



Chemical Formulas

- A *chemical formula* gives the numbers and types of atoms that are found in a substance.
- When the substance is a discrete molecule, then the chemical formula is also its molecular formula.

Fe (iron) is a chemical formula

Fe₂O₃ is a molecular formula



The Elements

- The chemical formulas of most of the elements are simply their elemental symbol:

Na (sodium)

Fe (iron)

He (helium)

U (uranium)

- These chemical formulas are said to be monatomic—only an atom in chemical formula



The Elements

- There are seven elements that occur naturally as diatomic molecules—molecules that contain two atoms:

H₂ (hydrogen) N₂ (nitrogen)

O₂ (oxygen) F₂ (fluorine)

Cl₂ (chlorine) Br₂ (bromine)

I₂ (iodine)

- The last four elements in this list are in the same family of the Periodic Table



Binary Compounds

- A binary compound is one composed of only two different types of atoms.

Rules for binary compound formulas

1. Element to left in Periodic Table comes first except for hydrogen:

KCl

PCl₃

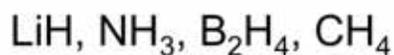
Al₂S₃

Fe₃O₄

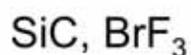


Binary Compounds

2. Hydrogen comes last unless other element is from group 16 or 17:

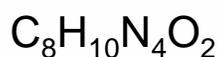
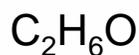


3. If both elements are from the same group, the lower element comes first:



Other Compounds

- For compounds with three or more elements *that are not ionic*, if it contains carbon, this comes first followed by hydrogen. Other elements are then listed in alphabetical order:





Other Compounds

- However, the preceding rule is often ignored when writing organic formulas (molecules containing carbon, hydrogen, and maybe other elements) in order to give a better idea of how the atoms are connected:

C_2H_6O is the molecular formula for ethanol, but nobody ever writes it this way—instead the formula is written C_2H_5OH to indicate one H atom is connected to the O atom.



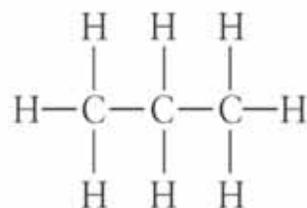
Structural Formulas

- Very often, chemists use structural formulas to show where the atoms in a molecule are positioned. The atoms are connected to each other with **bonds**.
- Bonds represent the attractive forces that hold molecules together.
- There are three types of structural formulas: line structures, ball-and-stick models, and spacing-filling models.



Line Structures

- Lines represent the bonds between atoms



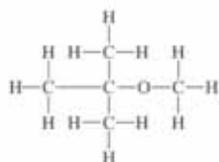
Line structure of propane, C_3H_8



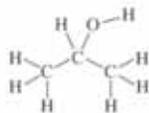
Line Structures

- For organic molecules, the carbon atoms are often not shown.
- C-H bonds are also omitted in line structures.

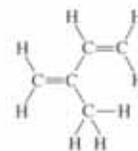
Line Structures



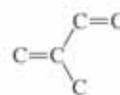
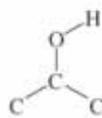
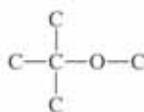
$C_5H_{12}O$
MTBE
(a key antiknock ingredient
in gasoline)



Isopropanol
(rubbing alcohol)



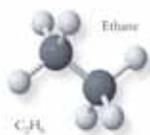
C_5H_8
Isoprene
(the building block of
natural rubber)



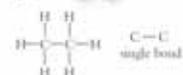
Ball-and-Stick Models

- Atoms are represented by balls that are either color-coded or labeled with the appropriate element.

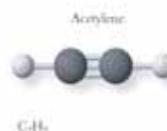
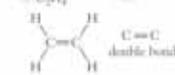
(Color code is given on p. 7 of textbook)



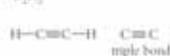
C_2H_6



C_2H_4

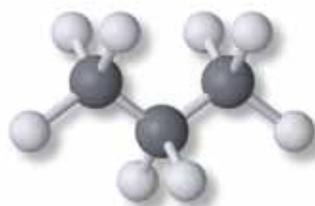


C_2H_2

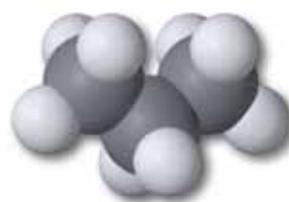


Space-Filling Models

- Atoms are represented by balls that are color-coded and are approximately the correct relative size of the atoms.
- This gives a better perspective of the space available in a molecule.



Ball-and-stick model



Space-filling model

Comparison of Structural Models

Molecule	Water	Ammonia	Methane	Ethanol
Chemical formula	H_2O	NH_3	CH_4	C_2H_5OH
Structural formula	$H-O-H$	$\begin{array}{c} H \\ \\ H-N-H \end{array}$	$\begin{array}{c} H \\ \\ H-C-H \\ \\ H \end{array}$	$\begin{array}{c} H & H \\ & \\ H-C & -C-O-H \\ & \\ H & H \end{array}$
Ball-and-stick model				
Space-filling model				



Nonmetallic Binary Compounds

3. When more than one atom appears in chemical formula, name is prefixed by number of atoms present

CO: carbon monoxide

SiO₂: silicon dioxide

NI₃: nitrogen triiodide

CCl₄: carbon tetrachloride

PCl₅: phosphorous pentachloride

SF₆: sulfur hexafluoride

IF₇: iodine heptafluoride



Nonmetallic Binary Compounds

A Series of Nitrogen Oxides

NO: nitrogen oxide (nitrogen monoxide)

NO₂: nitrogen dioxide

NO₃: nitrogen trioxide

N₂O: dinitrogen oxide (nitrous oxide)

N₂O₃: dinitrogen trioxide

N₂O₄: dinitrogen tetroxide

N₂O₅: dinitrogen pentoxide



Binary Compounds with Hydrogen

- When hydrogen combines with elements from groups 1 or 17, a diatomic molecule results.
- The molecule is named according to the previous rules for nonmetallic binary compounds:

NaH: sodium hydride

HCl: hydrogen chloride

LiH: lithium hydride



Binary Compounds with Hydrogen

- When hydrogen combines with elements from groups 2 or 16, the resulting molecule contains 2 H atoms.
- The molecule is named according to the previous rules for nonmetallic binary compounds, but the *di* is omitted:

H₂S: hydrogen sulfide

CaH₂: calcium hydride

- Exception is oxygen:

H₂O: water H₂O₂: hydrogen peroxide



Ionic Compounds

- Ions are atoms or molecules that have a net electrical charge
- Species may either lose electrons to become positively charged (cations) or gain electrons to become negatively charged (anions)

Na^+ sodium ion

Cl^- chloride ion

NH_4^+ ammonium ion

NO_3^- nitrate ion

PO_4^{3-} phosphate ion

Mg^{2+} magnesium



Ionic Compounds

- The positive charge of a cation is equal to the number of electrons lost by the species to form an ion
- The negative charge of an anion is equal to the number of electrons gained by the species to form an ion



Ionic Compounds

- Metals usually form cations
- Transition metals may form cations with various positive charges:



- The positive charge on a metal atom is frequently referred to as its oxidation state

Fe(II) iron has an oxidation state of 2

Fe(III) iron has an oxidation state of 3



Ionic Compounds

- Group 16 and 17 elements usually form anions.

S^{2-} sulfide ion F^- fluoride ion

O^{2-} oxide ion Br^- bromide ion

- Polyatomic ions are also very common—composed of molecular ions, not atomic ions.

Polyatomic Ions and Their Names

<u>Formula</u>	<u>Name</u>	<u>Formula</u>	<u>Name</u>
NH_4^+	ammonium	NO_3^-	nitrate
H_3O^+	hydronium	NO_2^-	nitrite
Hg_2^+	mercury(I)	PO_4^{3-}	phosphate
OH^-	hydroxide	MnO_4^-	permanganate
CN^-	cyanide	CrO_4^{2-}	chromate
CO_3^{2-}	carbonate	$\text{Cr}_2\text{O}_7^{2-}$	dichromate
CH_3CO_2^-	acetate	ClO_4^-	perchlorate
$\text{C}_2\text{O}_4^{2-}$	oxalate	ClO_3^-	chlorate
SO_4^{2-}	sulfate	ClO_2^-	chlorite
SO_3^{2-}	sulfite	ClO^-	hypochlorite

Hydrates

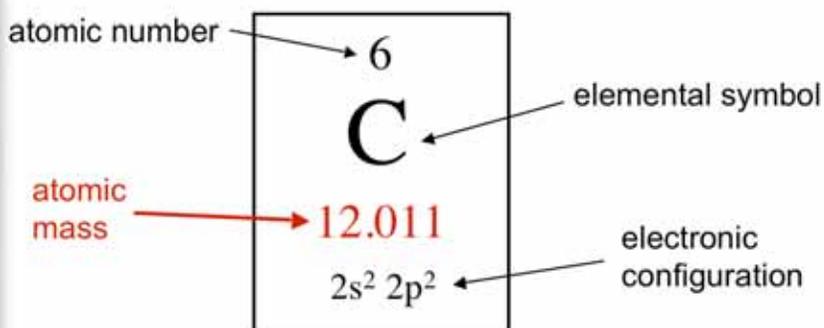
- Many ionic compounds have a set number of water molecules associated with them in the solid phase. These are called hydrates.
- Hydrates are denoted with the number of water molecules in the structure by including $\bullet n\text{H}_2\text{O}$ in the formula (n = number of water molecules)

$\text{CuSO}_4 \bullet 5\text{H}_2\text{O}$ copper(II) sulfate pentahydrate

$\text{Al}(\text{NO}_3)_3 \bullet 9\text{H}_2\text{O}$ aluminum nitrate nonahydrate

Molar Mass (Molecular Weight)

- *Atomic mass* of an element listed in the Periodic Table is the mass of one mole of the naturally occurring element.



Molar Mass (Molecular Weight)

- *Molecular mass* of a molecule is the sum of the atomic masses of all atoms comprising that molecule.

H₂:

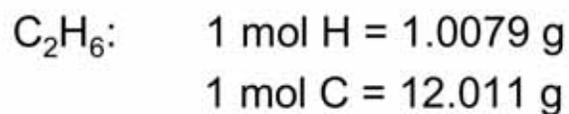
$$1 \text{ mol H} = 1.0079 \text{ g}$$

$$2 \text{ mol H} = 1 \text{ mol H}_2$$

$$\left(\frac{2 \text{ mol H}}{1 \text{ mol H}_2} \right) \left(\frac{1.0079 \text{ g}}{1 \text{ mol H}} \right) = \frac{2.0158 \text{ g}}{\text{mol H}_2}$$



Molar Mass (Molecular Weight)



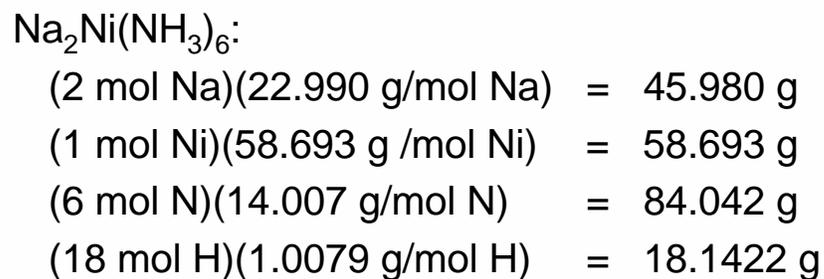
$$\begin{array}{r} (2 \text{ mol C}) (12.011 \text{ g/mol C}) = 24.022 \text{ g} \\ (6 \text{ mol H}) (1.0079 \text{ g/mol H}) = 6.0474 \text{ g} \\ \hline \end{array}$$

$$1 \text{ mol } C_2H_6 \text{ (molar mass)} = 30.069 \text{ g}$$

note use of significant figures!



Molar Mass (Molecular Weight)



$$1 \text{ mol } Na_2Ni(NH_3)_6 = 206.827 \text{ g}$$

note use of significant figures!

Mole-Mass Conversions

- Using molar mass, we can now calculate the number of moles or the mass of any compound if we know the other quantity.

How many moles in 6.358 g H₂?

$$6.358 \text{ g H}_2 \frac{(1 \text{ mol H}_2)}{(2.0158 \text{ g})} = 3.154 \text{ mol H}_2$$

Mole-Mass Conversions

What is the mass of 23.706 mol C₂H₆?

$$23.706 \text{ mol C}_2\text{H}_6 \frac{(30.069 \text{ g})}{(1 \text{ mol C}_2\text{H}_6)} = 712.82 \text{ g C}_2\text{H}_6$$

∞ mass ⇒ moles: divide by molar mass

∞ moles ⇒ mass: multiply by molar mass



Percent Composition

- We are sometimes given the percent of each element present in a compound by mass. This can be determined experimentally by elemental analysis using mass spectrometry or atomic absorption spectrometry.
- The percentages must add to 100%
- From the percent composition, we can then determine the empirical formula of a compound.



Empirical Formula

- If we know the percentage of each element in a chemical compound, we can then determine its *empirical formula*—the chemical formula of the compound with the fewest possible number of atoms.

dinitrogen tetroxide

empirical formula: NO_2

molecular formula: N_2O_4



Empirical Formula

- The empirical formula may be different from the molecular formula
- Glucose has a percent composition of
40.00% carbon
6.71% hydrogen
53.29% oxygen
- Resulting empirical formula: CH_2O
- Molecular formula of glucose: $\text{C}_6\text{H}_{12}\text{O}_6$



Empirical Formula

A compound was determined to contain 61.52% C, 5.16% H, 10.25% N, and 23.07% O. What is the compound's empirical formula?

1. Assume 100 g of compound; find moles of each element

$$61.52 \text{ g C} / 12.011 \text{ g mol}^{-1} \text{ C} = 5.122 \text{ mol C}$$

$$5.16 \text{ g H} / 1.0079 \text{ g mol}^{-1} \text{ H} = 5.12 \text{ mol H}$$

$$10.25 \text{ g N} / 14.007 \text{ g mol}^{-1} \text{ N} = 0.7318 \text{ mol N}$$

$$23.07 \text{ g O} / 15.999 \text{ g mol}^{-1} \text{ O} = 1.442 \text{ mol O}$$



Empirical Formula

2. Divide moles of each element by smallest mole value to determine number of atoms in empirical formula

N has only 0.7318 moles—N has the smallest mole value in the compound

$$\text{C: } 5.122 \text{ mol} / 0.7318 \text{ mol} = 6.999$$

$$\text{H: } 5.12 \text{ mol} / 0.7318 \text{ mol} = 7.00$$

$$\text{N: } 0.7318 \text{ mol} / 0.7318 \text{ mol} = 1.000$$

$$\text{O: } 1.442 \text{ mol} / 0.7318 \text{ mol} = 1.970$$

Empirical formula = $\text{C}_7\text{H}_7\text{NO}_2$



Empirical Formula

If you are given the masses of the elements in a compound instead of the percent composition, you can go through a similar process to determine the empirical formula:

1. Calculate moles of each element

2. Divide by smallest value to determine empirical formula