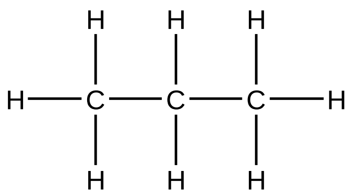
CHEMICAL FORMULAE (ANSWERS)

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).

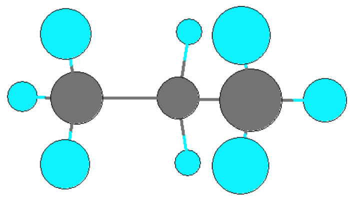
Empirical formula = the kinds of elements found in the compound and the ratio of their atoms.
Molecular formula = the kinds of elements found in the compound and the numbers of their atoms.
Structural formula = the kinds of elements found in the compound, the numbers of their atoms, order of atom attachment, 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

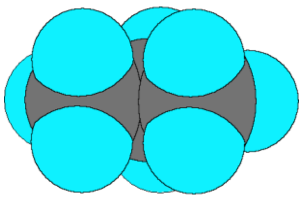
1.



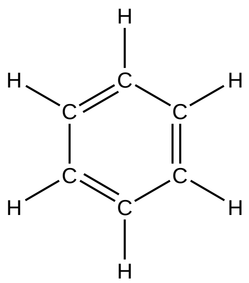
structural



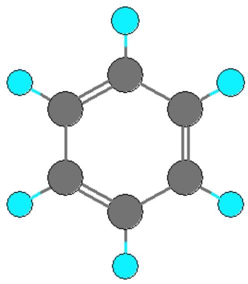
ball-and-stick



space-filling



2. structural



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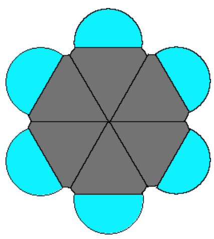

space-filling

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 **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 see table 3.2, p. 89 (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^- = hydrogen carbonate.

-ate ion: chlorate = ClO_3^{-1}
-ate ion + 1 O ⇒ same charge, per- prefix, perchlorate = ClO_4^{-1}
-ate ion – 1 O ⇒ same charge, -ite suffix, chlorite = ClO_2^{-1}
-ate ion – 2 O ⇒ 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 **$FePO_4$**
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 $\mathbf{BF_3}$
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)$Fe_2(SO4)_3$	q)Cu_2O	r)$CoSO_4.7H_2O$	s)$KMnO_4$	t)MnO_2	u)H_2SO_3

a) potassium chloride b) hydrogen chloride c)hydrochloric acid d) sodium carbonate e) sodium hydrogen carbonate f) carbon monoxide g) carbon dioxide h) sulphur dioxide i) sulphur trioxide j) phosphorous pentachloride k) sulphuric acid l) sodium hypochlorite m) iodine trichloride n) ammonium chloride o) iron(II) sulphate p) iron(III) sulphate q) copper(I) oxide r) cobalt(II) sulphate heptahydrate s) potassium manganate(VII) t) manganese(IV) oxide u) sulphurous acid.

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) ⟹ $C_9H_8O_4$

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)

(a)_KNO_2____

(b)_ $Na_2S_2O_3$____
(c) __C_2H_5Br____

a) 5.85/39.1 = 0.15 mole K; 2.1 / 14.01 = 0.15 mole N; 4.8/16 = 0.3 $K_{0.15}N_{0.15}O_{0.3}$ = KNO_2

b) 3.22 / 22.99 = 0.14 mole Na; 4.48 / 32.07 = 0.16 mole S; 3.16 / 16 = 0.21 = $Na_{0.14}S_{0.16}O_{0.21}$ = $Na_2S_2O_3$

Assume 100g so 22/12.01 = 1.83 mole C; 4.6 / 1.01 = 4.55 mole H; 73.4 / 79.9 = 1.09 mole Br $C_{1.83}H_{4.55}Br_{1.09}$ = C_2H_5Br

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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) .

5 x 12.01 3 x 1.01 = 63.08__252/63.08 = = 4 so molecular formula = 4 x (C_5H_3) = $C_{20}H_{12}$____

____ [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**.

40/12.01 = C = 3.33; 6.73/1.01 = 6.66 H; 16/52.28 = 3.27 O. CH_2O = 30.03 so n = 60.02/30.03 = 2 so molecular formula = 2 x (CH_2O) = $C_2H_4O_2$____

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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_20. Calculate the empirical formula.

Ans = C_2H_5

1.60 / 44.01 = 0.0364 moles CO_2 = 0.0364 moles C; 0.819/18.02 = 0.0454 moles H_20 = 2 x 0.0454 = 0.0908 moles H so $C_{0.0364}$ $H_{0.0908}$ = $CH_{2.5}$ = C_2H_5 (make whole number)

b) Upon combustion, a 0.8009g sample of compound containing carbon , hydrogen and oxygen produced 1.6004g CO_2 and 0.6551g H_20. Calculate the empirical formula of the compound.

1.6004 / 44.01 = 0.0364 moles CO_2; 0.6551 / 18.01 = 0.0364 moles H_2O.

= 0.0364 moles C; 2 x 0.0364 = 0.0728 moles H so mass C and H = 0.0364 x 12.01 = 0.437 g C and 0.0728 x 1.008 = 0.0734 g H; Mass O = 0.8009 -(0.437 + 0.0734) = 0.2905 g O. So moles O = 0.2905 / 16 = 0.0182 moles O = $C_{0.0364}H_{0.0728}O_{0.0182}$ =
C_2H_4O____

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____[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
  - ✓ Δ = heat
  - ✓ hν = 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).

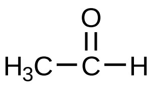
Name of hydrocarbon = base name (number of C atoms) + suffix (number of multiple bonds)

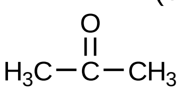
Base names: C = 1 = meth-, 2 = eth-, 3 = prop-, 4 = but-, 5 = pent-, 6 = hex-, 7 = hept-, 8 = oct-, 9 = non-, 10 = dec-. E.g. C = 3 = propane.

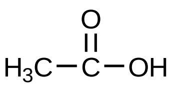
C-C = alkane e.g. $CH_3CH_2CH_2$ = propane
C=C = alkene e.g. $CH_2{=}CHCH_3$ = propene
$C{\equiv}C$ = alkyne e.g. $HC{\equiv}CCH_3$

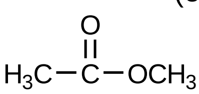
Family = a group of compounds with the same functional group:

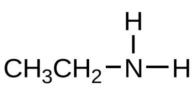
alcohol — $CH_3CH_2\text{-}OH$ (ethanol)
ether — $CH_3CH_2\text{-}O\text{-}CH_2CH_3$ (diethyl ether)

aldehyde  (ethanal)

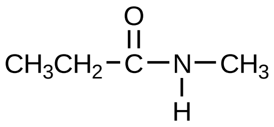
ketone  (propanone or acetone)

carboxylic acid  (ethanoic or acetic acid)

ester  (methyl ethanoate)

amine  (ethyl amine)

amide
(e.g. protein linkage)



(*N*-methylpropanamide)