⊞—Utilities

⊞—rat

⊞—Chem Bal

$ChemSign := 1$ $TOL := 10^{-12}$

⊟—Examples

Balancing equations using null space

Example

$R := [$ "KAu(CN)4" "KAu(CN)2Cl2" "KHCl2" "Fe4(CN)12Fe3(CN)6" "PtCl3(H2O)7" $]$

$R := augment(R, [$ "Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2" "K3.99Fe(CN)6" "HAuCl3" "NO2" $])$

Function call $A := ChemAtoms(R)$ $B := ChemBal(R)$

$A =$

	"KAu(CN)4"	"KAu(CN)2Cl2"	"KHCl2"	"Fe4(CN)12Fe3(CN)6"	"PtCl3(H2O)7"	"Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2"	"K3.99Fe(CN)6"	"HAuCl3"	"NO2"
"C"	4	2	0	18	0	10	6	0	0
"N"	4	2	0	18	0	8	6	0	1
"K"	1	1	1	0	0	0	3.99	0	0
"Au"	1	1	0	0	0	0	0	1	0
"Cl"	0	2	2	0	3	0	0	3	0
"H"	0	0	1	0	14	24	0	1	0
"Fe"	0	0	0	7	0	0	1	0	0
"O"	0	0	0	0	7	10	0	0	2
"Pt"	0	0	0	0	1	2	0	0	0

$strsplit(B_1, " -> ") =$ "2793 KAu(CN)4 + 5179 KAu(CN)2Cl2 + 3200 KHCl2 + 400 Fe4(CN)12Fe3(CN)6 + 2386 PtCl3(H2O)7"
"1193 Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2 + 2800 K3.99Fe(CN)6 + 7972 HAuCl3 + 2386 NO2"

By "hand", main math involved: $B := null(A_{[2..10][2..10]})$ $[N\ D] := rat\left(\frac{B}{\min(|\overrightarrow{B}|)}\right)$ $C := lcm(D) \cdot \frac{\overrightarrow{N}}{D}$

Results

$$B = \begin{bmatrix} -0.2457 \\ -0.4556 \\ -0.2815 \\ -0.0352 \\ -0.2099 \\ 0.1049 \\ 0.2463 \\ 0.7013 \\ 0.2099 \end{bmatrix} \quad C = \begin{bmatrix} -2793 \\ -5179 \\ -3200 \\ -400 \\ -2386 \\ 1193 \\ 2800 \\ 7972 \\ 2386 \end{bmatrix} \quad R^T = \begin{bmatrix} \text{"KAu(CN)4"} \\ \text{"KAu(CN)2Cl2"} \\ \text{"KHCl2"} \\ \text{"Fe4(CN)12Fe3(CN)6"} \\ \text{"PtCl3(H2O)7"} \\ \text{"Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2"} \\ \text{"K3.99Fe(CN)6"} \\ \text{"HAuCl3"} \\ \text{"NO2"} \end{bmatrix}$$

Example

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

$R := augment(R, [$ "Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2" "Cs3.99Yb(CN)6" "HRuF2.97" "NO2" $])$

Function call $A := ChemAtoms(R)$ $B := ChemBal(R)$

$A =$

	"Yb4(CN)12Yb3(CN)6"	"CsRu(CN)2F2"	"CsRu(CN)4"	"CsHF2"	"PtF3(H2O)7"	"Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2"	"Cs3.99Yb(CN)6"	"HRuF2.97"	"NO2"
"C"	18	2	4	0	0	10	6	0	0
"N"	18	2	4	0	0	8	6	0	1
"Yb"	7	0	0	0	0	0	1	0	0
"Cs"	0	1	1	1	0	0	3.99	0	0
"Ru"	0	1	1	0	0	0	0	1	0
"F"	0	2	0	2	3	0	0	2.97	0
"H"	0	0	0	1	14	24	0	1	0
"O"	0	0	0	0	7	10	0	0	2
"Pt"	0	0	0	0	1	2	0	0	0

$strsplit(B_1, " -> ") =$ "39600 Yb4(CN)12Yb3(CN)6 + 508735 CsRu(CN)2F2 + 288465 CsRu(CN)4 + 308828 CsHF2 + 244186 PtF3(H2O)7"
"122093 Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2 + 277200 Cs3.99Yb(CN)6 + 797200 HRuF2.97 + 244186 NO2"

By "hand", main math involved:

$$B := null\left(A_{[2..10][2..10]}\right) \qquad [N\ D] := rat\left(\frac{B}{\min\left(\left|\overrightarrow{B}\right|\right)}\right) \qquad C := lcm(D)\cdot\frac{\overrightarrow{N}}{D}$$

Results

$$B = \begin{bmatrix} -0.0349 \\ -0.4487 \\ -0.2544 \\ -0.2724 \\ -0.2154 \\ 0.1077 \\ 0.2445 \\ 0.7031 \\ 0.2154 \end{bmatrix} \qquad C = \begin{bmatrix} -39600 \\ -508735 \\ -288465 \\ -308828 \\ -244186 \\ 122093 \\ 277200 \\ 797200 \\ 244186 \end{bmatrix} \qquad R^{T} = \begin{bmatrix} \text{"Yb4(CN)12Yb3(CN)6"} \\ \text{"CsRu(CN)2F2"} \\ \text{"CsRu(CN)4"} \\ \text{"CsHF2"} \\ \text{"PtF3(H2O)7"} \\ \text{"Pt2(NH3)4(C5H4ON)2(NO3)2(H2O)2"} \\ \text{"Cs3.99Yb(CN)6"} \\ \text{"HRuF2.97"} \\ \text{"NO2"} \end{bmatrix}$$

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