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

Fe_2O_3 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:

  H_2 (hydrogen) N_2 (nitrogen)

  O_2 (oxygen) F_2 (fluorine)

  Cl_2 (chlorine) Br_2 (bromine)

  I_2 (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

   PCl_3

   Al_2S_3

   Fe_3O_4

Binary Compounds

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

   LiH, NH_3, B_2H_4, CH_4

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

   SiC, BrF_3

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:

  C_2H_6O

  C_4H_9BrO

  CH_3Cl

  $C_8H_{10}N_4O_2$

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:

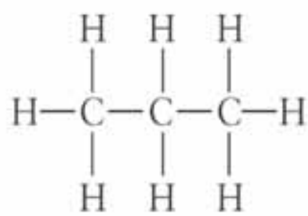
  C_2H_6O is the molecular formula for ethanol, but nobody ever writes it this way—instead the formula is written C_2H_5OH to indicate one H atom is connected to the O atom.

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

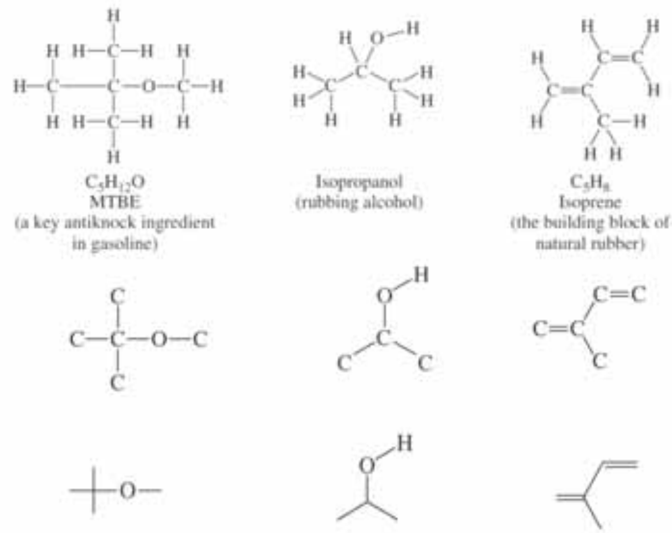


Line structure of propane, C_3H_8

Line Structures

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

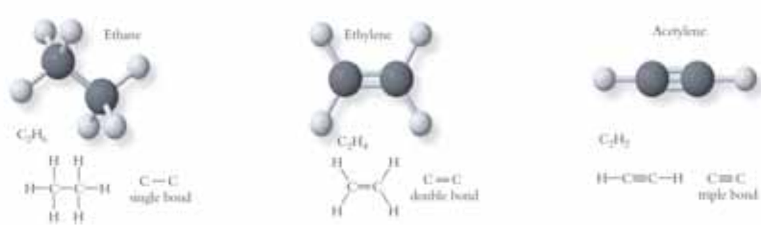
Line Structures



Ball-and-Stick Models

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

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



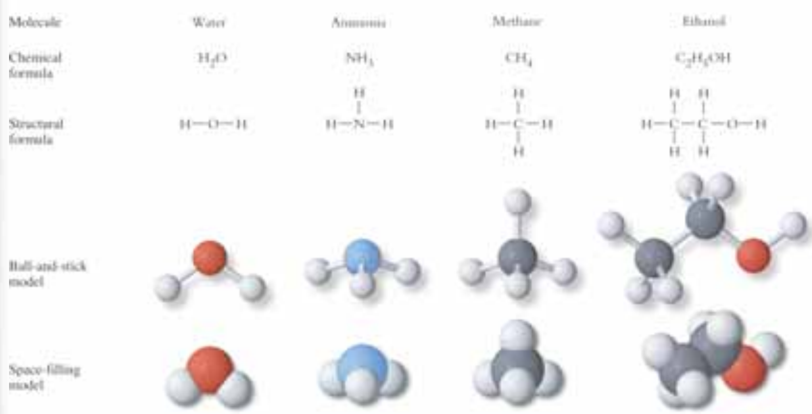
Space-Filling Models

- Atoms are represent 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

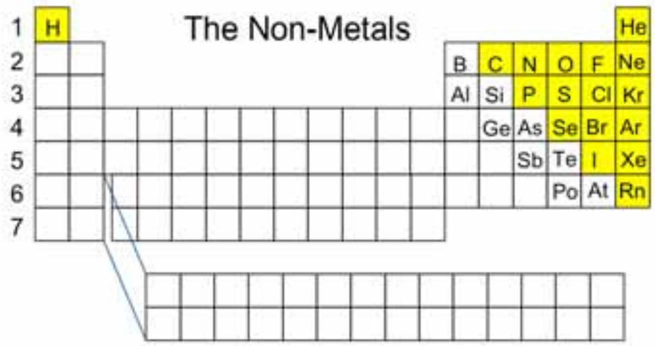
Comparison of Structural Models



Naming Chemical Compounds

Nonmetallic Binary Compounds

- Molecules composed of only two different non-metals



Nonmetallic Binary Compounds

1. Element that appears first retains its elemental name.
2. Second element begins with root derived from name and ends with *-ide*

As: arsenide	Br: bromide
C: carbide	Cl: chloride
O: oxide	F: fluoride
H: hydride	I: iodide
N: nitride	S: sulfide

Nonmetallic Binary Compounds

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

   CO: carbon monoxide

   SiO_2: silicon dioxide

   NI_3: nitrogen triiodide

   CCl_4: carbon tetrachloride

   PCl_5: phosphorous pentachloride

   SF_6: sulfur hexafluoride

   IF_7: iodine heptafluoride

Nonmetallic Binary Compounds

<u>A Series of Nitrogen Oxides</u>

NO: nitrogen oxide (nitrogen monoxide)

NO_2: nitrogen dioxide

NO_3: nitrogen trioxide

N_2O: dinitrogen oxide (nitrous oxide)

N_2O_3: dinitrogen trioxide

N_2O_4: dinitrogen tetroxide

N_2O_5: 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:

  H_2S: hydrogen sulfide

  CaH_2: calcium hydride
- Exception is oxygen:

  H_2O: water H_2O_2: hydrogen peroxide

Ionic Compounds

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

Na^+ sodium ion	Cl^- chlroide 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:

  Fe^{2+} or Fe^{3+}

- 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

Formula	Name	Formula	Name
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	$Cr_2O_7^{2-}$	dichromate
$CH_3CO_2^-$	acetate	ClO_4^-	perchlorate
$C_2O_4^{2-}$	oxalate	ClO_3^-	chlorate
SO_4^{2-}	sulfate	ClO_2^-	chlorite
SO_3^{2-}	sulfite	ClO^-	hypochlorite

Hydrates

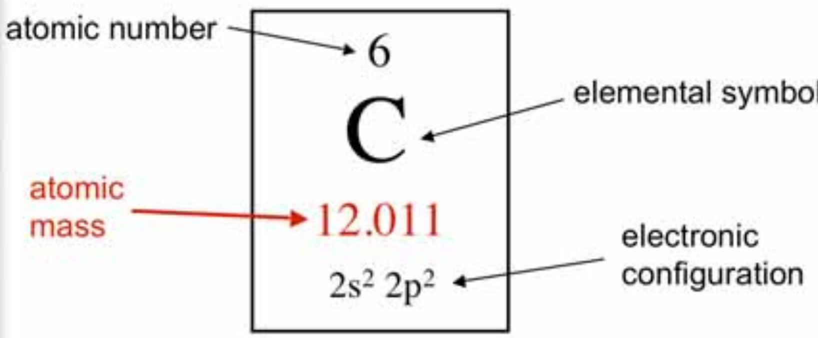
- Many ionic compounds have a set number of water molecules associated with them in the solid phase. These are called hydrates.
- Hydrates are denoted with the number of water molecules in the structure by including $\bullet nH_2O$ in the formula (n = number of water molecules)

$CuSO_4 \bullet 5H_2O$ copper(II) sulfate pentahydrate

$Al(NO_3)_3 \bullet 9H_2O$ 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.

  H_2:

  1 mol H = 1.0079 g

  2 mol H = 1 mol H_2

$$\left(\frac{2\ \cancel{\text{mol H}}}{1\,\text{mol}\ H_2}\right)\left(\frac{1.0079\ \text{g}}{1\ \cancel{\text{mol H}}}\right)=\frac{2.0158\ \text{g}}{\text{mol}\ H_2}$$

Molar Mass (Molecular Weight)

C_2H_6: 1 mol H = 1.0079 g
1 mol C = 12.011 g

(2 mol C) (12.011 g /mol C) = 24.022 g
(6 mol H) (1.0079 g/mol H) = 6.0474 g

1 mol C_2H_6 (molar mass) = 30.069 g

note use of significant figures!

Molar Mass (Molecular Weight)

$Na_2Ni(NH_3)_6$:

(2 mol Na)(22.990 g/mol Na)	=	45.980 g
(1 mol Ni)(58.693 g /mol Ni)	=	58.693 g
(6 mol N)(14.007 g/mol N)	=	84.042 g
(18 mol H)(1.0079 g/mol H)	=	18.1422 g

1 mol $Na_2Ni(NH_3)_6$ = 206.827 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 H_2?

$$6.358\ \text{g}\ H_2 \ \frac{(1\ \text{mol}\ H_2)}{(2.0158\ \text{g})} = 3.154\ \text{mol}\ H_2$$

Mole-Mass Conversions

What is the mass of 23.706 mol C_2H_6?

$$23.706\ \text{mol}\ C_2H_6 \ \frac{(30.069\ \text{g})}{(1\ \text{mol}\ C_2H_6)}$$

$$= 712.82\ \text{g}\ C_2H_6$$

∞ 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: $C_6H_{12}O_6$

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 g C / 12.011 g mol^{-1} C = 5.122 mol C

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

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

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

C: 5.122 mol / 0.7318 mol = 6.999

H: 5.12 mol / 0.7318 mol = 7.00

N: 0.7318 mol / 0.7318 mol = 1.000

O: 1.442 mol / 0.7318 mol = 1.970

Empirical formula = $C_7H_7NO_2$

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