Mass-Mass Stoichiometry Math for MIS

Nov 8, 2019

$2Na + 2HCl \rightarrow 2NaCl + H_2$

→ any value to including 0 & ℕ? use ℤ+?

Types

ElementT = { H, He, Li, Be, B, C, ... } ← not strings

ex Na, N, Cl

MoleculeT = tuple of (num: ℕ, elem: ElementT)

(1, Na), (1, N), (2, N)

CompoundT = set of MoleculeT ← this says order doesn't matter

~~CompoundT = tuple of (num: ℕ, Molec: MoleculeT)~~
~~tuple of (num: ℕ, Compound: CompoundT)~~

{ (1, Na) }
{ (1, N), (1, C
{ (1, Na), (1,
{ (2, N) }

~~Eq~~
~~Stoichiometry~~ coeff
StoichiometricT = tuple of (~~num~~: ℕ, Compound: CompoundT)

{2, { (1, Na) }
{2, { (1, N), (1,
{2, { (1, Na), (1
{1, { (2, N) }

ChemicalEqT = set of ~~Compound~~ StoichiometricT

ReactionT = sequence [2] of ChemicalEqT

Functions

functor type (signature)

atomicMass : ElementT → ℝ
atomicMass(e) ≡ (e = H ⇒ 1.0079 | e = He ⇒ 4.0026 | ...)

---

numAtomsInMolec : MoleculeT × ElementT → ℕ
numAtomsInMolec(m, e) ≡ (m.elem = e ⇒ m.num | m.elem ≠ e ⇒ 0)

---

numAtomsInCompound : CompoundT × ElementT → ℕ
numAtomsInCompound(C, e) ≡ +(m : MoleculeT | m ∈ C • numAtomsInMolec(m,

Gries & Schneider notation → (*)(x : T | R • E)

---

numAtomsInStoichiometric : StoichiometricT × ElementT → ℕ
numAtomsInStoichiometric(S, e) ≡ S.coeff * numAtomsInCompound
(S.Compound, e