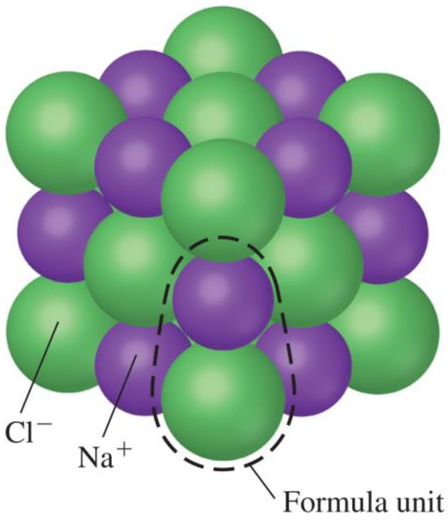
Petrucci • Harwood • Herring • Madura

Ninth Edition

GENERAL CHEMISTRY

Principles and Modern Applications



Chapter 3: Chemical Compounds

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University of Windsor, Canada

Contents

Contents

- *Focus On Mass Spectrometry-Determining Molecular Formulas*

- Molecular Compounds

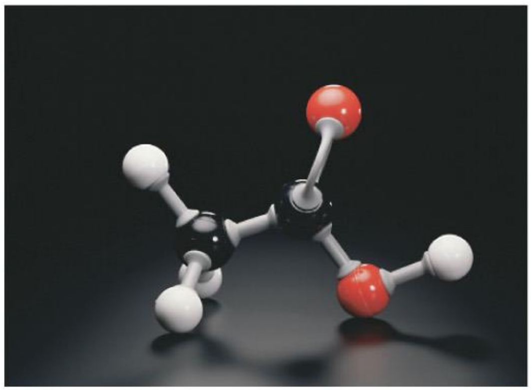
The two elements present

H_2O

Lack of subscript means one atom of O per molecule

Two H atoms per molecule

Molecular compounds

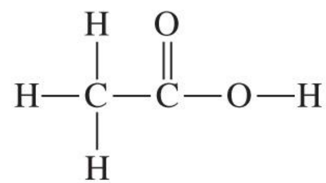


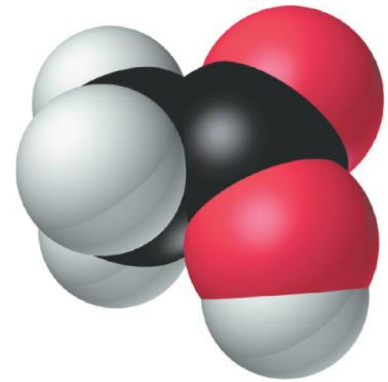
Molecular model:
("ball-and-stick")

Empirical formula: CH_2O

Molecular formula: $C_2H_4O_2$

Structural formula:

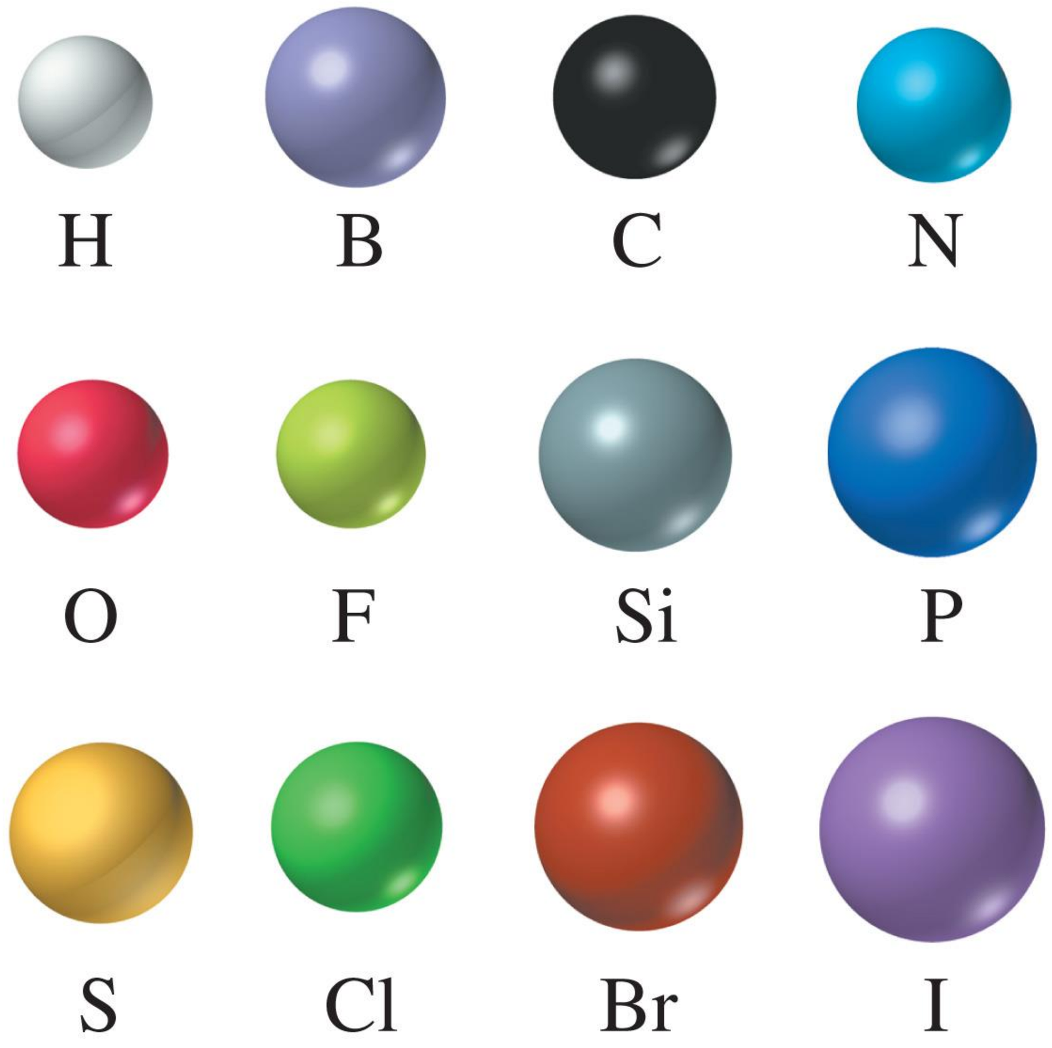




Molecular model:
("space-filling")

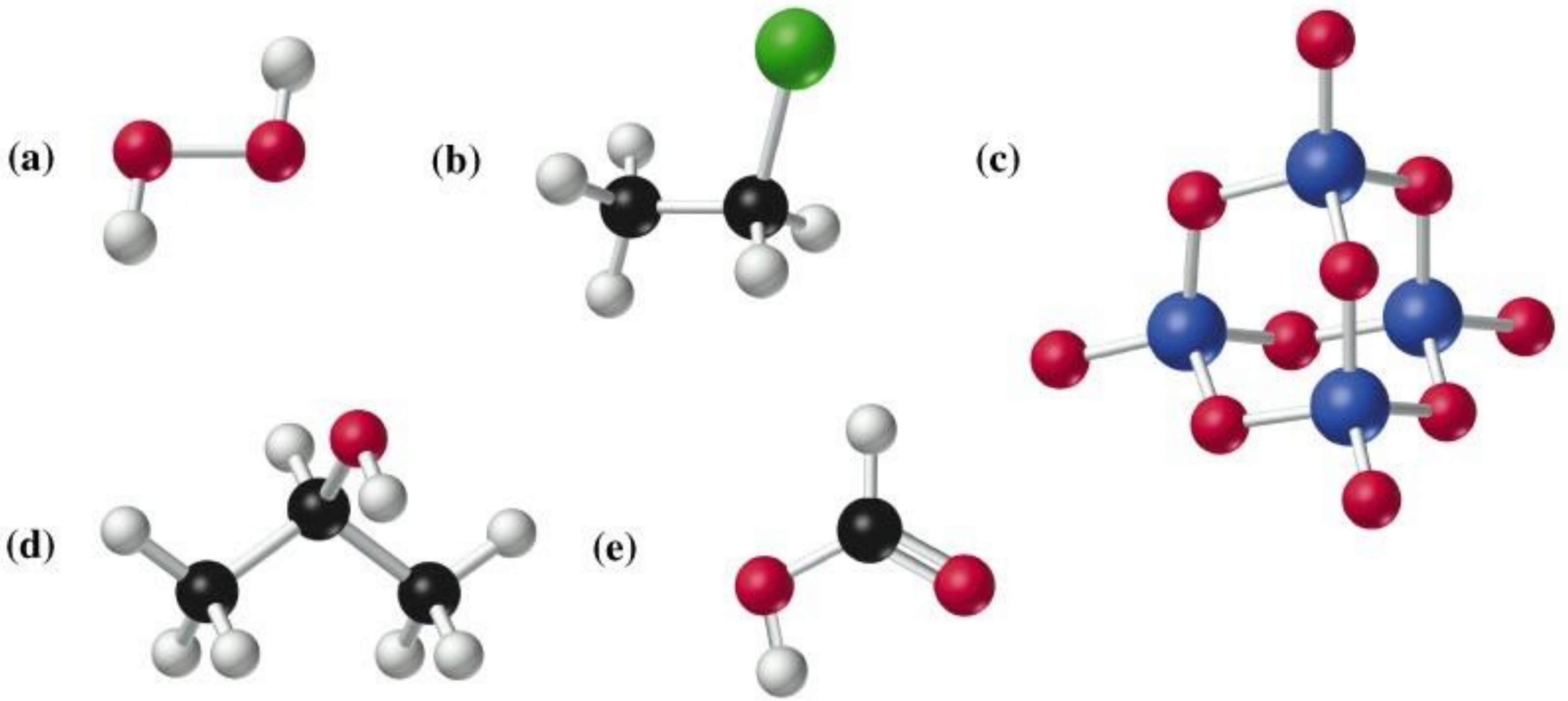
1 👎/inch
0.4 👎/cm

Standard Color Scheme



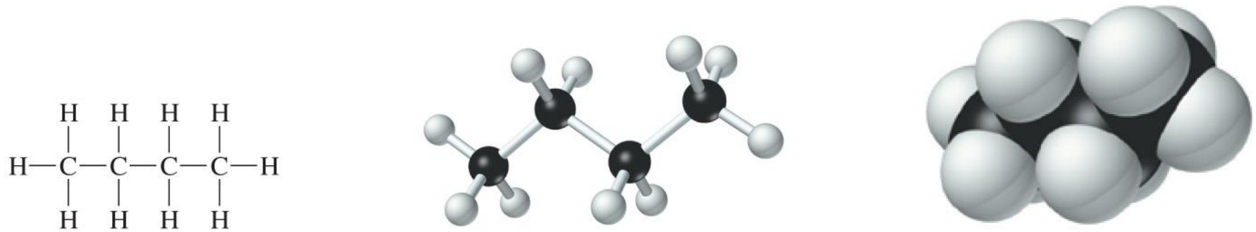
Some Organic and Inorganic Molecules

H_2O_2 CH_3CH_2Cl P_4O_{10}

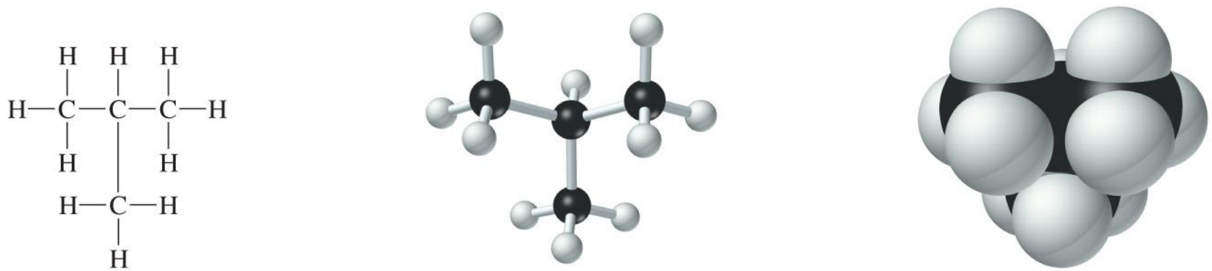


$CH_3CH(OH)CH_3$ HCO_2H

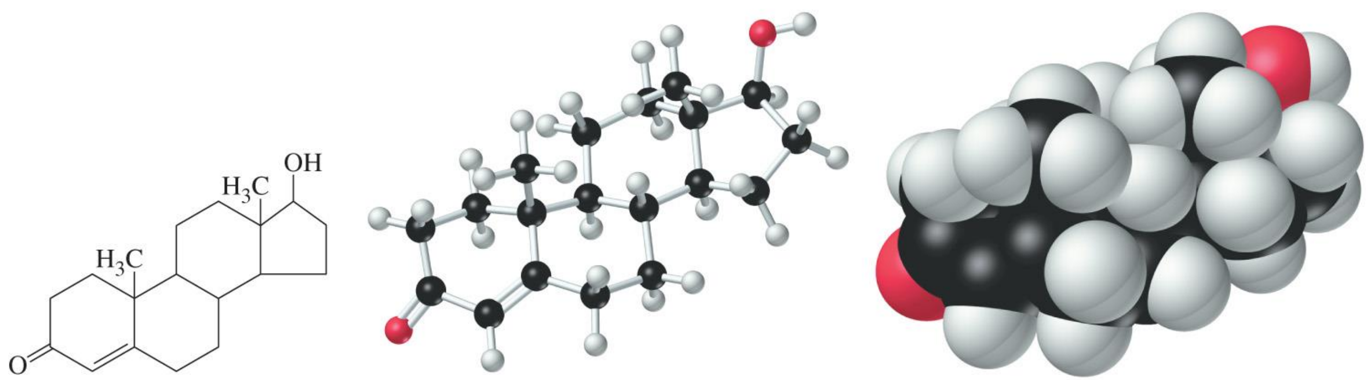
Organic Compounds



(a) Butane



(b) Methylpropane



(c) Testosterone

Ionic Compounds

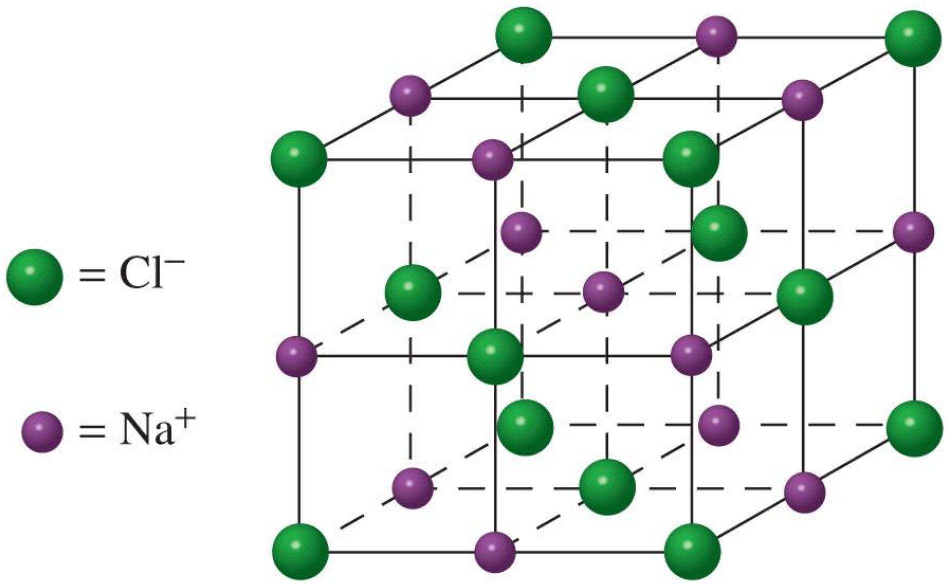
- Atoms of almost all elements can gain *or* lose electrons to form charged species called **ions**.
- Compounds composed of ions are known as **ionic compounds**.

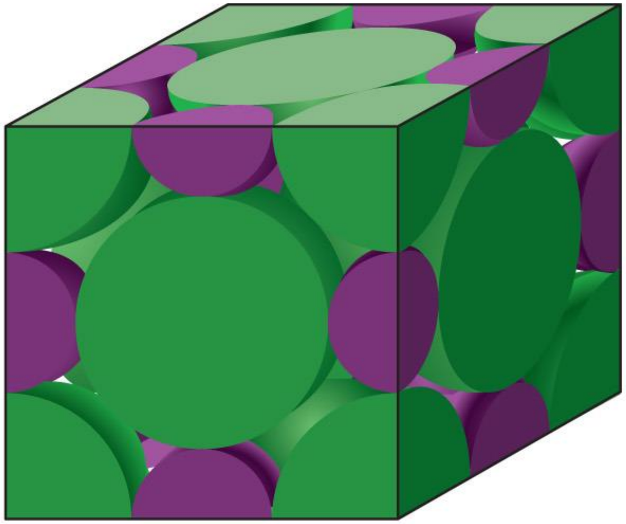
  - Metals tend to lose electrons to form positively charged ions called **cations**.
  - Non-metals tend to gain electrons to form negatively charged ions called **anions**.

Sodium Chloride

An extended array of Na^+ and Cl^- ions

The simplest formula unit is NaCl





3-2 The Mole Concept and Chemical Calculations

- Formula mass
  - the mass of a formula unit in atomic mass units (u)
- Molecular mass
  - a formula mass of a *molecular compound*
- Weighted average mass
  - add up the weighted average atomic masses
- Exact Mass
  - add up the isotopic masses (see mass spectrometry)

EXAMPLE 3-2

Combining Several Factors in a Calculation Involving Molar Mass. The volatile liquid ethyl mercaptan, C_2H_5SH is one of the most odoriferous substances known. It is sometimes added to natural gas to make gas leaks detectable. How many C_2H_5SH molecules are contained in a 1.0 μL sample given the following information?

The density is 0.84 g/mL, a drop of liquid is about 0.05 mL and 1.0 μL is only 0.02 of a drop.

EXAMPLE 7-3

Solution.

The strategy to follow can be laid out in a flow diagram.

$$\mu L \xrightarrow{10^{-6}\ L/\mu L} L \xrightarrow{10^{3}\ mL/L} mL \xrightarrow{0.84\ g/mL} g \xrightarrow{\frac{1\ mol}{62.1\ g}} mol \xrightarrow{6.02\ 10^{23}\ molec/mol} molecules$$

The factors in each conversion may be added above the arrows.

Don't worry if your conversion factors are upside down, fix them when you write the equations by making sure the units cancel properly.

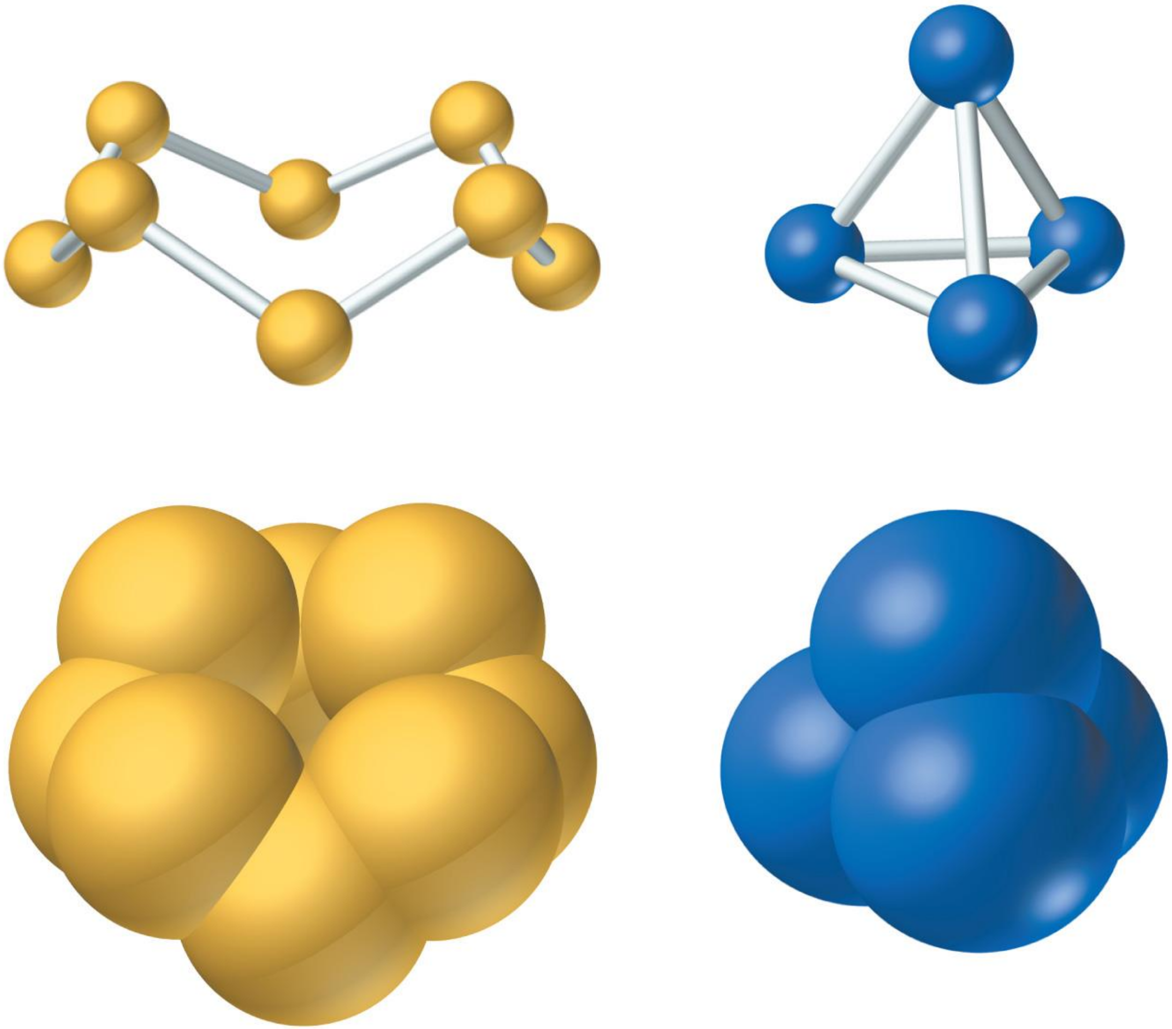
Using the strategy and the conversion factors, write the equation:

$$1\,\cancel{\mu L} \times 10^{-6}\,\cancel{L}/\cancel{\mu L} \times 10^{3}\,\cancel{mL}/\cancel{L} \times 0.84\,\cancel{g}/\cancel{mL} \times \frac{1\,\cancel{mol}}{62.1\,\cancel{g}} \times 6.02 \times 10^{23}\,\text{molec}/\cancel{mol}$$

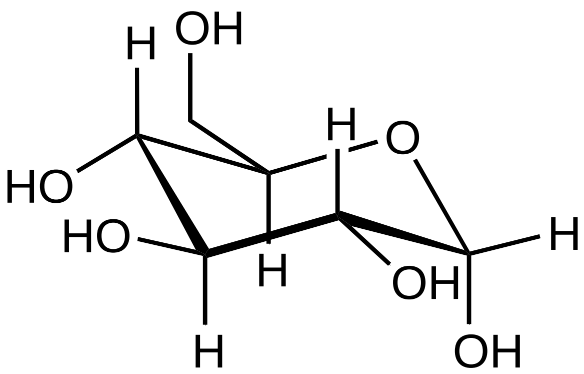
Check the units cancel and *only then* calculate.

$$= 8.1 \times 10^{18}\ \text{molecules}$$

Inorganic Molecules



Molecular Mass



Glucose

Molecular formula $C_6H_{12}O_6$

Empirical formula CH_2O

Molecular Mass: Use the naturally occurring mixture of isotopes,

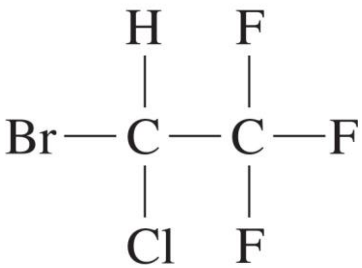
$$\mathbf{6} \times 12.01 + \mathbf{12} \times 1.01 + \mathbf{6} \times 16.00 = 180.18$$

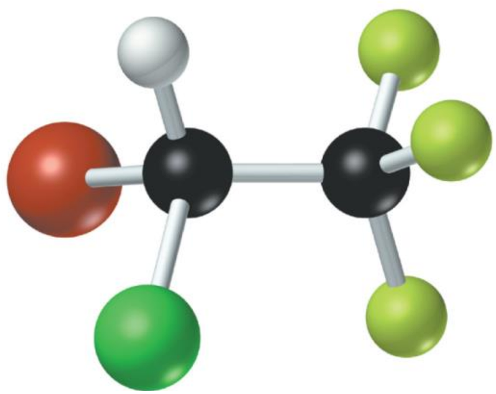
Exact Mass: Use the most abundant isotopes,

$$\mathbf{6} \times 12.000000 + \mathbf{12} \times 1.007825 + \mathbf{6} \times 15.994915$$

$$= 180.06339$$

3-3 Composition of Chemical Compounds





Halothane $C_2HBrClF_3$

Mole ratio $n_C/n_{halothane}$

Mass ratio $m_C/m_{halothane}$

$$M(C_2HBrClF_3) = 2M_C + M_H + M_{Br} + M_{Cl} + 3M_F$$

$$= (2 \times 12.01) + 1.01 + 79.90 + 35.45 + (3 \times 19.00)$$

$$= 197.38 \text{ g/mol}$$

EXAMPLE 7-3

Calculating the Mass Percent Composition of a Compound

What is the mass percent composition of halothane, $C_2HBrClF_3$?

Calculate the molecular mass

$$M(C_2HBrClF_3) = 197.38 \text{ g/mol}$$

For one mole of compound, formulate the mass ratio and convert to percent:

$$\%C = \frac{\left(2 \text{ mol C} \times \left(\dfrac{12.01 \text{ g C}}{1 \text{ mol C}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 12.17\%$$

EXAMPLE 7-3

$$\%H = \frac{\left(1 \text{ mol H} \times \left(\frac{1.01 \text{ g H}}{1 \text{ mol H}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 0.51\% \text{ H}$$

$$\%Br = \frac{\left(1 \text{ mol Br} \times \left(\frac{79.90 \text{ g Br}}{1 \text{ mol Br}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 40.48\% \text{ Br}$$

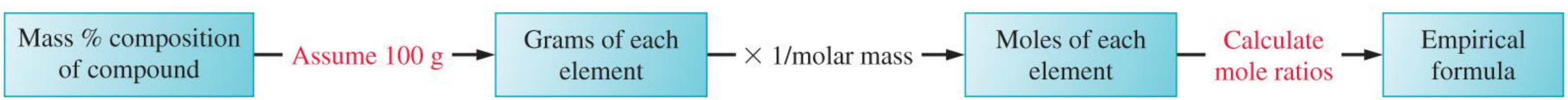
$$\%Cl = \frac{\left(1 \text{ mol C} \times \left(\frac{35.45 \text{ g Cl}}{1 \text{ mol Cl}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 17.96\% \text{ Cl}$$

$$\%F = \frac{\left(3 \text{ mol C} \times \left(\frac{19.00 \text{ g F}}{1 \text{ mol F}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 28.88\% \text{ F}$$

Establishing Formulas from Experimentally Determined Percent Composition

5 Step approach:

1. Choose an arbitrary sample size (100g).
2. Convert masses to amounts in moles.
3. Write a formula.
4. Convert formula to small whole numbers.
5. Multiply all subscripts by a small whole number to make the subscripts integral.



EXAMPLE 3-5

Determining the Empirical and Molecular Formulas of a Compound from Its Mass Percent Composition

Dibutyl succinate is an insect repellent used against household ants and roaches. Its composition is 62.58% C, 9.63% H and 27.79% O. Its experimentally determined molecular mass is 230 u. What are the empirical and molecular formulas of dibutyl succinate?

Step 1: Determine the mass of each element in a 100g sample.

C 62.58 g   H 9.63 g   O 27.79 g

EXAMPLE 3-5

Step 2: Convert masses to amounts in moles.

$$n_C = 62.58\,g\,C \times \frac{1\,mol\,C}{12.011\,g\,C} = 5.210\,mol\,C$$

$$n_H = 9.63\,g\,H \times \frac{1\,mol\,H}{1.008\,g\,H} = 9.55\,mol\,H$$

$$n_O = 27.79\,g\,O \times \frac{1\,mol\,O}{15.999\,g\,O} = 1.737\,mol\,O$$

Step 3: Write a tentative formula. $C_{5.21}H_{9.55}O_{1.74}$

Step 4: Convert to small whole numbers. $C_{2.99}H_{5.49}O$

EXAMPLE 3-5

Step 5: Convert to a small whole number ratio.

Multiply $\times$ 2 to get $C_{5.98}H_{10.98}O_2$

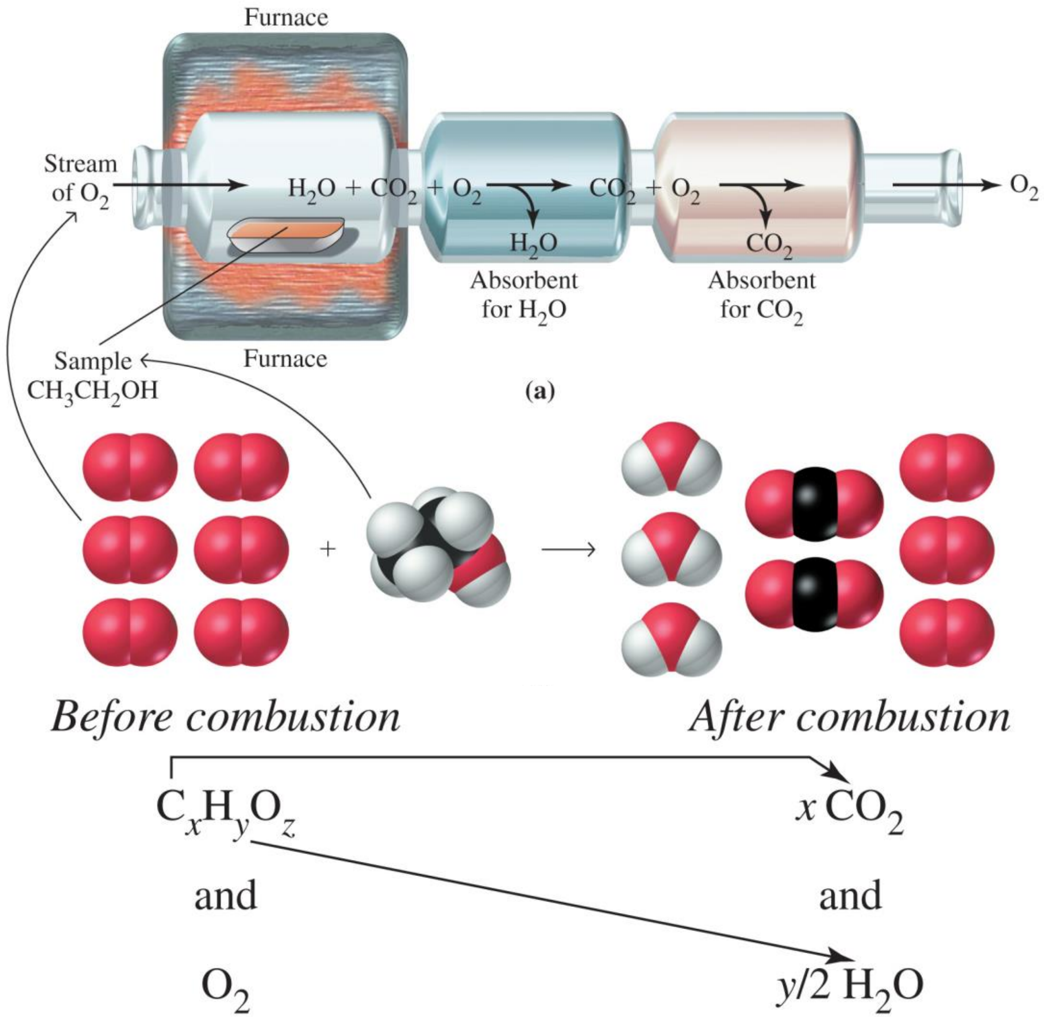
The empirical formula is $C_6H_{11}O_2$

Step 6: Determine the molecular formula.

Empirical formula mass is 115 u.
Molecular formula mass is 230 u.

The molecular formula is $C_{12}H_{22}O_4$

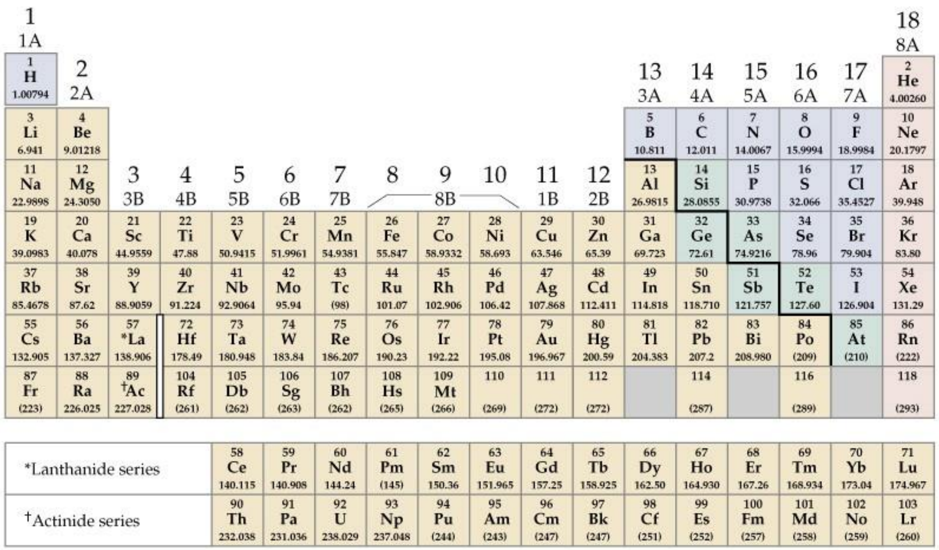
Combustion Analysis



3-4 Oxidation States: A Useful Tool in Describing Chemical Compounds

Metals tend to lose electrons.

$Na \rightarrow Na^{+} + e^{-}$



Non-metals tend to gain electrons.

$Cl + e^{-} \rightarrow Cl^{-}$

Reducing agents

Oxidizing agents

We use the Oxidation State to keep track of the number of electrons that have been gained or lost by an element.

Rules for Oxidation States

1. The oxidation state (OS) of an individual atom in a free element is 0.

2. The total of the OS in all atoms in:
   i. Neutral species is 0.
   ii. Ionic species is equal to the charge on the ion.

3. In their compounds, the alkali metals and the alkaline earths have OS of +1 and +2 respectively.

4. In compounds the OS of fluorine is *always* –1

Rules for Oxidation States

5. In compounds, the OS of hydrogen is *usually* +1

6. In compounds, the OS of oxygen is *usually* –2.

7. In binary (two-element) compounds with metals:
   i. Halogens have OS of –1,
   ii. Group 16 have OS of –2 and
   iii. Group 15 have OS of –3.

EXAMPLE 3-7

Assigning Oxidation States What is the oxidation state of the underlined element in each of the following? a) P_4; b) Al_2O_3; c) MnO_4^-; d) NaH.

a) P_4 is an element. P OS = 0

b) Al_2O_3: O is –2. O_3 is –6. Since (+6)/2=(+3), Al OS = +3.

c) MnO_4^-: net OS = -1, O_4 is –8. Mn OS = +7.

d) NaH: net OS = 0, rule 3 beats rule 5, Na OS = +1 and H OS = -1.

3-5 Naming Compounds: Organic and Inorganic Compounds

Trivial names are used for common compounds.

A systematic method of naming compounds is known as a system of *nomenclature*.

Organic compounds

Inorganic compounds

Lead (IV) oxide

Lead (II) oxide

3-6 Names and Formulas of Inorganic Compounds

Binary Compounds of Metals and Nonmetals

Name unchanged

$NaCl$ = Sodium chloride

“ide” ending

MgI_2 = Magnesium iodide

Al_2O_3 = Aluminum oxide

TABLE 3.1 Some Simple Ions

Name	Symbol	Name	Symbol
Positive ions (cations)			
Lithium ion	Li^+	Chromium(II) ion	Cr^{2+}
Sodium ion	Na^+	Chromium(III) ion	Cr^{3+}
Potassium ion	K^+	Iron(II) ion	Fe^{2+}
Rubidium ion	Rb^+	Iron(III) ion	Fe^{3+}
Cesium ion	Cs^+	Cobalt(II) ion	Co^{2+}
Magnesium ion	Mg^{2+}	Cobalt(III) ion	Co^{3+}
Calcium ion	Ca^{2+}	Copper(I) ion	Cu^+
Strontium ion	Sr^{2+}	Copper(II) ion	Cu^{2+}
Barium ion	Ba^{2+}	Mercury(I) ion	Hg_2^{2+}
Aluminum ion	Al^{3+}	Mercury(II) ion	Hg^{2+}
Zinc ion	Zn^{2+}	Tin(II) ion	Sn^{2+}
Silver ion	Ag^+	Lead(II) ion	Pb^{2+}
Negative ions (anions)			
Hydride ion	H^-	Iodide ion	I^-
Fluoride ion	F^-	Oxide ion	O^{2-}
Chloride ion	Cl^-	Sulfide ion	S^{2-}
Bromide ion	Br^-	Nitride ion	N^{3-}

Binary Compounds of Two Non-Metals

Molecular compounds

usually write the positive OS element first.

HCl hydrogen chloride

Some pairs form more than one compound

mono	1	penta	5
di	2	hexa	6
tri	3	hepta	7
tetra	4	octa	8

TABLE 3.2 Naming Binary Molecular Compounds

Formula	Name[a]
BCl_3	Boron trichloride
CCl_4	Carbon tetrachloride
CO	Carbon monoxide
CO_2	Carbon dioxide
NO	Nitrogen monoxide
NO_2	Nitrogen dioxide
N_2O	Dinitrogen monoxide
N_2O_3	Dinitrogen trioxide
N_2O_4	Dinitrogen tetroxide
N_2O_5	Dinitrogen pentoxide
PCl_3	Phosphorus trichloride
PCl_5	Phosphorus pentachloride
SF_6	Sulfur hexafluoride

[a] When the prefix ends in *a* or *o* and the element name begins with *a* or *o*, the final vowel of the prefix is dropped for ease of pronunciation. For example, carbon *mon*oxide, not carbon *mono*oxide, and dinitrogen *tetr*oxide, not dinitrogen *tetra*oxide. However, PI_3 is phosphorus *tri*iodide, not phosphorus *tr*iodide.

Binary Acids

Acids produce H^+ when dissolved in water.

They are compounds that ionize in water.

Emphasize the fact that a molecule is an acid by altering the name.

HCl	hydrogen chloride	hydrochloric acid
HF	hydrogen fluoride	hydrofluoric acid

TABLE 3.3 Some Common Polyatomic Ions

Name	Formula	Typical Compound	Name	Formula	Typical Compound
Cation			**Anions**		
Ammonium ion	NH_4^+	NH_4Cl	Nitrite ion	NO_2^-	$NaNO_2$
Anions			Nitrate ion	NO_3^-	$NaNO_3$
Acetate ion	$C_2H_3O_2^-$	$NaC_2H_3O_2$	Oxalate ion	$C_2O_4^{2-}$	$Na_2C_2O_4$
Carbonate ion	CO_3^{2-}	Na_2CO_3	Permanganate ion	MnO_4^-	$NaMnO_4$
Hydrogen carbonate ion[a] (or bicarbonate ion)	HCO_3^-	$NaHCO_3$	Phosphate ion	PO_4^{3-}	Na_3PO_4
			Hydrogen phosphate ion[a]	HPO_4^{2-}	Na_2HPO_4
Hypochlorite ion	ClO^-	$NaClO$	Dihydrogen phosphate ion[a]	$H_2PO_4^-$	NaH_2PO_4
Chlorite ion	ClO_2^-	$NaClO_2$	Sulfite ion	SO_3^{2-}	Na_2SO_3
Chlorate ion	ClO_3^-	$NaClO_3$	Hydrogen sulfite ion[a] (or bisulfite ion)	HSO_3^-	$NaHSO_3$
Perchlorate ion	ClO_4^-	$NaClO_4$			
Chromate ion	CrO_4^{2-}	Na_2CrO_4	Sulfate ion	SO_4^{2-}	Na_2SO_4
Dichromate ion	$Cr_2O_7^{2-}$	$Na_2Cr_2O_7$	Hydrogen sulfate ion[a] (or bisulfate ion)	HSO_4^-	$NaHSO_4$
Cyanide ion	CN^-	$NaCN$			
Hydroxide ion	OH^-	$NaOH$	Thiosulfate ion	$S_2O_3^{2-}$	$Na_2S_2O_3$

[a] These anion names are sometimes written as a single word—for example, hydrogencarbonate, hydrogenphosphate, and so forth.

TABLE 3.4 Nomenclature of Some Oxoacids and Their Salts

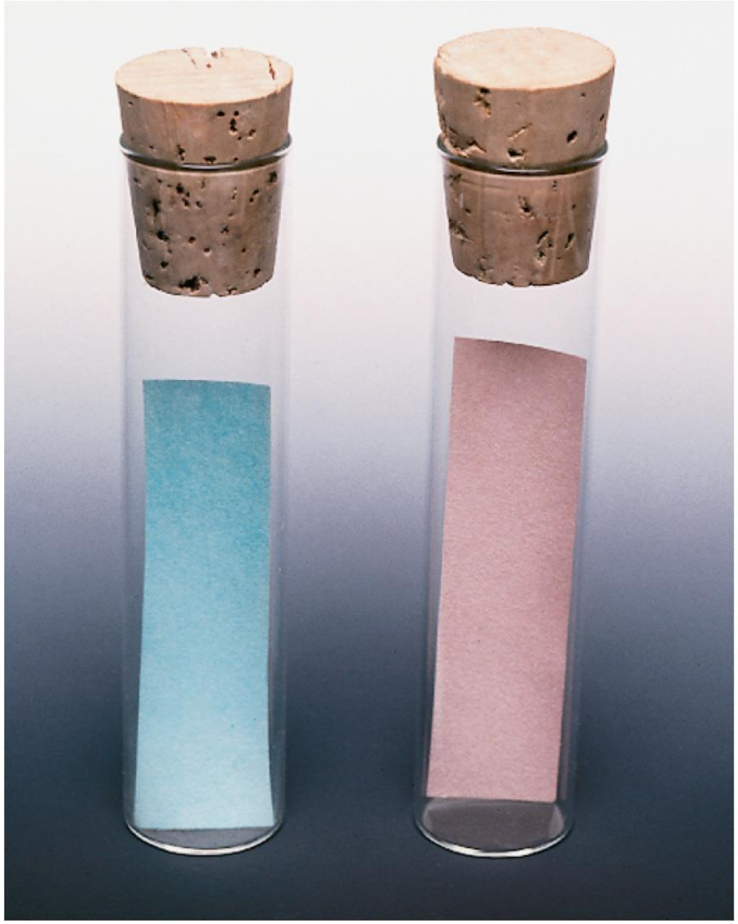
Oxidation State	Formula of Acid[a]	Name of Acid[b]	Formula of Salt[b]	Name of Salt
Cl: +1	$HClO$	*Hypo*chlor*ous* acid	$NaClO$	Sodium *hypo*chlor*ite*
Cl: +3	$HClO_2$	Chlor*ous* acid	$NaClO_2$	Sodium chlor*ite*
Cl: +5	$HClO_3$	Chlor*ic* acid	$NaClO_3$	Sodium chlor*ate*
Cl: +7	$HClO_4$	*Per*chlor*ic* acid	$NaClO_4$	Sodium *per*chlor*ate*
N: +3	HNO_2	Nitr*ous* acid	$NaNO_2$	Sodium nitr*ite*
N: +5	HNO_3	Nitr*ic* acid	$NaNO_3$	Sodium nitr*ate*
S: +4	H_2SO_3	Sulfur*ous* acid	Na_2SO_3	Sodium sulf*ite*
S: +6	H_2SO_4	Sulfur*ic* acid	Na_2SO_4	Sodium sulf*ate*

[a] In all these acids, H atoms are bonded to O atoms, not the central nonmetal atom. Often formulas are written to reflect this fact, for instance, HOCl instead of HClO and HOClO instead of $HClO_2$.

[b] In general, the *-ic* and *-ate* names are assigned to compounds in which the central nonmetal atom has an oxidation state equal to the periodic table group number minus 10. Halogen compounds are exceptional in that the *-ic* and *-ate* names are assigned to compounds in which the halogen has an oxidation state of +5 (even though the group number is 17).

Some Compounds of Greater Complexity

- Effect of Moisture
  - Blue anhydrous
    - $CoCl_2$
  - Pink hexahydrate
    - $CoCl_2 \cdot 6\ H_2O$



$$\%H_2O = \frac{\left(6 \text{ mol } H_2O \times \left(\frac{18.02 \text{ g } H_2O}{1 \text{ mol } H_2O}\right)\right)}{237.9 \text{ g } CoCl_2 \cdot 6\ H_2O} \times 100\%$$

$$= 45.45\%\ H_2O$$

3-7 Names and Formulas of Organic Compounds

Organic compounds abound in nature

Fats, carbohydrates and proteins are foods.

Propane, gasoline, kerosene, oil.

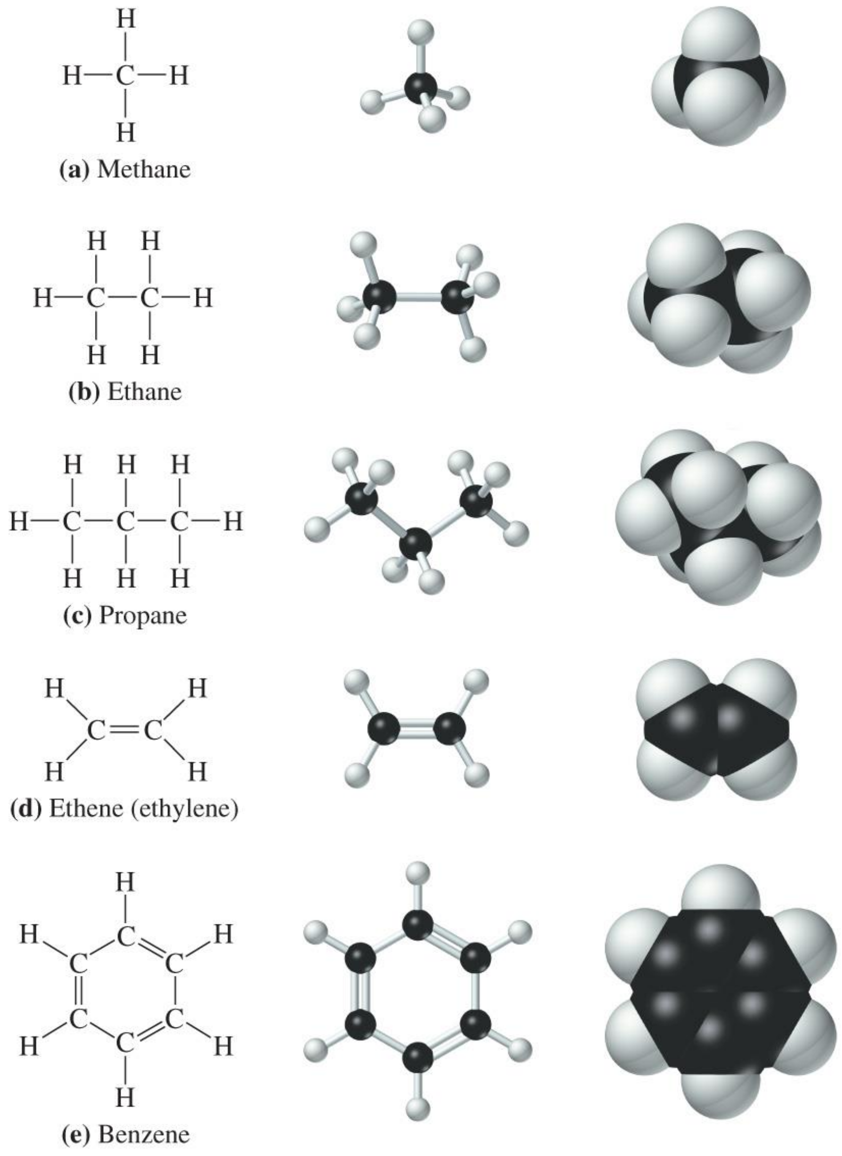
Drugs and plastics

Carbon atoms form chains and rings and act as the framework of molecules.

TABLE 3.5 Word stem (or prefix) indicating the number of carbon atoms in simple organic molecules

Stem (or prefix)	Number of C Atoms
Meth-	1
Eth-	2
Prop-	3
But-	4
Pent-	5
Hex-	6
Hept-	7
Oct-	8
Non-	9
Dec-	10

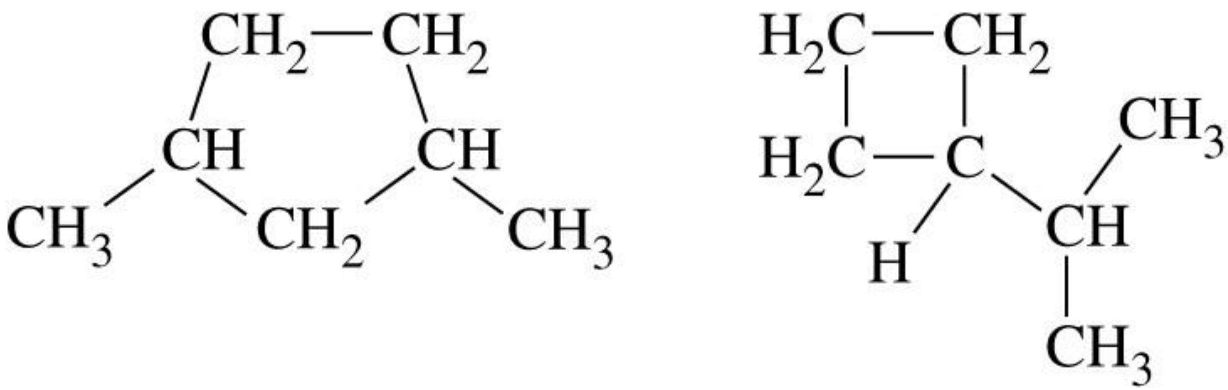
Visualizations of some Hydrocarbons



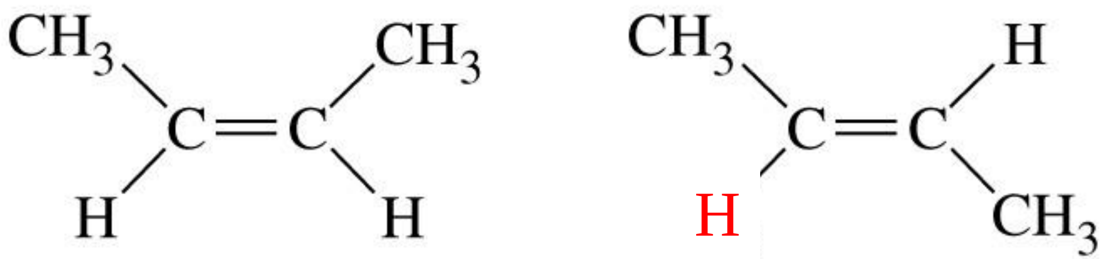
Isomers

Isomers have the same molecular formula but have different arrangements of atoms in space. Are the following pairs isomers?

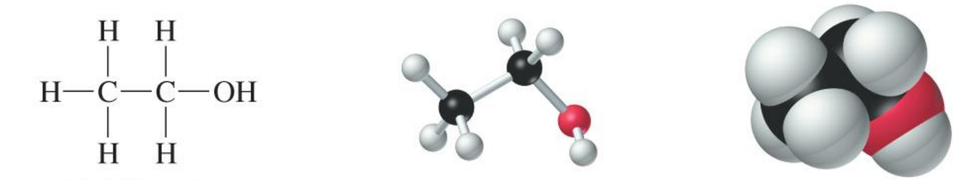
(a)



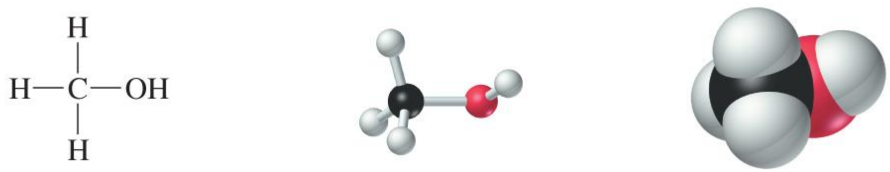
(c)



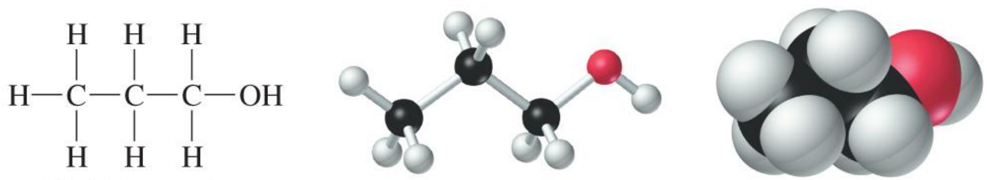
Functional Groups – Alcohols



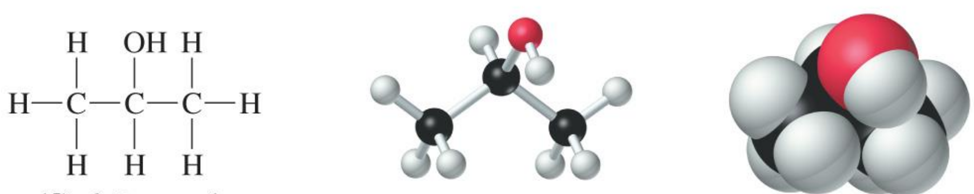
(a) Ethanol, or Ethyl alcohol



(b) Methanol, or Methyl alcohol

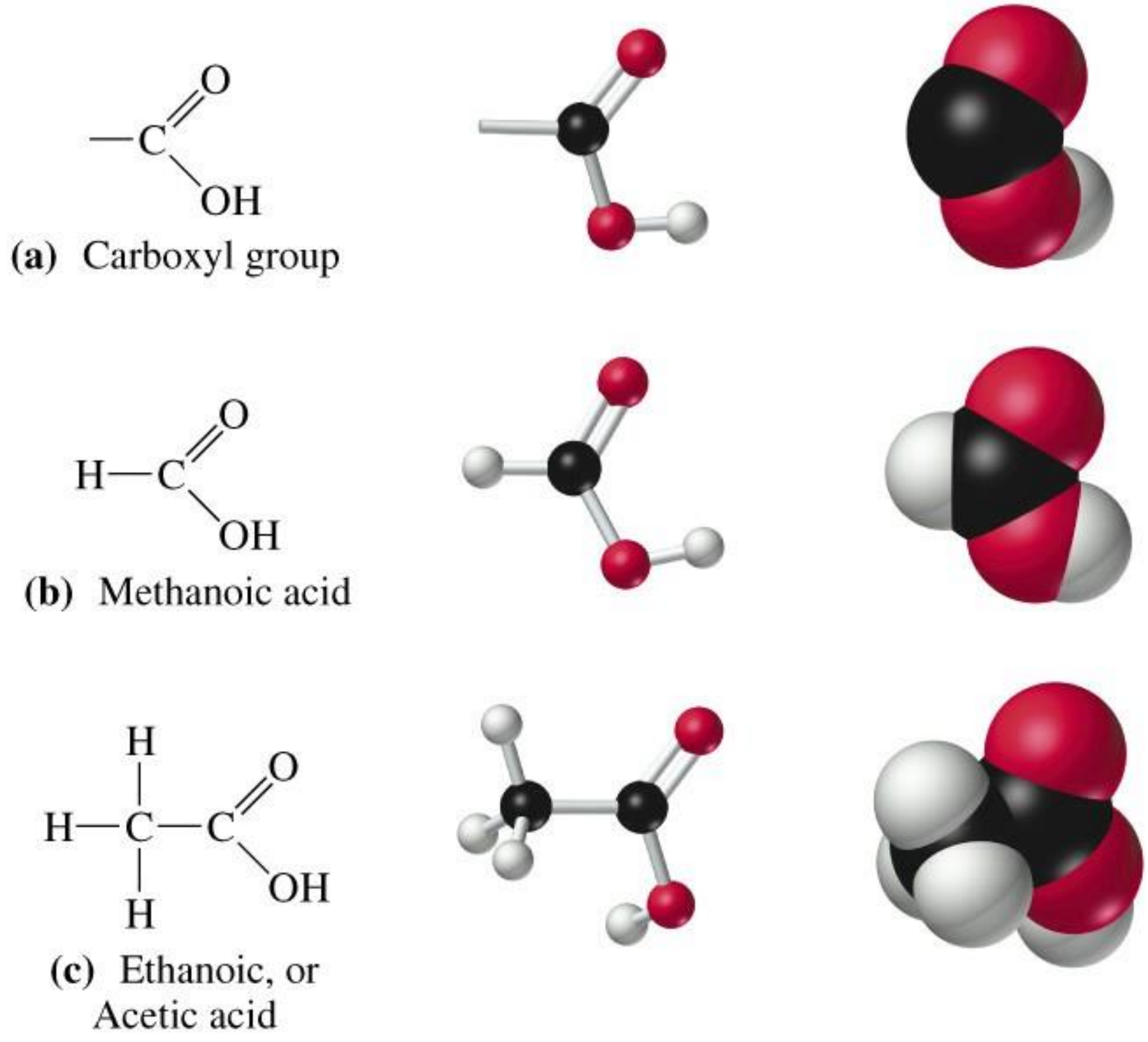


(c) 1-Propanol, or Propyl alcohol



(d) 2-Propanol, or Isopropyl alcohol

Functional Groups – Carboxylic Acid



End of Chapter Questions

- Individuals have individual learning styles.
  - You may have more than one style for different types of learning.

    - Seeing
    - Listening
    - Reading
    - Writing

- Take notes and actively listen.
- Participate in your learning process!