical Name
N_2O_5	dinitrogen pentoxide, not dinitrogen pentaoxide
PCI₅	phosphorus pentachloride , not monophosphorus pentachloride
СО	carbon monoxide, not monocarbon monooxide

In N_2O_5 , the name dinitrogen pentaoxide is incorrect by virtue of rule number 5, although if you will read older references, this system of nomenclature was allowed and accepted. However, the common practice today is to drop "a" or "o" in the prefix if the name of the element starts with a vowel. In PCI₅, monophosphorus pentachloride is incorrect by virtue of rule 4. Lastly, for CO, monocarbon monooxide is incorrect by virtue of rules 4 and 5.

b. Writing Chemical Formula of Binary Covalent Compounds

Rule 1:	Identify the chemical symbol of the element.
Rule 2:	Take note of the prefix used for each element, and write the corresponding number as a subscript of that element.
Rule 3:	When writing the chemical formula, make sure to write the less electronegative element first. The most electronegative element in the periodic table is fluorine (F). Hence, you can make it a convention that the farther the element is from fluorine, the less electronegative it is.



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Examples:

Chemical Name	Chemical Formula		
oxygen difluoride	O is less electronegative than F; there is one O atom and two F atoms, hence the chemical formula is \mathbf{OF}_2 , not F_2O		
tetraphosphorus decoxide	P is less electronegative than F; there are four atoms of P and 10 atoms of O, hence the chemical formula is P_4O_{10} , not $O_{10}P_4$		
sulfur hexaflouride	S is less electronegative than F; there is one S atom and 6 F atoms, hence the chemical formula is \mathbf{SF}_{6} , not $F_{6}S$		
dioxygen difluoride	O is less electronegative than F; there are two O atoms and two F atoms, hence the chemical formula is O ₂ F ₂ , not F ₂ O ₂		

Always remember to write first the symbol for the less electronegative element in the chemical formula, followed by the more electronegative species. Fortunately, it is not a common mistake since **most of the time, the less electronegative element is written first in the chemical name**, so you can really use it as a guide.

2. Binary Ionic Compounds

A **binary ionic compound** is a compound that is composed of a single type of cation and a single type of anion.

a. Naming Binary Ionic Compounds

Naming binary ionic compounds is a little more complicated than the nomenclature of binary covalent compounds due to the presence of cations with multiple oxidation states. If the cation exhibits only one oxidation state, then the compound is a Type I binary ionic compound. In contrast, if the cation exhibits at least two oxidation states, then the compound is a Type II binary ionic compound.



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i. Type I Binary Ionic Compounds

Rule 1:	The cation is always named first, while the anion is always named second.
Rule 2:	Monoatomic cations are named as if they are elements. Meanwhile, the monoatomic anion takes the root of the element name + - <i>ide</i> .
Rule 3:	Polyatomic cations and anions have special and unique names and you should familiarize yourself with all of them.
Rule 4:	The prefixes being used in the nomenclature of covalent compounds are not usually used in the nomenclature of ionic compounds.

The table below provides the list of the most common polyatomic ions that you can encounter. It will be hard to remember them all at once, so it is suggested that you familiarize yourself with them by reading them repeatedly every day (familiarization is the key!).

lon	Name	lon	Name
NH_4^+	ammonium	SO4 ²⁻	sulfate
⁻OH	hydroxide	HSO_4^-	hydrogen sulfate/bisulfate
$C_2H_3O_2^-$	acetate	SO3 ²⁻	sulfite
NO_3^-	nitrate	HSO_3^-	hydrogen sulfite/bisulfite
NO_2^-	nitrite	CO ₃ ²⁻	carbonate
CN⁻	cyanide	HCO₃ [−]	hydrogen carbonate/bicarbonate
MnO₄ [−]	permanganate	CrO ₄ ^{2–}	chromate



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O2 ²⁻	peroxide	Cr ₂ O ₇ ²⁻	dichromate
S ₂ O ₃ ²⁻	thiosulfate	AsO ₄ ^{3–}	arsenate
CIO-	hypochlorite	PO ₃ ^{3–}	phosphite
CIO_2^-	chlorite	PO4 ³⁻	phosphate
CIO ₃ ⁻	chlorate	HPO4 ²⁻	hydrogen phosphate/biphosphate
CIO ₄ ⁻	perchlorate	$H_2PO_4^-$	dihydrogen phosphate

Examples:

Chemical Name	Chemical Formula
sodium chloride	NaCl
ammonium bromide	NH₄Br
barium hydroxide, not barium dihydroxi	Ba(OH) ₂
ammonium sulfate, not diammonium sul	$(NH_4)_2SO_4$

One of the most common mistakes committed when naming ionic compounds is the use of prefixes used for naming binary covalent compounds. Keep in mind that those prefixes are NEVER used when naming ionic compounds. Hence, the correct name of $Ba(OH)_2$ is barium hydroxide and not barium dihydroxide. The same is true for naming $(NH_4)_2SO_4$.

ii. Type II Binary Ionic Compounds

Rule 1:The cation is always named first, while the anion is always named
second.



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- Rule 2: In naming the cation using the systematic method, identify the oxidation state of the cation, and write the oxidation state (in roman numeral) adjacent to the name of the cation
 Rule 3: In naming the cation using the stock system, identify the oxidation state of the cation. If the oxidation state of the cation is less than the other oxidation state, the cation is named as the element root name + -ous. On the other hand, if the oxidation state of the cation is greater than the other oxidation state, the cation is named as the element root name element root name + -ic.
 Rule 4: Name the monoatomic anion by taking the root of the element name + -ide. Use corresponding names for polyatomic anions.
- Rule 5:The prefixes being used in the nomenclature of covalent compounds
are not usually used in the nomenclature of ionic compounds.

As you can see, it's getting more and more complicated as we proceed. First, you were asked to familiarize the prefixes, then the polyatomic ions, and now, the stock and systematic names! It is challenging, but again, familiarization is the key!

Metal ion	Stock Name	Systematic Name
Pb ²⁺	plumbous	lead(II)
Pb ⁴⁺	plumbic	lead(IV)
Fe ²⁺	ferrous	iron(II)
Fe ³⁺	ferric	iron(III)
Co ²⁺	cobaltous	cobalt(II)
C0 ³⁺	cobaltic	cobalt(III)



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Cu⁺	cuprous	copper(I)
Cu ²⁺	cupric	copper(II)

Examples:

Compound Formula	Stock Name	Systematic Name
	cupric chloride	copper(II) chloride
FeSO₄	ferrous sulfate	iron(II) sulfate
SnBr₄	stannic bromide	tin(IV) bromide
Pb(OH) ₂	plumbous hydroxide	lead(II) hydroxide

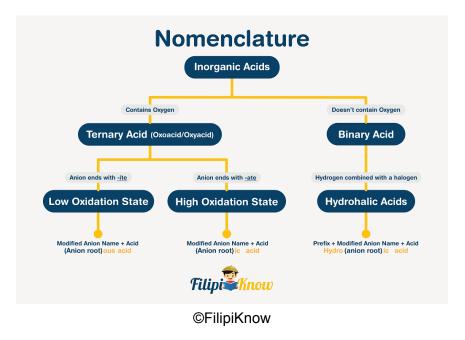
Nowadays, stock names are less preferably used because of their ambiguity, specifically for cations with more than two oxidation states. For example, Mn can have oxidation states of +2, +3, +4, +6, and +7. The use of stock names for these cases makes the name confusing since it is not known which among the Mn^{2+} , Mn^{3+} , Mn^{4+} , Mn^{6+} , and Mn^{7+} is the manganous and manganic ion.

Let us now proceed with the nomenclature of inorganic acids. By definition, acids are compounds that release (directly or indirectly) free H_3O^+ in an aqueous solution. The schematic diagram shown below efficiently describes how the naming of inorganic acids is carried out.



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Examples:

Chemical Formula	Chemical Name
HCI	there is no oxygen atom in the anion, hence the name is hydrochloric acid
HBr	there is no oxygen atom in the anion, hence the name is hydrobromic acid
HNO ₃	there are oxygen atoms in the anion, and the anion name is a nitrate, hence, the name of the acid is nitric acid
H_2SO_4	there are oxygen atoms in the anion, and the anion name is sulfate, hence, the name of the acid is sulfuric acid



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HNO ₂	there are oxygen atoms in the anion, and the anion name is nitrite, hence, the name of the acid is nitrous acid
H_2SO_3	there are oxygen atoms in the anion, and the anion name is sulfite, hence, the name of the acid is sulfurous acid

Additional polyatomic anions that you can commonly encounter in the nomenclature of inorganic acids are shown below.

Formula	Name	Formula	Name	Formula	Name
CIO-	hypochlorite	BrO⁻	hypobromite	IO [_]	hypoiodite
CIO_2^-	chlorite	BrO_2^-	bromite	IO_2^-	iodite
ClO₃ [−]	chlorate	BrO ₃ ⁻	bromate	IO_3^-	iodate
CIO_4^-	perchlorate	BrO ₄ ⁻	perbromate	IO_4^-	periodate

b. Writing Chemical Formula of Binary Ionic Compounds

- Rule 1:Separately write the cation and anion, indicating their correct
charge.
- Rule 2:Using the criss-cross method, take the absolute value of the
charge of the cation, and write it as a subscript of the anion. In
the same way, take the absolute value of the charge of the
anion and write it as the subscript of the cation.
- **Rule 3:** For polyatomic ions, write parenthesis if necessary.



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Rule 4:The subscripts of the anion and cation must be written in the
lowest possible terms. As an example, the formula of ferrous
sulfate is written as $FeSO_4$, instead of $Fe_2(SO_4)_2$ since the
subscripts of both ions are 2. In the same manner, the formula
of tin(IV) sulfate is $Sn(SO_4)_2$ instead of $Sn_2(SO_4)_4$.

Examples:

Chemical Name	lons involved	Chemical Formula
calcium hydroxide	Ca²⁺, ⁻OH	Ca(OH) ₂
ammonium chloride	NH₄⁺, CI⁻	NH₄CI
barium phosphate	Ba ²⁺ , PO ₄ ³⁻	Ba ₃ (PO ₄) ₂
ferrous dichromate	Fe ²⁺ , Cr ₂ O ₇ ²⁻	FeCr ₂ O ₇
lead(II) iodide	Pb²+, I⁻	Pbl ₂
cupric nitrate	Cu ²⁺ , NO ₃ ⁻	Cu(NO ₃) ₂

The trick here that you need to remember is to always write the cation first (with its correct charge) followed by the anion (with its correct charge) like what was done in the second column.

Next, whatever the charge of the cation is, take its absolute value and make it the subscript of the anion. Then, take the absolute value of the charge of the anion and make it the subscript of the cation. Make sure to include parentheses if the ion is polyatomic! For example, in calcium hydroxide, there is a huge difference between $Ca(OH)_2$ (the correct formula) and $CaOH_2$ (non-existent).

Another thing that you need to remember is to always write the subscript of the chemical formula to the lowest possible terms. For example, by following the rules described for calcium



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hydroxide, the formula of ferrous dichromate should be $(Fe)_2(Cr_2O_7)_2$. However, due to this additional rule, the correct formula is $FeCr_2O_7$.

But before you write in the lowest possible terms, always make sure that you are dealing with an ionic compound, because this rule does not apply to binary covalent compounds. For example, P_4O_{10} (a binary covalent compound) cannot be written as P_2O_5 ! Try to name these compounds and you will see that these two are distinct from one another!

Determining Oxidation Number

An **oxidation number** is a number (can be positive, negative, or zero) assigned to a certain element to indicate its degree of oxidation or reduction. You will realize the importance of determining the oxidation number in the nomenclature of binary ionic compounds, and in balancing redox reactions.

Certain rules were established to allow us to determine the oxidation number of a certain element easily. This material will walk you through the step-by-step process (with illustration) of determining the oxidation numbers of a certain element in a compound.

Rules in Assigning Oxidation Numbers

- Rule 1:Free/uncombined elements have oxidation numbers equal to zero. Example: H2,Al, Fe, Zn, N2 all have zero oxidation numbers.
- **Rule 2:** Monoatomic ions have oxidation numbers equal to their charge. Example: The oxidation number of Fe²⁺ is +2, and the oxidation number of Cl⁻ is -1.
- Rule 3:In its ionic form, the oxidation number of Group I elements (except H) is always
+1, while the oxidation number of Group II elements is always +2.
- **Rule 4:** The oxidation number of H is +1. However, when it is combined with metal in hydride compounds, its oxidation number is -1. Example: In lithium hydride, LiH, the oxidation number of H is -1.



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 peroxide anion (O₂²⁻), wherein its oxidation number is -1. Rule 7: Halogens have negative oxidation numbers when it forms halide compound However, when it forms oxygen-containing compounds, its oxidation number positive. Rule 8: For polyatomic ions, the algebraic sum of the oxidation number of each elemis equal to the charge of the ion. Rule 9: In neutral compounds, the algebraic sum of the oxidation numbers of all the 	Rule 5:	In all of its compounds, AI has an oxidation number of +3. Also, F has an oxidation number of -1 in all of its compounds.
 However, when it forms oxygen-containing compounds, its oxidation number positive. Rule 8: For polyatomic ions, the algebraic sum of the oxidation number of each elem is equal to the charge of the ion. Rule 9: In neutral compounds, the algebraic sum of the oxidation numbers of all the 	Rule 6:	The oxidation number of oxygen is -2, except for hydrogen peroxide (H_2O_2) or peroxide anion $(O_2^{2^-})$, wherein its oxidation number is -1.
is equal to the charge of the ion. Rule 9: In neutral compounds, the algebraic sum of the oxidation numbers of all the	Rule 7:	Halogens have negative oxidation numbers when it forms halide compounds. However, when it forms oxygen-containing compounds, its oxidation number is positive.
	Rule 8:	For polyatomic ions, the algebraic sum of the oxidation number of each element is equal to the charge of the ion.
elements is equal to zero.	Rule 9:	In neutral compounds, the algebraic sum of the oxidation numbers of all the elements is equal to zero.

Sample Problems:

Determine the oxidation number of highlighted atoms in the following species:

- 1. **He**
- 2. K**Mn**O₄
- 3. $Cr_2O_7^{2-}$
- 4. $C_6H_{12}O_6$

Solutions:

1. Helium (He) is a free element, therefore, by virtue of rule 1, its oxidation number is zero.

2. In KMnO₄, the K is a Group 1 cation and its oxidation number is +1 by virtue of rule 3. On the other hand, O has an oxidation number of -2 by virtue of rule 6, but since there are four oxygen atoms, each has an oxidation number of -2, then the total oxidation number contributed by the oxidation atoms is (4)(-2) = -8.



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Finally, since $KMnO_4$ is a neutral compound, then the algebraic sum of the oxidation numbers of K, Mn, and O must be zero in accordance with rule 9.

+1 x -8 KMnO4

(+1) + x + (-8) = 0

x = -1 + 8 = +7

Therefore, the oxidation number of Mn is +7.

3. By virtue of rule 6, O has an oxidation number of -2, but since there are 7 O atoms, then (7)(-2) = -14. By virtue of rule 8, the algebraic sum of the oxidation numbers of Cr and O should be equal to -2. Hence:



2x + (-14) = -2

2x = -2 + 14 = +12

x = +12/2 = +6

Why 2x, you ask? Well, we are looking for the oxidation number of Cr, and it so happens that there are 2 Cr atoms in the chemical formula, hence 2x.

Based on the computation above, the oxidation number of Cr is +6.

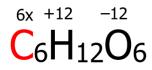


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4. By virtue of rule 6, the oxidation number of O is -2, hence (6)(-2) = -12. Furthermore, the oxidation number of H is +1 by virtue of rule 4, giving us (12)(+1) = +12. Finally, the algebraic sum of the oxidation numbers of C, H, and O must be equal to zero according to rule 9.



6x + (-12) + (+12) = 0

6x + 0 = 0

x = 0

Hence, the oxidation number of C is 0.

Representation of Compounds

As you may have noticed by now, the elemental composition of compounds is one of the information that can be obtained from its chemical formula. In water (H_2O), for example, you can immediately say that per molecule of water, there are two atoms of hydrogen and an oxygen atom. This follows that in every mole of water, there are 2 moles of hydrogen and 1 mole of oxygen. This can then be ultimately expressed to mass to get the *percent composition by mass*.

Percent composition by mass is the percent by mass of each element in a compound. *What is its importance*, you ask?

Well, one of the most famous applications of this concept is the verification of a reagent's purity. For example, a certain chemical manufacturing company claims that it can synthesize pure NH_4NO_3 . One way chemists can verify this claim is to isolate one of the elements from the compound in its weighable form, then compare the experimental mass to the calculated mass. If the experimental data matches the calculated value, then the manufacturer's claim is true.



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To compute the percent composition by mass of a certain element in the compound, the formula shown below can be used:

% composition of an element = $\frac{n \times Molar \text{ mass of the element}}{Molar \text{ mass of the compound}} \times 100$

where n is the number of moles of the element per mole of the compound. Let us work with some examples to better understand this concept.

Sample Problem 1:

Calculate the weight percent of C (MM = 12 g/mol), H (MM = 1 g/mol), and O (MM = 16 g/mol) in $C_6H_{12}O_6$ (MM = 180 g/mol).

Solution:

Solving for the percent composition of C (n = 6):

% composition of $C = \frac{6 \times 12 \, g/mol}{180 \, g/mol} \times 100 = 40 \%$

Meanwhile, the percentage composition of H (n = 12) is:

% composition of $H = \frac{12 x 1 g/mol}{180 g/mol} x 100 = 6.7 \%$

Finally, we can solve for the percent composition of O in two ways. First, you can solve by using the formula of the percent composition (n = 6):





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% composition of $O = \frac{6 \times 16 \ g/mol}{180 \ g/mol} \times 100 = 53.3 \%$

Alternatively, since there are only C, H, and O in the chemical formula of $C_6H_{12}O_6$, you can just subtract the sum of % C and % H to 100 %.

% composition of 0 = 100 - (40% + 6.7%) = 53.3%

Sample Problem 2:

Ammonium nitrate (NH_4NO_3 ; MM = 80 g/mol) is widely used in agriculture as a nitrogen-rich fertilizer. How many grams of N (MM = 14 g/mol) is present in a 100g pure NH₄NO₃?

Solution:

Based on the chemical formula, we can readily say that there are 2 moles of N per mole of NH_4NO_3 . This means that n = 2. Using the formula to calculate % composition of N by mass:

% composition of $N = \frac{n \times Molar \max of N}{Molar \max of NH_4 NO_3} \times 100$ % composition of $N = \frac{2 \times 14 g/mol}{80 g/mol} \times 100 = 35.0$ %

Since N is 35.0 % by mass with respect to NH₄NO₃, that also means that there are 35 g N per 100 g of pure NH₄NO₃.

Writing Lewis Structure and Molecular Geometry

By definition, **molecular geometry** is the orientation of atoms of a molecule in space.





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Is it really important to study the 3D structure of the compounds? Well, the answer is a big YES, since the compound's geometry itself can directly affect the physical and chemical properties of a compound. This may include melting point, boiling point, density, and even reactivity.

For you to be able to draw correct molecular geometries, the most important prerequisite is you should know how to draw Lewis structures of chemical species. **Lewis structures**, also known as the **electron dot structure**, is a simple diagram showing the bond between two atoms, as well as the lone pairs around each atom in a chemical species.

Written below is the set of rules that you can use as a guide in writing the Lewis structures.

Steps in Writing Lewis Structures

Step 1: Identify the central atom. The central atom is usually the least electronegative atom among the atoms in the compound. The most electronegative element in the periodic table is fluorine (F). Hence, you can make it a convention that the farther the element is from fluorine, the less electronegative it is. However, H can never be the central atom, as H can only hold 1 covalent bond. Once you have identified the central atom, all the other atom(s) will be the substituent atom(s).

Step 2: Count the total number of valence electrons. The carbon group has 4 valence electrons, the nitrogen group has 5, the chalcogens (also known as the oxygen group) have 6, the halogen group has 7, and the noble gases have 8 valence electrons. In addition, hydrogen (H) has 1 valence electron, while beryllium (Be) has 2 valence electrons.

Step 3: For negatively-charged species, add the charge to the total number of electrons. Meanwhile, for positively-charged species, subtract the charge from the total number of electrons.

Step 4: Draw a single bond first between the central atom and the substituent atom(s). Each bond is counted as 2 electrons. After subtracting the bonding electrons from the total number of electrons, distribute the remaining electrons among the substituent atom(s) first until each atom is already surrounded by 8 electrons. This rule is known as the **octet rule**. C, N, and O are strict followers of the octet rule. Hence, when these atoms are the central atom, you should make sure that there are only 8 electrons around these atoms. There are some exceptions though, all



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of which will be discussed in the examples to be presented below. If there are still electrons remaining, they must be distributed to the central atom.

Step 5: For charged species, the structure must be enclosed in a square bracket, with its net charge written as a superscript.

Let us work with some examples to better understand these steps.

Sample Problem 1:

Draw the Lewis structure of phosphorus pentachloride, PCI₅.

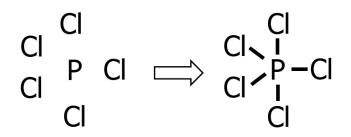
Solution:

Step 1: P is less electronegative than Cl since it is farther from F, hence P is the central atom and Cl is the substituent atom.

Step 2: P belongs to the nitrogen group, while CI is a halogen. Hence:

- valence electrons from P: 1 x 5e⁻ = 5e⁻
- valence electrons from CI: 5 x 7e⁻ = 35e⁻
- total number of valence e⁻: 5e⁻ + 35e⁻ = 40e⁻

Step 3: The species being considered is a neutral species, hence no electron will be added or subtracted.



Step 4: Since we've already drawn 5 bonds, that means we already used 10 electrons (recall that each covalent bond consists of 2 e⁻) out of 40e⁻. Hence, we only need to distribute 30e⁻.

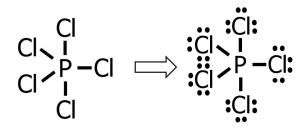


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Distributing these 30e⁻ to the substituent atom first until 8e⁻ are present around each atom, we will have:



As you can see, we used up all the remaining 30e⁻ so that there will be 8e⁻ around each one of the chlorine atoms. Since there are no more electrons to distribute, then we've already drawn the Lewis structure of the compound. One thing you can notice in our Lewis structure is that the central atom does not follow the octet rule (notice that there are 10e⁻ around the P atom). Such cases are known as an **expanded octet**. This usually occurs if the central atom is P, S, and the noble gases.

Sample Problem 2:

Draw the Lewis structure of ammonium ion, NH₄⁺.

Solution:

Step 1: Since H can never be the central atom, then N will be the central atom of NH₄⁺.

Step 2: N belongs to the nitrogen group, while H only has 1 valence electron. Hence:

- valence electrons from N: 1 x 5e⁻ = 5e⁻
- valence electrons from H: 4 x 1e⁻ = 4e⁻
- total number of valence e⁻: 5e⁻ + 4e⁻ = 9e⁻

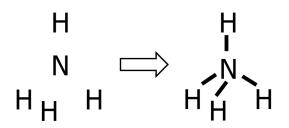
Step 3: The species being considered is a cation with a +1 charge. Therefore, we need to subtract 1 from the total number of valence electrons, leaving us with 8e⁻.



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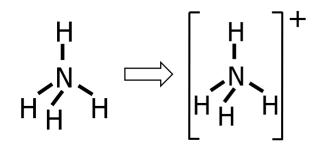


Compounds



Step 4: Since we've already drawn 4 bonds, that means we already used 8e⁻ out of 8e⁻. Therefore, there is nothing left to distribute. Take note that there are only 2e⁻ around the H atoms, which is completely okay since H can hold up to 2e⁻ only. Meanwhile, N has 8e⁻ around it, so the octet rule was satisfied.

Step 5: Finally, since NH_4^+ is a cation, we need to enclose the Lewis structure inside of a square bracket and write the charge as a superscript.



Aside from the expanded octet, another violation of the octet rule is the **incomplete octet**, which is commonly exhibited by beryllium compounds.

Try drawing the Lewis structure of $BeCl_2$. You will notice that although the Cl atoms have $8e^-$ around it, Be only has $4e^-$, hence, an incomplete octet. Aside from those, another violation of the octet rule is the **duet rule**, which is applicable only to hydrogen atoms since H can only hold a maximum of 2 electrons in its <u>1s orbital</u>.

So far, we've only discussed single covalent bonds. *How about double and triple bonds? How do we know if we need to draw multiple bonds?* To answer this question, you will need to know the concept of a formal charge.



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By definition, a **formal charge** is the electrical charge difference between the valence electron in an isolated atom and the number of electrons assigned to that atom in a Lewis structure. Mathematically, the formal charge can be determined using the formula:

Formal Charge = $V - N - \frac{B}{2}$

where V is the number of valence electrons of the atom, N is the number of nonbonding electrons around that atom in a Lewis structure, while B is the number of bonding electrons around the same atom in the Lewis structure.

Let us work with the sample problem below to better demonstrate how to determine formal charges and how it can be used to identify if multiple bonds are needed in a Lewis structure.

Sample Problem 3:

Draw the Lewis structure of sulfate ion, SO_4^{2-} .

Solution:

Step 1: Since S is farther from F, then S will be the central atom of SO_4^{2-} .

Step 2: Both O and S are chalcogens, therefore:

- valence electrons from S: 1 x 6e⁻ = 6e⁻
- valence electrons from O: 4 x 6e⁻ = 24e⁻
- total number of valence e⁻: 6e⁻ + 24e⁻ = 30e⁻

Step 3: The species being considered is an anion with a charge of —2, therefore, we need to add 2e⁻ to the total number of valence electrons, leaving us with 32e⁻.

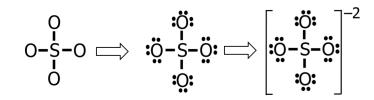
Steps 4-5: Using the knowledge that we have so far, the Lewis structure of SO_4^{2-} is shown in the figure below:



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Seems good, right? All the electrons were distributed, and all the atoms obey the octet rule. However, you will find something unusual if you determine the formal charge of each atom in this Lewis structure.

To solve for the formal charges of each atom, it is worth noting that sulfur, being a chalcogen, has 6 valence electrons, hence V = 6. In the Lewis structure that we currently have, there are no nonbonding electrons around the sulfur (N = 0), while there are 4 bonding electrons (B = 8). Hence, solving for the formal charge we have:

Formal Charge of
$$S = 6 - 0 - \frac{8}{2} = + 2$$

On the other hand, for oxygen, V = 6, N = 6, and B = 2. Therefore:

Formal Charge of
$$0 = 6 - 6 - \frac{2}{2} = -1$$

An ideal Lewis structure for any compound is a structure wherein the formal charge of all the atoms involved is, as much as possible, equal to or close to zero. So far, the formal charge of S in our current Lewis structure is +2, while all the oxygen atoms have a formal charge of -1.

Now, let me just do my stuff here, and let's see what happens to the previous structure that we have.

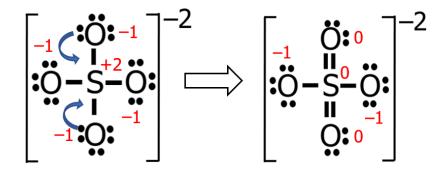


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The numbers printed in red are the formal charges before and after the transformation. *What did I do?* Well, I just converted two nonbonding electron pairs (as the blue arrows suggest) into two bonding electron pairs. This makes the formal charges of three atoms zero (if you cannot believe it, you can solve it and see for yourself).

Hence, the more appropriate Lewis structure of SO_4^{2-} is the latest version that we have. Take note that the algebraic sum of the formal charges is equal to zero for neutral molecules, while for ions, it should be equal to the charge of that ion.

TIPS: There is an easier way to determine the formal charge. You can think of an imaginary circle (or you can actually draw it if it is allowed to write on the questionnaire) around a certain atom, including all the lone pairs around it as well as the tip of the bond/s near it. Then, count the number of nonbonding electrons + bonding electrons around it, wherein each tip of the bond is counted as 1 electron only. Subtract this from the number of valence electrons of that atom and you can immediately obtain the formal charge.

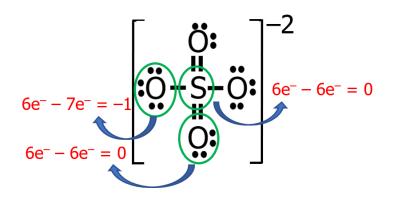
Try to determine the formal charge of the atoms in our previous examples and check if we draw the Lewis structure correctly!



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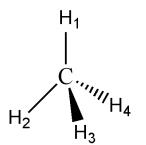
Compounds



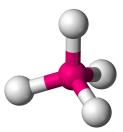
Now that you know how to draw the Lewis structure, it's time to level up the structure from Lewis structure to molecular geometry.

In a Lewis structure, the orientation of atoms in space is not being considered, making this structure a planar structure. However, not all molecules are flat. You might be asking yourself *"If molecules have 3D structures, how are we supposed to write them on flat paper?"* Good thing for us, there is what we call a solid wedge and a dashed (or broken) wedge.

A **solid wedge** denotes a covalent bond towards the viewer. You can also visualize it as if the atom on the other side of the solid wedge pops out of the paper. Whereas a **dashed wedge** represents a bond that is directed away from the viewer. **Solid lines**, on the other hand, represent a bond that is lying flat on the paper.



Molecular geometry of CH₄



Ball and Stick model



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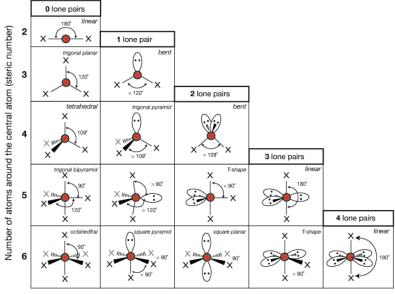


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In the structure of carbon tetrahydride above, more popularly known as methane, the hydrogens labeled 1 and 2 are on the surface of the paper, H_3 is directed towards you, while H_4 is directed away from you. Molecules assume geometries like this because they orient the substituent atoms in such a way that the distance between the two adjacent atoms is as far as possible.

Recall the bonding pairs that form the covalent bond are made up of electrons. To minimize the repulsive forces between these bonding pairs, the bonds must be oriented as far as possible. This approach to the study of molecular geometry is called the *valence-shell electron-pair repulsion (VSEPR) model*.

Shown in the table below are the most common electron pair geometries. For simplicity, we will just consider molecules of the form AX_mE_n , where A is the central atom, m is the steric number or the number of substituent atom X, and n is the number of lone pairs (E) on the central atom.



A table of VSEPR geometries by Dr. Jeff Cruzan is licensed under CC BY-NC-SA 3.0

Take note that lone pairs are not drawn with a solid line, and solid and broken wedges. The figure above presented it that way just to show that lone pairs assume a position that will maximize the distance between bonding and nonbonding electrons.



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Let us work with some examples to better demonstrate this concept.

Sample Problem 4:

Identify and draw the molecular geometry of CIF₃.

Solution:

Step 1: Without a doubt, CI will be our central atom since F is the most electronegative element in the periodic table.

Step 2: Both CI and F are halogens, therefore:

- valence electrons from CI: 1 x 7e⁻ = 7e⁻
- valence electrons from F: 3 x 7e⁻ = 21e⁻
- total number of valence e⁻: 7e⁻ + 21e⁻ = 28e⁻

Step 3: The species being considered is a neutral compound. Therefore, no electrons will be added or subtracted, leaving us with 28e⁻.

Steps 4-5: Using the knowledge that we have so far, you know that there will be two lone pairs on the CI atom for us to be able to distribute all 28e⁻. Furthermore, upon determination of formal charges, you will realize that no multiple bonds are necessary.

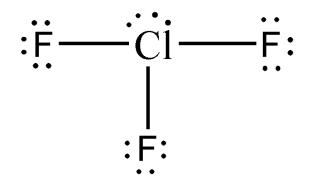
Hence, considering that the type of molecule is AX_3E_2 , the molecular geometry of CIF_3 is T-shaped.



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Compounds



Take note that the two pairs of nonbonding electrons were not drawn with solid wedge and broken wedge, although it should be apparent to you that to minimize repulsive forces, one lone pair is situated somewhat towards you, while the other lone pair is directed away from you.

Additional Information: Electron Pair Geometry

In determining molecular geometry, we treat the lone pairs around the central atom as if they are not there. However, there is a type of chemical geometry that treats the lone pair as if it is a substituent atom. This is the **electron pair geometry**. With this, CIF_3 has a molecular geometry of T-shaped, but its electron pair geometry is trigonal bipyramidal.

Sample Problem 5:

Identify and draw the molecular geometry of PCI₅ and SO₄²⁻.

Solution:

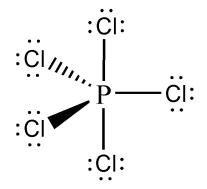
We've already constructed the Lewis structure of PCI_5 from the previous sample problem (i.e., Sample Problem 1). From there, we have determined that PCI_5 is an AX₅ type of molecule. Hence, its molecular geometry is trigonal bipyramidal, and should be drawn as follows:



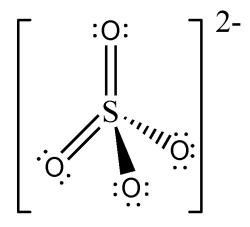
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Meanwhile, the Lewis structure of SO_4^{2-} was identified in Sample Problem 3, and we know for a fact that SO_4^{2-} is an AX₄ type of molecule. Therefore, its molecular geometry is tetrahedral, and should be drawn as follows:



Take note that there is no way to draw multiple bonds using solid and broken wedges; hence, you should orient your drawing such that the multiple bonds will lie on the plane of the paper, like what we did in this example.



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Intermolecular Forces of Attraction

So far, we've only discussed the types of chemical bonds that hold two atoms together in a compound. Such forces of attraction are called intramolecular forces (*intra*- means within). In this section, we will discuss the forces between molecules, which are also known as the **intermolecular forces of attraction**, commonly abbreviated as IMFA (*inter*- means between).

You might ask again, "Is it really important to study the forces that hold two molecules together?" Well for starters, some physical properties of compounds (i.e., melting point, boiling point, vapor pressure, etc.) can be explained largely by the IMFA that these compounds exhibit. For example, why does CCl_4 (BP: 76.72 °C) with a molar mass of almost 9x that of water (BP: 100 °C) boil at a lower temperature? IMFA can explain that.

In general, there are three types of IMFA, namely: London dispersion Forces (LDF), dipole-dipole forces (DDF), and hydrogen bonding (H-Bonding).

London dispersion forces are a type of IMFA that is present in all substances, regardless of type, polarity, molar mass, and the like. It is also the weakest type of IMFA, and its occurrence is attributed to the fact that all substances, even the nonpolar ones, exhibit dipole moments momentarily.

By definition, the **dipole moment** is the product of charge and the distance between the charges in a molecule. We will not quantify dipole moments in this material, but you need to know that dipole moments alone dictate whether a certain compound is polar or nonpolar.

Polar compounds have a net dipole moment, while nonpolar compounds have no net dipole moment. As a result, it is very crucial that you know how to determine if a compound has a net dipole moment or none. One of the prerequisites to do so is that you should know how to draw its molecular geometry.

Let us work with some examples to demonstrate how to determine if a compound is polar or nonpolar using the net dipole moment.



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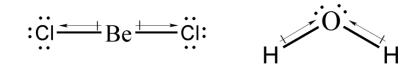
Compounds

Sample Problem 1:

Determine whether BeCl₂ and H₂O are polar or nonpolar.

Solution:

Using the knowledge that we have so far, we know that $BeCl_2$ will exhibit linear geometry, whereas H_2O will exhibit a V-shaped structure. We can determine if the compound is polar or not by drawing a dipole arrow (see figure below) and adding them vectorially. If all the dipole arrows cancel out, then the compound is nonpolar. Otherwise, it is polar.



Dipole arrows are drawn such that the head is pointing at the more electronegative atom. As you can see, adding the dipole moments of $BeCl_2$ results in the cancellation of one another, which makes BeC_{12} a nonpolar compound. Meanwhile, adding the dipole moments of H_2O results in a net dipole moment that goes upward, hence water is a polar molecule.

Now, what do we mean by instantaneous dipole moments in LDF? Well, remember that covalent bonds are not rigid. Meaning, atoms can sway back and forth or up and down. In one specific instance, the bond of $BeCl_2$ can look like what is shown below.



Notice that at that instant, BeCl₂ has a momentary net dipole moment that points downward, giving rise to the London dispersion forces. Nonpolar compounds always have instantaneous dipole moments; however, these instantaneous dipoles cancel one another, making these compounds nonpolar.



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Manual determination of polarity is tedious and time-consuming. To save time, you can use the table below as a guide. However, keep in mind that this is only applicable to compounds of type AX_mE_n , or those compounds with one type of substituent atoms only. If there is more than one type of substituent atom involved, then you have no choice but to determine the polarity manually.

Molecule Type/s	Molecular Geometry	Polarity	Examples
AX ₂	linear	nonpolar	BeCl ₂ , HgCl ₂
AX ₃	trigonal planar	nonpolar	BF ₃
AX_2E , AX_2E_2	bent/V-shaped	polar	H_2O , SO_2
AX ₄	tetrahedral	nonpolar	CH_4 , NH_4^+
AX ₃ E	trigonal pyramidal	polar	NH ₃ , PCI ₃
AX ₅	trigonal bipyramidal	nonpolar	PCI ₅
AX4E	seesaw	polar	SF_4
AX_3E_2	T-shaped	polar	CIF ₃
AX_6	octahedral	nonpolar	SF_6
AX₅E	Square pyramidal	polar	BrF_5
AX_4E_2	square planar	nonpolar	XeF ₄

The next type of IMFA is the **dipole-dipole force (DDF)**, which exists only for polar substances. Collectively, LDF and DDF are known as **van der Waals interactions**.



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DDF is a stronger type of IMFA relative to LDF. A special type of DDF is hydrogen bonding, which is exhibited only by compounds wherein a hydrogen atom is directly bonded to N, O, and F, although recent studies suggest that H₂S also exhibits H-bonding.

Now, how do we use the compound's IMFA to predict some of its physical properties? Across compounds of relatively the same molar mass, stronger IMFA generally entails higher boiling point and melting point, higher viscosity, higher surface tension, and lower vapor pressure.

Sample Problem 2:

Arrange the following set of compounds in order of increasing boiling point.

- 1. F₂ (MM = 38 g/mol), Br₂ (MM = 160 g/mol), H₂ (MM = 2 g/mol)
- 2. Ne (MM = 20 g/mol), HCl (MM = 37 g/mol), H_2O (MM = 18 g/mol)

Solution:

In (a), all compounds are linear and nonpolar, hence we can rank them in order of increasing boiling point based on their molar mass. In general, among compounds that exhibit the same type of IMFA, the higher the molar mass, the higher the boiling point. Hence, the correct sequence is $H_2 < F_2 < Br_2$. True enough, H_2 boils at –252.9 °C, F_2 boils at –188 °C, while Br_2 boils at 58.8 °C.

Meanwhile, among compounds with relatively the same molar mass, the IMFA will dictate the trend in boiling point. Ne, being a nonpolar substance, exhibits only LDF. Meanwhile, HCI is a polar compound that exhibits both LDF and DDF, while H₂O is also a polar compound that exhibits LDF, DDF, and hydrogen bonding. As a result, the correct sequence is Ne < HCI < H₂O. This is supported by literature values since Ne boils at –246 °C, HCI at –85.05 °C, and water at 100 °C.



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