
 ☒—Utilities

 ☒—rat

 ☒—Chem Bal

ChemSign := 1

TOL := 10^{-12}

 ☒—Examples

Balancing equations using null space

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

ChemMass (R) = [55.847 31.9988 159.6922] $\frac{\text{g}}{\text{mol}}$

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

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'.

General procedure is, given a list of compounds

R := ["NH4ClO4(s)" "Al(s)" "Al2O3(s)" "AlCl3(s)" "H2O(g)" "N2(g)"]

Find the Atoms in one compound

 $R_1 = \text{"NH4ClO4(s)"}$

$$\text{ChemAtoms} (R_1) = \begin{bmatrix} \text{"N"} & 1 \\ \text{"H"} & 4 \\ \text{"Cl"} & 1 \\ \text{"O"} & 4 \end{bmatrix}$$

Doing that for each compound, we get a Matrix with compositions

$$A := \text{ChemAtoms} (R) = \begin{bmatrix} "" & \text{"NH4ClO4(s)"} & \text{"Al(s)"} & \text{"Al2O3(s)"} & \text{"AlCl3(s)"} & \text{"H2O(g)"} & \text{"N2(g)"} \\ \text{"N"} & 1 & 0 & 0 & 0 & 0 & 2 \\ \text{"H"} & 4 & 0 & 0 & 0 & 2 & 0 \\ \text{"Cl"} & 1 & 0 & 0 & 3 & 0 & 0 \\ \text{"O"} & 4 & 0 & 3 & 0 & 1 & 0 \\ \text{"Al"} & 0 & 1 & 2 & 1 & 0 & 0 \end{bmatrix}$$

Basis for the Null space of the compositions

$$B := \text{null} \left(A \begin{bmatrix} 2 \dots \text{rows} (A) \end{bmatrix} \begin{bmatrix} 2 \dots \text{cols} (A) \end{bmatrix} \right) = \begin{bmatrix} 0.3413 \\ 0.5689 \\ -0.2276 \\ -0.1138 \\ -0.6827 \\ -0.1707 \end{bmatrix}$$

B are the coefficients for balance the equation. Final step is try to convert it to integers. rat returns Num and Den as the best rational approximation for B, and lcm is the Euclidean least common multiplier.

$$\begin{bmatrix} N & D \end{bmatrix} := \text{rat} \left(\frac{B}{\min(|B|)} \right) = \begin{bmatrix} 3 \\ 5 \\ -2 \\ -1 \\ -6 \\ -3 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 2 \end{bmatrix} \quad \text{lcm}(D) \cdot \frac{N}{D} = \begin{bmatrix} 6 \\ 10 \\ -4 \\ -2 \\ -12 \\ -3 \end{bmatrix} \quad \text{coeffs of} \quad R^T = \begin{bmatrix} \text{"NH4ClO4(s)"} \\ \text{"Al(s)"} \\ \text{"Al2O3(s)"} \\ \text{"AlCl3(s)"} \\ \text{"H2O(g)"} \\ \text{"N2(g)"} \end{bmatrix}$$

ChemBal (R) = ["4 Al2O3(s) + 2 AlCl3(s) + 12 H2O(g) + 3 N2(g) -> 6 NH4ClO4(s) + 10 Al(s)"]

Examples

$$R := [\text{"(NH}_4\text{)}_2\text{Cr}_2\text{O}_7\text{(s)} \text{ "Cr}_2\text{O}_3\text{(s)} \text{ "N}_2\text{(g)} \text{ "H}_2\text{O(g)} \text{ "}]$$

$$\text{ChemBal}(R) = [\text{"(NH}_4\text{)}_2\text{Cr}_2\text{O}_7\text{(s)} \rightarrow \text{Cr}_2\text{O}_3\text{(s)} + \text{N}_2\text{(g)} + 4 \text{ H}_2\text{O(g)} \text{ " } -1 \ 1 \ 1]$$

$$R := [\text{"Al(s)} \text{ "NH}_4\text{ClO}_4\text{(s)} \text{ "Al}_2\text{O}_3\text{(s)} \text{ "AlCl}_3\text{(s)} \text{ "H}_2\text{O(g)} \text{ "N}_2\text{(g)} \text{ "}]$$

$$\text{ChemBal}(R) = [\text{"4 Al}_2\text{O}_3\text{(s)} + 2 \text{ AlCl}_3\text{(s)} + 12 \text{ H}_2\text{O(g)} + 3 \text{ N}_2\text{(g)} \rightarrow 10 \text{ Al(s)} + 6 \text{ NH}_4\text{ClO}_4\text{(s)} \text{ "}]$$

$$R := [\text{"C}_8\text{H}_{18}\text{(g)} \text{ "O}_2\text{(g)} \text{ "CO}_2\text{(g)} \text{ "H}_2\text{O(l)} \text{ "}]$$

$$\text{ChemBal}(R) = [\text{"16 CO}_2\text{(g)} + 18 \text{ H}_2\text{O(l)} \rightarrow 2 \text{ C}_8\text{H}_{18}\text{(g)} + 25 \text{ O}_2\text{(g)} \text{ " } 2 \ 25 \ -16]$$

$$R := [\text{"C}_7\text{H}_{16}\text{(g)} \text{ "O}_2\text{(g)} \text{ "CO}_2\text{(g)} \text{ "H}_2\text{O(l)} \text{ "}]$$

$$\text{ChemBal}(R) = [\text{"7 CO}_2\text{(g)} + 8 \text{ H}_2\text{O(l)} \rightarrow \text{C}_7\text{H}_{16}\text{(g)} + 11 \text{ O}_2\text{(g)} \text{ " } 1 \ 11 \ -7 \ -8]$$

$$R := [\text{"Pb(NO}_3\text{)}_2\text{(aq)} \text{ "NaCl(aq)} \text{ "NaNO}_3\text{(aq)} \text{ "PbCl}_2\text{(s)} \text{ "}]$$

$$\text{ChemBal}(R) = [\text{"Pb(NO}_3\text{)}_2\text{(aq)} + 2 \text{ NaCl(aq)} \rightarrow 2 \text{ NaNO}_3\text{(aq)} + \text{PbCl}_2\text{(s)} \text{ " } -1]$$

$$R := [\text{"C}_2\text{H}_5\text{OH(l)} \text{ "O}_2\text{(g)} \text{ "CO}_2\text{(g)} \text{ "H}_2\text{O(l)} \text{ "}]$$

$$\text{ChemBal}(R) = [\text{"2 CO}_2\text{(g)} + 3 \text{ H}_2\text{O(l)} \rightarrow \text{C}_2\text{H}_5\text{OH(l)} + 3 \text{ O}_2\text{(g)} \text{ " } 1 \ 3 \ -2 \ -3]$$
Reactions with ions

$$R := [\text{"Fe}^{+2} \text{ "Cr}_2\text{O}_7^{-2} \text{ "H}^+ \text{ "Fe}^{+3} \text{ "Cr}^{+3} \text{ "H}_2\text{O} \text{ "}]$$

$$\text{ChemAtoms}(R) = \begin{bmatrix} & \text{"Fe}^{+2} \text{ "Cr}_2\text{O}_7^{-2} \text{ "H}^+ \text{ "Fe}^{+3} \text{ "Cr}^{+3} \text{ "H}_2\text{O} \text{ " \\ "Fe" & 1 & 0 & 0 & 1 & 0 & 0 \\ "Q" & 2 & -2 & 1 & 3 & 3 & 0 \\ "Cr" & 0 & 2 & 0 & 0 & 1 & 0 \\ "O" & 0 & 7 & 0 & 0 & 0 & 1 \\ "H" & 0 & 0 & 1 & 0 & 0 & 2 \end{bmatrix} \quad \leftarrow Q \text{ are the charges.}$$

$$\text{ChemBal}(R) = [\text{"6 Fe}^{+3} + 2 \text{ Cr}^{+3} + 7 \text{ H}_2\text{O} \rightarrow 6 \text{ Fe}^{+2} + \text{Cr}_2\text{O}_7^{-2} + 14 \text{ H}^+ \text{ " } 6]$$

$$R := [\text{"Cr}_2\text{O}_7^{-2} \text{ "H}^+ \text{ "I}^- \text{ "Cr}^{+3} \text{ "I}_2 \text{ "H}_2\text{O} \text{ "}]$$

$$\text{ChemAtoms}(R) = \begin{bmatrix} & \text{"Cr}_2\text{O}_7^{-2} \text{ "H}^+ \text{ "I}^- \text{ "Cr}^{+3} \text{ "I}_2 \text{ "H}_2\text{O} \text{ " \\ "Cr" & 2 & 0 & 0 & 1 & 0 & 0 \\ "O" & 7 & 0 & 0 & 0 & 0 & 1 \\ "Q" & -2 & 1 & -1 & 3 & 0 & 0 \\ "H" & 0 & 1 & 0 & 0 & 0 & 2 \\ "I" & 0 & 0 & 1 & 0 & 2 & 0 \end{bmatrix}$$

$$\text{ChemBal}(R) = [\text{"Cr}_2\text{O}_7^{-2} + 14 \text{ H}^+ + 6 \text{ I}^- \rightarrow 2 \text{ Cr}^{+3} + 3 \text{ I}_2 + 7 \text{ H}_2\text{O} \text{ " } -1 \ -14]$$

$$R := [\text{"MnO}_4^- \text{ "SnO}_2^{-2} \text{ "MnO}_2 \text{ "SnO}_3^{-2} \text{ "OH}^- \text{ "H}_2\text{O} \text{ "}]$$

$$\text{ChemBal}(R) = [\text{"2 MnO}_2 + 3 \text{ SnO}_3\text{-2} + 2 \text{ OH}^- \rightarrow 2 \text{ MnO}_4^- + 3 \text{ SnO}_2\text{-2} + \text{H}_2\text{O}" }]$$

$$R := [\text{"H}^+ \text{ "Cr2O7-2" "C}_2\text{H}_5\text{OH" "Cr+3" "CO}_2 \text{ "H}_2\text{O}" }]$$

$$\text{ChemBal}(R) = [\text{"4 Cr+3 + 2 CO}_2 + 11 \text{ H}_2\text{O} \rightarrow 16 \text{ H}^+ + 2 \text{ Cr2O7-2} + \text{C}_2\text{H}_5\text{OH}" }]$$

Miscellaneous samples

$$R := [\text{"C}_2\text{H}_6 \text{ "O}_2 \text{ "CO}_2 \text{ "H}_2\text{O}" }]$$

$$\text{ChemBal}(R) = [\text{"4 CO}_2 + 6 \text{ H}_2\text{O} \rightarrow 2 \text{ C}_2\text{H}_6 + 7 \text{ O}_2" \text{ 2 7 -4 -6}]$$

$$R := [\text{"C}_2\text{H}_6 \text{ "O}_2 \text{ "CO}_2 \text{ "H}_2\text{O}" }]$$

$$\text{ChemBal}(R) = [\text{"4 CO}_2 + 6 \text{ H}_2\text{O} \rightarrow 2 \text{ C}_2\text{H}_6 + 7 \text{ O}_2" \text{ 2 7 -4 -6}]$$

$$R := [\text{"NaOH" "H}_2\text{SO}_4 \text{ "Na}_2\text{SO}_4 \text{ "H}_2\text{O}" }]$$

$$\text{ChemBal}(R) = [\text{"Na}_2\text{SO}_4 + 2 \text{ H}_2\text{O} \rightarrow 2 \text{ NaOH} + \text{H}_2\text{SO}_4" \text{ 2 1 -1 -2}]$$

$$R := [\text{"NaCl" "SO}_2 \text{ "H}_2\text{O" "O}_2 \text{ "Na}_2\text{SO}_4 \text{ "HCl}" }]$$

$$\text{ChemBal}(R) = [\text{"2 Na}_2\text{SO}_4 + 4 \text{ HCl} \rightarrow 4 \text{ NaCl} + 2 \text{ SO}_2 + 2 \text{ H}_2\text{O} + \text{O}_2" \text{ 4 2 2 1}]$$

$$R := [\text{"H}_3\text{PO}_4 \text{ "(NH}_4)_2\text{MoO}_4 \text{ "HNO}_3 \text{ "(NH}_4)_3\text{PO}_4(\text{MoO}_3)_{12} \text{ "N}_2\text{H}_4\text{O}_3 \text{ "H}_2\text{O}" }]$$

$$\text{ChemBal}(R) = [\text{"(NH}_4)_3\text{PO}_4(\text{MoO}_3)_{12} + 21 \text{ N}_2\text{H}_4\text{O}_3 + 12 \text{ H}_2\text{O} \rightarrow \text{H}_3\text{PO}_4 + 12 \text{ (NH}_4)_2\text{MoO}_4 + 21 \text{ HNO}_3" \text{ 1 12 21 -1}]$$

$$R := [\text{"MgN}_2\text{O}_6 \text{ "Mg" "N}_2 \text{ "O}_2" }]$$

$$\text{ChemBal}(R) = [\text{"Mg} + \text{N}_2 + 3 \text{ O}_2 \rightarrow \text{MgN}_2\text{O}_6" \text{ 1 -1 -1 -3}]$$

$$R := [\text{"K}_4\text{Fe(CN)}_6 \text{ "H}_2\text{SO}_4 \text{ "H}_2\text{O" "K}_2\text{SO}_4 \text{ "FeSO}_4 \text{ "(NH}_4)_2\text{SO}_4 \text{ "CO}" }]$$

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

$$\text{ChemBal}(R) = [\text{"2 K}_2\text{SO}_4 + \text{FeSO}_4 + 3 \text{ (NH}_4)_2\text{SO}_4 + 6 \text{ CO} \rightarrow \text{K}_4\text{Fe(CN)}_6 + 6 \text{ H}_2\text{SO}_4 + 6 \text{ H}_2\text{O}" \text{ 1 6 6 -2}]$$

$$R := [\text{"K}_4\text{FeC}_6\text{N}_6 \text{ "KMnO}_4 \text{ "H}_2\text{SO}_4 \text{ "KHSO}_4 \text{ "Fe}_2\text{S}_3\text{O}_{12} \text{ "MnSO}_4 \text{ "HNO}_3 \text{ "CO}_2 \text{ "H}_2\text{O}" }]$$

$$B := \text{ChemBal}(R) \quad B_{[2..9]}^T = [10 \ 122 \ 299 \ -162 \ -5 \ -122 \ -60 \ -60]$$

$$B_1 = \text{"162 KHSO}_4 + 5 \text{ Fe}_2\text{S}_3\text{O}_{12} + 122 \text{ MnSO}_4 + 60 \text{ HNO}_3 + 60 \text{ CO}_2 + 188 \text{ H}_2\text{O} \rightarrow 10 \text{ K}_4\text{FeC}_6\text{N}_6 + 122 \text{ KMnO}_4 + 299 \text{ H}_2\text{SO}_4"$$

A := ChemAtoms (R) =	" "	"K4FeC6N6"	"KMnO4"	"H2SO4"	"KHSO4"	"Fe2S3O12"	"MnSO4"	"HNO3"	"CO2"	"H2O"
	"K"	4	1	0	1	0	0	0	0	0
	"Fe"	1	0	0	0	2	0	0	0	0
	"C"	6	0	0	0	0	0	0	1	0
	"N"	6	0	0	0	0	0	1	0	0
	"Mn"	0	1	0	0	0	1	0	0	0
	"O"	0	4	4	4	12	4	3	2	1
	"H"	0	0	2	1	0	0	1	0	2
	"S"	0	0	1	1	3	1	0	0	0

```
R1 := [ "H2" "Ca(CN)2" "NaAlF4" "FeSO4" "MgSiO3" "KI" "H3PO4" "PbCrO4" "BrCl" "CF2Cl2" "SO2" ]
```

```
R2 := [ "PbBr2" "CrCl3" "MgCO3" "KAl(OH)4" "Fe(SCN)3" "PI3" "NaSiO3" "CaF2" "H2O" ]
```

$$R := \text{augment}(R1, R2) \quad B := \text{ChemBal}(R)$$

$$B_1[2 \dots \text{cols}(B)] = [119 \ 18 \ 6 \ 12 \ 6 \ 6 \ 2 \ 12 \ 24 \ 6 \ 24 \ -12 \ -12 \ -6 \ -6 \ -12 \ -2 \ -6 \ -18 \ -110]$$

```
substr (B1, 1, 98) = "12 PbBr2 + 12 CrCl3 + 6 MgCO3 + 6 KAl(OH)4 + 12 Fe(SCN)3 + 2 PI3 + 6 NaSiO3 + 18 CaF2 + 110 H2O ->"
```

$$\text{substr}(B_1, 97, 114) = \text{"} \rightarrow 119 \text{ H}_2 + 18 \text{ Ca(CN)}_2 + 6 \text{ NaAlF}_4 + 12 \text{ FeSO}_4 + 6 \text{ MgSiO}_3 + 6 \text{ KI} + 2 \text{ H}_3\text{PO}_4 + 12 \text{ PbCrO}_4 + 24 \text{ BrCl} + 6 \text{ CF}_2\text{Cl}_2 + 24 \text{ SO}_2 \text{"}$$

Issues

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 := [ "CO" "CO2" "H2" "CH4" "H2O" ]
```

$$A := \text{ChemAtoms}(R) = \begin{bmatrix} "" & "CO" & "CO_2" & "H_2" & "CH_4" & "H_2O" \\ "C" & 1 & 1 & 0 & 1 & 0 \\ "O" & 1 & 2 & 0 & 0 & 1 \\ "H" & 0 & 0 & 2 & 4 & 2 \end{bmatrix}$$

[illegible]

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

```
R := [ "FeS2" "HNO3" "Fe2S3O12" "NO" "H2S04" ]
```

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

$$\text{ChemAtoms}(\mathbf{R}) = \begin{bmatrix} "" & \text{"FeS2"} & \text{"HNO3"} & \text{"Fe2S3O12"} & \text{"NO"} & \text{"H2SO4"} \\ \text{"Fe"} & 1 & 0 & 2 & 0 & 0 \\ \text{"S"} & 2 & 0 & 3 & 0 & 1 \\ \text{"H"} & 0 & 1 & 0 & 0 & 2 \\ \text{"N"} & 0 & 1 & 0 & 1 & 0 \\ \text{"O"} & 0 & 3 & 12 & 1 & 4 \end{bmatrix}$$