

☒—Utilities

☒—rat

☒—Chem Bal

ChemSign := 1 TOL := 10⁻¹²

☒—Examples

Balancing equations using null space

Example

$R := [\text{"KAu(CN)4"} \text{"KAu(CN)2Cl2"} \text{"KHC12"} \text{"Fe4(CN)12Fe3(CN)6"} \text{"PtCl3(H2O)7"}]$

$R := \text{augment}(R, [\text{"Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2"} \text{"K4Fe(CN)6"} \text{"HAuCl3"} \text{"NO2"}])$

Function call

$A := \text{ChemAtoms}(R)$ $B := \text{ChemBal}(R)$

$$A = \begin{bmatrix} \text{"C"} & 4 & 2 & 0 & 18 & 0 & 10 & 6 & 0 & 0 \\ \text{"N"} & 4 & 2 & 0 & 18 & 0 & 8 & 6 & 0 & 1 \\ \text{"K"} & 1 & 1 & 1 & 0 & 0 & 0 & 4 & 0 & 0 \\ \text{"Au"} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ \text{"Cl"} & 0 & 2 & 2 & 0 & 3 & 0 & 0 & 3 & 0 \\ \text{"H"} & 0 & 0 & 1 & 0 & 14 & 24 & 0 & 1 & 0 \\ \text{"Fe"} & 0 & 0 & 0 & 7 & 0 & 0 & 1 & 0 & 0 \\ \text{"O"} & 0 & 0 & 0 & 0 & 7 & 10 & 0 & 0 & 2 \\ \text{"Pt"} & 0 & 0 & 0 & 0 & 1 & 2 & 0 & 0 & 0 \end{bmatrix}$$

$\text{strsplit}(B_1, " \rightarrow ") = [\text{"3 Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2 + 7 K4Fe(CN)6 + 20 HAUCl3 + 6 NO2"} \text{"7 KAu(CN)4 + 13 KAu(CN)2Cl2 + 8 KHC12 + Fe4(CN)12Fe3(CN)6 + 6 PtCl3(H2O)7"}]$

By "hand", main math involved:

$$B := \text{null}(A [2..10][2..10]) \quad [N \ D] := \text{rat}\left(\frac{B}{\min(|B|)}\right) \quad C := \text{Lcm}(D) \cdot \frac{N}{D}$$

Results

$$B = \begin{bmatrix} 0.2455 \\ 0.4559 \\ 0.2806 \\ 0.0351 \\ 0.2104 \\ -0.1052 \\ -0.2455 \\ -0.7014 \\ -0.2104 \end{bmatrix} \quad C = \begin{bmatrix} 7 \\ 13 \\ 8 \\ 1 \\ 6 \\ -3 \\ -7 \\ -20 \\ -6 \end{bmatrix} \quad R^T = \begin{bmatrix} \text{"KAu(CN)4"} \\ \text{"KAu(CN)2Cl2"} \\ \text{"KHC12"} \\ \text{"Fe4(CN)12Fe3(CN)6"} \\ \text{"PtCl3(H2O)7"} \\ \text{"Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2"} \\ \text{"K4Fe(CN)6"} \\ \text{"HAuCl3"} \\ \text{"NO2"} \end{bmatrix}$$

Example

$R := [\text{"Yb4(CN)12Yb3(CN)6"} \text{"CsRu(CN)2F2"} \text{"CsRu(CN)4"} \text{"CsHF2"} \text{"PtF3(H2O)7"}]$

$R := \text{augment}(R, [\text{"Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2"} \text{"Cs4Yb(CN)6"} \text{"HRuF3"} \text{"NO2"}])$

Function call

$A := \text{ChemAtoms}(R)$ $B := \text{ChemBal}(R)$

$$A = \begin{bmatrix} \text{"C"} & 18 & 2 & 4 & 0 & 0 & 10 & 6 & 0 & 0 \\ \text{"N"} & 18 & 2 & 4 & 0 & 0 & 8 & 6 & 0 & 1 \\ \text{"Yb"} & 7 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \text{"Cs"} & 0 & 1 & 1 & 1 & 0 & 0 & 4 & 0 & 0 \\ \text{"Ru"} & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ \text{"F"} & 0 & 2 & 0 & 2 & 3 & 0 & 0 & 3 & 0 \\ \text{"H"} & 0 & 0 & 0 & 1 & 14 & 24 & 0 & 1 & 0 \\ \text{"O"} & 0 & 0 & 0 & 0 & 7 & 10 & 0 & 0 & 2 \\ \text{"Pt"} & 0 & 0 & 0 & 0 & 1 & 2 & 0 & 0 & 0 \end{bmatrix}$$

$\text{strsplit}(B_1, " \rightarrow ") = [\text{"3 Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2 + 7 Cs4Yb(CN)6 + 20 HRuF3 + 6 NO2"} \text{"Yb4(CN)12Yb3(CN)6 + 13 CsRu(CN)2F2 + 7 CsRu(CN)4 + 8 CsHF2 + 6 PtF3(H2O)7"}]$

By "hand", main math
involved:

$$B := null \left(A \begin{matrix} [2..10] \\ [2..10] \end{matrix} \right) \quad [N \ D] := rat \left(\frac{B}{\min(|B|)} \right) \quad C := Lcm(D) \cdot \frac{\vec{N}}{D}$$

Results

$$B = \begin{bmatrix} 0.0351 \\ 0.4559 \\ 0.2455 \\ 0.2806 \\ 0.2104 \\ -0.1052 \\ -0.2455 \\ -0.7014 \\ -0.2104 \end{bmatrix} \quad C = \begin{bmatrix} 1 \\ 13 \\ 7 \\ 8 \\ 6 \\ -3 \\ -7 \\ -20 \\ -6 \end{bmatrix} \quad R^T = \begin{bmatrix} \text{"Yb4(CN)12Yb3(CN)6"} \\ \text{"CsRu(CN)2F2"} \\ \text{"CsRu(CN)4"} \\ \text{"CsHF2"} \\ \text{"PtF3(H2O)7"} \\ \text{"Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2"} \\ \text{"Cs4Yb(CN)6"} \\ \text{"HRuF3"} \\ \text{"NO2"} \end{bmatrix}$$

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