# 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. $Cl_2$, $H_2$, $P_4$).
**compounds** are generally represented with a **chemical formula**. **Molecular compounds** contain non-metals (e.g. $H_2O$, HCl) and **ionic compounds** contain *cations* and *anions* (e.g. NaCl, $Na_2SO_4$).

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

| Molecule | Empirical formula | Molecular formula |
|---|---|---|
| 1. propane | $C_3H_8$ | $C_3H_8$ |
| 2. benzene | CH | $C_6H_6$ |

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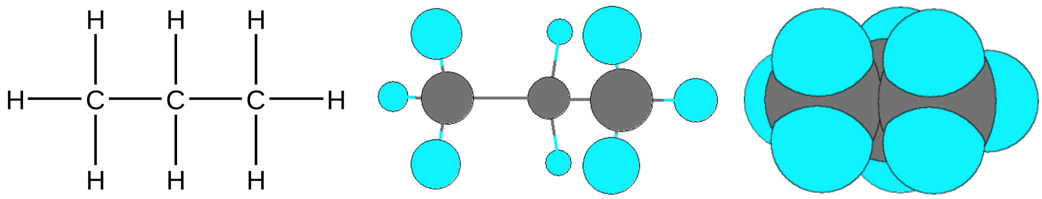
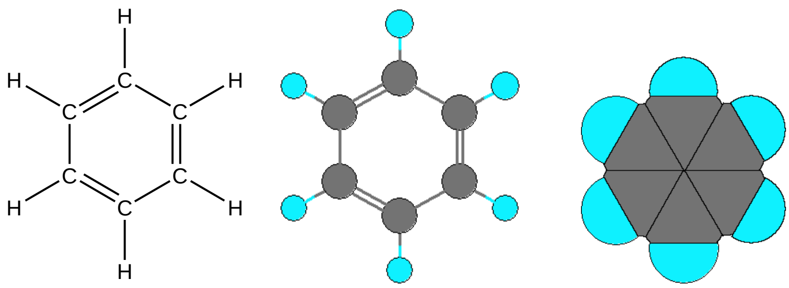


**structural** **ball-and-stick** **space-filling**



**2. structural** **ball-and-stick** **space-filling**

## 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 $Al^{3+}$ Group 3A
2. Write the symbol for the nonmetal anion and its charge $O^{2-}$ Group 6A

3. Charge (without sign) becomes subscript for other ion $Al^{3+}O^{2-}$
4. Reduce subscripts to smallest whole number ratio $\mathbf{Al_2O_3}$
5. Check that the total charge of the cations cancels the total charge of the anions
Al = (2)·(+3) = +6; O = (3)·(-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**

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

**hydrates** = cystalline ionic compounds containing a specific number of waters for each formula unit e.g. $CuSO_4.6H_2O$ = copper(II) sulphate hexahydrate (blue colour). After heating, it becomes $CuSO_4$ (anydrous 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 ⇒ 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. HCl(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).

<u>Naming Binary Acids</u>
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

<u>Naming Oxyacids</u>
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)HCl(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)$Fe_2(SO_4)_3$ | q)$Cu_2O$ | r)$CoSO_4.7H_2O$ | s)$KMnO_4$ | t)$MnO_2$ | u)$H_2SO_3$ |

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**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 $H_2O$ = 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 $H_2O$ contains 2 moles of H and 1 mole of O. Molar Mass = 1 mole $H_2O$ = 2(1.01 g H) + 16.00 g O = 18.02 g, so: Molar Mass of $H_2O$ is 18.02 g/mole or gmol$^{-1}$.**

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

$$\frac{\text{part}}{\text{whole}} \times 100\%$$

**$C_2Cl_4F_2$** % Cl by mass = ? $\frac{141.8 \text{ g/mol}}{203.8 \text{ g.mol}} \times 100\% = 69.58\%$

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 mol C $\frac{4.48}{1.008}$ = 4.44 mol H $\frac{35.53}{16.00}$ = 2.220 mol O

Pseudoformula: $C_{4.996}H_{4.44}O_{2.220}$

$C_{\frac{4.996}{2.220}}H_{\frac{4.44}{2.220}}O_{\frac{2.220}{2.220}}$

= $C_{2.25}H_2O_1$ x 4 (make whole numbers) $\Longrightarrow$ $C_9H_8O_4$

As $C_9H_8O_4$ = 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)

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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) .

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______________________________________________ [ans = $C_{20}H_{12}$]

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

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## 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 $CO_2$ and 0.1159 g of $H_2O$. **What is the empirical formula for menthol?** (x is a multiplication operator).

$$0.2829 \text{ g of } CO_2 \times \frac{1 \text{ mol } CO_2}{44.0\text{g } CO_2} = 0.006430 \text{ mol } CO_2 \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 0.006430 \text{ mol C}$$

$$0.1159 \text{ g of } H_2O \times \frac{1 \text{ mol } H_2O}{18.0\text{g } H_2O} = 0.006439 \text{ mol } H_20 \times \frac{2 \text{ mol H}}{1 \text{ mol } H_20} = 0.01288 \text{ mol H}$$

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

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

$$0.001288 \text{ mol H} \times \frac{1.0\text{g H}}{1 \text{ mol H}} = 0.01288\text{g H}$$

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

Total= mass C + mass H + mass O

0.1005g= 0.07716 g C + 0.01288 g H + mass O

mass O = 0.01046g 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 mol C / 0.0006538 =9.83 ≈ 10
0.01288 mol H / 0.0006538 = 19.70 ≈ 20
0.0006538 mol O / 0.0006538 = 1

Empirical Formula **$C_{10}H_{20}O$**

### PRACTICE EXAMPLE THREE

**a) Upon combustion, a compound containing only carbon a hydrogen produced 1.60g $CO_2$ and 0.819g $H_2O$. Calculate the empirical formula.**

**b) Upon combustion, a 0.8009g sample of compound containing carbon , hydrogen and oxygen produced 1.6004g $CO_2$ and 0.6551g $H_2O$. Calculate the empirical formula of the compound.**

[ $C_2H_4O$ ]

**CHEMICAL REACTIONS**

$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2\ H_2O(g)$

- 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
  - ✓ $\Delta$ = 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 nitogen. 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, $C_2H_5OH$, ethanoic or acetic acid $CH_3CO_2H$). They contain covalent bonding. Carbon covalently bonded to a metal is also known, such as a transition metal (organometallic compound e.g. $CH_3CH_2MgCl$ ethylmagnesium chloride).

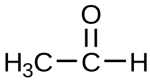
Name of hydrocarbon = base name (number of C atoms) + suffix (number of multiple bonds)

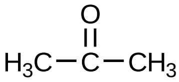
Base names: C = 1 = meth-, 2 = eth-, 3 = prop-, 4 = but-, 5 = pent-, 6 = hex-, 7 = hept-, 8 = oct-, 9 = non-, 10 = dec-. E.g. C = 3 = propane.

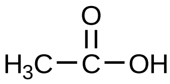
C-C = alkane e.g. $CH_3CH_2CH_2$ = propane
C=C = alkene e.g. $CH_2{=}CHCH_3$ = propene
$C{\equiv}C$ = alkyne e.g. $HC{\equiv}CCH_3$

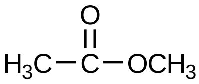
Family = a group of compounds with the same functional group.

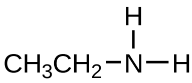
alcohol — $CH_3CH_2$-OH (ethanol)
ether — $CH_3CH_2$-O-$CH_2CH_3$ (diethyl ether)

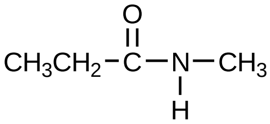
aldehyde  (ethanal)

ketone  (propanone or acetone)

carboxylic acid  (ethanoic or acetic acid)

ester  (methyl ethanoate)

amine  (ethyl amine)

amide
(e.g. protein linkage) 

(*N*-methylpropanamide)