

Examples

Molecular Mass

$$\text{ChemMass} ("Fe2O3") = 159.6922 \frac{\text{kg}}{\text{mol}}$$

Balancing equations using null space

$$R := ["Fe" "O2" "Fe2O3"]$$

$$\text{ChemAtoms} (R) = \begin{bmatrix} "" & "Fe" & "O2" & "Fe2O3" \\ "Fe" & 1 & 0 & 2 \\ "O" & 0 & 2 & 3 \end{bmatrix}$$

$$\text{ChemBal} (R) = ["2 Fe2O3 -> 4 Fe + 3 O2" 4 3 -2]$$

ChemAtoms give the matrix for solve for the null space, which can be rounded to integer values. Positive values are products, negative are reactants. You can change this with 'ChemSign:=-1'.

$$C := \text{null} \left(\text{ChemAtoms} (R)_{[2..3][2..4]} \right) = \begin{bmatrix} 0.7428 \\ 0.5571 \\ -0.3714 \end{bmatrix} \xrightarrow{\text{round} (5.3852 \cdot C, 0)} \begin{bmatrix} 4 \\ 3 \\ -2 \end{bmatrix}$$

$$R := ["C2H6" "O2" "CO2" "H2O"]$$

$$\text{ChemAtoms} (R) = \begin{bmatrix} "" & "C2H6" & "O2" & "CO2" & "H2O" \\ "C" & 2 & 0 & 1 & 0 \\ "H" & 6 & 0 & 0 & 2 \\ "O" & 0 & 2 & 2 & 1 \end{bmatrix}$$

$$\text{ChemBal} (R) = ["4 CO2 + 6 H2O -> 2 C2H6 + 7 O2" 2 7 -4 -6]$$

$$R := ["C2H6" "O2" "CO2" "H2O"]$$

$$\text{ChemAtoms} (R) = \begin{bmatrix} "" & "C2H6" & "O2" & "CO2" & "H2O" \\ "C" & 2 & 0 & 1 & 0 \\ "H" & 6 & 0 & 0 & 2 \\ "O" & 0 & 2 & 2 & 1 \end{bmatrix}$$

$$\text{ChemBal} (R) = ["4 CO2 + 6 H2O -> 2 C2H6 + 7 O2" 2 7 -4 -6]$$

$$R := ["NaOH" "H2SO4" "Na2SO4" "H2O"]$$

$$\text{ChemBal} (R) = [" Na2SO4 + 2 H2O -> 2 NaOH + H2SO4" 2 1 -1 -2]$$

$$R := ["NaCl" "SO2" "H2O" "O2" "Na2SO4" "HCl"]$$

$$\text{ChemBal} (R) = ["2 Na2SO4 + 4 HCl -> 4 NaCl + 2 SO2 + 2 H2O + O2" 4 2 2 1 ...]$$

ToDo: include parenthesis into compounds. Right now you can't.

Balance $\text{K}_4\text{Fe}(\text{CN})_6 + 6 \text{H}_2\text{SO}_4 + 6 \text{H}_2\text{O} = 2 \text{K}_2\text{SO}_4 + \text{FeSO}_4 + 3 (\text{NH}_4)_2\text{SO}_4 + 6 \text{CO}$

$R := [\text{"K}_4\text{FeC}_6\text{N}_6" \text{"H}_2\text{SO}_4" \text{"H}_2\text{O}" \text{"K}_2\text{SO}_4" \text{"FeSO}_4" \text{"N}_2\text{H}_8\text{SO}_4" \text{"CO"}]$

$$A := \text{ChemAtoms} (R) = \begin{bmatrix} "" & \text{"K}_4\text{FeC}_6\text{N}_6" & \text{"H}_2\text{SO}_4" & \text{"H}_2\text{O}" & \text{"K}_2\text{SO}_4" & \text{"FeSO}_4" & \text{"N}_2\text{H}_8\text{SO}_4" & \text{"CO"} \\ \text{"K"} & 4 & 0 & 0 & 2 & 0 & 0 & 0 \\ \text{"Fe"} & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ \text{"C"} & 6 & 0 & 0 & 0 & 0 & 0 & 1 \\ \text{"N"} & 6 & 0 & 0 & 0 & 0 & 2 & 0 \\ \text{"H"} & 0 & 2 & 2 & 0 & 0 & 8 & 0 \\ \text{"S"} & 0 & 1 & 0 & 1 & 1 & 1 & 0 \\ \text{"O"} & 0 & 4 & 1 & 4 & 4 & 4 & 1 \end{bmatrix}$$

$$\text{ChemBal} (R) = [\text{" K}_4\text{FeC}_6\text{N}_6 + 6 \text{H}_2\text{SO}_4 + 6 \text{H}_2\text{O} -> 2 \text{K}_2\text{SO}_4 + \text{FeSO}_4 + 3 \text{N}_2\text{H}_8\text{SO}_4 + 6 \text{CO}" -1 -6 -6 2 ...]$$

Two solutions: I don't know what can do here very well because usually it means that can be more than one reaction, but I don't understand this case..

$R := [\text{"CO"} \text{"CO}_2" \text{"H}_2" \text{"CH}_4" \text{"H}_2\text{O}"]$

$$C\$:= \text{ChemAtoms} (R) = \begin{bmatrix} "" & \text{"CO"} & \text{"CO}_2" & \text{"H}_2" & \text{"CH}_4" & \text{"H}_2\text{O}" \\ \text{"C"} & 1 & 1 & 0 & 1 & 0 \\ \text{"O"} & 1 & 2 & 0 & 0 & 1 \\ \text{"H"} & 0 & 0 & 2 & 4 & 2 \end{bmatrix}$$

$$C := \text{null} \left(\text{ChemAtoms} (R) \begin{bmatrix} 2..4 \\ 2..6 \end{bmatrix} \right) = \begin{bmatrix} 0.662790490127092 & -0.353286470586764 \\ -0.351617456828673 & 0.429019197409211 \\ 0.581901643066585 & 0.656217377876552 \\ -0.311173033298419 & -0.075732726822447 \\ 0.040444423530254 & -0.504751924231658 \end{bmatrix}$$

No solutions: Here the error msg it's ok, can't be reactions with this compounds.

$R := [\text{"FeS}_2" \text{"HNO}_3" \text{"Fe}_2\text{S}_3\text{O}_{12}" \text{"NO"} \text{"H}_2\text{SO}_4"]$

$$\text{ChemBal} (R) = \blacksquare$$

$$\text{ChemAtoms} (R) = \begin{bmatrix} "" & \text{"FeS}_2" & \text{"HNO}_3" & \text{"Fe}_2\text{S}_3\text{O}_{12}" & \text{"NO"} & \text{"H}_2\text{SO}_4" \\ \text{"Fe"} & 1 & 0 & 2 & 0 & 0 \\ \text{"S"} & 2 & 0 & 3 & 0 & 1 \\ \text{"H"} & 0 & 1 & 0 & 0 & 2 \\ \text{"N"} & 0 & 1 & 0 & 1 & 0 \\ \text{"O"} & 0 & 3 & 12 & 1 & 4 \end{bmatrix}$$

Alvaro