

CHEMICAL FORMULAE AND EQUATIONS

ionic bonds = electrons have been transferred between atoms, resulting in oppositely charged ions that attract each other. Contain cations and anions.

covalent bonds = two atoms share some of their electrons.

Atomic element = one atom e.g. Ne, Xe

Molecular element = elements whose particles are multi-atom molecules (e.g. Cl₂, H₂, P₄).

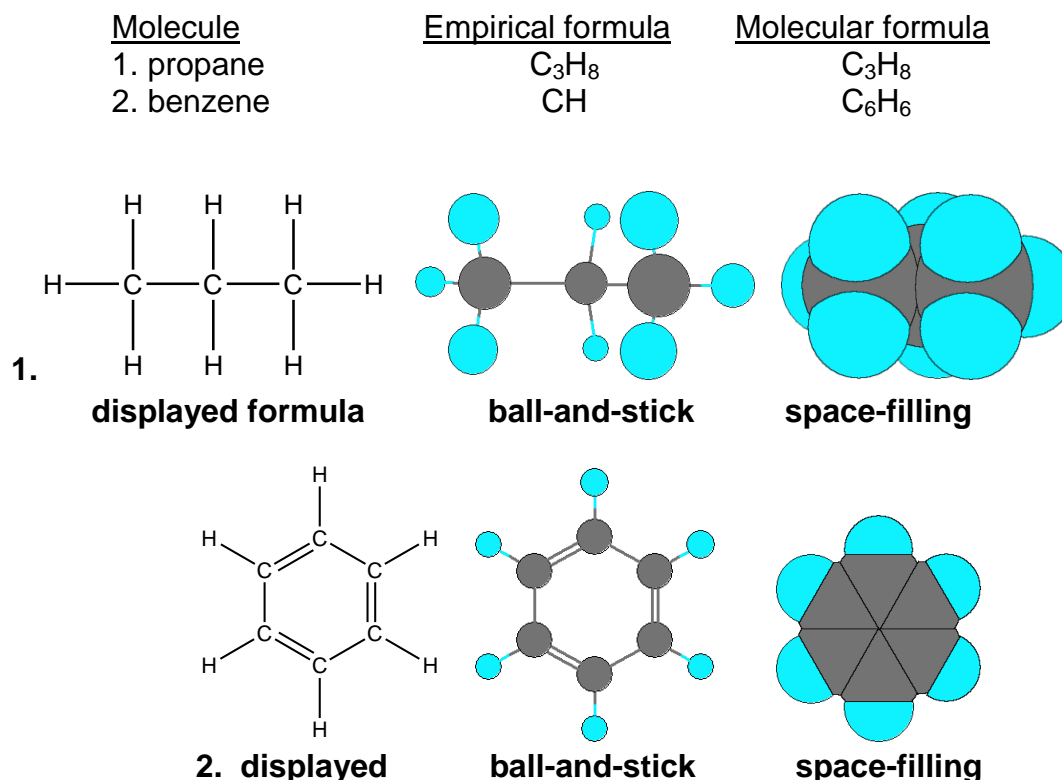
compounds are generally represented with a **chemical formula**. **Molecular compounds** contain non-metals (e.g. H₂O, HCl) and **ionic compounds** contain *cations* and *anions* (e.g. NaCl, Na₂SO₄).

Empirical formula = the kinds of elements found in the compound and the ratio of their atoms.

Molecular formula = the kinds of elements found in the compound and the numbers of their atoms.

Structural formula = the kinds of elements found in the compound, the numbers of their atoms, order of atom attachment, and the kind of attachment: CH₃CH₂OH: ethanol; CH₂=CHCH₂Br: 3-bromoprop-1-ene (traditional name allyl bromide).

Models show the 3-dimensional structure along with all the other information given in structural formula.



WRITING IONIC FORMULAS

Write the formula of a compound made from aluminum ions and oxide ions

1. Write the symbol for the metal cation and its charge Al³⁺ Group 3A

- Write the symbol for the nonmetal anion and its charge O^{2-} Group 6A
- Charge (without sign) becomes subscript for other ion $Al^{3+}O^{2-}$
- Reduce subscripts to smallest whole number ratio Al_2O_3
- Check that the total charge of the cations cancels the total charge of the anions
 $Al = (2) \cdot (+3) = +6$; $O = (3) \cdot (-2) = -6$

✓ If **cation** is:

- metal with invariant charge = metal name
- metal with variable charge = metal name(charge)
- polyatomic ion = name of polyatomic ion

✓ If **anion** is:

- nonmetal = stem of nonmetal name + ide
- polyatomic ion = name of polyatomic ion

e.g. $CuSO_4$ = copper(II) sulphate; Cu_2O = copper(I) oxide; CrO_3 = chromium (VI) oxide; $K_2Cr_2O_7$ potassium chromate(VI).

Metals with invariant charge; (e.g. Na^+ , Ca^{2+}); metals that form cations with different charges; common monoatomic anions (e.g. Cl^- , chloride, O^{2-} = oxide); common polyatomic ions (e.g. CH_3COO^- or $C_2H_3O_2^-$ = acetate; NO_3^- = nitrate, SO_4^{2-} = sulphate).

elements in the same column form similar polyatomic ions

same number of O's and same charge

ClO_3^- = chlorate \ BrO_3^- = bromate

if the polyatomic ion starts with H, add hydrogen- prefix before name and add 1 to the charge: CO_3^{2-} = carbonate \ HCO_3^{2-} = hydrogen carbonate.

-ate ion: chlorate = ClO_3^{-1}

-ate ion + 1 O \Rightarrow same charge, per- prefix, perchlorate = ClO_4^{-1}

-ate ion - 1 O \Rightarrow same charge, -ite suffix, chlorite = ClO_2^{-1}

-ate ion - 2 O \Rightarrow same charge, hypo- prefix, -ite suffix, hypochlorite = ClO^{-1}

Writing Formula for Ionic Compounds Containing Polyatomic Ion: Iron(III) phosphate

- Write the symbol for the cation and its charge Fe^{3+}
- Write the symbol for the anion and its charge PO_4^{3-}
- Charge (without sign) becomes subscript for other ion $Fe^{3+}PO_4^{3-}$ $Fe_3(PO_4)_3$
- Reduce subscripts to smallest whole number ratio **$FePO_4$**
- Check that the total charge of the cations cancels the total charge of the anions
 $Fe = (1) \cdot (+3) = +3$; $PO_4 = (1) \cdot (-3) = -3$

hydrates = crystalline ionic compounds containing a specific number of waters for each formula unit e.g. $CuSO_4 \cdot 6H_2O$ = copper(II) sulphate hexahydrate (blue colour). After heating, it becomes $CuSO_4$ (anhydrous copper(II) sulphate - colourless).

Naming Molecular Compounds

E.g. Naming BF_3

1. Name the first element: boron
2. Name the second element with an -ide: fluorine \Rightarrow fluoride
3. Add a prefix to each name to indicate the subscript
monoboron, trifluoride
4. Write the first element with prefix, then the second element with prefix
5. Drop prefix mono from first element: **boron trifluoride**

1 = mono-*not used on first nonmetal*, 2 = di-, 3 = tri-, 4 = tetra-, 5 = penta-, 6 = hexa-, 7 = hepta-, 8 = octa-, 9 = nona-, 10 = deca-.

acids = molecular compounds that form H^+ when dissolved in water
to indicate the compound is dissolved in water (**aq**) is written after the formula
not named as acid if not dissolved in water

binary acids have H^{+1} cation and nonmetal anion: contain only two different elements (e.g. $\text{HCl}(\text{aq})$ = hydrochloric acid)

oxyacids have H^{+1} cation and polyatomic anion: contain oxygen (e.g. H_2SO_4 sulphuric acid, H_2SO_3 sulphurous acid, HNO_3 , nitric acid).

Naming Binary Acids

write a hydro prefix

follow with the nonmetal name

change ending on nonmetal name to -ic

write the word acid at the end of the name

Naming Oxyacids

if polyatomic ion name ends in -ate, then change ending to -ic suffix

if polyatomic ion name ends in -ite, then change ending to -ous suffix

write word acid at end of all names

PRACTICE EXAMPLE ONE

Name the following compounds:

- | | | | | | | |
|--------------------|---------------------------------|----------------------------|--|---------------------|-------------------|----------------------------|
| a) KCl | b) HCl | c) $\text{HCl}(\text{aq})$ | d) Na_2CO_3 | e) NaHCO_3 | f) CO | g) CO_2 |
| h) SO_2 | i) SO_3 | j) PCl_5 | k) H_2SO_4 | l) NaClO | m) ICl_3 | n) NH_4Cl |
| o) FeSO_4 | p) $\text{Fe}_2(\text{SO}_4)_3$ | q) Cu_2O | r) $\text{CoSO}_4 \cdot 7\text{H}_2\text{O}$ | s) KMnO_4 | t) MnO_2 | u) H_2SO_3 |

Formula Mass = the mass of an individual molecule or formula unit; also known as **molecular mass** or **molecular weight** = sum of the masses of the atoms in a single molecule or formula unit.

mass of 1 molecule of H₂O = 2(1.01 amu H) + 16.00 amu O = **18.02 amu**

The relative masses of molecules can be calculated from atomic masses. Since 1 mole of H₂O contains 2 moles of H and 1 mole of O. Molar Mass = 1 mole H₂O = 2(1.01 g H) + 16.00 g O = 18.02 g, so: Molar Mass of H₂O is 18.02 g/mole or gmol⁻¹.

Percent composition = % of each element in a compound by mass =

$$\frac{\text{part}}{\text{whole}} \times 100\% \quad \text{C}_2\text{Cl}_4\text{F}_2 \text{ \% Cl by mass} = ? \quad \frac{141.8 \text{ g/mol}}{203.8 \text{ g.mol}} \times 100\% = 69.58\%$$

Benzaldehyde is 79.2% carbon. What mass of benzaldehyde contains 19.8 g of C?

Solution: 100g benzaldehyde contains 79.2 g carbon

$$19.8 \text{ g C} \times \frac{100\text{g benzaldehyde}}{79.2 \text{ g C}} = 25.0 \text{ g benzaldehyde}$$

FINDING AN EMPIRICAL FORMULA & MOLECULAR FORMULA

1. convert the percentages to grams
2. assume you start with 100 g of the compound
3. skip if already grams
4. convert grams to moles
5. use molar mass of each element
6. write a pseudoformula using moles as subscripts
7. divide all by smallest number of moles
8. if result is within 0.1 of whole number, round to whole number
9. multiply all mole ratios by number to make all whole numbers
10. if ratio 0.5, multiply all by 2; if ratio 0.33 or 0.67, multiply all by 3; if ratio 0.25 or 0.75, multiply all by 4; etc.
11. skip if already whole numbers

- The **molecular formula** is a **multiple** of the **empirical formula**
- To determine the molecular formula you need to know the empirical formula and the **molar mass** of the compound

Laboratory analysis of aspirin determined the following mass percent composition. C = 60.00%, H = 4.48%, O = 35.53%. Find the empirical formula. If the molar mass is 180.17 g/mol, then workout the molecular formula.

Solution: in 100 g of aspirin there are 60.00 g C, 4.48 g H, and 35.53 g O.

1 mole C = 12.01 g C, 1 mole H = 1.008 g H, 1 mole O = 16.00 g O.

$$\frac{60.00}{12.01} = 4.996 \text{ mol C} \quad \frac{4.48}{1.008} = 4.44 \text{ mol H} \quad \frac{35.53}{16.00} = 2.220 \text{ mol O}$$

Pseudoformula: $\text{C}_{4.996} \text{H}_{4.44} \text{O}_{2.220}$

$$\begin{array}{ccc} \text{C} & \frac{4.996}{2.220} & \text{H} & \frac{4.44}{2.220} & \text{O} & \frac{2.220}{2.220} \\ & 2.220 & & 2.220 & & 2.220 \end{array}$$

$$= \text{C}_{2.25} \text{H}_2 \text{O}_1 \times 4 \text{ (make whole numbers)} \rightleftharpoons \text{C}_9 \text{H}_8 \text{O}_4$$

As $\text{C}_9\text{H}_8\text{O}_4 = n = 1 = 180.17$, then there is no need to multiply so this is **the molecular formula**.

PRACTICE EXAMPLE TWO

Find the empirical formulae of the following compounds which contained:

- (a) 5.85 g K; 2.10 g N; 4.80 g O
- (b) 3.22 g Na; 4.48 g S; 3.36 g O
- (c) 22.0% C; 4.6% H; 73.4% Br (by mass)

Benzopyrene has a molar mass of 252 g and an empirical formula of C_5H_3 . What is its molecular formula? (C = 12.01, H=1.01) .

[ans = $\text{C}_{20}\text{H}_{12}$]

A compound containing 40% carbon, 6.73% hydrogen and 52.28% oxygen was shown to have a molar mass of 60.06 g mol^{-1} by mass spectrometry. Use this information to work out its **molecular formula**.

COMBUSTION ANALYSIS

Menthol, the substance we can smell in mentholated cough drops, is composed of C, H, and O. A 0.1005 g sample of menthol is combusted, producing 0.2829 g of CO₂ and 0.1159 g of H₂O. **What is the empirical formula for menthol?** (x is a multiplication operator).

$$0.2829 \text{ g of CO}_2 \times \frac{1 \text{ mol CO}_2}{44.0 \text{ g CO}_2} = 0.006430 \text{ mol CO}_2 \times \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} = 0.006430 \text{ mol C}$$

$$0.1159 \text{ g of H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.0 \text{ g H}_2\text{O}} = 0.006439 \text{ mol H}_2\text{O} \times \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} = 0.01288 \text{ mol H}$$

Now we need to convert the moles to grams of these elements

$$0.006430 \text{ mol C} \times \frac{12.0 \text{ g C}}{1 \text{ mol C}} = 0.07716 \text{ g C}$$

$$0.01288 \text{ mol H} \times \frac{1.0 \text{ g H}}{1 \text{ mol H}} = 0.01288 \text{ g H}$$

Find the mass of Oxygen by subtracting the C and H from the total mass of the sample

$$\text{Total} = \text{mass C} + \text{mass H} + \text{mass O}$$

$$0.1005 \text{ g} = 0.07716 \text{ g C} + 0.01288 \text{ g H} + \text{mass O}$$

$$\text{mass O} = 0.01046 \text{ g O}$$

Convert to moles of O

$$0.01046 \text{ g O} \times \frac{1 \text{ mol O}}{16.0 \text{ g O}} = 0.0006538 \text{ mol O}$$

Finally find the mole ratio by dividing by the smallest quantity

$$0.006430 \text{ mol C} / 0.0006538 = 9.83 \approx 10$$

$$0.01288 \text{ mol H} / 0.0006538 = 19.70 \approx 20$$

$$0.0006538 \text{ mol O} / 0.0006538 = 1$$

Empirical Formula **C₁₀H₂₀O**

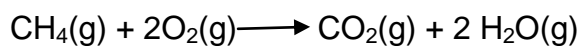
PRACTICE EXAMPLE THREE

a) Upon combustion, a compound containing only carbon hydrogen produced 1.60g CO₂ and 0.819g H₂O. Calculate the empirical formula.

b) Upon combustion, a 0.8009g sample of compound containing carbon , hydrogen and oxygen produced 1.6004g CO₂ and 0.6551g H₂O. Calculate the empirical formula of the compound.

[C₂H₄O]

CHEMICAL REACTIONS



- this equation is balanced, meaning that there are equal numbers of atoms of each element on the reactant and product sides
 - ✓ to obtain the number of atoms of an element, multiply the subscript by the coefficient
- symbols used to indicate state after chemical
 - ✓ (g) = gas; (l) = liquid; (s) = solid
 - (aq) = aqueous = dissolved in water
- energy symbols used above the arrow for decomposition reactions
 - ✓ Δ = heat
 - ✓ $h\nu$ = light
 - ✓ shock = mechanical
 - ✓ elec = electrical

APPENDIX 1: ORGANIC COMPOUNDS (REFERENCE GUIDE)

Organic compounds are composed of carbon and hydrogen and sometimes a few other elements. Many organic compounds contain carbon, hydrogen, oxygen and/or nitrogen. Organic compounds may be divided into hydrocarbons containing carbon and hydrogen (e.g. methane CH_4 , ethene, C_2H_4) and functionalised hydrocarbons containing carbon, hydrogen and at least one other element - usually a non-metal (e.g. ethanol, $\text{C}_2\text{H}_5\text{OH}$, ethanoic or acetic acid $\text{CH}_3\text{CO}_2\text{H}$). They contain covalent bonding. Carbon covalently bonded to a metal is also known, such as a transition metal (organometallic compound e.g. $\text{CH}_3\text{CH}_2\text{MgCl}$ ethylmagnesium chloride).

Name of hydrocarbon = base name (number of C atoms) + suffix (number of multiple bonds)

Base names: C = 1 = meth-, 2 = eth-, 3 = prop-, 4 = but-, 5 = pent-, 6 = hex-, 7 = hept-, 8 = oct-, 9 = non-, 10 = dec-. E.g. C = 3 = propane.

C-C = alkane e.g. $\text{CH}_3\text{CH}_2\text{CH}_2$ = propane

C=C = alkene e.g. $\text{CH}_2=\text{CHCH}_3$ = propene

$\text{C}\equiv\text{C}$ = alkyne e.g. $\text{HC}\equiv\text{CCH}_3$

Family = a group of compounds with the same functional group.

alcohol	$\text{CH}_3\text{CH}_2\text{-OH}$ (ethanol)
ether	$\text{CH}_3\text{CH}_2\text{-O-CH}_2\text{CH}_3$ (diethyl ether)
aldehyde	$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{C}-\text{H} \end{array}$ (ethanal)
ketone	$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{C}-\text{CH}_3 \end{array}$ (propanone or acetone)
carboxylic acid	$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{C}-\text{OH} \end{array}$ (ethanoic or acetic acid)
ester	$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{C}-\text{OCH}_3 \end{array}$ (methyl ethanoate)
amine	$\begin{array}{c} \text{H} \\ \\ \text{CH}_3\text{CH}_2-\text{N}-\text{H} \end{array}$ (ethyl amine)
amide (e.g. protein linkage)	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{CH}_2-\text{C}-\text{N}-\text{CH}_3 \\ \\ \text{H} \end{array}$ (<i>N</i> -methylpropanamide)

