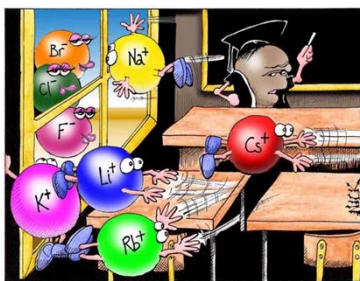
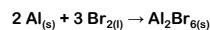


Molecules, Ions and their Compounds



"Perhaps one of you gentlemen would mind telling me just what it is outside the window that you find so attractive..?"



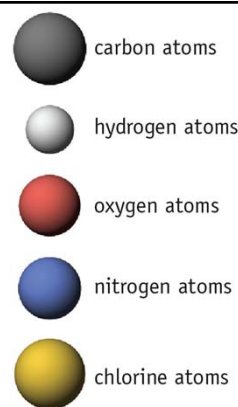
aluminum + bromine → aluminum bromide

Note: Aluminum reacts with halogens heavier than chlorine to produce "dimers" (in their liquid and gas phases) that are more consistent with the physical and chemical properties of molecules than ionic compounds.

Representing Formulas

NAME	MOLECULAR FORMULA	CONDENSED FORMULA	STRUCTURAL FORMULA	MOLECULAR MODEL
Ethanol	C ₂ H ₆ O	CH ₃ CH ₂ OH	<pre> H H H-C - C - O - H H H </pre>	
Dimethyl ether	C ₂ H ₆ O	CH ₃ OCH ₃	<pre> H H H-C - O - C - H H H </pre>	

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Colors commonly used for representing atoms

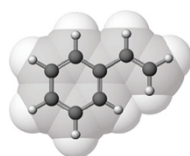
(Sometimes sulfur is represented by yellow and chlorine by green)

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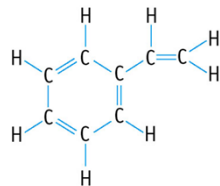
The styrene molecule is the building block of polystyrene, a material used for drinking cups and building insulation. What is the molecular formula for styrene?



Condensed formula



Molecular model



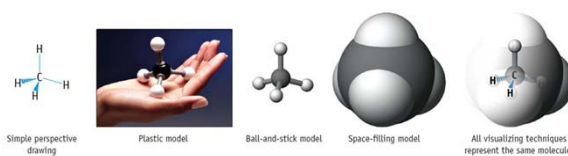
Structural formula



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Molecular Model Representations:

See ACDLabs: ChemsKetch at the web site



Simple perspective drawing

Plastic model

Ball-and-stick model

Space-filling model

All visualizing techniques represent the same molecule.

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Question:
Cysteine, whose molecular model and structural formula are illustrated here, is an important amino acid and a constituent of many living things. What is its molecular formula?

$C_3NH_7SO_2$

Ionic Compounds: Formulas, Names and Properties

Common Name	Name	Formula	Ions Involved
Calcite	Calcium carbonate	CaCO ₃	Ca ²⁺ , CO ₃ ²⁻
Fluorite	Calcium fluoride	CaF ₂	Ca ²⁺ , F ⁻
Gypsum	Calcium sulfate dihydrate	CaSO ₄ · 2 H ₂ O	Ca ²⁺ , SO ₄ ²⁻
Hematite	Iron(III) oxide	Fe ₂ O ₃	Fe ³⁺ , O ²⁻
Orpiment	Arsenic sulfide	As ₂ S ₃	As ³⁺ , S ²⁻

Definition: Compounds that are bound together by electrostatic attractions produced by the transfer of electrons between species in the compound.

Ionic Compounds

- Generally form between metals and nonmetals
- The bond between atoms forms from a transfer of electrons from one atom to another.
- The one that loses electrons becomes positively charged and is called a "cation".
- The one that gains electrons becomes negatively charged and is called an "anion".
- There is no such thing as an ionic "molecule" because the compound exists as a repeating pattern of positive and negative ions (i.e. an ionic crystal).

Cations (positively charged particles) and Anions (negatively charged particles)

(a)

$$F = k(n^+)(n^-)/d^2$$

(b)

(c)

As ion charge increases, force of attraction increases.

As distance increases, force of attraction decreases.

Given that in the electrostatic force equation the constant $k = 8.988 \times 10^9 \text{ Nm}^2/\text{C}^2$ and the ion radii for magnesium and oxygen are 65pm and 140pm, respectively, determine the force between the two atoms in the compound magnesium oxide. ($q_e = 1.602 \times 10^{-19} \text{ C}$)

Answer:

$$F = 8.988 \times 10^9 \text{ Nm}^2/\text{C}^2 (2)(1.602 \times 10^{-19} \text{ C})(2)(1.602 \times 10^{-19} \text{ C}) / (2.05 \times 10^{-10} \text{ m})^2$$

$$= 2.20 \times 10^{-8} \text{ N}$$

Ionic Compound

A compound consisting of a positively charged component (cation) and a negatively charged component (anion)

Any charged particle is known generically as an "ion".

Ions form from the transfer of one or more electrons from one species to another

The charged particles are electrostatically attracted to one another forming a crystalline structure with a repeating pattern of positive and negative particles.

Usually fixed charge in ionic compounds

Metals
Transition metals
Metalloids
Nonmetals

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Many transition and post-transition metals have more than one possible charge.

Empirical Formula - Provides information about the (quantity) ratio of combined elements in a compound written in lowest terms.

Ex. Rb_2O (Two rubidium atoms combine with one oxygen atom)

-When writing the formula for an ionic compound, the cation is always listed first.

- In the formation of an ionic compound, all electrons must be accounted for. You cannot have any "leftovers" (i.e. the compound must be overall electrically neutral)

-Often you can use the "crisscross" method to determine the ratio of elements in the compound.

Just remember to reduce where necessary.

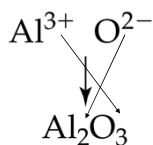


Table 3.1 Formulas and Names of Some Common Polyatomic Ions

Formula	Name	Formula	Name
CATION: Positive Ion			
NH_4^+	ammonium ion	You should memorize these	
ANIONS: Negative Ions			
Based on a Group 4A element		Based on a Group 7A element	
CN^-	cyanide ion	ClO^-	hypochlorite ion
CH_3CO_2^-	acetate ion	ClO_2^-	chlorite ion
CO_3^{2-}	carbonate ion	ClO_3^-	chlorate ion
HCO_3^-	hydrogen carbonate ion (or bicarbonate ion)	ClO_4^-	perchlorate ion
Based on a Group 5A element		Based on a transition metal	
NO_2^-	nitrite ion	CrO_4^{2-}	chromate ion
NO_3^-	nitrate ion	$\text{Cr}_2\text{O}_7^{2-}$	dichromate ion
PO_4^{3-}	phosphate ion	MnO_4^-	permanganate ion
HPO_4^{2-}	hydrogen phosphate ion		
H_2PO_4^-	dihydrogen phosphate ion		
Based on a Group 6A element			
OH^-	hydroxide ion		
SO_3^{2-}	sulfite ion		
SO_4^{2-}	sulfate ion		
HSO_4^-	hydrogen sulfate ion (or bisulfate ion)		

increasing oxygen content

per . . . ate
. . . ate
. . . ite
hypo . . . ite

Polyatomic ions: Groups of covalently bonded atoms that carry an overall charge.

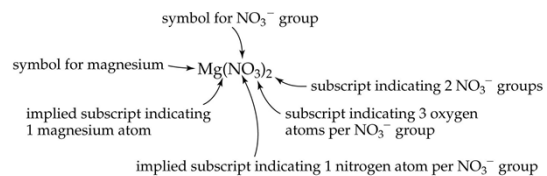
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-With polyatomic ions, the charge is over the whole group of atoms:



-The identity of the polyatomic ion MUST be preserved. Use parentheses if you need more than one. DON'T just multiply thru.

(i.e. $\text{Ca}(\text{NO}_3)_2$, NOT CaN_2O_6)



Naming Ionic Compounds

Type 1. Cation and anion with fixed charge:

Example: Name the compound MgF_2

Answer: magnesium fluoride

Name the cation then name the anion with the ending changed to "ide".

Type 2. Cation with variable charge:

Example: Name the compound FeCl_3

Answer: ferric chloride (trivial) or

Iron(III)chloride (Stock/IUPAC/Standardized)

For trivial naming, the suffix "ic" on the cation means the higher of two charges and "ous" means the lower.

When using the trivial name for "polyvalent" atoms, use the Latin derivative when available (i.e. say plumbous NOT leadous) (exception: Mercurous, not Hydrargyrous)

Type 3. Ionic compounds that contain polyatomic ions.

Example: Name $\text{Sr}(\text{NO}_3)_2$

Answer: strontium nitrate

Use the polyatomic ion name directly without modification

Naming Ionic Compounds		
Notes: 1. Compounds where electrons are transferred between elements (usually between metals and nonmetals) 2. When writing formulas for these compounds the charges between the cation and anion must be balanced to that the overall compound is <i>neutral</i> .		
Combinations you will encounter:	Rules:	Example:
Metal with a fixed charge paired with a nonmetal	1. Name the metal 2. Name the nonmetal with the ending changed to -ide	NaCl Sodium chloride
Metal with a fixed charge paired with a polyatomic anion	1. Name the metal 2. Name the polyatomic anion	Mg(NO ₃) ₂ Magnesium nitrate
Metal with a variable charge paired with a nonmetal	1. Name the metal using: Roman numeral for charge or Latin derivative (if available) with -ic or -ous ending 2. Name the nonmetal with the ending changed to -ide	FeCl ₃ Iron(III)chloride Ferric chloride
Metal with a variable charge paired with a polyatomic anion	1. Name the metal using: Roman numeral for charge or Latin derivative (if available) with -ic or -ous ending 2. Name the polyatomic anion	Sr(NO ₃) ₂ Strontium nitrate
Polyatomic cation paired with a polyatomic anion	1. Name the polyatomic cation 2. Name the polyatomic anion	NH ₄ NO ₃ Ammonium nitrate

Exercises 3.4 (page 109) and 3.5 (page 111)

Exercise 3.4

a) Give the number and identity of the constituent ions in each of the following ionic compounds: NaF, Cu(NO₃)₂, NaCH₃CO₂.

b) Iron, a transition metal, forms ions having at least two different charges. Write the formulas of the compounds formed between two different iron cations and chloride ions.

c) Write the formulas of all neutral ionic compounds that can be formed by combining the cations Na⁺ and Ba²⁺ with the anions S²⁻ and PO₄³⁻.

Exercise 3.5

1. Give the formula for each of the following ionic compounds:

a) ammonium nitrate b) cobalt(II)sulfate c) nickel(II)cyanide
d) vanadium(III)oxide e) barium acetate f) calcium hypochlorite

2. Name the following ionic compounds:

a) MgBr₂ b) Li₂CO₃ c) KHSO₃ d) KMnO₄
e) (NH₄)₂S f) CuCl and CuCl₂

Answers:

Exercise 3.4

a) Give the number and identity of the constituent ions in each of the following ionic compounds: NaF, Cu(NO₃)₂, NaCH₃CO₂.

1 - Na⁺, 1 - F⁻; 1 - Cu²⁺, 2 - NO₃⁻; 1 - Na⁺, 1 - CH₃CO₂⁻

b) Iron, a transition metal, forms ions having at least two different charges. Write the formulas of the compounds formed between two different iron cations and chloride ions. **FeCl₂; FeCl₃**

c) Write the formulas of all neutral ionic compounds that can be formed by combining the cations Na⁺ and Ba²⁺ with the anions S²⁻ and PO₄³⁻.

Na₂S; Na₃PO₄; BaS; Ba₃(PO₄)₂

Exercise 3.5

1. Give the formula for each of the following ionic compounds:

a) ammonium nitrate b) cobalt(II)sulfate c) nickel(II)cyanide
d) vanadium(III)oxide e) barium acetate f) calcium hypochlorite

a) NH₄NO₃ b) CoSO₄ c) Ni(CN)₂; d) V₂O₃ e) Ba(CH₃CO₂)₂ f) Ca(ClO)₂

2. Name the following ionic compounds:

a) MgBr₂ b) Li₂CO₃ c) KHSO₃ d) KMnO₄
e) (NH₄)₂S f) CuCl and CuCl₂

**a) magnesium bromide b) lithium carbonate c) potassium bisulfite
(potassium hydrogen sulfite) d) potassium permanganate
e) ammonium sulfide f) copper(I)chloride (cuprous chloride);
copper(II)chloride (cupric chloride)**



CO

CO₂

Binary Molecular Compounds:

Covalent bonds (shared electrons)

Why would nonmetal-nonmetal compounds want to share electrons?

Examples:

NO N₂O NO₂ N₂O₄

The number and type of each element present must be designated.

We must use prefixes

1-mono 6-hex
2-di 7-hept
3-tri 8-oct
4-tetra 9-non
5-pent 10-dec

Don't use mono for the first occurring element in the compound.

Name these compounds: SF₆, Cl₂O₇, CF₄

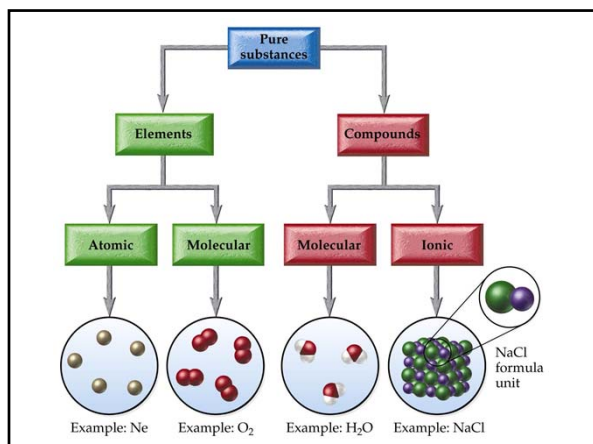
Compare CH ₄ , NH ₃ , H ₂ O.	
	<p>The elements of covalent compounds are listed in order of increasing electronegativity</p>

Naming Covalent Compounds (Molecules)

Notes:

1. Compounds where electrons are shared and no ions form (usually between nonmetals and nonmetals)
2. These compounds are the ONLY ones that use prefixes (mono, di, tri, etc.)

Combinations you will encounter:	Rules:	Example:
Nonmetal element paired with a nonmetal element	1. Name the first occurring element using the prefix corresponding to the subscript (except mono-) 2. Name the second occurring element using the prefix corresponding to the subscript and changing the ending to -ide	Cl ₂ O ₇ Dichlorine heptoxide



Molecular Mass (molecular weight): The sum of the masses of the atoms represented in a molecular formula (in u).

Formula Mass (formula weight): The sum of the masses of the atoms or ions present in a formula unit (i.e. the empirical formula of an ionic compound)(in u).

1 mole = The quantity of things as there are atoms in exactly 12.0g of the C-12 isotope.

This must be determined experimentally.

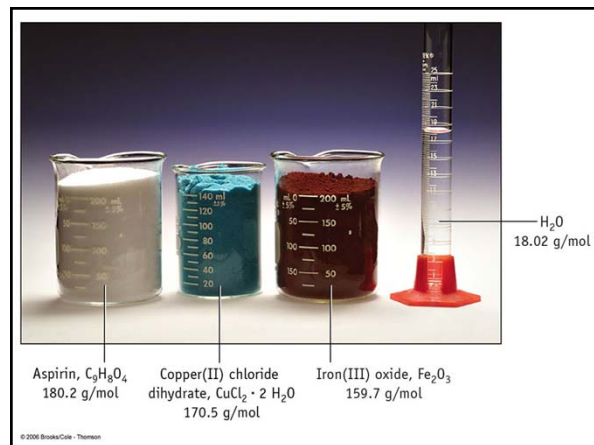
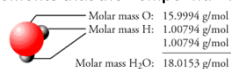
N_A (Avogadro's number) = 6.022×10^{23} = 1 mole

Mass number of an element:

- 1) Taken in amu's (u) = atomic mass (mass of 1 atom)
- 2) Taken in grams (g) = molar mass (mass of 1 mole of atoms)

24.30Mg If you have 24.30g of Mg you have 6.022×10^{23} atoms of Mg or 1mole

Determining the molar mass of a compound: Add the molar masses of the individual elements that the compound contains.



The mole is the bridge between masses you can measure and quantities you could never hope to count. The mole is useful in determining the amount substances to use in a chemical reaction.

Grams $\xleftrightarrow{\text{(multiply by MM)}} \text{Moles} \xleftrightarrow{\text{(divide by } N_A)} \text{Basic Units (atoms, molecules, formula units, etc.)}$
 (divide by MM) (multiply by N_A)

Example:

Determine the number of oxygen atoms contained in 25.00g of magnesium phosphate.

Example:

Determine the number of oxygen atoms contained in 25.00g of magnesium phosphate.

Answer:



$$25.00\text{g} / 262.8577\text{g/mol} = .0951\text{mol}$$

$$.0951\text{mol} \times 6.022 \times 10^{23} = 5.727 \times 10^{22}$$

$$5.727 \times 10^{22} \times 8 = \mathbf{4.582 \times 10^{23} \text{ atoms O}}$$

Mass Percent Composition: Determines the mass percentage of each element in the compound

$$\text{Mass \%} = (\text{Total mass of element in compound} / \text{Mass of compound}) \times 100$$

Examples:

1. Determine the mass percentage of oxygen in carbon dioxide.
2. A compound is analyzed and found to contain 22.59%N and 77.41%O by mass. Determine the empirical formula for the compound.
3. It is determined through mass spectroscopy that the true mass of the molecule falls between 120-130u. What is the molecular formula for the compound?

Answers:

1. Carbon dioxide is CO_2

$$\text{Mass \% O} = (2\text{O}/\text{CO}_2) = (32.0/44.01) \times 100 = 72.7\% \text{ oxygen}$$

2. In 100.g sample

$$\text{N} = 22.59\text{g}/14.01\text{g/mol} = 1.61\text{mol}$$

$$\text{O} = 77.41\text{g}/16.00\text{g/mol} = 4.84\text{mol O}$$

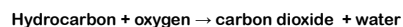


3. N_2O_6

Combustion Analysis

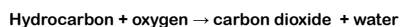
In an analysis of a hydrocarbon containing C, H and O, a 5.00g sample of the substance was combusted from which 9.571g of CO_2 and 5.867g of H_2O were produced. Determine the empirical formula of the hydrocarbon.

General formula:



In an analysis of a hydrocarbon containing C, H and O, a 5.00g sample of the substance was combusted from which 9.571g of CO_2 and 5.867g of H_2O were produced. Determine the empirical formula of the hydrocarbon.

General formula:



Answer:

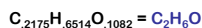
$$\text{Mass \% H in H}_2\text{O} = 11.19\%$$

$$\text{Mass \% C in CO}_2 = 27.29\%$$

$$\text{Mass H} = .1119(5.867\text{g}) = .6565\text{g} = .6514\text{mol H}$$

$$\text{Mass C} = .2729(9.571\text{g}) = 2.612\text{g} = .2175\text{mol C}$$

$$\text{Mass O} = 5.00 - .6565 - 2.612 = 1.7315\text{g} = .1082\text{mol O}$$



Determining the formula of a hydrated Compound

Example:

Hydrated nickel(II)chloride is a beautiful green, crystalline compound. When heated strongly, this compound is dehydrated. If 0.235g of $\text{NiCl}_2 \cdot x\text{H}_2\text{O}$ gives 0.128g of NiCl_2 on heating, what is the value of x?

Determining the formula of a hydrated Compound

Example:

Hydrated nickel(II)chloride is a beautiful green, crystalline compound. When heated strongly, this compound is dehydrated. If 0.235g of $\text{NiCl}_2 \cdot x\text{H}_2\text{O}$ gives 0.128g of NiCl_2 on heating, what is the value of x ?

Answer:

$$0.128\text{g NiCl}_2 / 129.599\text{g/mol} = 9.88 \times 10^{-4}\text{mol NiCl}_2$$

$$\text{gH}_2\text{O} = 0.235\text{g} - .128\text{g} = .107\text{g H}_2\text{O}$$

$$\text{Mol H}_2\text{O} = .107\text{g} / 18.0153\text{g/mol} = 5.939 \times 10^{-3}\text{mol H}_2\text{O}$$

$$\text{Ratio H}_2\text{O/NiCl}_2 = 5.939 \times 10^{-3} / 9.88 \times 10^{-4} = 6.0$$

$$\text{Formula is NiCl}_2 \cdot 6\text{H}_2\text{O} \quad x = 6$$

