

STOICHIOMETRY FUNDAMENTALS

Three types of stoichiometric relations. Each has set of stoichiometric coefficients which relate consumption/formation of a compound to other reactants and products in a particular reaction:

Molar:

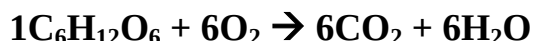


where A_i are reactants for $i = 1 \rightarrow k$ and products for $i = k+1 \rightarrow m$

And a_i are stoichiometric coefficients

Characteristics of molar stoichiometric relations:

Example:



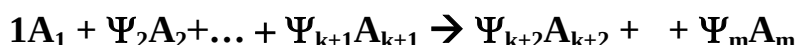
Units: moles, molecules

Element mass is conserved

Charge is conserved

Typically, stoichiometric coefficients are normalized to a reference reactant or product, which then has a stoichiometric coefficient of “1.”

Mass:



Where Ψ_i are stoichiometric coefficients

$$\text{And } \Psi_i = \frac{a_i (\text{MW of } A_i)}{a_1 (\text{MW of } A_1)} \text{ for } i = 2 \rightarrow m$$

Note that mass stoichiometric coefficients are normalized by the molecular weight of the reference compound (typically reactant 1).

Units: mass (grams, kilograms)

Charge and element mass is not conserved

Total mass of reactants = total mass of products

That is:

$$\sum_{i=1}^k \Psi_i = \sum_{i=k+1}^m \Psi_i$$

Example:



Reference compound is glucose, MW = 180

$$\Psi_1 = 1$$

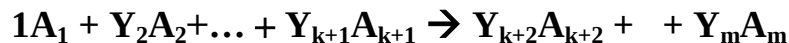
$$\Psi_2 = 6(32)/180 = 1.067 \text{ g-O}_2/\text{g-glucose}$$

$$\Psi_3 = 6(44)/180 = 1.467 \text{ g-CO}_2/\text{g-glucose}$$

$$\Psi_4 = 6(18)/180 = 0.60 \text{ g-H}_2\text{O/g-glucose}$$

$$\begin{aligned} \text{balance: } 1 + 1.067 &= 2.067 \\ 1.467 + 0.6 &= 2.067 \end{aligned}$$

COD (electron):



where the reference compound is COD and the stoichiometric coefficients, Y_i are in units of mass COD

$$\text{Y}_1 = 1$$

$$\text{Y}_i = \frac{a_i(\text{MW} - A_i)(\text{COD}_i)}{a_1(\text{MW} - A_1)(\text{COD}_1)} = \Psi_i \frac{\text{COD}_i}{\text{COD}_1}$$

Where COD_i is the COD equivalent of the i th compound. For example the COD equivalent of glucose is $6 \cdot 32 / 180 = 1.067 \text{ g-COD/g-glucose}$ (see molar stoichiometry above).

Other useful COD equivalents: $\text{COD}_{\text{cells}} (\text{C}_5\text{H}_7\text{NO}_2) = 5(32)/113 = 1.42 \text{ g-COD/g-cells}$

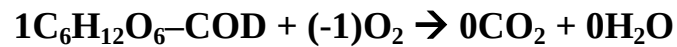
$$\text{COD}_{\text{O}_2} = -1 \text{ g-COD/g-O}_2$$

COD equivalent of water, CO_2 , and any other compound not involved in exchange of electrons is zero.

Units: g-COD

COD mass is conserved

Example:



$$\begin{array}{l} \text{Balance:} \quad 1 - 1 = 0 \\ \quad \quad \quad 0 + 0 = 0 \end{array}$$