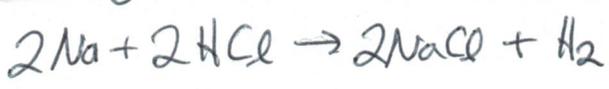


Mass-Mass Stoichiometry Math for MIS

Nov 8, 2019

→ only value to include 0 or N? use Z+?



Types

Element T = $\{ \text{H, He, Li, Be, B, C, ...} \}$ ← not strings

ex Na, H, Cl

^{Mol}Molecule T = tuple of (num: N, elem: Element T)

(1, Na), (1, H), (2, H)

Compound T = Set of Molecule T ← this says order doesn't matter

~~Component T = tuple of (num: N, Molec: Molecule T)~~
~~tuple of (num: N, Compound: Compound T)~~

$\{ \text{Na} \}$
 $\{ (1, \text{H}), (1, \text{Cl}) \}$
 $\{ (1, \text{Na}), (1, \text{H}) \}$
 $\{ (2, \text{H}) \}$

Etc

Stoichiometry

Stoichiometric T = tuple of (num: N, Compound: Compound T)

(2, $\{ (1, \text{Na}) \}$)
 (2, $\{ (1, \text{H}), (1, \text{Cl}) \}$)
 (2, $\{ (1, \text{Na}), (1, \text{H}) \}$)
 (1, $\{ (2, \text{H}) \}$)

Chemical Eq T = set of Compound Stoichiometric T

Reaction T = sequence [2] of Chemical Eq T

Functions

← function type (signature)

atomic Mass: Element T → R

atomic Mass (e) ≡ (e = H ⇒ 1.0079 | e = He ⇒ 4.0026 | ...)

num Atoms In Molec: Molecule T × Element T → N

num Atoms In Molec (M, e) ≡ (m.elem = e ⇒ m.num | m.elem ≠ e ⇒ 0)

num Atoms In Compound C: Compound T × Element T → N

num Atoms In Compound (C, e) ≡ $\sum (m: \text{Molecule T} \mid m \in C \cdot \text{num Atoms In Molec}(m, e))$

Gros & Schneider notation → $\otimes (x: T \mid R \cdot E)$

num Atoms In Stoichiometric: Stoichiometric T × Element T → N

num Atoms In Stoichiometric (S, e) ≡ S.coeff * num Atoms In Compound (S.Compound.e)