

Stoichiometry

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Chemical equations

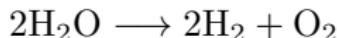
- ▶ a chemical reaction involves p reactants, q products (molecules)
- ▶ expressed as



- reactants R_1, \dots, R_p , products P_1, \dots, P_q
- coefficients $a_1, \dots, a_p, b_1, \dots, b_q > 0$
- ▶ coefficients usually integers, but can be scaled
 - e.g., multiplying all coefficients by 1/2 doesn't change the reaction

Example

electrolysis of water:



- ▶ one reactant: water (H_2O)
- ▶ two products: hydrogen (H_2) and oxygen (O_2)
- ▶ reaction consumes 2 water molecules and produces 2 hydrogen molecules and 1 oxygen molecule

Balancing equations

- ▶ each molecule (reactant/product) contains specific numbers of (types of) atoms, given in its formula
 - e.g., H_2O contains two H and one O
- ▶ *conservation of mass*: total number of each type of atom in a chemical equation must *balance*
- ▶ for each atom, total number on LHS must equal total on RHS
- ▶ e.g., electrolysis reaction is balanced:
 - 4 units of H on LHS and RHS
 - 2 units of O on LHS and RHS
- ▶ finding (nonzero) coefficients to achieve balance is called *balancing equations*

Reactant and product matrices

- ▶ consider reaction with m types of atoms, p reactants, q products
- ▶ $m \times p$ reactant matrix R is defined by

R_{ij} = number of atoms of type i in reactant R_j ,

$$i = 1, \dots, m, \quad j = 1, \dots, p$$

- ▶ with $a = (a_1, \dots, a_p)$ (vector of reactant coefficients)

Ra = (vector of) total numbers of atoms of each type in reactants

- ▶ define product $m \times q$ matrix P in similar way
- ▶ m -vector Pb is total numbers of atoms of each type in products
- ▶ conservation of mass is $Ra = Pb$

Balancing equations via linear equations

- ▶ conservation of mass is $\begin{bmatrix} R & -P \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 0$
- ▶ simple solution is $a = b = 0$
- ▶ to find a nonzero solution, set any coefficient (say, a_1) to be 1
- ▶ balancing chemical equations can be expressed as solving a set of $m + 1$ linear equations in $p + q$ variables

$$\begin{bmatrix} R & -P \\ e_1^T & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = e_{m+1}$$

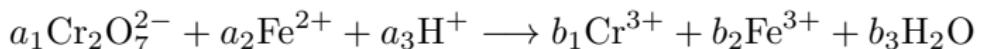
(we ignore here that a_i and b_i should be nonnegative integers)

Conservation of charge

- ▶ can extend to include charge, e.g., $\text{Cr}_2\text{O}_7^{2-}$ has charge -2
- ▶ *conservation of charge*: total charge on each side of reaction must balance
- ▶ we can simply treat charge as another type of atom to balance

Example

- ▶ reaction to balance



- ▶ 5 atoms/charge: as Cr, O, Fe, H, charge
- ▶ reactant and product matrix:

$$R = \begin{bmatrix} 2 & 0 & 0 \\ 7 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -2 & 2 & 1 \end{bmatrix}, \quad P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \\ 3 & 3 & 0 \end{bmatrix}$$

Balancing equations example

- balancing: system of equations (including $a_1 = 1$ constraint)

$$\begin{bmatrix} 2 & 0 & 0 & -1 & 0 & 0 \\ 7 & 0 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -2 \\ -2 & 2 & 1 & -3 & -3 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Balancing equations example

- ▶ solving the system yields

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 6 \\ 14 \\ 2 \\ 6 \\ 7 \end{bmatrix}$$

- ▶ the balanced equation is

