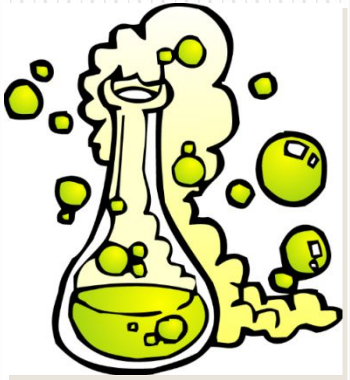
Chemical Formulas and Nomenclature命名法 of compounds

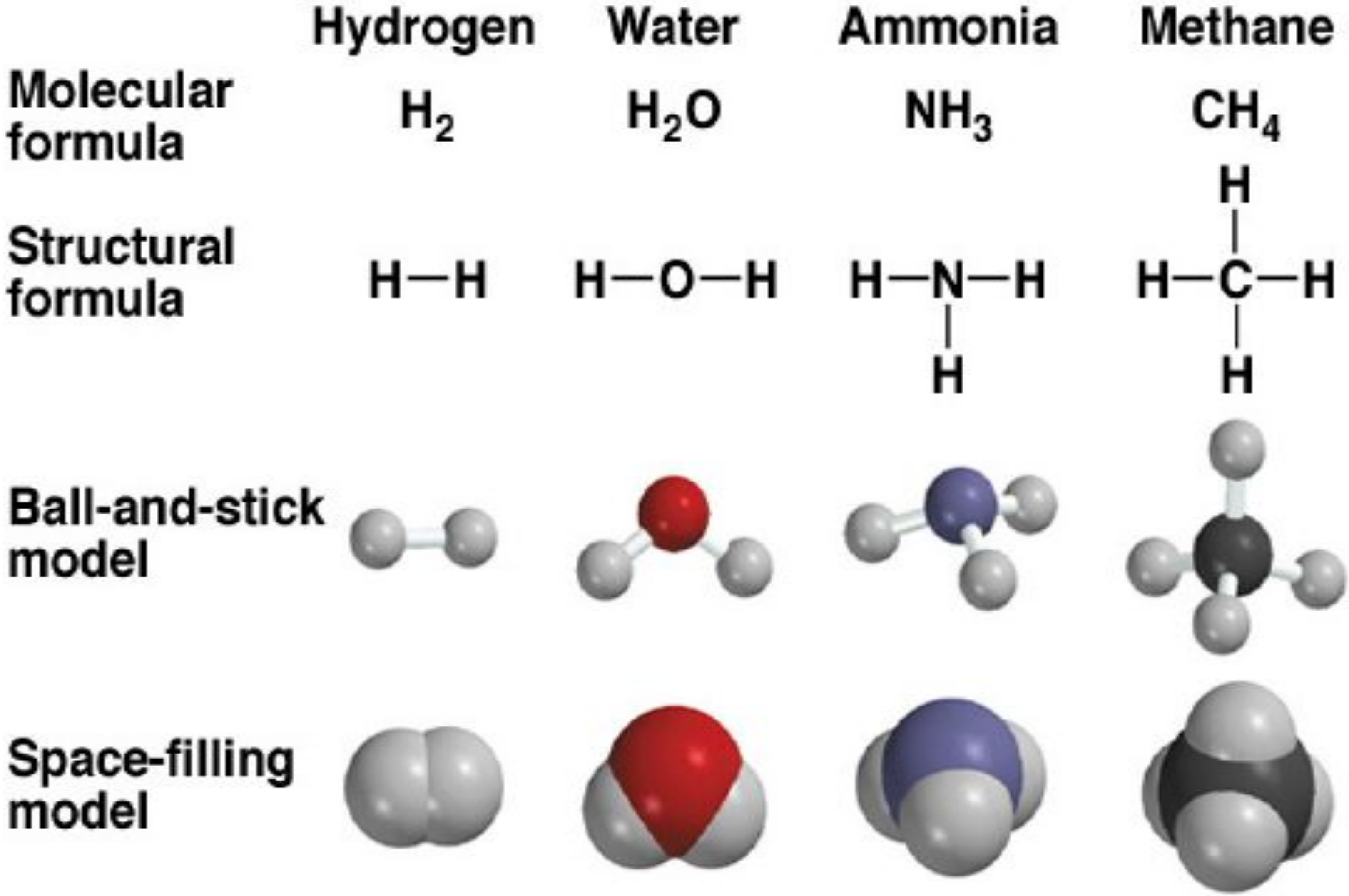


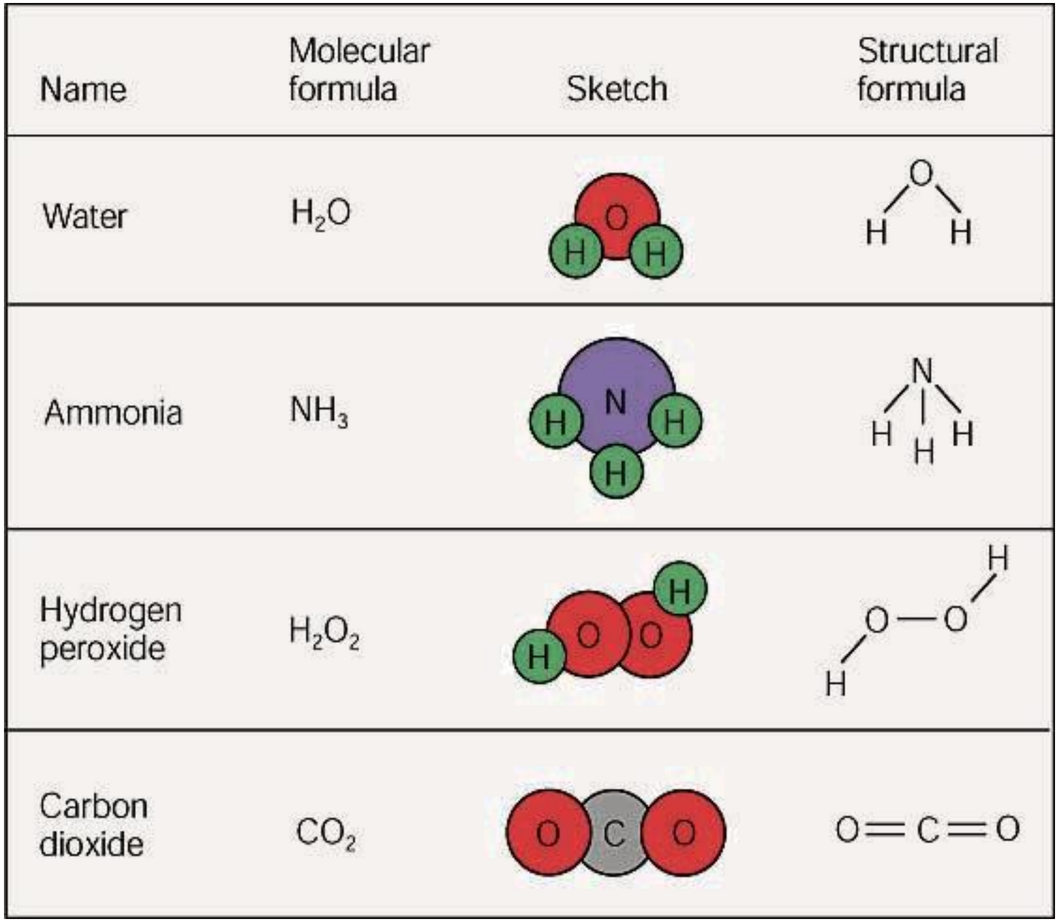
Chemical Formulas

- A ***molecular formula*** shows the ***exact number*** of atoms of each element in the smallest unit of a substance (true formula)
- An ***empirical formula*** shows the ***simplest*** whole-number ratio of the atoms in substance (simplest formula)
- A ***structural Formula*** shows the relative **arrangements** of atoms in a molecule.

molecular	empirical
H_2O	H_2O
$C_6H_{12}O_6$	CH_2O
O_3	O
N_2H_4	NH_2

Standard Types of Formulas and Models





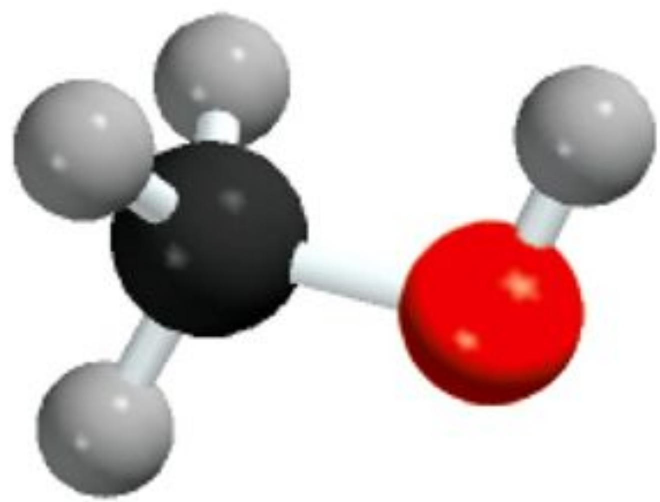
Name	Molecular formula	Sketch	Structural formula
Water	H_2O		H–O–H
Ammonia	NH_3		NH_3 (N bonded to three H)
Hydrogen peroxide	H_2O_2		H–O–O–H
Carbon dioxide	CO_2		O=C=O

If you know the name of an ingredient, you can write a chemical formula, and the percent composition of a particular substance can be calculated from the formula. This can be useful information for consumer decisions.

Example 2.2

DCM, Worked Examples

Write the molecular formula of methanol, an organic solvent and antifreeze, from its ball-and-stick model, shown in the margin.

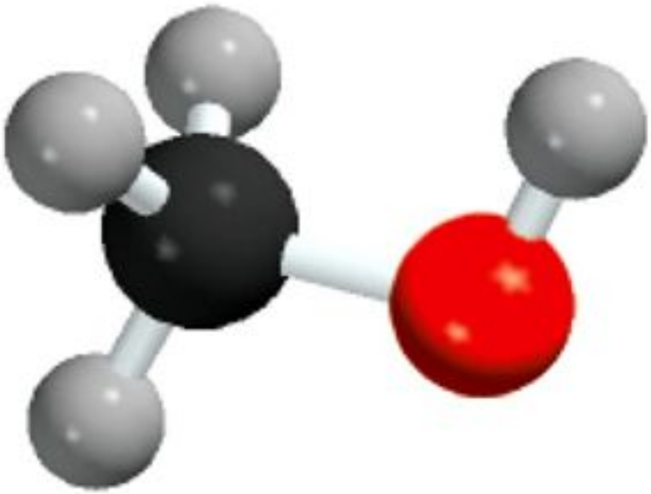


Example 2.2

DCM, Worked Examples

Write the molecular formula of methanol, an organic solvent and antifreeze, from its ball-and-stick model, shown in the margin.

Solution Refer to the labels (also see back endpapers). There are four H atoms, one C atom, and one O atom. Therefore, the molecular formula is CH_4O. However, the standard way of writing the molecular formula for methanol is CH_3OH because it shows how the atoms are joined in the molecule.



Example 2.3

DCM, Worked Examples

Write the empirical formulas for the following molecules: (a) acetylene (C_2H_2), which is used in welding torches; (b) glucose ($C_6H_{12}O_6$), a substance known as blood sugar; and (c) nitrous oxide (N_2O), a gas that is used as an anesthetic gas ("laughing gas") and as an aerosol propellant for whipped creams.

Example 2.3

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Strategy Recall that to write the empirical formula, the subscripts in the molecular formula must be converted to the smallest possible whole numbers.

Solution

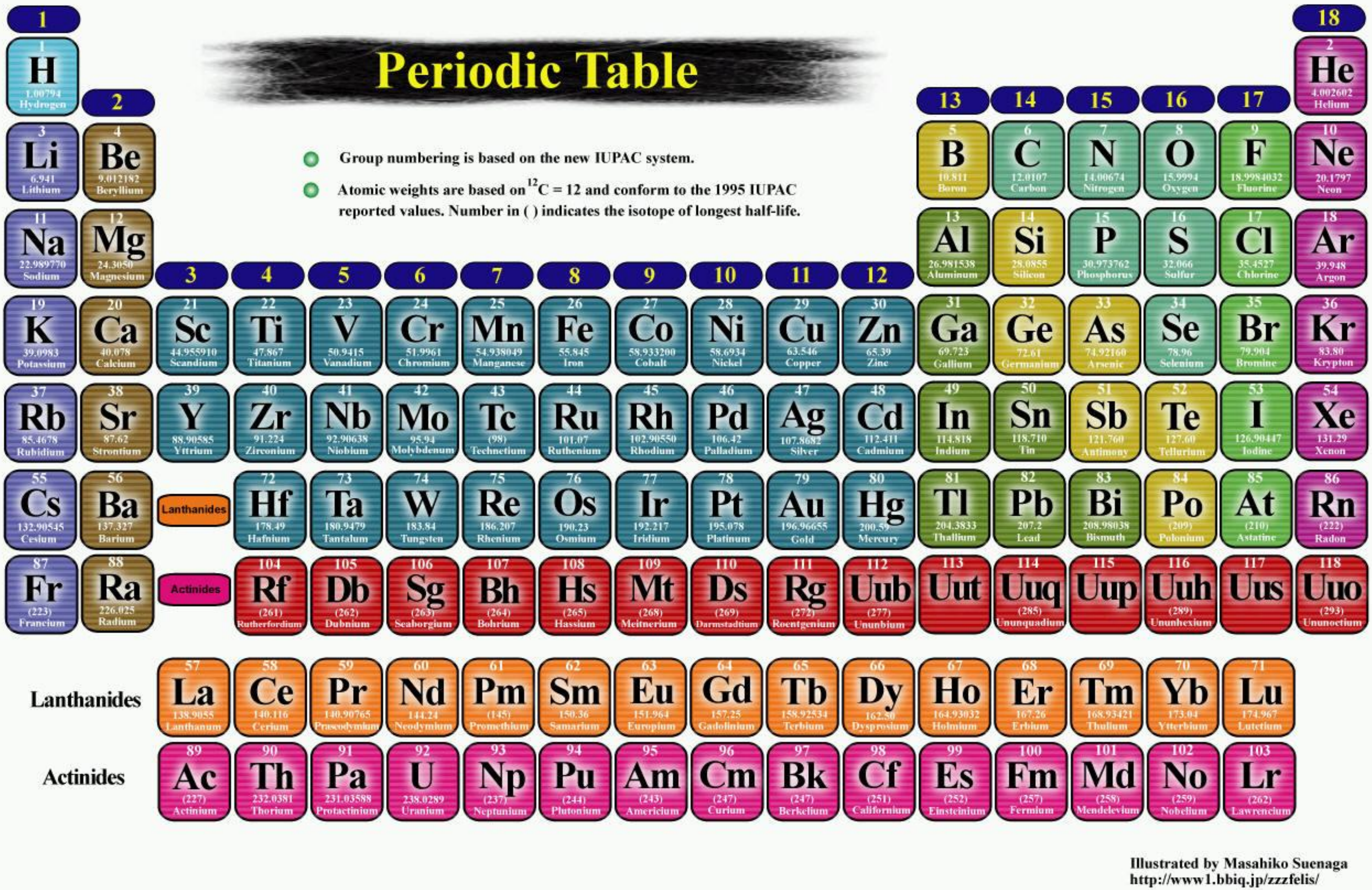
(a) There are two carbon atoms and two hydrogen atoms in acetylene. Dividing the subscripts by 2, we obtain the empirical formula CH.

(b) In glucose there are 6 carbon atoms, 12 hydrogen atoms, and 6 oxygen atoms. Dividing the subscripts by 6, we obtain the empirical formula CH_2O. Note that if we had divided the subscripts by 3, we would have obtained the formula $C_2H_4O_2$. Although the ratio of carbon to hydrogen to oxygen atoms in $C_2H_4O_2$ is the same as that in $C_6H_{12}O_6$ (1:2:1), $C_2H_4O_2$ is not the simplest formula because its subscripts are not in the smallest whole-number ratio.

(c) Because the subscripts in N_2O are already the smallest possible whole numbers, the empirical formula for nitrous oxide is the same as its molecular formula.

EXAMPLE 4.9 Empirical Formula from Percent Composition

Determine the empirical formula for the mineral chalcocite, which has the percent composition 79.8% Cu and 20.2% S.


Periodic Table
Group numbering is based on the new IUPAC system.
Atomic weights are based on 12C = 12 and conform to the 1995 IUPAC reported values. Number in ( ) indicates the isotope of longest half-life.
Lanthanides
Actinides
Illustrated by Masahiko Suenaga
http://www1.bbiq.jp/zzzfelis/

Solution:

If we assume the sample of chalcocite has a mass of 100 g, the masses of copper and sulfur will be numerically equal to their percent composition values:

$$79.8\% \text{ of } 100 \text{ g is } 79.8 \text{ g} = \text{mass Cu}$$
$$20.2\% \text{ of } 100 \text{ g is } 20.2 \text{ g} = \text{mass S}$$

Next we convert the mass of each element into its number of moles. The equivalence expressions arise from the molar masses of the elements:

$$1 \text{ mol Cu} = 63.55 \text{ g Cu}$$
$$1 \text{ mol S} = 32.06 \text{ g S}$$

We convert these expressions to ratios to convert mass to moles:

$$\frac{63.55 \text{ g Cu}}{1 \text{ mol Cu}} \text{ and } \frac{1 \text{ mol Cu}}{63.55 \text{ g Cu}}$$

$$\frac{32.06 \text{ g S}}{1 \text{ mol S}} \text{ and } \frac{1 \text{ mol S}}{32.06 \text{ g S}}$$

Since we need to cancel grams of each element and calculate moles, the second ratio is used in each case:

$$\text{mol Cu} = 79.8\ \cancel{\text{g Cu}} \times \frac{1\ \text{mol Cu}}{63.55\ \cancel{\text{g Cu}}} = 1.26\ \text{mol Cu}$$

$$\text{mol S} = 20.2\ \cancel{\text{g S}} \times \frac{1\ \text{mol S}}{32.06\ \cancel{\text{g S}}} = 0.630\ \text{mol S}$$

Finally, divide by the smaller of the two mole quantities:

$$\frac{\text{mol Cu}}{\text{mol S}} = \frac{1.26\ \text{mol Cu}}{0.630\ \text{mol S}} = \frac{2.00\ \text{Cu}}{1.00\ \text{S}}$$

Since 2 mol of copper are present for each 1 mol of sulfur, the empirical formula is Cu_2S.

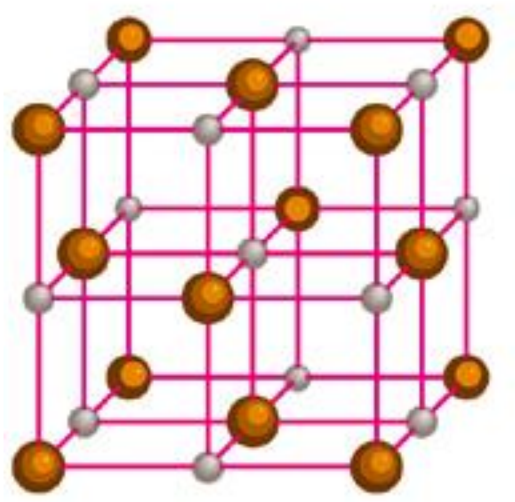
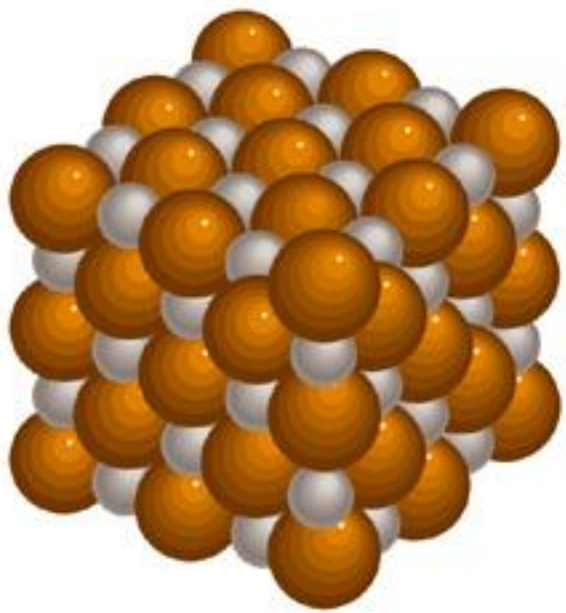
EXAMPLE 4.10 Empirical Formulas for More Than Two Elements

The mineral malachite is a beautiful green color, often with swirling bands of different intensity. It is often used in jewelry because of its attractive appearance. An analysis of malachite gives the following composition: 57.48% copper, 5.43% carbon, 0.91% hydrogen, and 36.18% oxygen. Determine the empirical formula of malachite.

Ionic compounds consist of a **combination of cations and anions (metal + nonmetal)**.

- the formula is always the same as the empirical formula.
- the **sum of the charges** on the cation(s) and anion(s) in each formula unit **must equal zero**.

The ionic compound NaCl


EXAMPLE 3.1 Ionic and Molecular Compounds

Based on their formulas, which of the following compounds are ionic?

(a) KCl (b) CO_2 (c) CaO (d) CCl_4

Solution:

We can determine if a compound is ionic by looking at the elements that compose it. An ionic compound is usually composed of ions from a metal and a nonmetal. Two of the compounds meet this criterion, KCl and CaO.

Formula of Ionic Compounds

2 x +3 = +6 3 x -2 = -6

Al_2O_3

Al^{3+} O^{2-}

1 x +2 = +2 2 x -1 = -2

$CaBr_2$

Ca^{2+} Br^{-}

1 x +2 = +2 1 x -2 = -2

Na_2CO_3

Na^{+} CO_3^{2-}

Example 2.4

DCM, Worked Examples

Write the formula of magnesium nitride, containing the Mg^{2+} and N^{3-} ions.

EXAMPLE 3.6 Formulas for Ionic Compounds

Write the formulas for compounds containing the following ions:

(a) calcium ion and nitride ion
(b) barium ion and nitrate ion
(c) potassium ion and sulfate ion

TABLE 2.3	Names and Formulas of Some Common Inorganic Cations and Anions
Cation	**Anion**
aluminum (Al^{3+})	bromide (Br^-)
ammonium (NH_4^+)	carbonate (CO_3^{2-})
barium (Ba^{2+})	chlorate (ClO_3^-)
cadmium (Cd^{2+})	chloride (Cl^-)
calcium (Ca^{2+})	chromate (CrO_4^{2-})
cesium (Cs^+)	cyanide (CN^-)
chromium(III) or chromic (Cr^{3+})	dichromate ($Cr_2O_7^{2-}$)
cobalt(II) or cobaltous (Co^{2+})	dihydrogen phosphate ($H_2PO_4^-$)
copper(I) or cuprous (Cu^+)	fluoride (F^-)
copper(II) or cupric (Cu^{2+})	hydride (H^-)
hydrogen (H^+)	hydrogen carbonate or bicarbonate (HCO_3^-)
iron(II) or ferrous (Fe^{2+})	hydrogen phosphate (HPO_4^{2-})
iron(III) or ferric (Fe^{3+})	hydrogen sulfate or bisulfate (HSO_4^-)
lead(II) or plumbous (Pb^{2+})	hydroxide (OH^-)
lithium (Li^+)	iodide (I^-)
magnesium (Mg^{2+})	nitrate (NO_3^-)
manganese(II) or manganous (Mn^{2+})	nitride (N^{3-})
mercury(I) or mercurous (Hg_2^{2+})*	nitrite (NO_2^-)
mercury(II) or mercuric (Hg^{2+})	oxide (O^{2-})
potassium (K^+)	permanganate (MnO_4^-)
rubidium (Rb^+)	peroxide (O_2^{2-})
silver (Ag^+)	phosphate (PO_4^{3-})
sodium (Na^+)	sulfate (SO_4^{2-})
strontium (Sr^{2+})	sulfide (S^{2-})
tin(II) or stannous (Sn^{2+})	sulfite (SO_3^{2-})
zinc (Zn^{2+})	thiocyanate (SCN^-)

Solution:

(a) Calcium ion and nitride ion are monatomic. Their charges can be determined from their positions in the periodic table. Calcium ion is expected to have a 2+ charge, and nitride ion is expected to have a 3− charge. Combining three calcium ions with two nitride ions yields a formula that has equal amounts of positive and negative charges: Ca_3N_2.

(b) Barium ion is a monatomic cation. Nitrate ion is a polyatomic anion. We can use the periodic table to predict the charge of the cation. The barium ion is expected to have a 2+ charge. From Table 3.4 we know that nitrate has a charge of 1−. It takes two nitrate ions for every one barium ion to give equal amounts of positive and negative charges: $Ba(NO_3)_2$.

(c) Potassium ion is a monatomic cation. Sulfate ion is a polyatomic anion. Based on its position in the periodic table, potassium ion is expected to have a 1+ charge. From Table 3.4 we know that the charge on sulfate ion is 2−. It takes two potassium ions for every one sulfate ion to yield equal amounts of positive and negative charges: K_2SO_4.

Chemical Nomenclature

- **Ionic Compounds**
  - **often a metal + nonmetal**
  - **anion (nonmetal), add "ide" to element name**

$BaCl_2$	barium chloride
K_2O	potassium oxide
$Mg(OH)_2$	magnesium hydroxide

- **Transition metal ionic compounds**
  - indicate charge on metal with Roman numerals羅馬數字

$FeCl_2$	2 Cl^- -2, so **Fe is +2**	iron(**II**) chloride
$FeCl_3$	3 Cl^- -3, so **Fe is +3**	iron(**III**) chloride
Cr_2S_3	3 S^{-2} -6, so **Cr is +3** (6/2)	chromium(**III**) sulfide

iron(II) chloride √

iron (II) chloride ×

TABLE 2.2 The "-ide" Nomenclature of Some Common Monatomic Anions According to Their Positions in the Periodic Table

Group 4A	Group 5A	Group 6A	Group 7A
C carbide (C^{4-})*	N nitride (N^{3-})	O oxide (O^{2-})	F fluoride (F^{-})
Si silicide (Si^{4-})	P phosphide (P^{3-})	S sulfide (S^{2-})	Cl chloride (Cl^{-})
		Se selenide (Se^{2-})	Br bromide (Br^{-})
		Te telluride (Te^{2-})	I iodide (I^{-})

*The word "carbide" is also used for the anion C_2^{2-}.

EXAMPLE 3.7 Naming Ionic Compounds

Name the compounds given by the formulas (a) Na_2O and (b) $Ca_3(PO_4)_2$.

Solution:

(a) The first compound, Na_2O, is composed of monatomic cations and anions whose charges can be predicted from the periodic table. We state the name of the metal ion first, followed by the root of the name for the nonmetal with an *–ide* ending: *sodium oxide.*

(b) The charge on a calcium ion can be predicted from the periodic table. The polyatomic ion is PO_4^{3-}, named phosphate ion. The name of the compound is *calcium phosphate.*

EXAMPLE 3.8 Naming Ionic Compounds Containing Metals with Multiple Charges

Name the compounds given by the formulas (a) $SnCl_2$ and (b) SnO_2.

Example 2.5

DCM, Worked Examples

Name the following compounds: (a) $Cu(NO_3)_2$, (b) KH_2PO_4, and (c) NH_4ClO_3.

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Cation	**Anion**
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cadmium (Cd^{2+})	chloride (Cl^-)
calcium (Ca^{2+})	chromate (CrO_4^{2-})
cesium (Cs^+)	cyanide (CN^-)
chromium(III) or chromic (Cr^{3+})	dichromate ($Cr_2O_7^{2-}$)
cobalt(II) or cobaltous (Co^{2+})	dihydrogen phosphate ($H_2PO_4^-$)
copper(I) or cuprous (Cu^+)	fluoride (F^-)
copper(II) or cupric (Cu^{2+})	hydride (H^-)
hydrogen (H^+)	hydrogen carbonate or bicarbonate (HCO_3^-)
iron(II) or ferrous (Fe^{2+})	hydrogen phosphate (HPO_4^{2-})
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lithium (Li^+)	iodide (I^-)
magnesium (Mg^{2+})	nitrate (NO_3^-)
manganese(II) or manganous (Mn^{2+})	nitride (N^{3-})
mercury(I) or mercurous (Hg_2^{2+})*	nitrite (NO_2^-)
mercury(II) or mercuric (Hg^{2+})	oxide (O^{2-})
potassium (K^+)	permanganate (MnO_4^-)
rubidium (Rb^+)	peroxide (O_2^{2-})
silver (Ag^+)	phosphate (PO_4^{3-})
sodium (Na^+)	sulfate (SO_4^{2-})
strontium (Sr^{2+})	sulfide (S^{2-})
tin(II) or stannous (Sn^{2+})	sulfite (SO_3^{2-})
zinc (Zn^{2+})	thiocyanate (SCN^-)

EXAMPLE 3.9 Formulas for Compounds Containing Metals That Exhibit Multiple Charges

Write the formulas for the compounds with the following names:

(a) iron(III) sulfide
(b) cobalt(II) nitrate

- **Molecular compounds**
  - nonmetals or nonmetals + metalloids
  - common names
    - H_2O, NH_3, CH_4, C_{60}
  - element further left in periodic table is 1st
  - element closest to bottom of group is 1st
  - **if more than one compound can be formed from the same elements, use prefixes to indicate number of each kind of atom**
  - last element ends in ***ide***

TABLE 2.4

Greek Prefixes Used in Naming Molecular Compounds

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

Molecular Compounds

HI — hydrogen iodide

NF_3 — nitrogen trifluoride

SO_2 — sulfur dioxide

N_2Cl_4

NO_2

TOXIC!

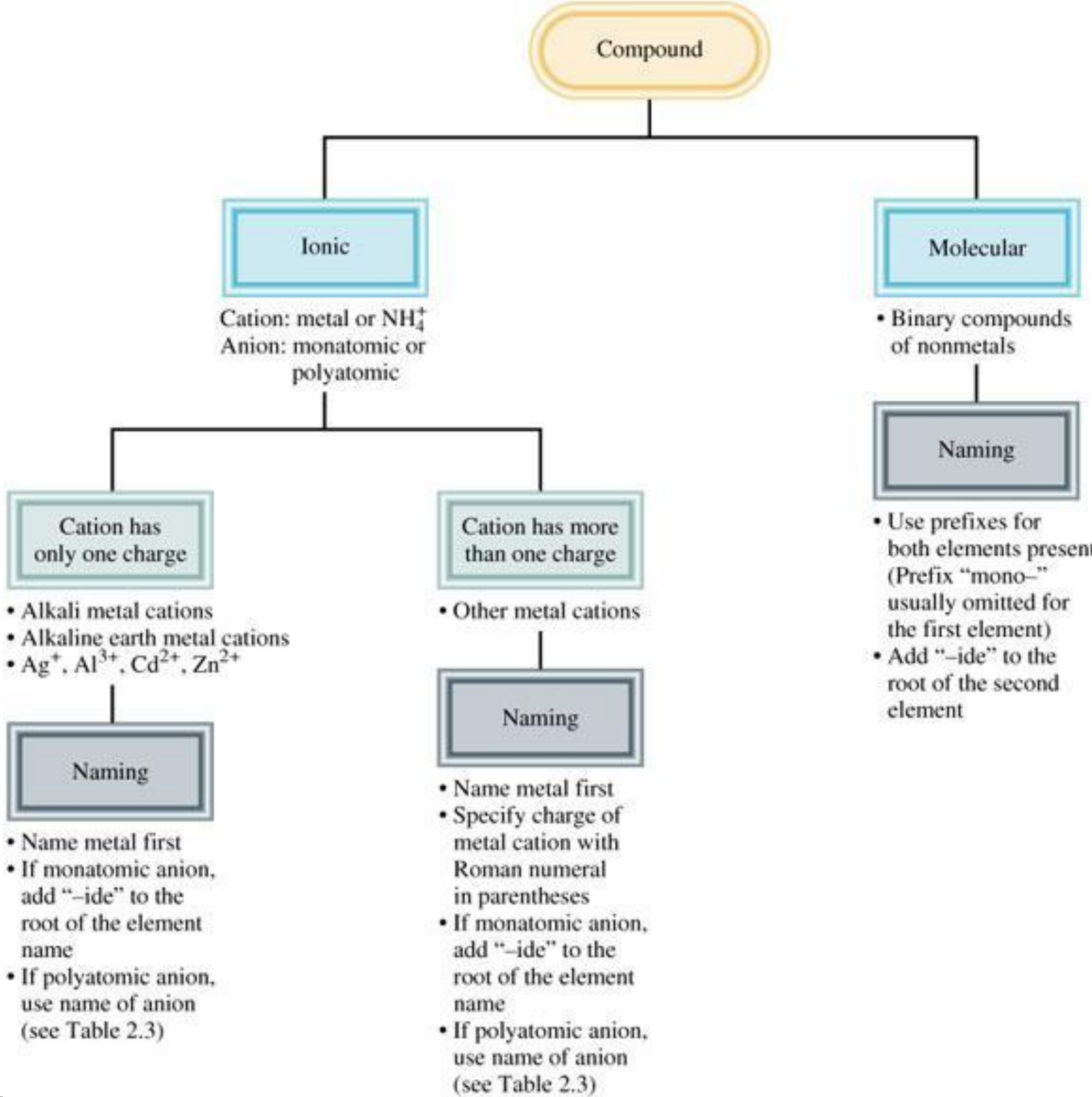
N_2O

Laughing Gas

Example 2.8

DCM, Worked Examples

Write chemical formulas for the following molecular compounds: (a) carbon disulfide and (b) disilicon hexabromide.


Compound
Ionic
Cation: metal or NH_4^+
Anion: monatomic or polyatomic
Molecular
• Binary compounds of nonmetals
Cation has only one charge
• Alkali metal cations
• Alkaline earth metal cations
• Ag^+, Al^{3+}, Cd^{2+}, Zn^{2+}
Cation has more than one charge
• Other metal cations
Naming
• Use prefixes for both elements present (Prefix "mono–" usually omitted for the first element)
• Add "–ide" to the root of the second element
Naming
• Name metal first
• If monatomic anion, add "–ide" to the root of the element name
• If polyatomic anion, use name of anion (see Table 2.3)
Naming
• Name metal first
• Specify charge of metal cation with Roman numeral in parentheses
• If monatomic anion, add "–ide" to the root of the element name
• If polyatomic anion, use name of anion (see Table 2.3)