CHEM103
General Chemistry

Chapter 3: Stoichiometry (化学计量): Calculations with Chemical Formulas and Equations

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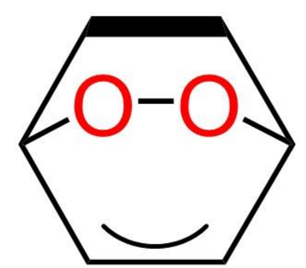
SUSTech



Assignments 1-2 & Mid-term EXAM

Please either **print** the Answer Sheet or **use** your paper; **write down** your answers on your sheet/paper.

Please submit your assignments to any of your TAs or me during the classes. Or you can submit your assignment to the folder **outside room 520**, **research building 1** (anytime you like).

Homework 1

Due date: **14 Sep. (Wed)**

Homework 2

Due date: **17 Sep. (Sat)**

Mid-term EXAM

13 Nov. 10-12 AM (Sun)

Review on Chapter 2

Atoms, Molecules & Ions

Atoms:

Atomic Theory; Atomic Structure (nucleus: electron, proton & neutron); Atomic Weight (atomic number; isotopes); Periodic Table (periods & groups)

Molecules:

Compounds; Chemical formula and empirical formula

Ions:

Cations, anions, ionic bonds

Naming of Inorganic & Organic Compounds

Outline of Chapter 3

Stoichiometry: Quantity of Substances; Balanced Chemical Formulas and Equations

Chemical Equations: Law of Conservation of Mass; Reactant & Product; States

Reaction Types: Combination, Decomposition & Combustion Reactions

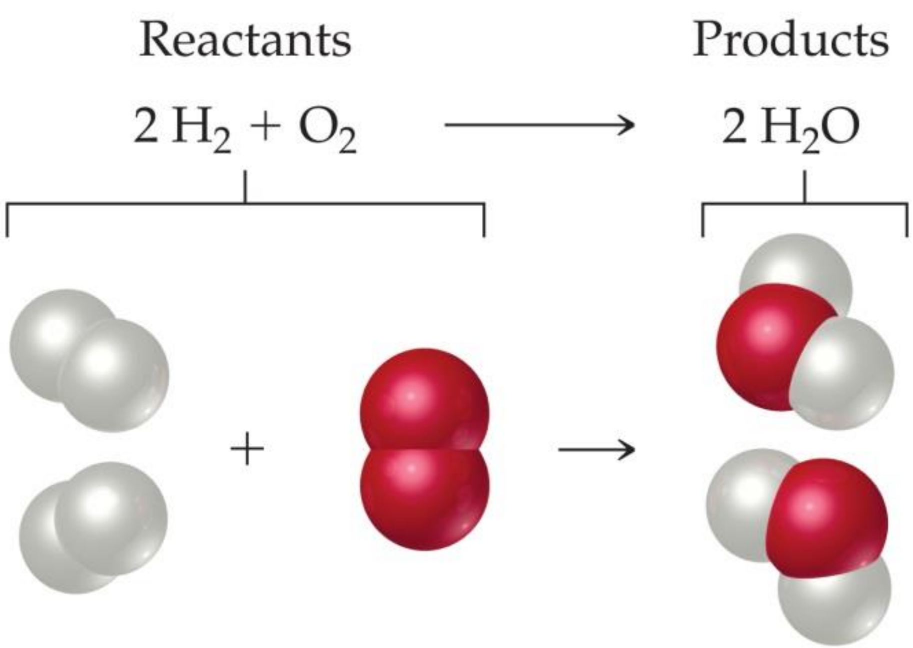
Weights: Formula Weight; Molecular Weight; Percent Composition

Moles: Avogadro's Number; Molar Mass; Moles

Stoichiometric Calculations: Limiting Reactants; Excess Reagent; Theoretical/Actual Yields

Chapter 3: Stoichiometry

- Study the **quantity** (数量) of substances **used** and **produced** in chemical reactions; *“Stoicheion”* & *“metron”*: Greek meaning of “element” & “measure”, respectively.
- Measure ozone (O_3, 臭氧) or greenhouse gas (温室气体) concentration (浓度) in the atmosphere.



(from NASA)

Law of Conservation of Mass

Stoichiometry is based on our understanding of **balanced chemical formulas** and **this law**.

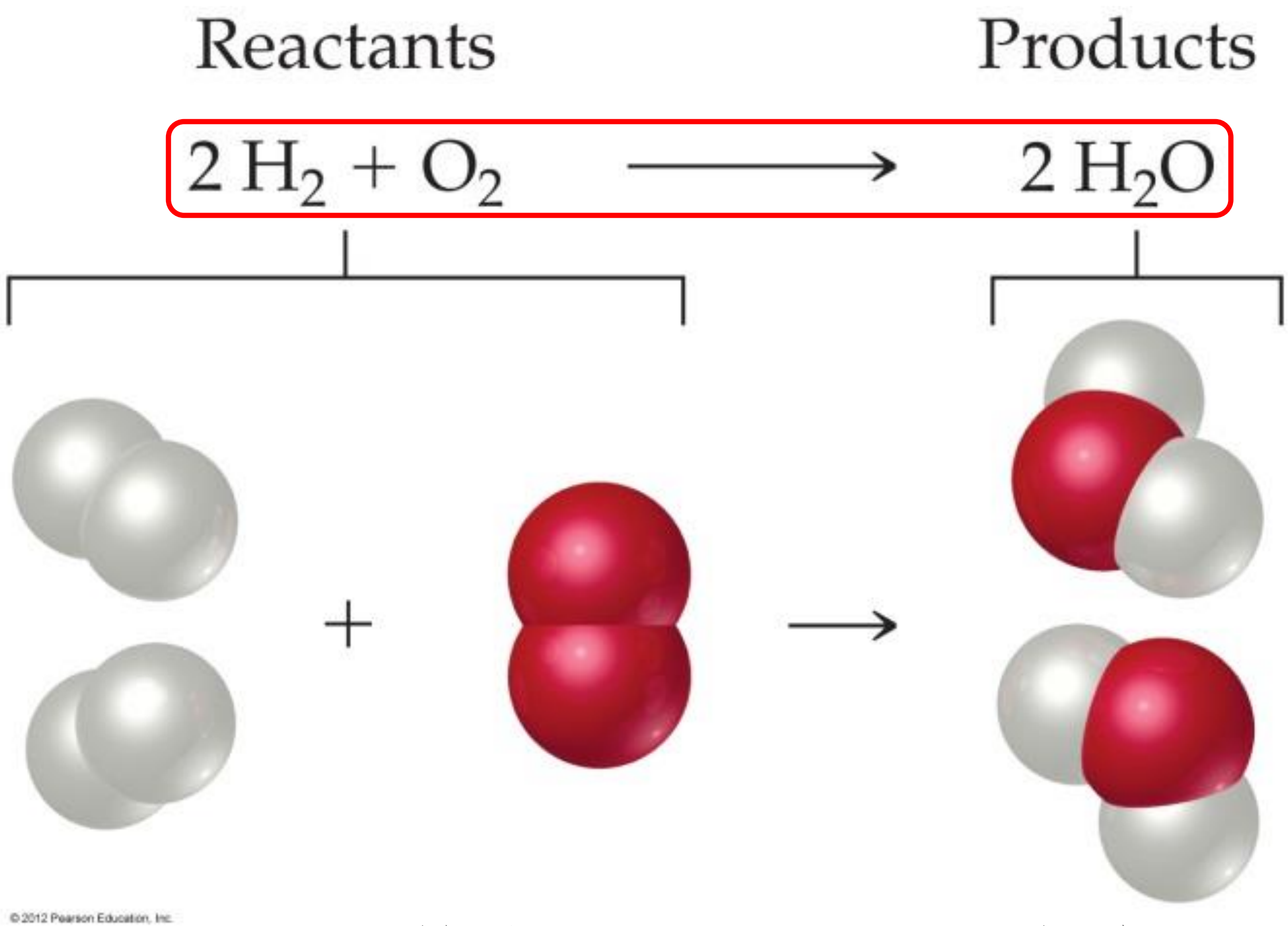
"We may lay it down as an incontestable (无可争辩) axiom (原则) that, in all the operations of art and nature, ***nothing is created****; an* ***equal amount of matter exists both before and after the experiment.*** *Upon this principle, the whole art of performing chemical experiments depends."* -- Antoine Lavoisier, 1789

Dalton's Postulates: Atoms are neither created nor destroyed during a chemical reaction.

Chemical Equations

Chemical Equations

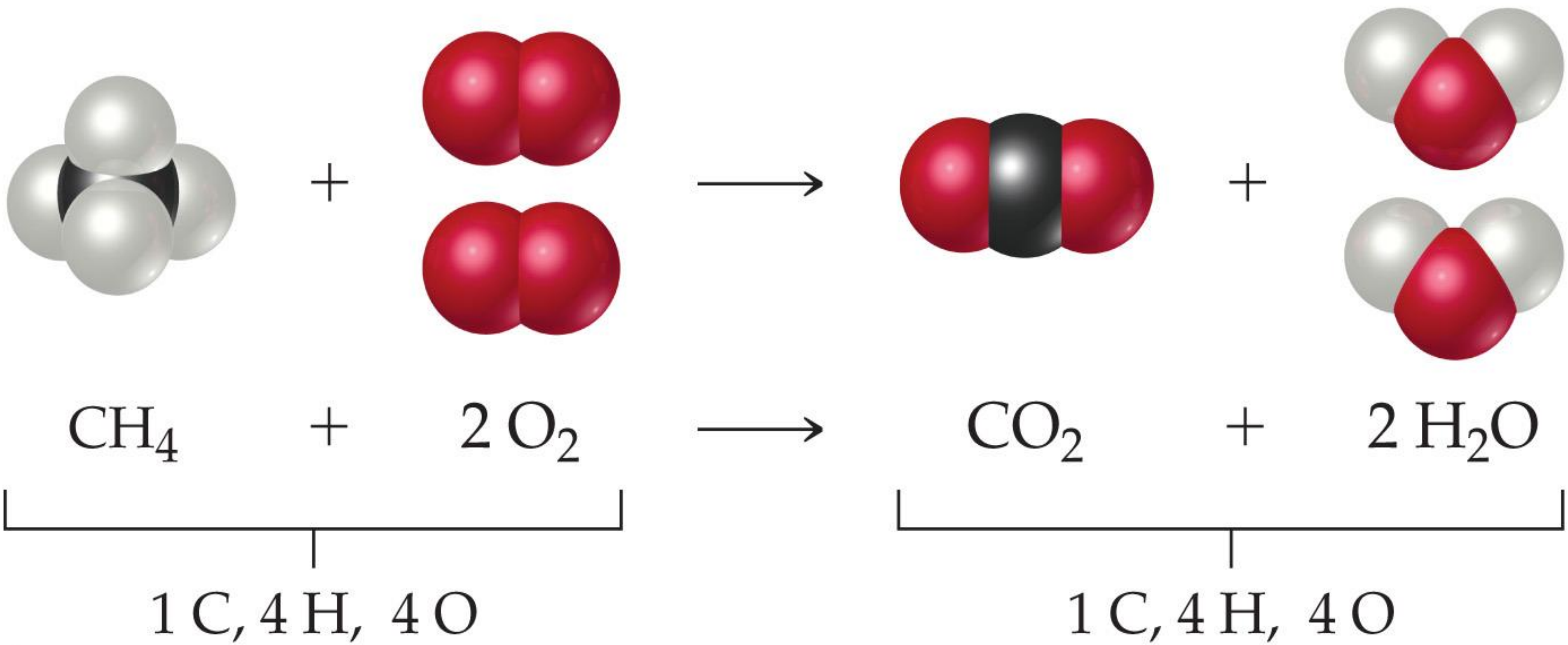
Chemical equations are concise representations of chemical reactions.



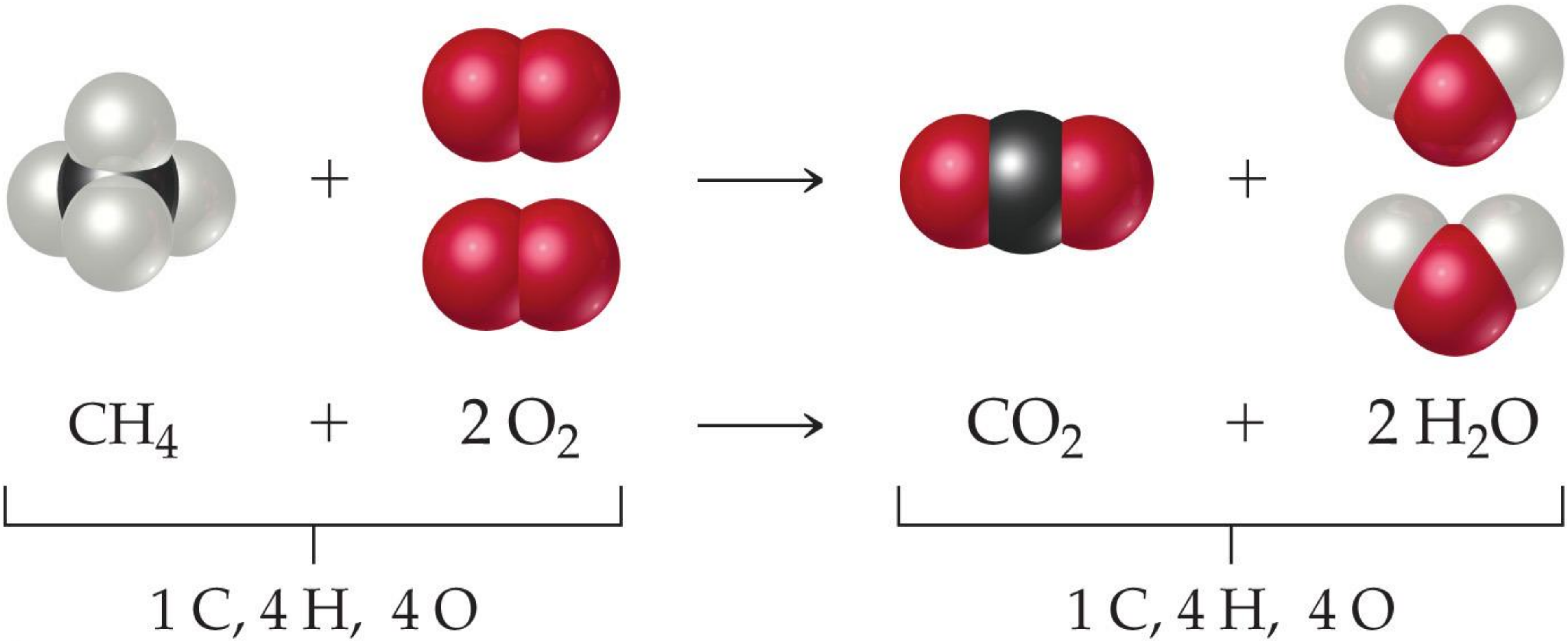
concise (简明) and precise (准确)

Anatomy (分析) of a Chemical Equation

$$CH_{4(g)} + 2O_{2(g)} \longrightarrow CO_{2(g)} + 2H_2O_{(g)}$$

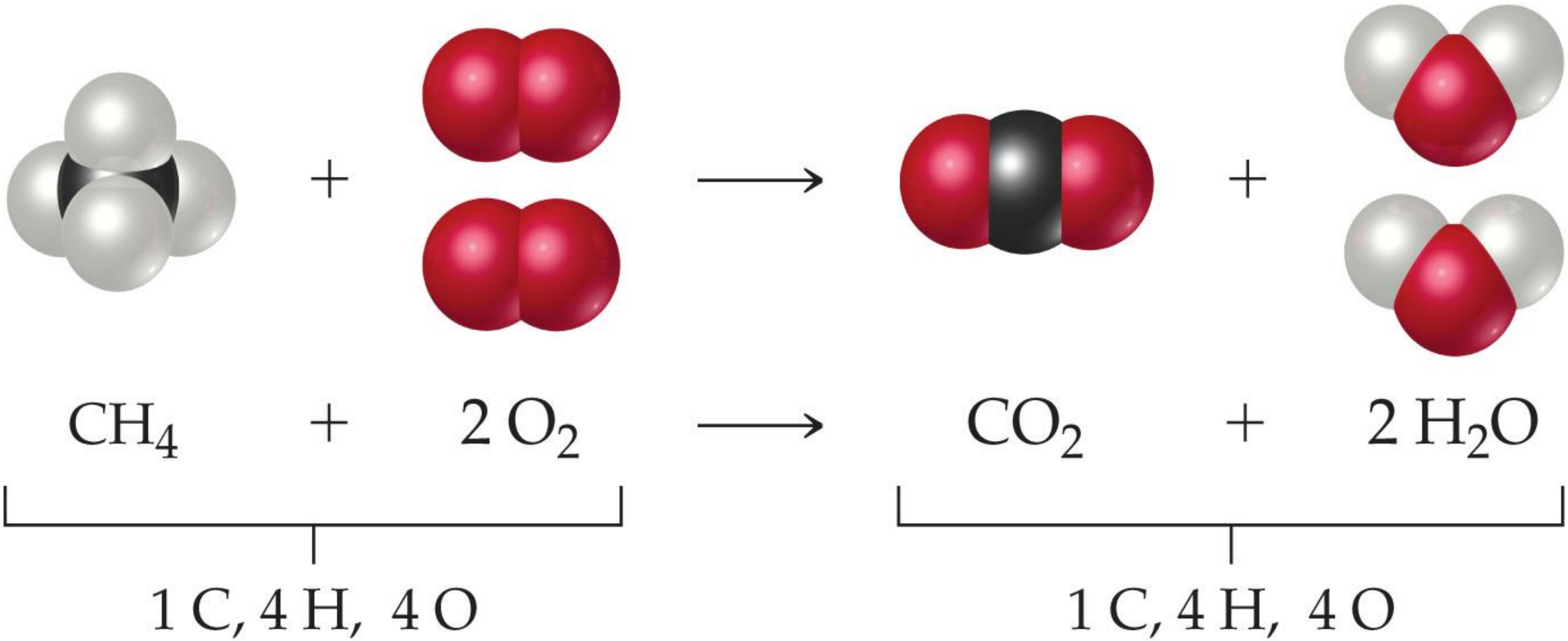


$CH_{4(g)} + 2O_{2(g)} \longrightarrow CO_{2(g)} + 2H_2O_{(g)}$



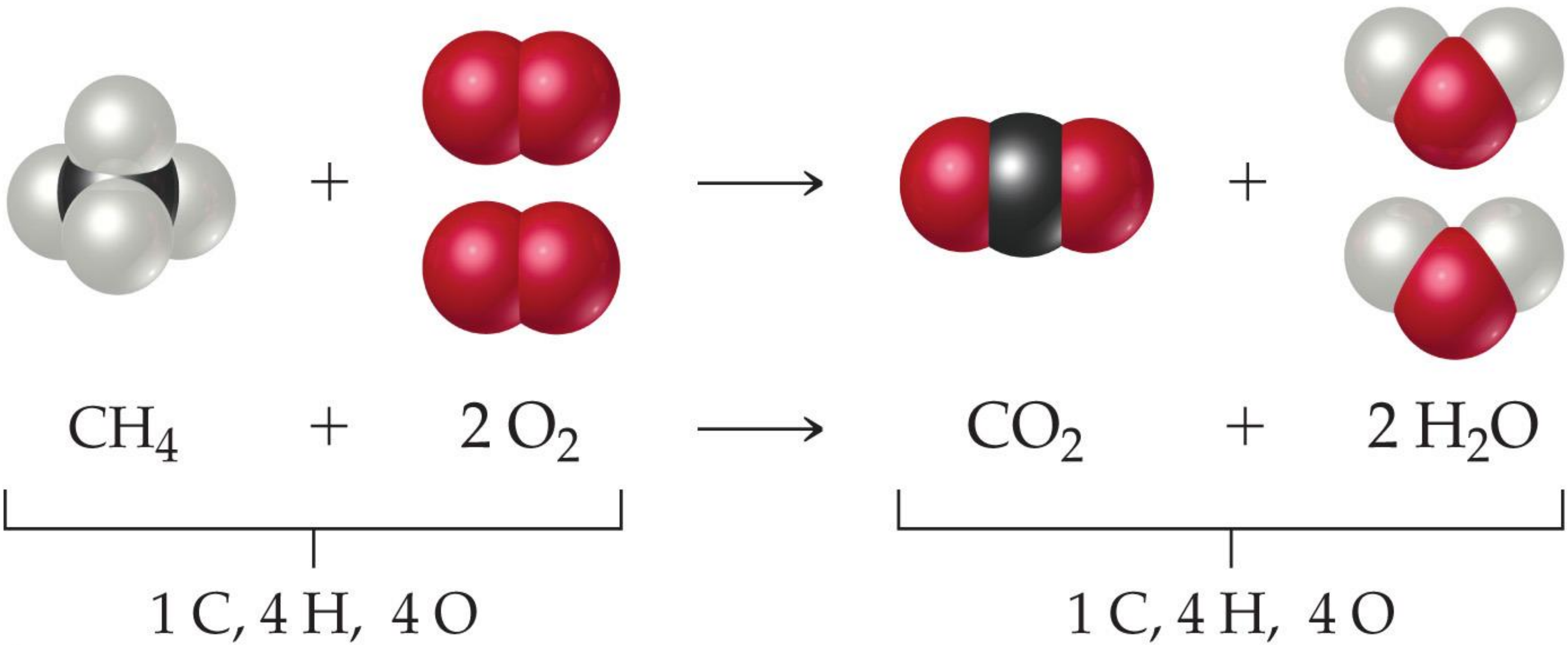
Reactants appear on the left side of the equation.

$$CH_{4(g)} + 2O_{2(g)} \longrightarrow CO_{2(g)} + 2H_2O_{(g)}$$



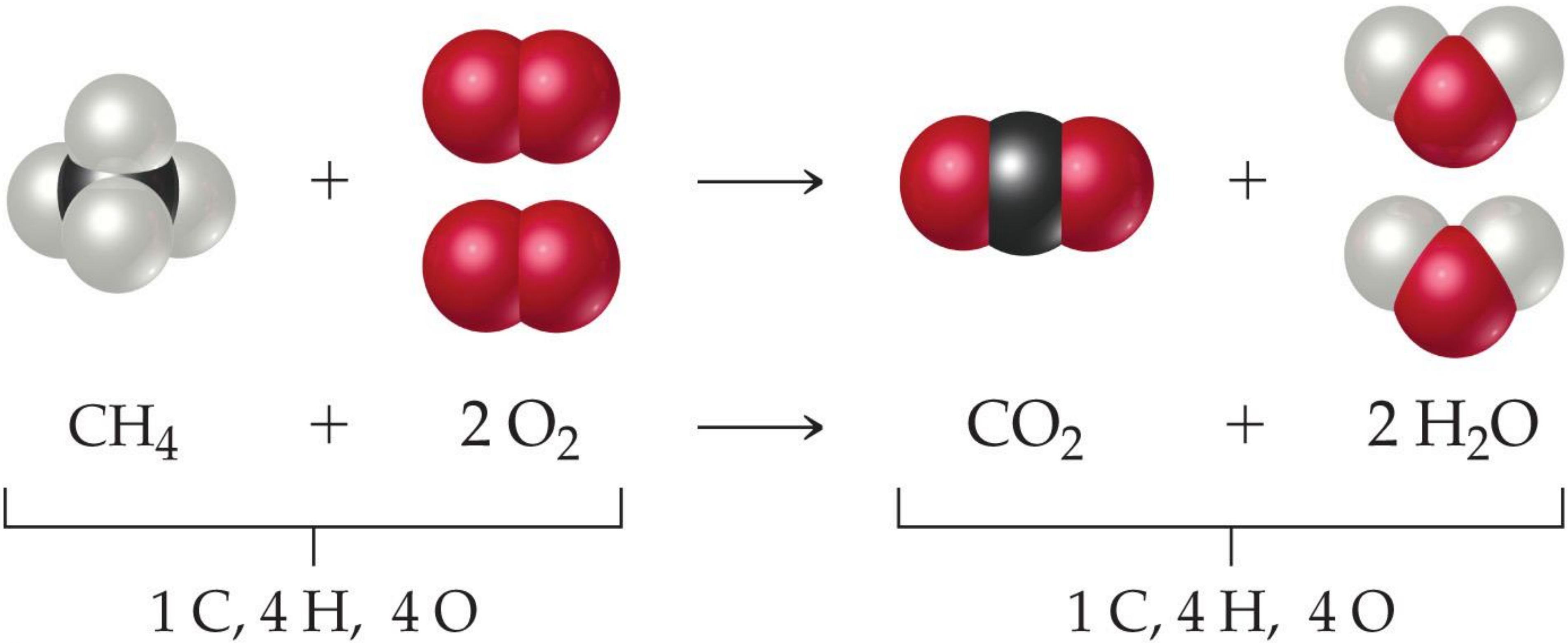
Products appear on the right side of the equation.

$CH_{4(g)} + 2O_{2(g)} \longrightarrow CO_{2(g)} + 2H_2O_{(g)}$



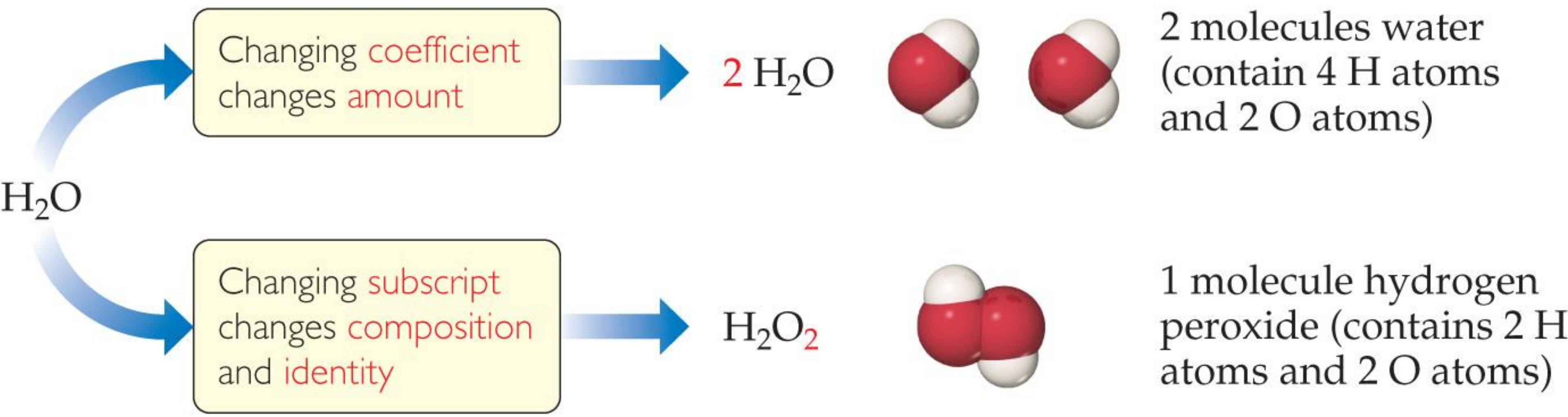
- The **states** (*g*, *l*, *aq* or *s*) of the reactants and products are written in parentheses to the right of each compound: *gas, liquid, aqueous (water) solution or solid*.

$$CH_{4(g)} + 2O_{2(g)} \longrightarrow CO_{2(g)} + 2H_2O_{(g)}$$



- **Coefficients** are inserted to balance the equation and indicate the **relative numbers** of **molecules** (equal numbers of each type of atoms on the both sides)
- The smallest possible whole number usually.

Coefficients（系数）and Subscripts



- **Coefficients** tell us the number/**amount** of **molecules** and balance the equation.
- **Subscripts** tell us the number of **atoms** of each **element** in **a** molecule (**composition**).

***Subscripts** & **Coefficients** have completely different meaning!*

Arrows (箭头) and Equal Symbols

$$NaOH(aq) \longrightarrow Na^{+}(aq) + OH^{-}(aq)$$

dissociates (nearly) **completely**: **irreversible** (不可逆) **process**.

$$CH_3COOH(aq) \rightleftharpoons CH_3COO^{-}(aq) + H^{+}(aq)$$

dissociates **partially**: **reversible** (可逆) **process** (**equilibrium** 平衡).

$$2H_2(g) + O_2(g) \;=\!=\!=\; 2H_2O(g) \quad \text{X}$$

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$$

$$4H + 2O \quad = \quad 4H + 2O$$

$$Mass(2H_2 + O_2) = Mass(2H_2O)$$

Stoichiometry

Reaction Types

- Combination (结合) Reactions
- Decomposition Reactions
- Combustion Reactions

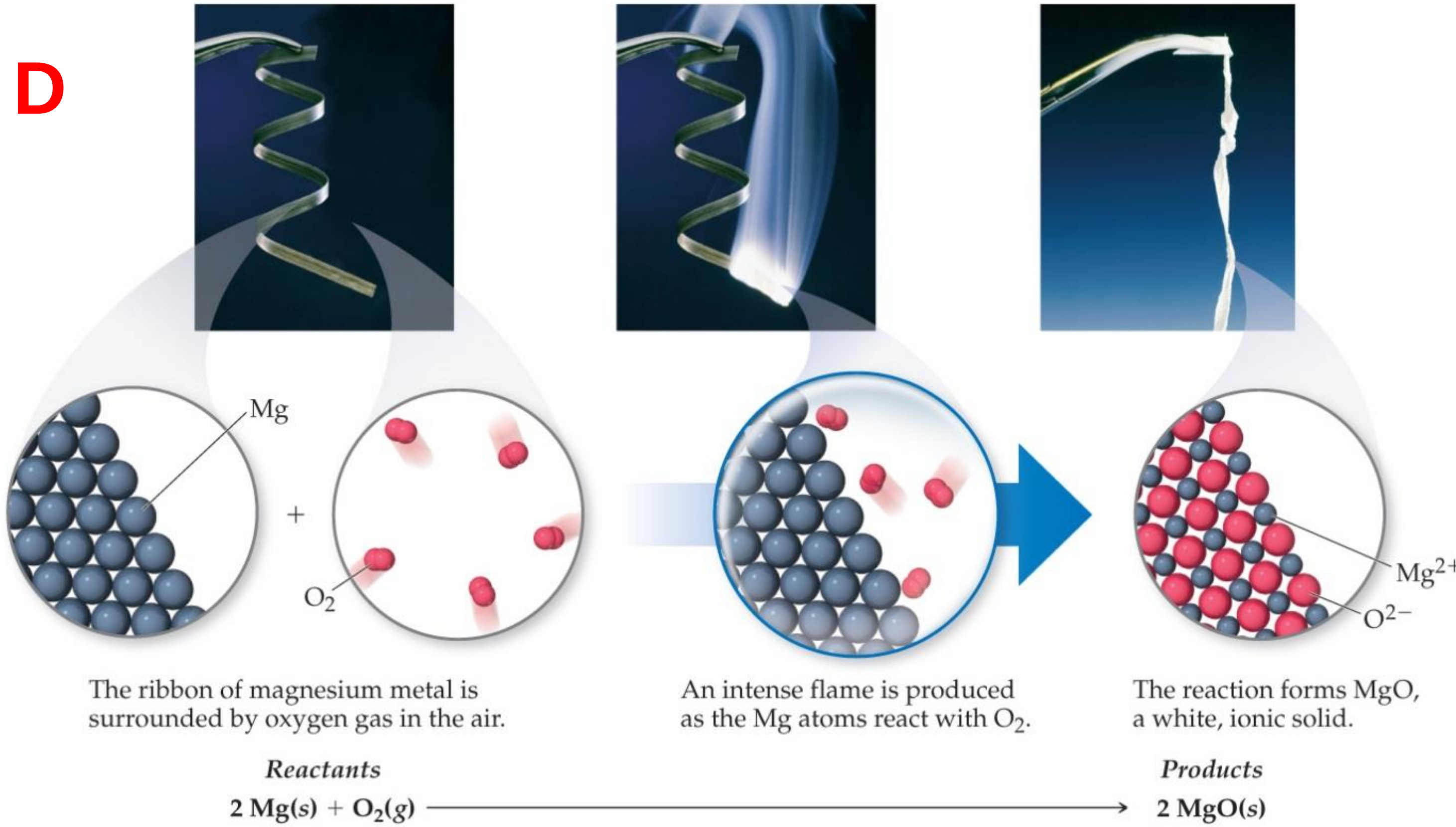
and many others…

Combination Reactions

Two or more substances react to form one product.

A + B → C

A + B + C → D



$?Mg(s) + ?O_2(g) \longrightarrow ?MgO(s)$ $(Mg^{2+}O^{2-})$

$?N_2(g) + ?H_2(g) \longrightarrow ?NH_3(g)$ (Haber process)

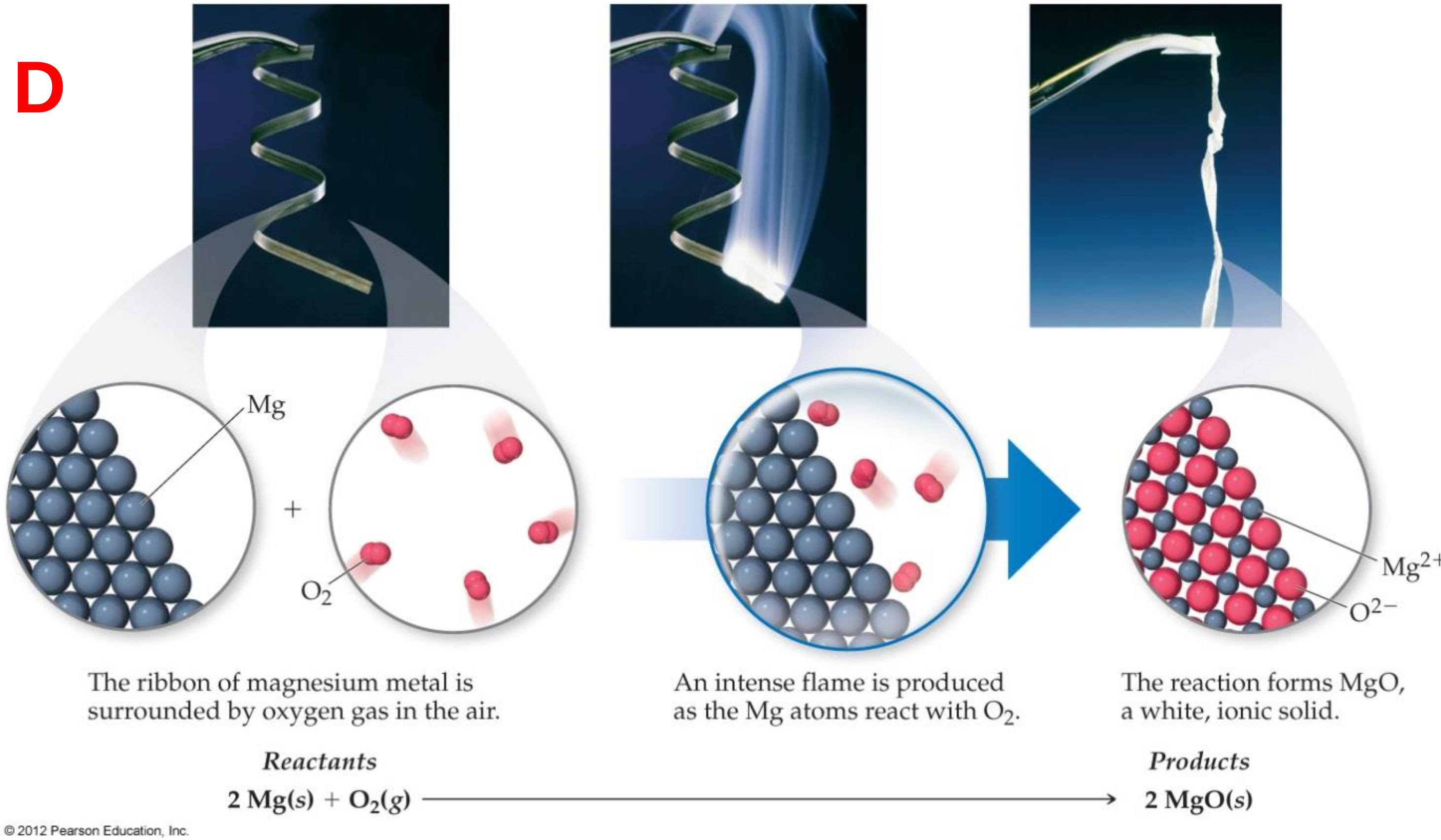
$C_3H_6(g) + Br_2(l) \longrightarrow C_3H_6Br_2(l)$

Combination Reactions

Two or more substances react to **form one** product.

A + B → C

A + B + C → D



$2Mg(s) + O_2(g) \longrightarrow 2MgO(s)$ $(Mg^{2+}O^{2-})$

$N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$ (Haber process)

$C_3H_6(g) + Br_2(l) \longrightarrow C_3H_6Br_2(l)$

Decomposition Reactions

One substance breaks down into **two or more** substances.

A → B + C

A → B + C + D

Decomposition of sodium azide:

(NaN_3, ~100g) → N_2 (~50 L)

$$?CaCO_3(s) \longrightarrow ?CaO(s) + ?CO_2(g)$$

$$?KClO_3(s) \longrightarrow ?KCl(s) + ?O_2(g)$$

$$?NaN_3(s) \longrightarrow ?Na(s) + ?N_2(g)$$

Stoichiometry

Decomposition Reactions

One substance breaks down into **two or more** substances.

A → B + C

A → B + C + D

Decomposition of sodium azide:

(NaN_3, ~100g) → N_2 (~50 L)

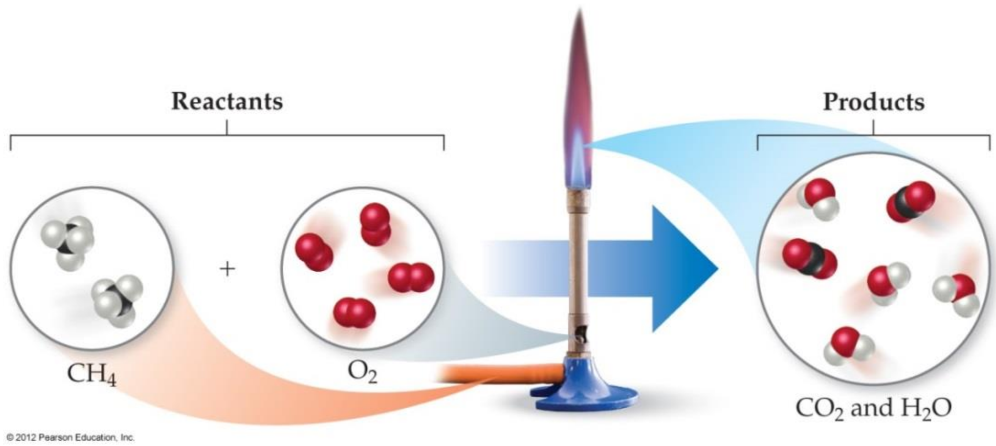
$$CaCO_3(s) \longrightarrow CaO(s) + CO_2(g)$$

$$2KClO_3(s) \longrightarrow 2KCl(s) + 3O_2(g)$$

$$2NaN_3(s) \longrightarrow 2Na(s) + 3N_2(g)$$

Stoichiometry

Combustion Reactions



- generally rapid reactions that produce a flame.
- most often involve hydrocarbons (C_xH_y) reacting with **oxygen** in the air.

$$C_xH_y(g) + \mathbf{O_2(g)}$$

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

$$C_3H_8(g) + 5O_2(g) \longrightarrow 3CO_2(g) + 4H_2O(g)$$

$$C_2H_5OH\ (g) + 3O_2(g) \longrightarrow 2CO_2(g) + 3H_2O(g)$$

For the reaction X $\rightarrow$ Y, X is referred to as the

a. yield.

b. reactant.

c. product.

d. coefficient.

$C_6H_6 + O_2 \rightarrow CO_2 + H_2O$

When this equation is correctly balanced, the coefficients are

a. 1, 7 $\rightarrow$ 6, 3.

b. 1, 8 $\rightarrow$ 6, 3.

c. 2, 15 $\rightarrow$ 12, 6.

d. 2, 16 $\rightarrow$ 12, 6.

GIVE IT SOME THOUGHT

If 20.00 g of a compound reacts completely with 30.00 g of another compound in a combination reaction, how many grams of product are formed?

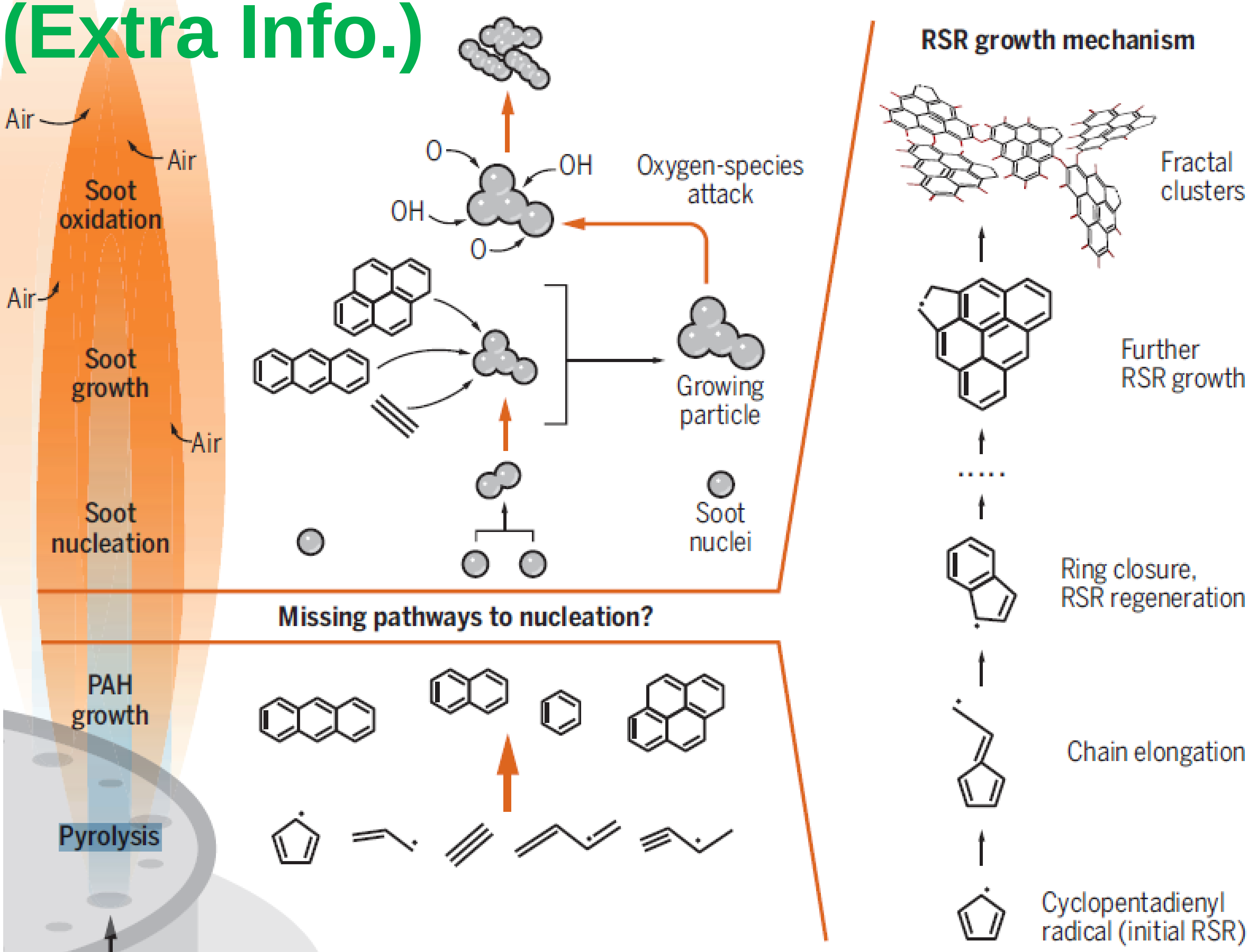
A. 10.00 g

B. 20.00 g

C. 30.00 g

D. $\boxed{\text{50.00 g}}$

(Extra Info.)



Flame zones
An overall picture of soot formation shows a flame that evolves from a blue fuel-rich zone to the orange soot zone.

Radicals to the rescue
Molecules such as cyclopentadiene (bottom) can form radicals that undergo chain reactions and build up large RSRs (middle) and ultimately fractal clusters of these larger molecules (top).

soot
煤烟

Science **2018**, *361*, 978.

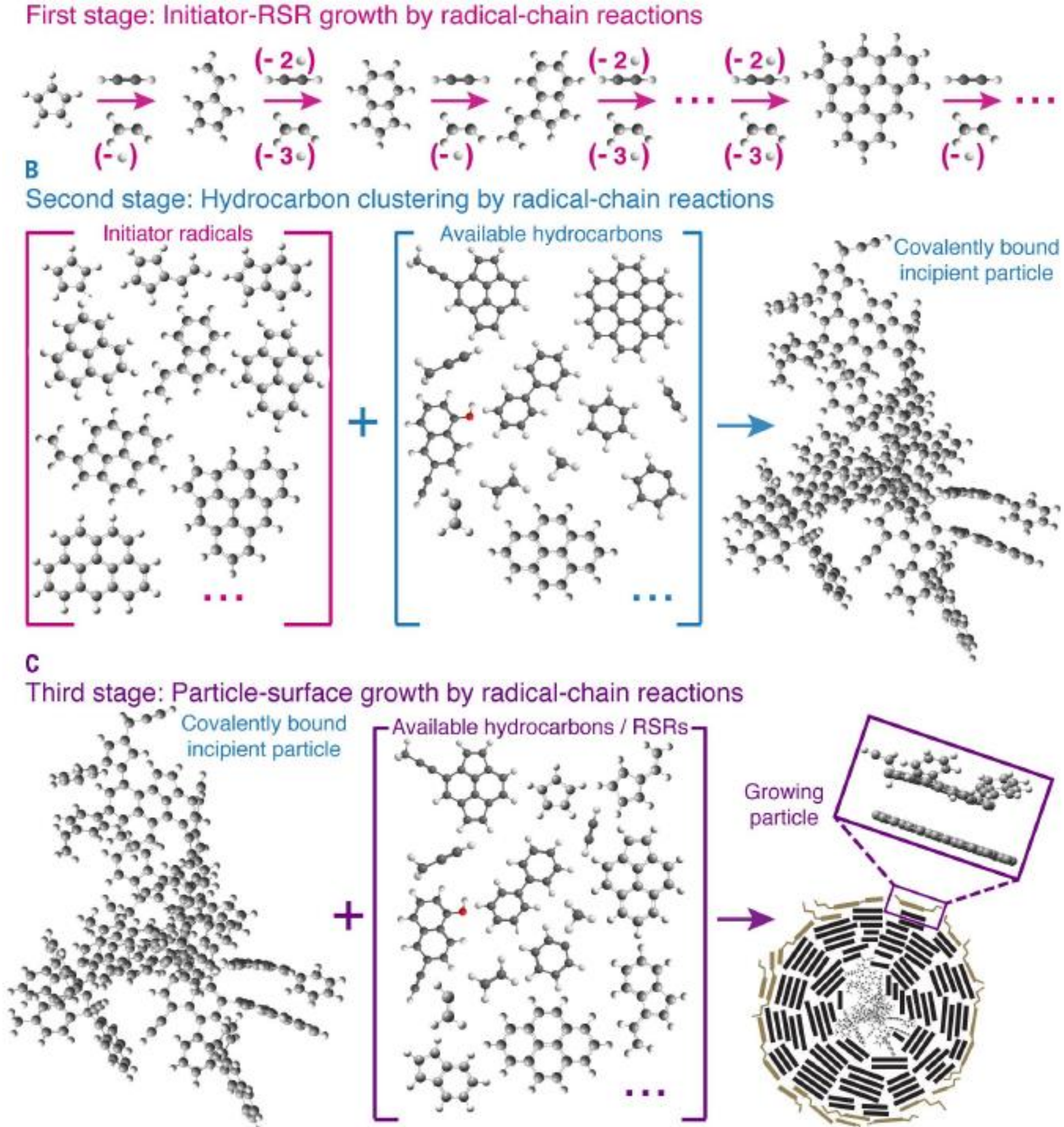
Stoichiometry

(Extra Info.)

COMBUSTION CHEMISTRY

Resonance-stabilized hydrocarbon-radical chain reactions may explain soot inception and growth

K. O. Johansson[1]*, M. P. Head-Gordon[2,3], P. E. Schrader[1], K. R. Wilson[3], H. A. Michelsen[1]*

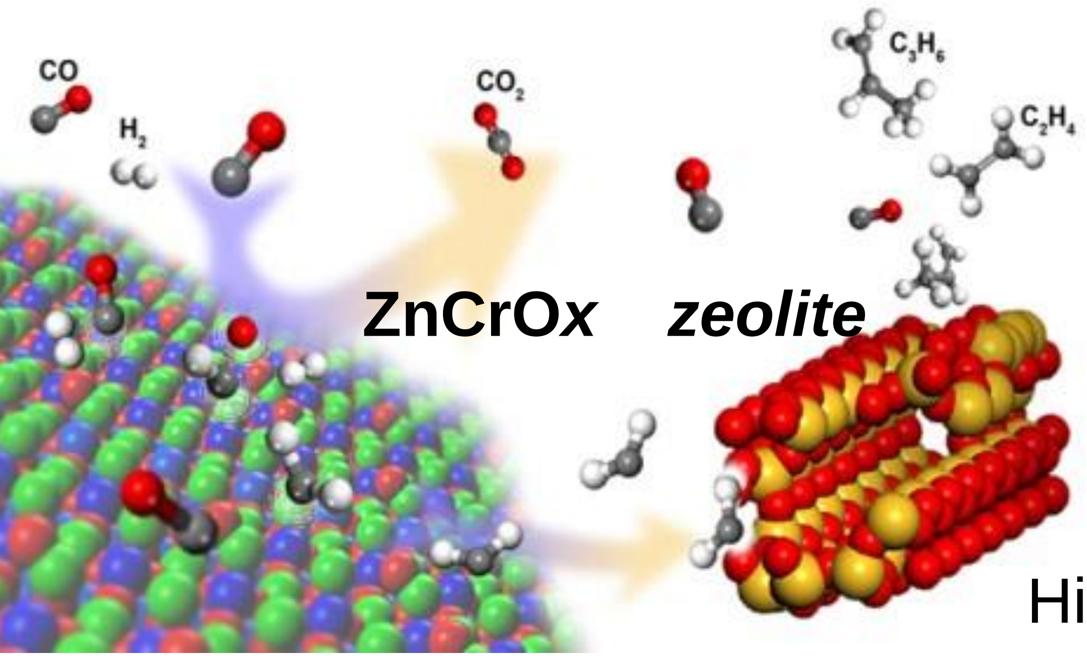


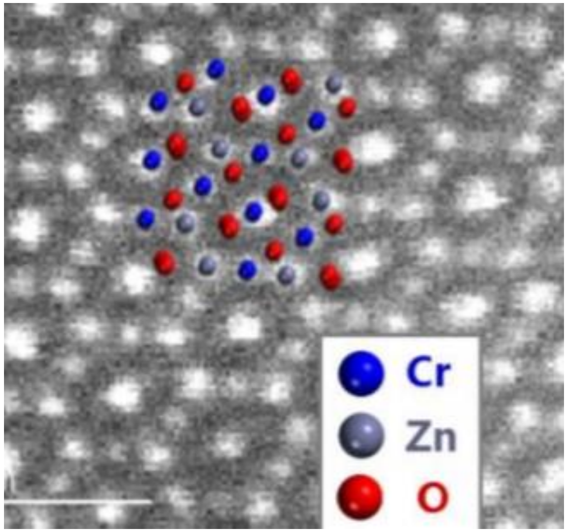
Science **2018**, *361*, 977.

Fischer–Tropsch process (Extra Info.)

$$(2n + 1)\ H_2 + n\ CO \rightarrow C_nH_{(2n+2)} + n\ H_2O$$

synthetic fuel/gas (燃料)





High resolution (S)TEM images

Science AAAS

Selective conversion of syngas to light olefins
Feng Jiao, Jinjing Li, Xiulian Pan, Jianping Xiao, Haobo Li, Hao Ma, Mingming Wei, Yang Pan, Zhongyue Zhou, Mingrun Li, Shu Miao, Jian Li, Yifeng Zhu, Dong Xiao, Ting He, Junhao Yang, Fei Qi, Qiang Fu and Xinhe Bao (March 3, 2016)
Science **351** (6277), 1065-1068. [doi: 10.1126/science.aaf1835]

Formula Weights

Formula Weight (FW)

- A **formula weight** (FW) of a substance is the sum of the atomic weights for the atoms of the substance in a **chemical formula** (CH_4 = 12.011 + 4*1.00794).
- FW of calcium chloride, $CaCl_2$:

$$
\begin{array}{r}
\text{Ca: } 1(40.08 \text{ amu}) \\
\underline{+\ \text{Cl: } 2(35.453 \text{ amu})} \\
110.99 \text{ amu}
\end{array}
$$

- Formula weights are generally reported for all, **especially ionic compounds** (which exist with a 3D order of ions: no simple group of atoms to call a molecule).

Molecular Weight (MW)

- A **molecular weight** is the sum of the atomic weights of the atoms in **a molecule**.
- For the molecule ethane, C_2H_6, the molecular weight would be:

$$
\begin{array}{rl}
C: & 2(12.011\text{ amu}) \\
+\ H: & 6(1.00794\text{ amu}) \\
\hline
 & 30.070\text{ amu}
\end{array}
$$

Percent Composition

One can find the percentage of the mass of **one** particular **element** in a compound by using this equation:

$$\% \text{ Element} = \frac{(\text{number of atoms of an element})(\text{its atomic weight})}{(\text{FW of the compound})} \times 100$$

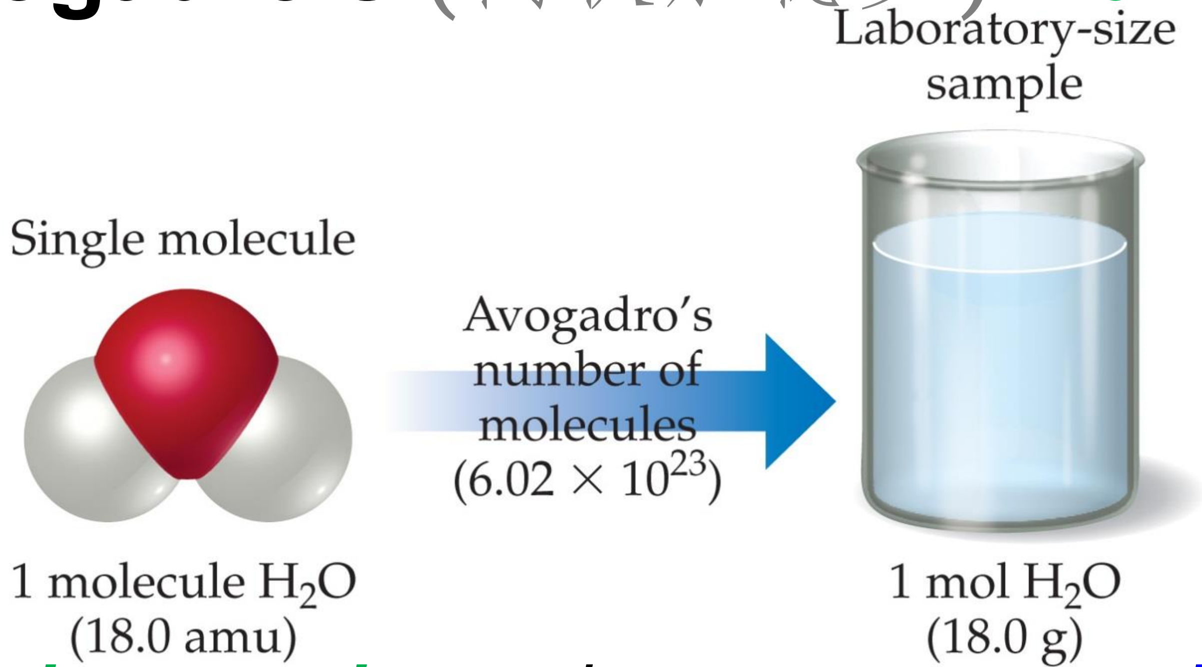
The percentage of carbon in ethane (C_2H_6):

$$\%C = \frac{(2)(12.011 \text{ amu})}{(30.070 \text{ amu})}$$

$$= \frac{24.022 \text{ amu}}{30.070 \text{ amu}} \times 100\% \;\; = 79.887\%$$

Moles (摩尔)

Avogadro's (阿伏加德罗) Number



(sub)-microscopic number *macroscopic number*

- From **experiments**, 1 mole (objects) = 6.02×10^{23} (objects), Avogadro's number (N_A).
- 1 mole He = 6.02×10^{23} He atoms; 1 mole O_2 = 6.02×10^{23} O_2 molecules = 2*6.02×10^{23} O atoms;
- **Different masses** for **different matter** with the **same** mol (amount/number of matter).

Stoichiometry

Molar Mass

By definition, a **molar mass** is the **mass** of 1 mol of a substance (i.e., g/mol).

→ How many grams of a substance per mole?
1 mole of ^{12}C has an exact mass of 12.000 g.

The **<u>value</u>** of **molar mass** of an element (g/mol) is same as that for the **atomic weight** (in amu) of the **element** on the periodic table e.g. Cl: 35.453 g/mol; Zn: 65.39 g/mol.

The **<u>value</u>** of **formula weight** (in amu) of a **substance** is the same number as its molar mass (in g/mol).
C_2H_6 = 30.070 g/mol; $CaCl_2$ = 110.99 g/mol.

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS§

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs

speed of light in vacuum	c	299 792 458 m s^{-1}	(exact)
Planck constant	h	6.626 070 15 x 10^{-34} J Hz^{-1}	(exact)
elementary charge	e	1.602 176 634 x 10^{-19} C	(exact)
Avogadro constant	N_A	6.022 140 76 x 10^{23} mol^{-1}	(exact)
Boltzmann constant	k	1.380 649 x 10^{-23} J K^{-1}	(exact)
electron volt	eV	1.602 176 634 x 10^{-19} J	(exact)
electron mass	m_e	9.109 383 70 x 10^{-31} kg	
energy equivalent	m_ec^2	0.510 998 950 MeV	
proton mass	m_p	1.672 621 924 x 10^{-27} kg	
energy equivalent	m_pc^2	938.272 088 MeV	
fine-structure constant	α	1/137.035 999	
Rydberg energy	$R_\infty hc$	13.605 693 1230 eV	
Newtonian constant of gravitation	G	6.674 x 10^{-11} m^3 kg^{-1} s^{-2}	

§For the most accurate values of these and other constants, visit pml.nist.gov/constants.

Physical Measurement Laboratory www.nist.gov/pml
Standard Reference Data www.nist.gov/srd

- Solids
- Liquids
- Gases
- Artificially Prepared

	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIII	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	
1 $^2S_{1/2}$ **H** Hydrogen 1.008 $1s$ 13.5984																	2 $^1S_0$ **He** Helium 4.0026 $1s^2$ 24.5874
3 $^2S_{1/2}$ **Li** Lithium 6.94 $1s^2 2s$ 5.3917	4 $^1S_0$ **Be** Beryllium 9.0122 $1s^2 2s^2$ 9.3227											5 $^2P^\circ_{1/2}$ **B** Boron 10.81 $1s^2 2s^2 2p$ 8.2980	6 $^3P_0$ **C** Carbon 12.011 $1s^2 2s^2 2p^2$ 11.2603	7 $^4S^\circ_{3/2}$ **N** Nitrogen 14.007 $1s^2 2s^2 2p^3$ 14.5341	8 $^3P_2$ **O** Oxygen 15.999 $1s^2 2s^2 2p^4$ 13.6181	9 $^2P^\circ_{3/2}$ **F** Fluorine 18.998 $1s^2 2s^2 2p^5$ 17.4228	10 $^1S_0$ **Ne** Neon 20.180 $1s^2 2s^2 2p^6$ 21.5645
11 $^2S_{1/2}$ **Na** Sodium 22.990 $[Ne]3s$ 5.1391	12 $^1S_0$ **Mg** Magnesium 24.305 $[Ne]3s^2$ 7.6462											13 $^2P^\circ_{1/2}$ **Al** Aluminum 26.982 $[Ne]3s^2 3p$ 5.9858	14 $^3P_0$ **Si** Silicon 28.085 $[Ne]3s^2 3p^2$ 8.1517	15 $^4S^\circ_{3/2}$ **P** Phosphorus 30.974 $[Ne]3s^2 3p^3$ 10.4867	16 $^3P_2$ **S** Sulfur 32.06 $[Ne]3s^2 3p^4$ 10.3600	17 $^2P^\circ_{3/2}$ **Cl** Chlorine 35.45 $[Ne]3s^2 3p^5$ 12.9676	18 $^1S_0$ **Ar** Argon 39.948 $[Ne]3s^2 3p^6$ 15.7596
19 $^2S_{1/2}$ **K** Potassium 39.098 $[Ar]4s$ 4.3407	20 $^1S_0$ **Ca** Calcium 40.078 $[Ar]4s^2$ 6.1132	21 $^2D_{3/2}$ **Sc** Scandium 44.956 $[Ar]3d4s^2$ 6.5615	22 $^3F_2$ **Ti** Titanium 47.867 $[Ar]3d^2 4s^2$ 6.8281	23 $^4F_{3/2}$ **V** Vanadium 50.942 $[Ar]3d^3 4s^2$ 6.7462	24 $^7S_3$ **Cr** Chromium 51.996 $[Ar]3d^5 4s$ 6.7665	25 $^6S_{5/2}$ **Mn** Manganese 54.938 $[Ar]3d^5 4s^2$ 7.4340	26 $^5D_4$ **Fe** Iron 55.845 $[Ar]3d^6 4s^2$ 7.9025	27 $^4F_{9/2}$ **Co** Cobalt 58.933 $[Ar]3d^7 4s^2$ 7.8810	28 $^3F_4$ **Ni** Nickel 58.693 $[Ar]3d^8 4s^2$ 7.6399	29 $^2S_{1/2}$ **Cu** Copper 63.546 $[Ar]3d^{10} 4s$ 7.7264	30 $^1S_0$ **Zn** Zinc 65.38 $[Ar]3d^{10} 4s^2$ 9.3942	31 $^2P^\circ_{1/2}$ **Ga** Gallium 69.723 $[Ar]3d^{10} 4s^2 4p$ 5.9993	32 $^3P_0$ **Ge** Germanium 72.630 $[Ar]3d^{10} 4s^2 4p^2$ 7.8994	33 $^4S^\circ_{3/2}$ **As** Arsenic 74.922 $[Ar]3d^{10} 4s^2 4p^3$ 9.7886	34 $^3P_2$ **Se** Selenium 78.971 $[Ar]3d^{10} 4s^2 4p^4$ 9.7524	35 $^2P^\circ_{3/2}$ **Br** Bromine 79.904 $[Ar]3d^{10} 4s^2 4p^5$ 11.8138	36 $^1S_0$ **Kr** Krypton 83.798 $[Ar]3d^{10} 4s^2 4p^6$ 13.9996
37 $^2S_{1/2}$ **Rb** Rubidium 85.468 $[Kr]5s$ 4.1771	38 $^1S_0$ **Sr** Strontium 87.62 $[Kr]5s^2$ 5.6949	39 $^2D_{3/2}$ **Y** Yttrium 88.906 $[Kr]4d5s^2$ 6.2173	40 $^3F_2$ **Zr** Zirconium 91.224 $[Kr]4d^2 5s^2$ 6.6341	41 $^6D_{1/2}$ **Nb** Niobium 92.906 $[Kr]4d^4 5s$ 6.7589	42 $^7S_3$ **Mo** Molybdenum 95.95 $[Kr]4d^5 5s$ 7.0924	43 $^6S_{5/2}$ **Tc** Technetium (97) $[Kr]4d^5 5s^2$ 7.1194	44 $^5F_5$ **Ru** Ruthenium 101.07 $[Kr]4d^7 5s$ 7.3605	45 $^4F_{9/2}$ **Rh** Rhodium 102.91 $[Kr]4d^8 5s$ 7.4589	46 $^1S_0$ **Pd** Palladium 106.42 $[Kr]4d^{10}$ 8.3369	47 $^2S_{1/2}$ **Ag** Silver 107.87 $[Kr]4d^{10} 5s$ 7.5762	48 $^1S_0$ **Cd** Cadmium 112.41 $[Kr]4d^{10} 5s^2$ 8.9938	49 $^2P^\circ_{1/2}$ **In** Indium 114.82 $[Kr]4d^{10} 5s^2 5p$ 5.7864	50 $^3P_0$ **Sn** Tin 118.71 $[Kr]4d^{10} 5s^2 5p^2$ 7.3439	51 $^4S^\circ_{3/2}$ **Sb** Antimony 121.76 $[Kr]4d^{10} 5s^2 5p^3$ 8.6084	52 $^3P_2$ **Te** Tellurium 127.60 $[Kr]4d^{10} 5s^2 5p^4$ 9.0097	53 $^2P^\circ_{3/2}$ **I** Iodine 126.90 $[Kr]4d^{10} 5s^2 5p^5$ 10.4513	54 $^1S_0$ **Xe** Xenon 131.29 $[Kr]4d^{10} 5s^2 5p^6$ 12.1298
55 $^2S_{1/2}$ **Cs** Cesium 132.91 $[Xe]6s$ 3.8939	56 $^1S_0$ **Ba** Barium 137.33 $[Xe]6s^2$ 5.2117		72 $^3F_2$ **Hf** Hafnium 178.49 $[Xe]4f^{14} 5d^2 6s^2$ 6.8251	73 $^4F_{3/2}$ **Ta** Tantalum 180.95 $[Xe]4f^{14} 5d^3 6s^2$ 7.5496	74 $^5D_0$ **W** Tungsten 183.84 $[Xe]4f^{14} 5d^4 6s^2$ 7.8640	75 $^6S_{5/2}$ **Re** Rhenium 186.21 $[Xe]4f^{14} 5d^5 6s^2$ 7.8335	76 $^5D_4$ **Os** Osmium 190.23 $[Xe]4f^{14} 5d^6 6s^2$ 8.4382	77 $^4F_{9/2}$ **Ir** Iridium 192.22 $[Xe]4f^{14} 5d^7 6s^2$ 8.9670	78 $^3D_3$ **Pt** Platinum 195.08 $[Xe]4f^{14} 5d^9 6s$ 8.9588	79 $^2S_{1/2}$ **Au** Gold 196.97 $[Xe]4f^{14} 5d^{10} 6s$ 9.2256	80 $^1S_0$ **Hg** Mercury 200.59 $[Xe]4f^{14} 5d^{10} 6s^2$ 10.4375	81 $^2P^\circ_{1/2}$ **Tl** Thallium 204.38 $[Hg]6p$ 6.1083	82 $^3P_0$ **Pb** Lead 207.2 $[Hg]6p^2$ 7.4167	83 $^4S^\circ_{3/2}$ **Bi** Bismuth 208.98 $[Hg]6p^3$ 7.2855	84 $^3P_2$ **Po** Polonium (209) $[Hg]6p^4$ 8.414	85 $^2P^\circ_{3/2}$ **At** Astatine (210) $[Hg]6p^5$ 9.3175	86 $^1S_0$ **Rn** Radon (222) $[Hg]6p^6$ 10.7485
87 $^2S_{1/2}$ **Fr** Francium (223) $[Rn]7s$ 4.0727	88 $^1S_0$ **Ra** Radium (226) $[Rn]7s^2$ 5.2784		104 $^3F_2$ **Rf** Rutherfordium (267) $[Rn]5f^{14} 6d^2 7s^2$ 6.02	105 $^4F_{3/2}$ **Db** Dubnium (268) $[Rn]5f^{14} 6d^3 7s^2$ 6.8	106 $_0$ **Sg** Seaborgium (269) $[Rn]5f^{14} 6d^4 7s^2$ 7.8	107 $_{5/2}$ **Bh** Bohrium (270) $[Rn]5f^{14} 6d^5 7s^2$ 7.7	108 $_4$ **Hs** Hassium (269) $[Rn]5f^{14} 6d^6 7s^2$ 7.6	109 **Mt** Meitnerium (278)	110 **Ds** Darmstadtium (281)	111 **Rg** Roentgenium (282)	112 **Cn** Copernicium (285)	113 **Nh** Nihonium (286)	114 **Fl** Flerovium (289)	115 **Mc** Moscovium (289)	116 **Lv** Livermorium (293)	117 **Ts** Tennessine (294)	118 **Og** Oganesson (294)

Lanthanides	57 $^2D_{3/2}$ **La** Lanthanum 138.91 $[Xe]5d6s^2$ 5.5769	58 $^1G^\circ_4$ **Ce** Cerium 140.12 $[Xe]4f5d6s^2$ 5.5386	59 $^4I^\circ_{9/2}$ **Pr** Praseodymium 140.91 $[Xe]4f^3 6s^2$ 5.4702	60 $^5I_4$ **Nd** Neodymium 144.24 $[Xe]4f^4 6s^2$ 5.5250	61 $^6H^\circ_{5/2}$ **Pm** Promethium (145) $[Xe]4f^5 6s^2$ 5.577	62 $^7F_0$ **Sm** Samarium 150.36 $[Xe]4f^6 6s^2$ 5.6437	63 $^8S^\circ_{7/2}$ **Eu** Europium 151.96 $[Xe]4f^7 6s^2$ 5.6704	64 $^9D^\circ_2$ **Gd** Gadolinium 157.25 $[Xe]4f^7 5d6s^2$ 6.1498	65 $^6H^\circ_{15/2}$ **Tb** Terbium 158.93 $[Xe]4f^9 6s^2$ 5.8638	66 $^5I_8$ **Dy** Dysprosium 162.50 $[Xe]4f^{10} 6s^2$ 5.9391	67 $^4I^\circ_{15/2}$ **Ho** Holmium 164.93 $[Xe]4f^{11} 6s^2$ 6.0215	68 $^3H_6$ **Er** Erbium 167.26 $[Xe]4f^{12} 6s^2$ 6.1077	69 $^2F^\circ_{7/2}$ **Tm** Thulium 168.93 $[Xe]4f^{13} 6s^2$ 6.1843	70 $^1S_0$ **Yb** Ytterbium 173.05 $[Xe]4f^{14} 6s^2$ 6.2542	71 $^2D_{3/2}$ **Lu** Lutetium 174.97 $[Xe]4f^{14} 5d6s^2$ 5.4259
Actinides	89 $^2D_{3/2}$ **Ac** Actinium (227) $[Rn]6d7s^2$ 5.3802	90 $^3F_2$ **Th** Thorium 232.04 $[Rn]6d^2 7s^2$ 6.3067	91 $^4K_{11/2}$ **Pa** Protactinium 231.04 $[Rn]5f^2 6d7s^2$ 5.89	92 $^5L^\circ_6$ **U** Uranium 238.03 $[Rn]5f^3 6d7s^2$ 6.1941	93 $^6L_{11/2}$ **Np** Neptunium (237) $[Rn]5f^4 6d7s^2$ 6.2655	94 $^7F_0$ **Pu** Plutonium (244) $[Rn]5f^6 7s^2$ 6.0258	95 $^8S^\circ_{7/2}$ **Am** Americium (243) $[Rn]5f^7 7s^2$ 5.9738	96 $^9D^\circ_2$ **Cm** Curium (247) $[Rn]5f^7 6d7s^2$ 5.9914	97 $^6H^\circ_{15/2}$ **Bk** Berkelium (247) $[Rn]5f^9 7s^2$ 6.1978	98 $^5I_8$ **Cf** Californium (251) $[Rn]5f^{10} 7s^2$ 6.2817	99 $^4I^\circ_{15/2}$ **Es** Einsteinium (252) $[Rn]5f^{11} 7s^2$ 6.3676	100 $^3H_6$ **Fm** Fermium (257) $[Rn]5f^{12} 7s^2$ 6.50	101 $^2F^\circ_{7/2}$ **Md** Mendelevium (258) $[Rn]5f^{13} 7s^2$ 6.58	102 $^1S_0$ **No** Nobelium (259) $[Rn]5f^{14} 7s^2$ 6.66	103 $^2P^\circ_{1/2}$ **Lr** Lawrencium (266) $[Rn]5f^{14} 7s^2 7p$ 4.96

Atomic Number — Ground State

58 $^1G^\circ_4$
Ce
Cerium
140.12
$[Xe]4f5d6s^2$
5.5386

mbol
ne
ard
nic
t† (u)
ound-state nfiguration
Ionization Energy (eV)

Table 3.2 Mole Relationships

Name of Substance	Formula	Formula Weight (amu)	Molar Mass (g/mol)	Number and Kind of Particles in One Mole
Atomic nitrogen	N	14.0	14.0	6.02×10^{23} N atoms
Molecular nitrogen	N_2	28.0	28.0	6.02×10^{23} N_2 molecules $2(6.02 \times 10^{23})$ N atoms
Silver	Ag	107.9	107.9	6.02×10^{23} Ag atoms
Silver ions	Ag^+	107.9[a]	107.9	6.02×10^{23} Ag^+ ions
Barium chloride	$BaCl_2$	208.2	208.2	6.02×10^{23} $BaCl_2$ formul 6.02×10^{23} Ba^{2+} ions $2(6.02 \times 10^{23})$ Cl^- ions

[a]Recall that the mass of an electron is more than 1800 times smaller than the masses of the proton and the neutron; thus, ions and atoms essentially the same mass.

- One mole of atoms, ions, or molecules contains Avogadro's number of those particles.
- One mole of molecules or formula units contains **Avogadro's number times the number** of atoms or ions of each element in the compound.

Atomic Mass vs. Molar Mass

The formula (or atomic) weight of a substance has the **same number/value** (相等数值) as its molar mass:
A.M. for ^{12}C = **12** amu; Molar mass for ^{12}C = **12** g/mol

However, atomic weight & molar mass have **different meanings, NOT equal**:
Atomic weight: **mass** (in amu; 1 amu = 1.66×10^{-24} g); "microscopic scale"
Molar mass: **mass/(moles of molecule)** (in g/mol); "macroscopic scale"
Formula weight (F.W.): total mass of **any substance** (e.g. atom, ion, metal, ionic compound, molecular compound,…etc) in a **chemical formula**;
Molecular weight (M.W.): if the substance is a **molecular compound**; F.W. is also OK in this case.

Interconversion of Moles

Moles provide a bridge from the molecular scale to the real-world scale (dimensional analysis).

Mass-to-mol (numbers), 1 mol/M.W.:

$$5.380 \text{ g } C_6H_{12}O_6 = 5.380 \text{ g} * \frac{1 \text{ mol}}{180.0 \text{ g}} = 0.02989 \text{ mol} (*6.02*10^{23}/1 \text{ mol})$$

$(= 0.1799*10^{23})$

Mol-to-mass, M.W./1 mol:

$$0.433 \text{ mol } Ca(NO_3)_2 = 0.433 \text{ mol} * \frac{164.1 \text{ g}}{1 \text{ mol}} = 71.1\text{g}$$

Report ALL your **numerical values** with correct significant figures, **not分数 (A/B**, use your calculator)!

GIVE IT SOME THOUGHT

a. Which has more mass, a mole of water (H_2O) or a mole of glucose ($C_6H_{12}O_6$)?

b. Which contains more molecules, a mole of water or a mole of glucose?

a.

A. Mole of glucose

B. Mole of water

b.

A. Mole of water

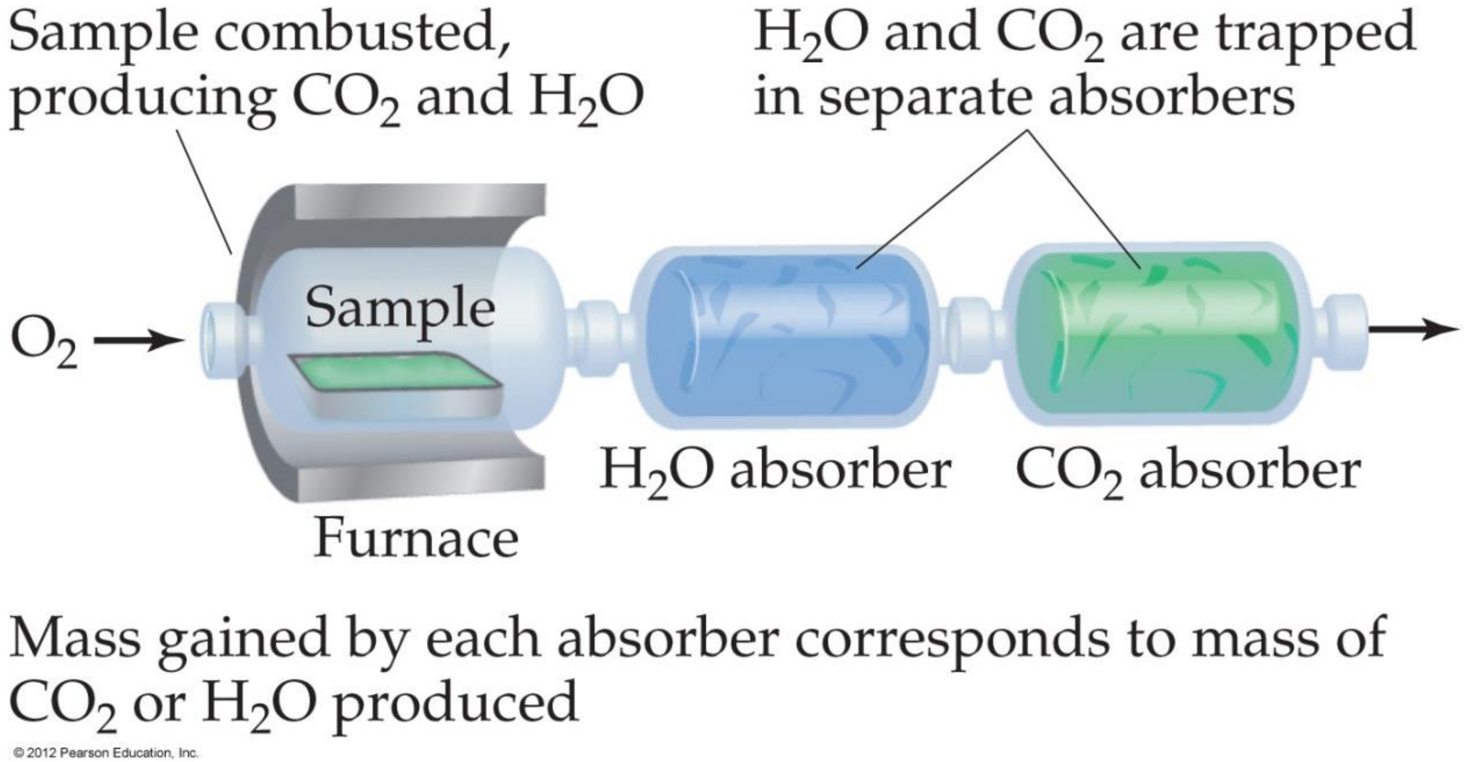
B. Mole of glucose

C. Requires Avogadro's number to answer question

D. They both contain the same number of molecules

Finding Empirical Formulas

Combustion Analysis: Empirical Formula



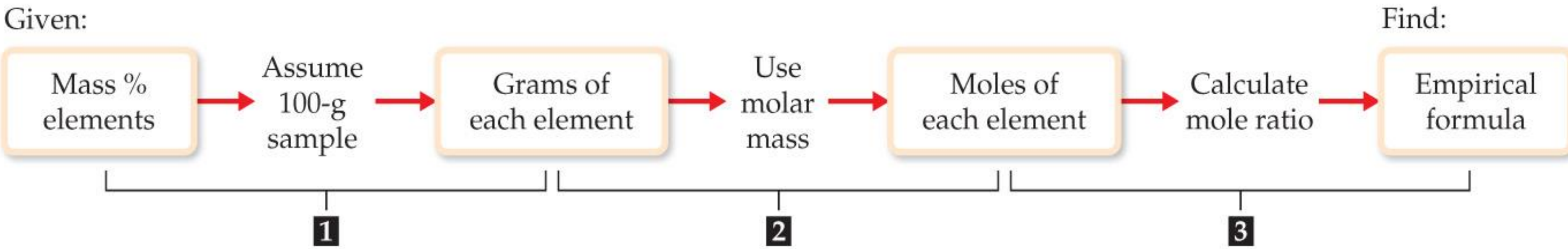
- Compounds containing C, H, and O are routinely analyzed through combustion in a chamber.

C (M_C) is determined from the mass of CO_2 produced.

H (M_H) is determined from the mass of H_2O produced.

O (M_O) is determined by difference between the amount of sample and that of C and H (**= M_{sample} - M_C - M_H**).

Calculating Empirical Formulas



One can calculate the empirical formula from the percent composition. E.g.

The compound *para*-aminobenzoic acid (PABA) is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula of PABA.

Assuming 100.00 g of *para*-aminobenzoic acid,

$$\text{C:} \quad 61.31\text{ g} \times \frac{1\text{ mol}}{12.01\text{ g}} = 5.105\text{ mol C}$$

$$\text{H:} \quad 5.14\text{ g} \times \frac{1\text{ mol}}{1.01\text{ g}} = 5.09\text{ mol H}$$

$$\text{N:} \quad 10.21\text{ g} \times \frac{1\text{ mol}}{14.01\text{ g}} = \mathbf{0.7288}\text{ mol N}$$

$$\text{O:} \quad 23.33\text{ g} \times \frac{1\text{ mol}}{16.00\text{ g}} = 1.456\text{ mol O}$$

Calculate the **mole ratio** by dividing by the **smallest number** of the mole (**0.7288** mol N):

$$C: \frac{5.105 \text{ mol}}{0.7288 \text{ mol}} = 7.005 \approx 7$$

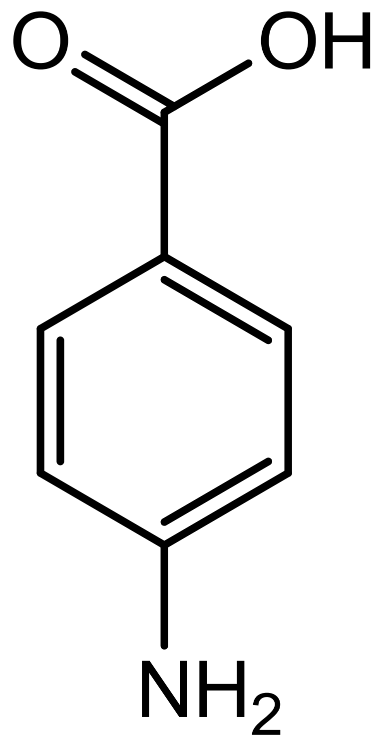
$$H: \frac{5.09 \text{ mol}}{0.7288 \text{ mol}} = 6.984 \approx 7$$

7*C + 7*H + N + 2*O

$$N: \frac{0.7288 \text{ mol}}{0.7288 \text{ mol}} = 1.000$$

$$O: \frac{1.458 \text{ mol}}{0.7288 \text{ mol}} = 2.001 \approx 2$$

The empirical formula: $C_7H_7NO_2$



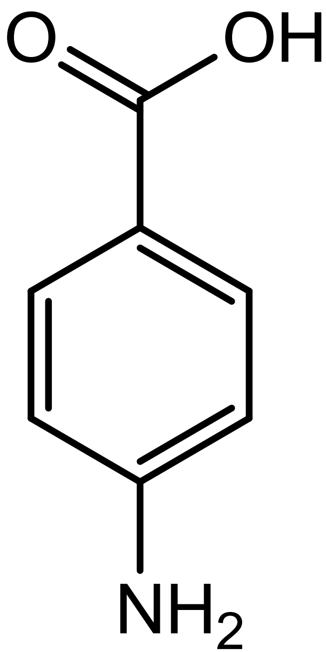
The structural formula

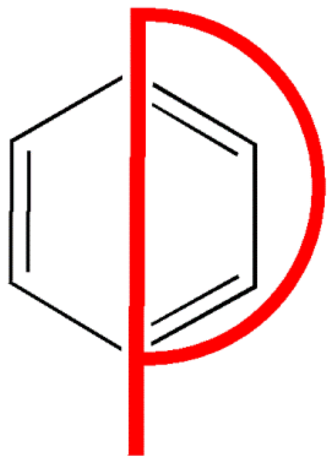
para-aminobenzoic acid

对氨基苯甲酸

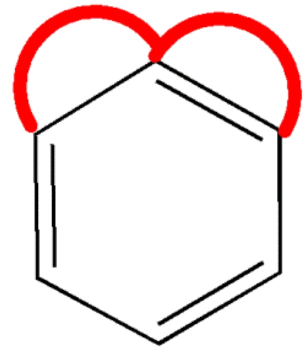
Q. What will we get, if we do not assume 100.00 g?

Extra info.: Para (对), Meta (间) & Ortho (邻)

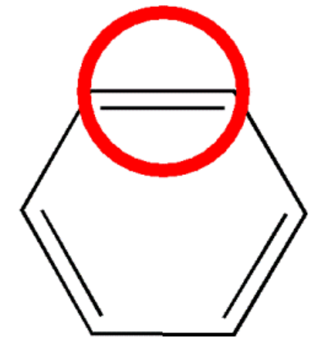




1,4 relationship
para



1,3 relationship
meta



1,2 relationship
ortho

para-aminobenzoic acid

对氨基苯甲酸

Stoichiometry

Determining a Molecular Formula

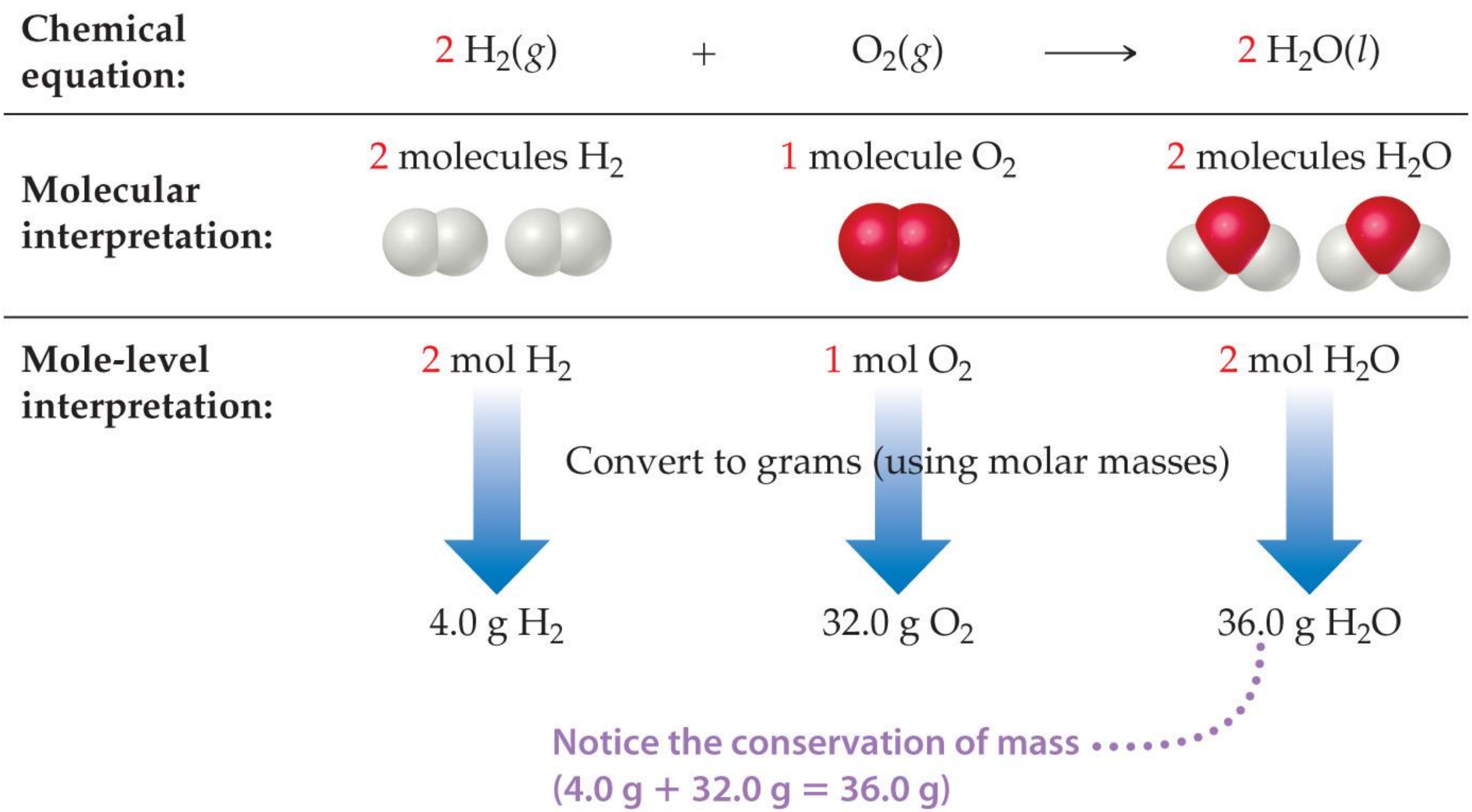
- the number of atoms in a **molecular formula (e.g. $X_nY_nZ_n$)** is a **multiple** (n = 1, 2 or above) of the number of atoms in an **empirical formula (e.g. XYZ)**.
- If we know the **empirical formula and a molar mass** (molecular weight) for the compound, we can determine the molecular formula (with **n** value).
- The empirical formula of a compound is CH; its molar mass is 78 g/mol.

Whole-number multiple (n) = 78/13 = 6

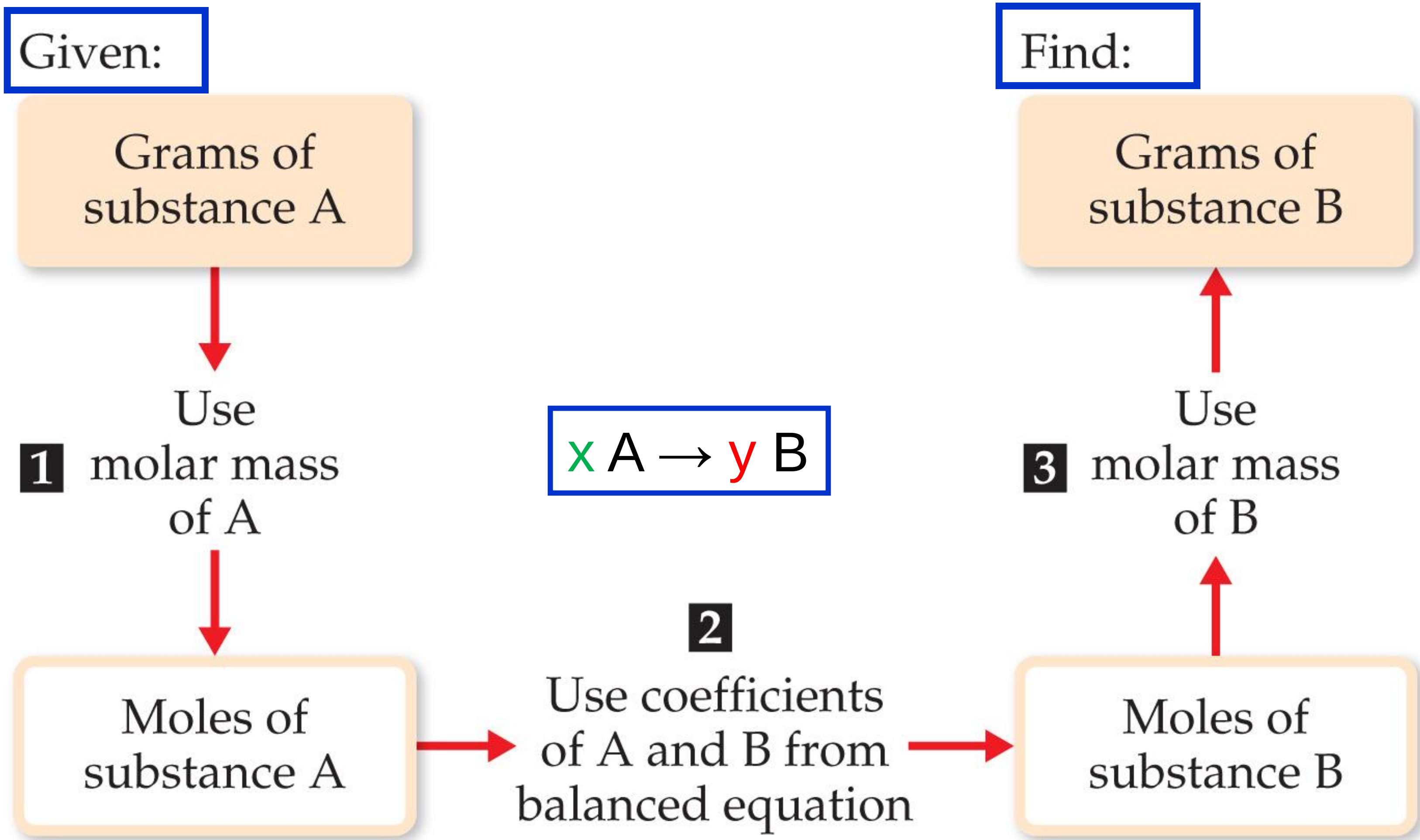
➔ molecular formula: C_6H_6

Stoichiometric Calculations

Stoichiometric Calculations

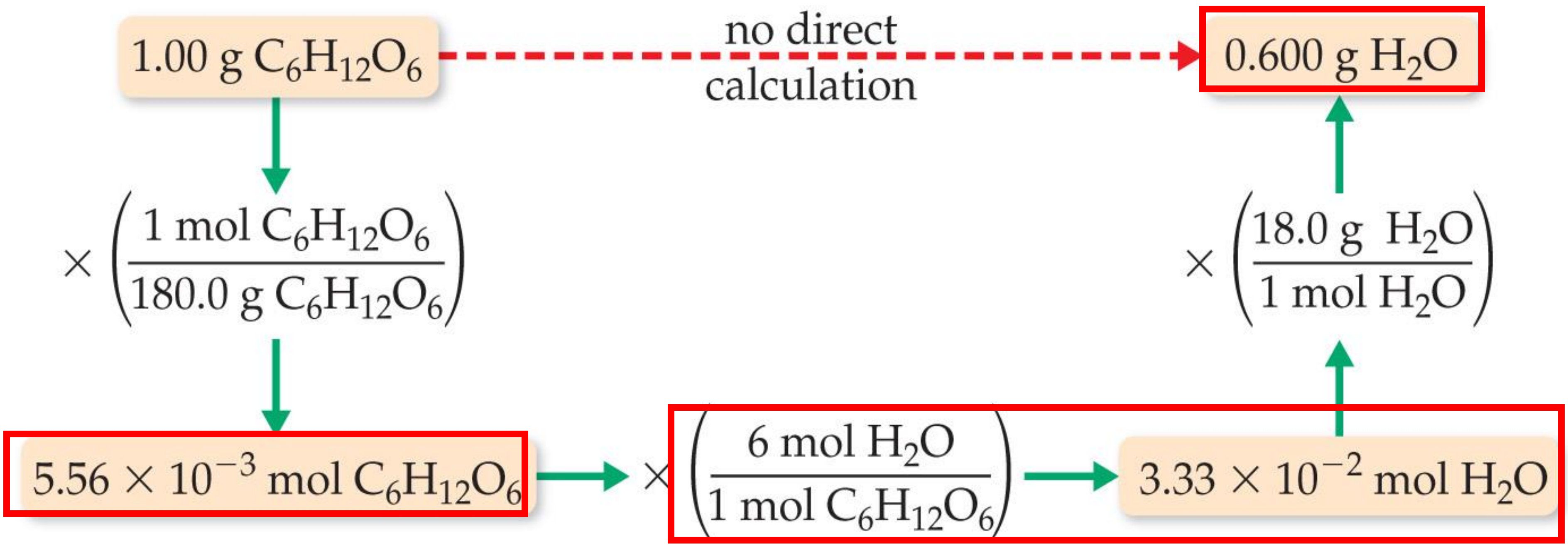


The coefficients in the balanced equation give the ratio of *moles* of the reactants and products.



From **mass of substance A**, we can use the **ratio of the coefficients** of A (x) and B (y) to calculate the mass of substance B formed in a chemical reaction.

1.00 g $C_6H_{12}O_6 + 6\ O_2 \longrightarrow 6\ CO_2 + 6\ H_2O$? g



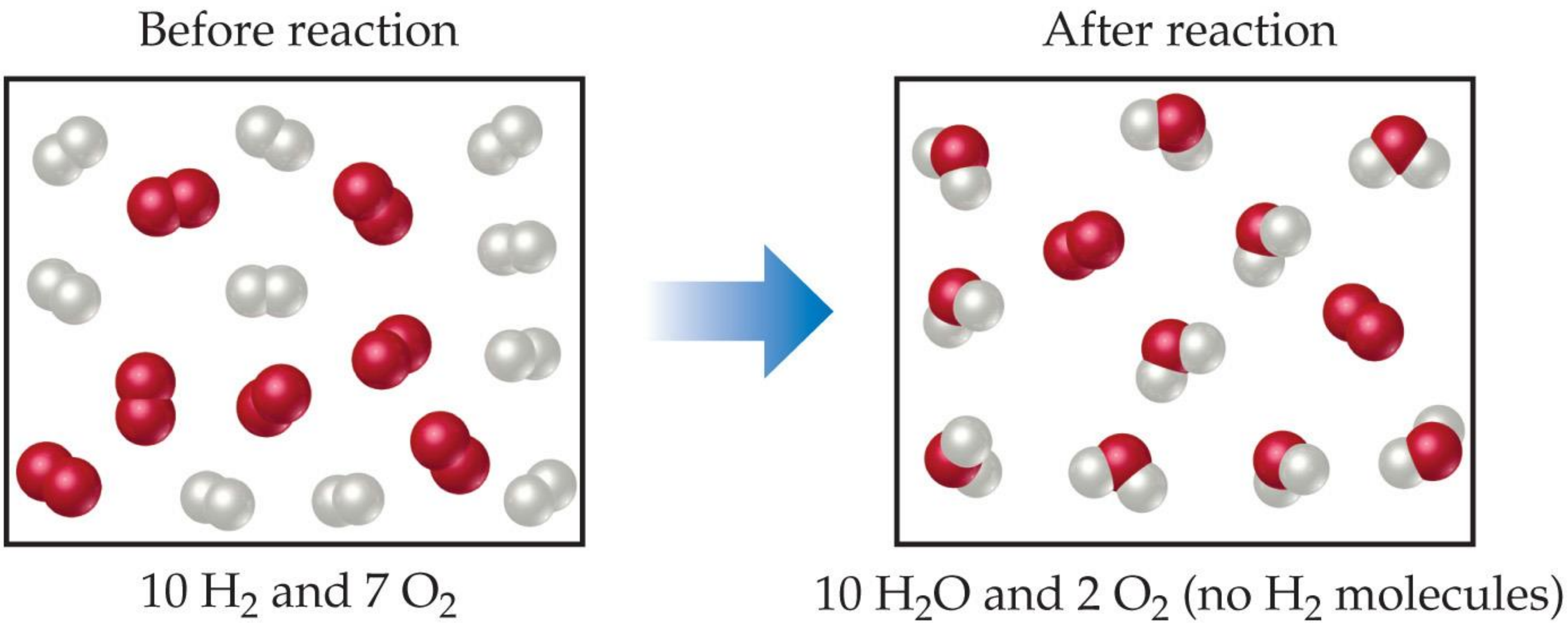
1.00 g of $C_6H_{12}O_6$

1. calculate no. of moles of $C_6H_{12}O_6$;
2. use the coefficients to determine no. moles of H_2O;
3. calculate grams of H_2O by its moles;

Stoichiometry

Limiting Reactant & Excess Reagent

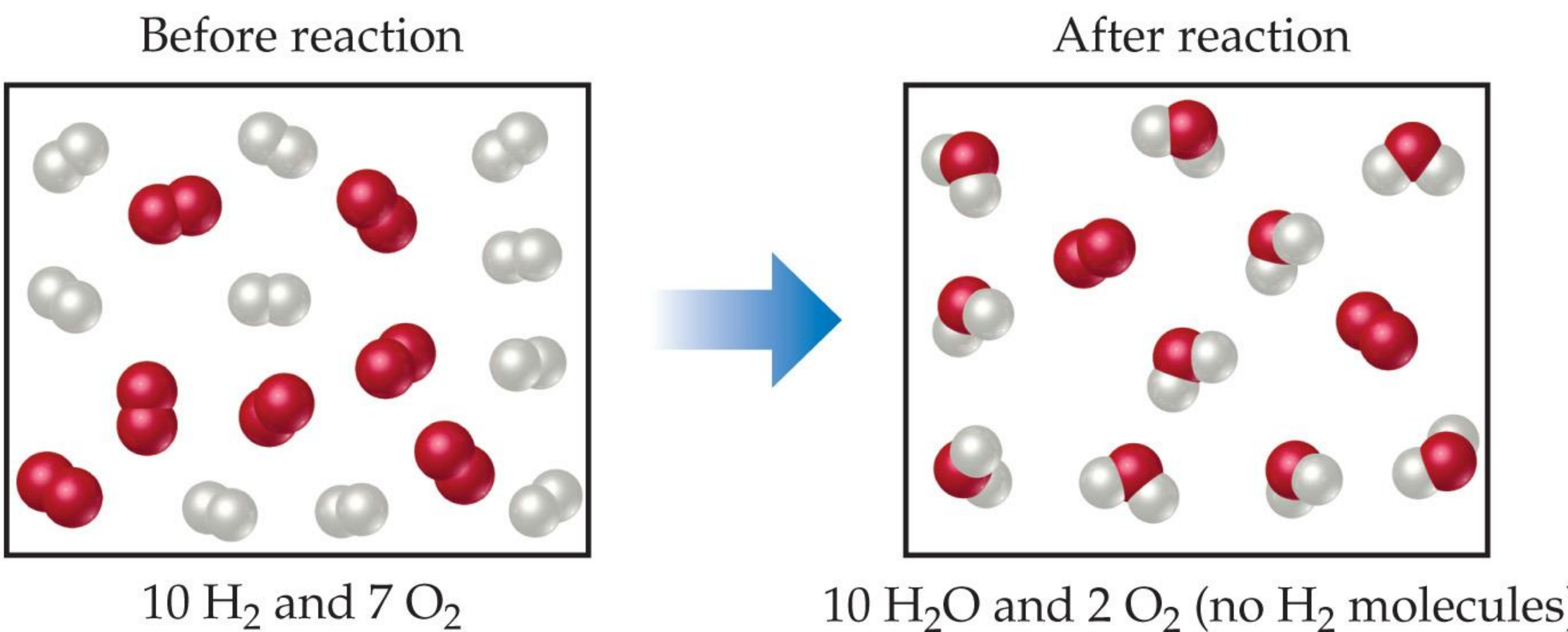
- The **limiting reactant** is the (not enough) reactant which is completely consumed first (i.e. H_2) and **affects** the **amount** of the **product(s)** formed.



- O_2 would be the **excess reagent**.

Theoretical & Actual Yields (产量)

- The **theoretical yield** is the **maximum amount of product** formed, if **all** of a **limiting reactant is used**.
- **Theoretical yield** is almost more than the **actual yield,** which is the amount one **actually produces and measures** (e.g. with side-reactions, <100 % isolation of all products).



Percent yield: compare the actual yield to the theoretical yield (ideally, 100%; **< 100 % in reality**).

$$\text{Percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%$$

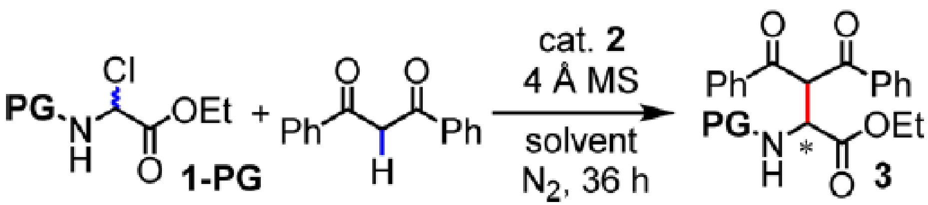
A Chemistry Research Paper:

Asymmetric Mannich Synthesis of α-Amino Esters by Anion-Binding Catalysis

Masayuki Wasa, Richard Y. Liu, Stéphane P. Roche, and Eric N. Jacobsen

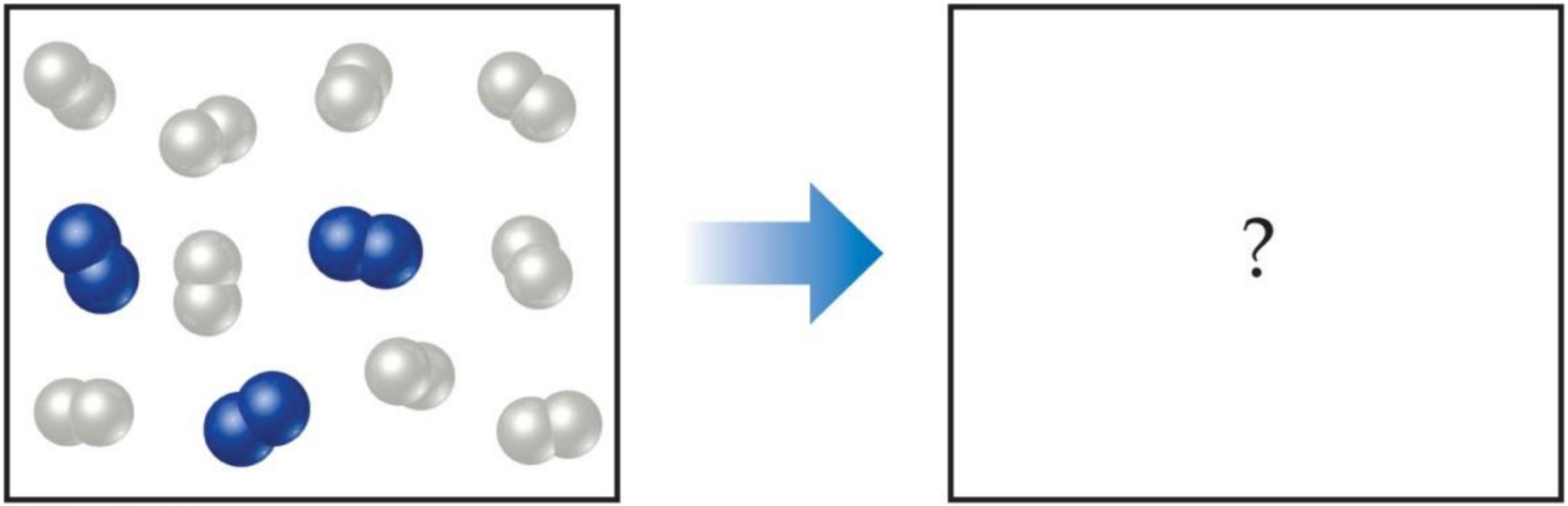
Publication Date (Web): September 1, 2014 (Communication)

DOI: 10.1021/ja5075163



PG	solvent	temp (°C)	yield (%)
Cbz	DCM	−30	90
Fmoc	DCM	−30	71
Troc	DCM	−30	83
MeO_2C–	DCM	−30	82
PhO_2C–	DCM	−30	50

In the following diagram, the white spheres represent hydrogen atoms and the blue spheres represent nitrogen atoms.



To be consistent with the law of conservation of mass, how many NH_3 molecules should be shown in the right (products) box?

Answer: Six NH_3 molecules.

The most important commercial process for converting N_2 from the air into nitrogen-containing compounds is based on the reaction of N_2 and H_2 to form ammonia (NH_3):

$$N_2(g) + 3\ H_2(g) \rightarrow 2\ NH_3(g)$$

How many moles of NH_3 can be formed from 3.0 mol of N_2 and 6.0 mol of H_2?

	$N_2(g)$	+	$3\ H_2(g)$	$\longrightarrow$	$2\ NH_3(g)$
Initial quantities:	3.0 mol		6.0 mol		0 mol
Change (reaction):	−2.0 mol		−6.0 mol		+4.0 mol
Final quantities:	1.0 mol		0 mol		$\boxed{4.0\text{ mol}}$

A certain alcohol contains only three elements, carbon, hydrogen, and oxygen. Combustion of a 10.00 gram sample of the alcohol produced 19.10 grams of CO_2 and 11.74 grams of H_2O. What is the empirical formula of the alcohol?

Express your answer as a chemical formula.

Mass of C in CO_2 = 19.10/(12.011+2*15.999)*12.011 g = 5.213 g

Mass of H in H_2O = 11.74/(2*1.008 + 15.999)*(2*1.008) g = 1.314 g

Mass of O = mass of sample – mass of C – mass of H = 10.00 g – 5.213 g – 1.314 g = 3.473 g

Mole of C = 5.213/12.011 mol = 0.4340 mol

Mole of H = 1.314/1.008 mol = 1.304 mol

Mole of O = 3.473/15.999 mol = **0.2171** mol

Relative mole of C = 0.4340/0.2171 = 1.999 ~ 2

Relative mole of H = 1.304/0.2171 = 6.005 ~ 6

Relative mole of O = 0.2171/0.2171 = 1

Empirical (chemical) formula = **C_2H_6O**

Sulfur and fluorine react in a combination reaction to produce sulfur hexafluoride:

$S(s) + 3F_2(g) \rightarrow SF_6(g)$

In a particular experiment, the percent yield is 79.0%. This means that in this experiment, a 7.90 g sample of fluorine yields ___________ g of SF_6.

Mole of F_2 = 7.90/(2*18.998) mol = 0.208 mol

Mole of SF_6 = 0.208**/3** mol = 0.0693 mol

Theoretical yield of SF_6: 0.0693*(32.06+6*18.998) g = 10.1 g

Actual yield of SF_6: 10.1 g *** 79.0 %** = 7.99 g

Lithium and nitrogen react in a combination reaction to produce lithium nitride:

$6Li(s) + N_2(g) \rightarrow 2Li_3N\,(s)$

In a particular experiment, 2.00 g samples of each reagent are reacted. The theoretical yield of lithium nitride is ___________ g.

Mole of Li = 2.00/(6.94) mol = 0.288 mol

Mole of N_2 = 2.00/(2*14.007) mol = 0.0714 mol

0.0480 (0.288/6) mol **$<$** 0.0714 mol

➔Li is a limiting reactant

Mole of Li_3N = 0.0480*2 mol = 0.0961 mol

Theoretical yield of Li_3N: 0.0961*(3*6.94+14.007) g = 3.34 g

If 147 grams of FeS_2 is allowed to react with 88 grams of O_2 according to the following equation, how many grams of Fe_2O_3 are produced?

$FeS_2 + O_2 \rightarrow Fe_2O_3 + SO_2$

Express your answer as an integer.

Write a balanced chemical equation:

$4FeS_2 + 11O_2 \rightarrow 2Fe_2O_3 + 8SO_2$

Mole of FeS_2 = 147/(55.845+2*32.06) mol = 1.23 mol

Mole of O_2 = 88/(2*15.999) mol = 2.8 mol

Coefficient ratio: 1.23/4 = **0.306**; 2.8/11 = **0.25**

➔ O_2 is a limiting reactant, while FeS_2 is an excess reagent;

mole of the product is determined by mole of the limiting reactant.

Mole of Fe_2O_3 = 88/(2*15.999)/11*2 mol

Mass of Fe_2O_3 = 88/(2*15.999)/11*2*(2*55.845+3*15.999) g

= 79.848 g ➔ 80 g

ML Prediction of Reactions (Extra Info.)

Neural Networks for the Prediction of Organic Chemistry Reactions

Jennifer N. Wei,[†] David Duvenaud,[‡] and Alán Aspuru-Guzik*[,†]

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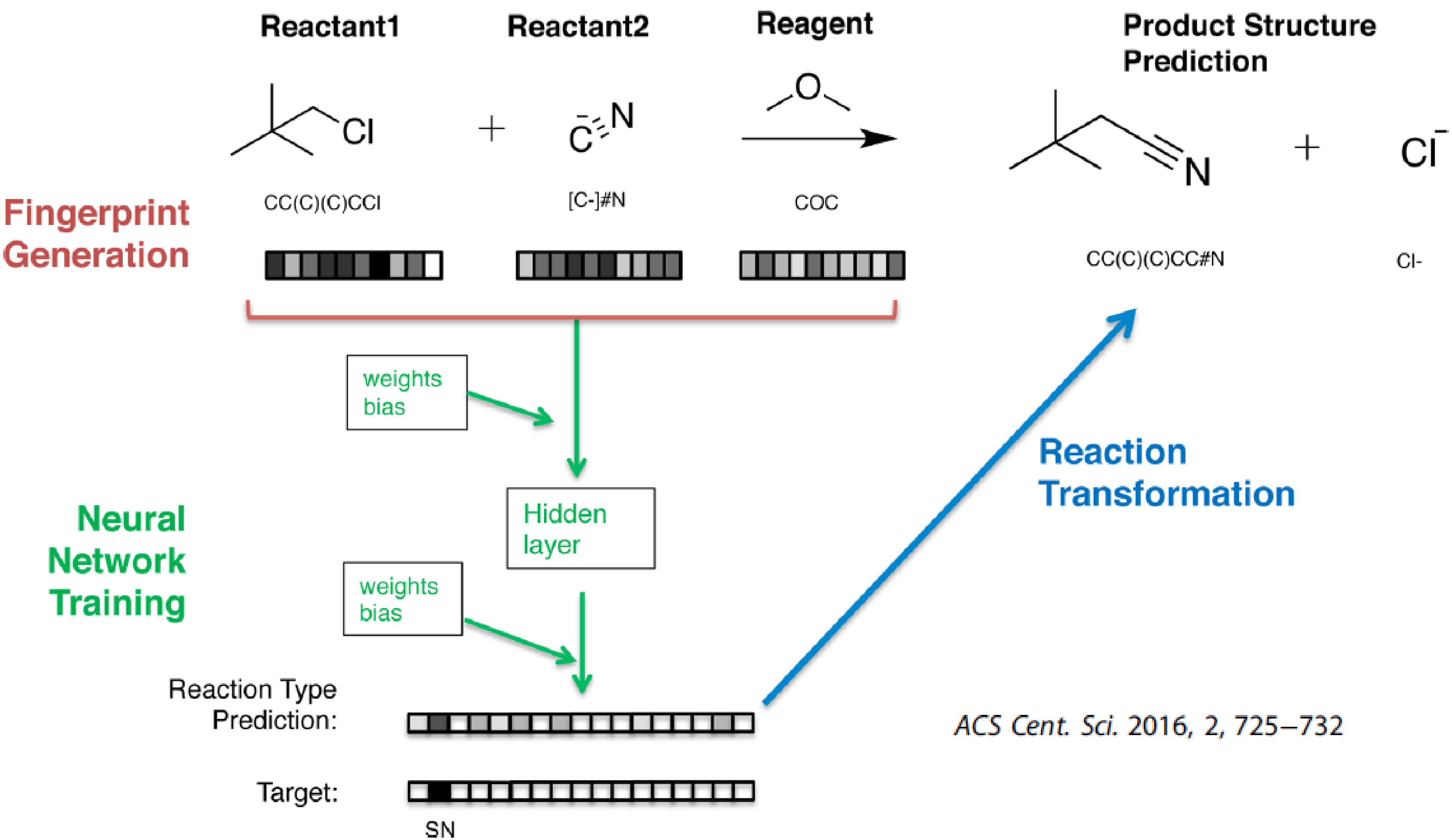
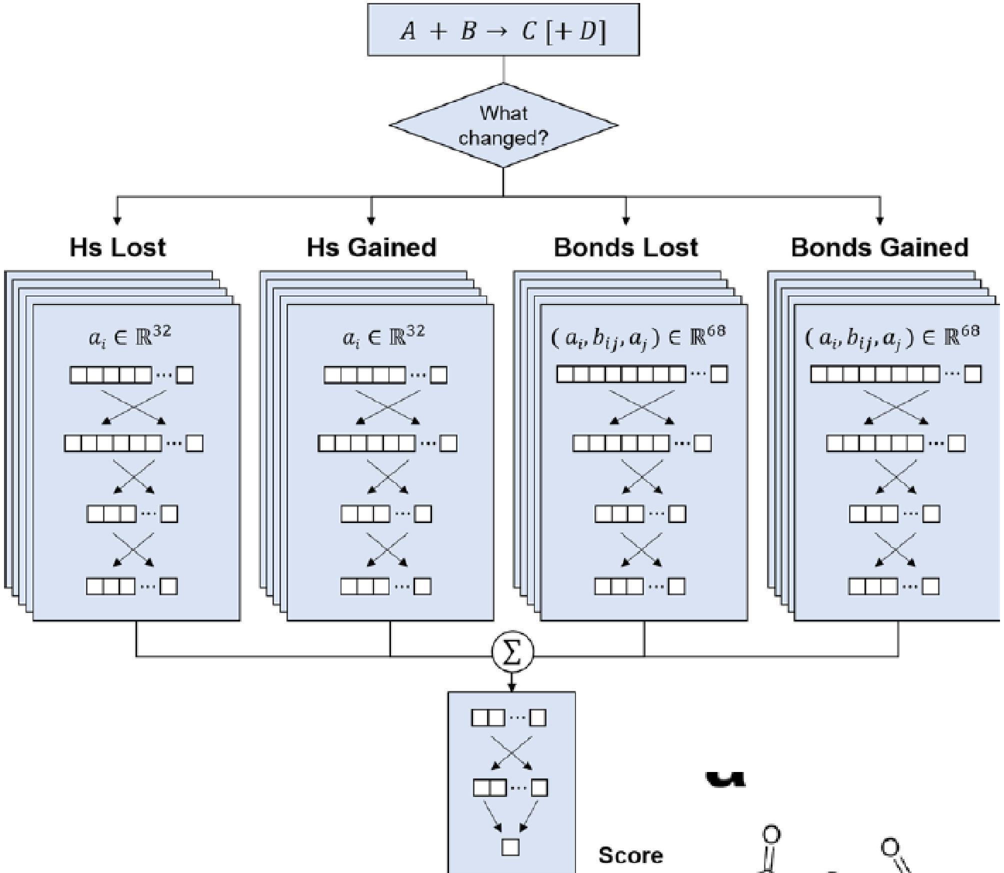


ACS Cent. Sci. 2016, 2, 725−732

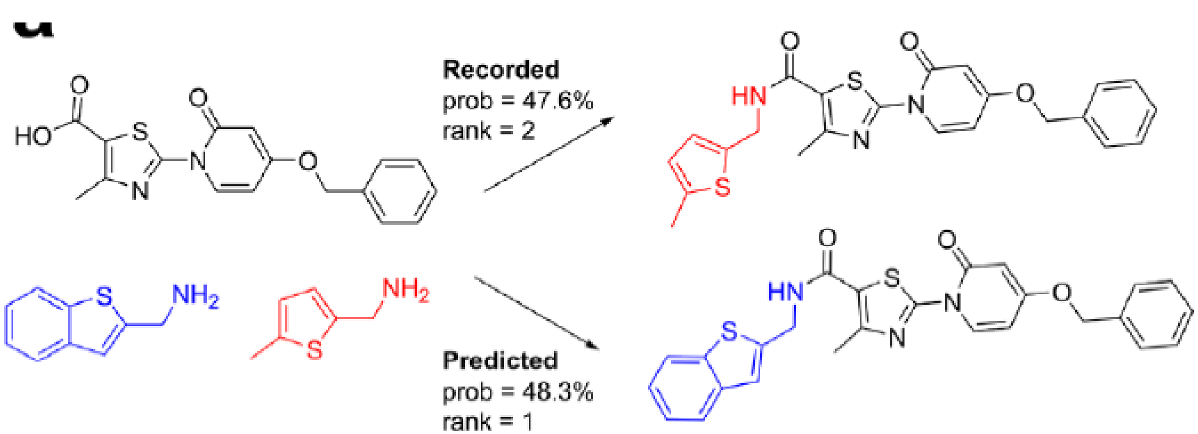
Prediction of Organic Reaction Outcomes Using Machine Learning

Connor W. Coley,[†] Regina Barzilay,[‡] Tommi S. Jaakkola,[‡] William H. Green,[*,†] and Klavs F. Jensen[*,†]

[†]Department of Chemical Engineering and [‡]Computer Science and Artificial Intelligence Laboratory, Massachusetts Institute of



ML Prediction of Reactions (Extra Info.)



ACS Cent. Sci. 2017, 3, 434–443

Quantitative interpretation explains machine learning models for chemical reaction prediction and uncovers bias

(Extra Info.)

Dávid Péter Kovács[1,2], William McCorkindale[1,2] & Alpha A. Lee[1]✉

[1] Cavendish Laboratory, University of Cambridge, Cambridge, UK.

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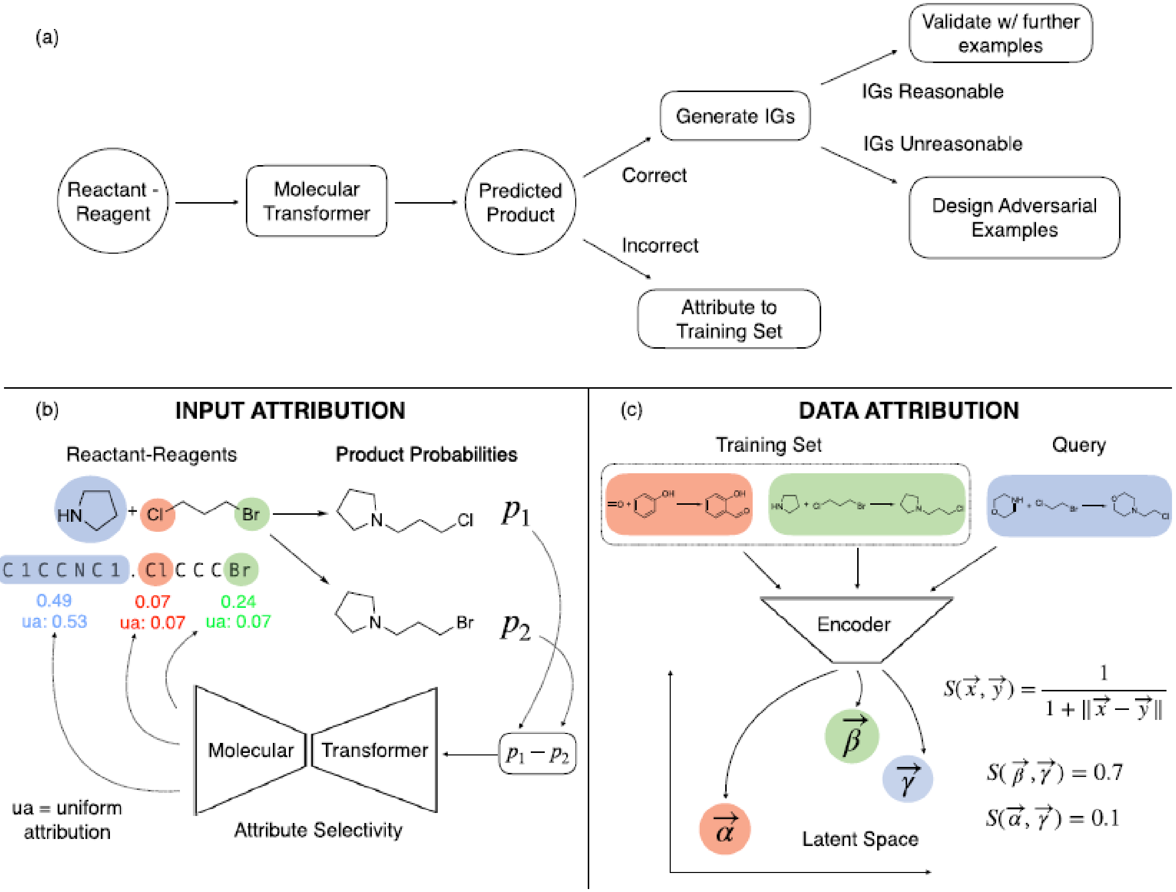

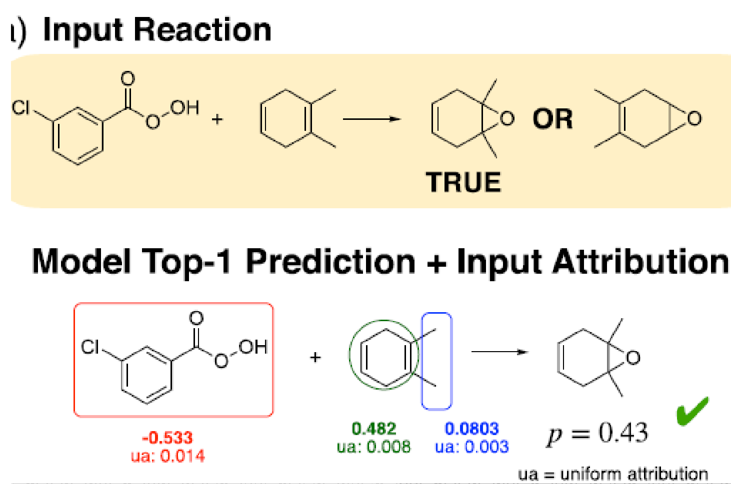

Key Summary

Stoichiometry: Quantity of Substances; Balanced Chemical Formulas and Equations

Chemical Equations: Law of Conservation of Mass; Reactant & Product; States

Reaction Types: Combination, Decomposition & Combustion Reactions

Formula Weights: Formula Weight; Molecular Weight; Percent Composition

Moles: Avogadro’s Number; Molar Mass; Moles

Stoichiometric Calculations: Limiting Reactants; Excess Reagent; Theoretical/Actual Yields

Thank You for Your Attention!

Any Questions?

Revision Exercises

The percentage by mass of phosphorus in Na_3PO_4 is

a. 44.0.
b. 11.7.
c. 26.7.
d. 18.9.

$$\boxed{\frac{31}{3x(23) + (31) + 4x(16)} \text{ x100\%}}$$

Ethanol contains 52.2% carbon, 13.0% hydrogen, and 34.8% oxygen by mass. The empirical formula of ethanol is

a. $C_2H_5O_2$
b. C_2H_6O
c. $C_2H_6O_2$
d. $C_3H_4O_2$

(C) 52.2/12 = 4.35
(H) 13/1 = 13
(O) 34.8/16 = 2.175

(C) 4.35/2.175 = 2
(H) 13/2.175 = 5.977 ≈ 6
(O) 2.175/2.175 = 1

Ribose (核糖) has a molecular weight of 150 grams per mole and the empirical formula CH_2O. The molecular formula of ribose is

a. $C_4H_8O_4$.
b. $C_5H_{10}O_5$.
c. $C_6H_{14}O_4$.
d. $C_6H_{12}O_6$.

Molecular formula = $(CH_2O)n$
Molecular weight = 150 g/mole
n(30) g/mole = 150 g/mole
n = 5

Stoichiometry

When 3.14 g of Compound X is completely combusted, 6.91 g of CO_2 and 2.26 g of H_2O form. The molecular formula of Compound X is

a. C_7H_{16}.

b. $C_6H_{12}O$.

c. $C_5H_8O_2$.

d. $C_4H_4O_3$.

Stoichiometry

$C_6H_6 + 2\ Br_2 \rightarrow C_6H_4Br_2 + 2\ HBr$

When 10.0 g of C_6H_6 and 30.0 g of Br_2 react as shown above, the limiting reactant is

(C: 12; H: 1; Br: 79.9)

a. Br_2.
b. C_6H_6.
c. HBr.
d. $C_6H_4Br_2$.

10.0g C_6H_6 = 10/(6x12+6) = 0.128 mole C_6H_6

30.0g Br_2 = 30/(2x79.9) = 0.188 mole Br_2

0.128 mole C_6H_6 requires 0.256 mole Br_2

$2\ Fe + 3\ Cl_2 \rightarrow 2\ FeCl_3$

When 10.0 g of iron and 20.0 g of chlorine react as shown, the theoretical yield of $FeCl_3$ is

Fe: 55.85; Cl:35.45)

a. 10.0 g.
b. 20.0 g.
c. 29.0 g.
d. 30.0 g.

10.0g Fe = 0.179 mole Fe

20.0g Cl_2 = 20/(2x35.45)
0.282 mole Cl_2

0.179 mole $FeCl_3$ will be formed
0.179x(55.85+3x35.45) = 29.0g

The percentage yield of a reaction is 100% x (Z), where Z is

a. theoretical yield / actual yield.
b. calculated yield / actual yield.
c. calculated yield / theoretical yield.
d. actual yield / theoretical yield.

$C_3H_4O_4 + 2\ C_2H_6O \rightarrow$
$C_7H_{12}O_4 + 2\ H_2O$

When 15.0 g of each reactant was mixed, 15.0 g of $C_7H_{12}O_2$ formed. The percentage yield of this product is

$C_3H_4O_4$: 104; C_2H_6O: 46; $C_7H_{12}O_2$: 160

a. 100%.
b. 75%.
c. 65%.
d. 50%.