Balancing Chemical Equations

Procedure for Balancing an Equation

$$\mathrm{CH_4 + O_2 \rightarrow CO_2 + H_2O}$$

Parsing

```
ElemS = [['C'], ['H'], ['O'], ['C'], ['O'], ['H'], ['O']]
FormulaS = [[['C'], 1], [['H'], 4]], [[['O'], 2]], [[['C'], 1], [['O'], 2]], [[['H'], 2], [['O'], 1]]]
ElementSideSet = [[['C'], ['H'], ['O']], [['C'], ['O'], ['H'], ['O']]]
Equation = [[[[['C'], 1], [['H'], 4]], [[['O'], 2]]], [[[['C'], 1], [['O'], 2]], [[['H'], 2], [['O'], 1]]]]
```

Matrix Tabulation

	CH_4	O_2	$-CO_2$	$-H_2O$
C	1	0	−1	0
H	4	0	0	−2
O	0	2	−2	−1

System of Linear Equations

$$\begin{cases} 1a + 0b - 1c - 0d &= 0 \\ 4a + 0b - 0c - 2d &= 0 \\ 0a + 2b - 2c - 1d &= 0 \end{cases}$$

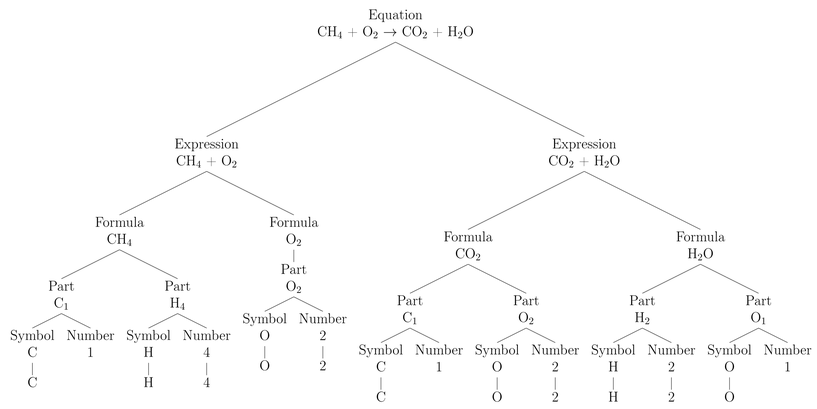
Solving

$$a = 1,\ b = 2,\ c = 1,\ d = 2$$

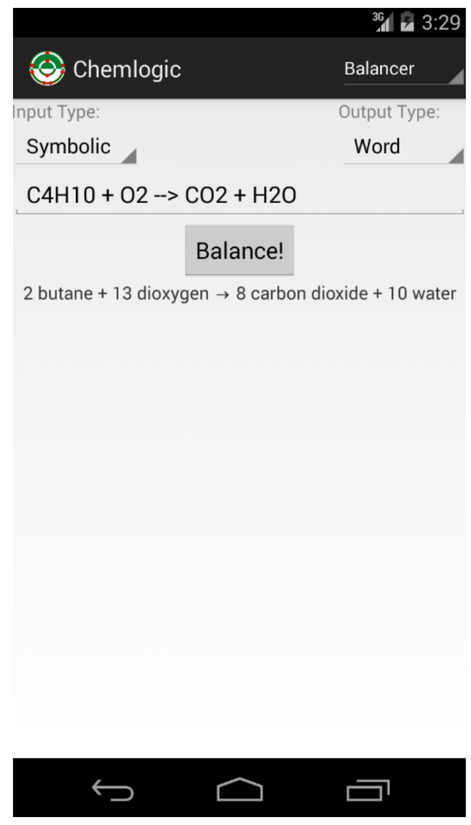
Reverse Parsing

$$\mathrm{CH_4 + \mathit{2}O_2 \rightarrow CO_2 + \mathit{2}H_2O}$$

The Abstract Syntax Tree for a Chemical Equation



Balancing an Equation Using the New Android App



Performing Stoichiometric Calculations

Procedure for Stoichiometric Calculations

$$\mathrm{20\,L\,CH_4 + 10\,L\,O_2 \rightarrow CO_2 + H_2O}$$

Queries: L excess, L excess, L produced, g produced

Parsing

```
FormulaS = [[['C'], 1], [['H'], 4]], [[['O'], 2]], [[['C'], 1], [['O'], 2]], [[['H'], 2], [['O'], 1]]]
QtyS = [[[20, 2], 'L']], [[[10, 2], 'L']], nil, nil]
QueryS = [[[[W, _], 'L']], excess], [[[X, _], 'L']], excess], [[[Y, _], 'L']], actual], [[[Z, _], g]], actual]]
```

Convert to Moles

```
QtyS = [[[0.8923, 2], mol]], [[[0.4462, 2], mol]], nil, nil]
```

Only One Reactant Quantity:

```
QtyIn = ...
FormulaIn = ...
```

More Than One Reactant Quantity:

Determine Limiting Reactant

```
FormulaLim = [[['O'], 2]]
QtyLim = [[[0.4462, 2], mol]]
```

Convert to Result Units

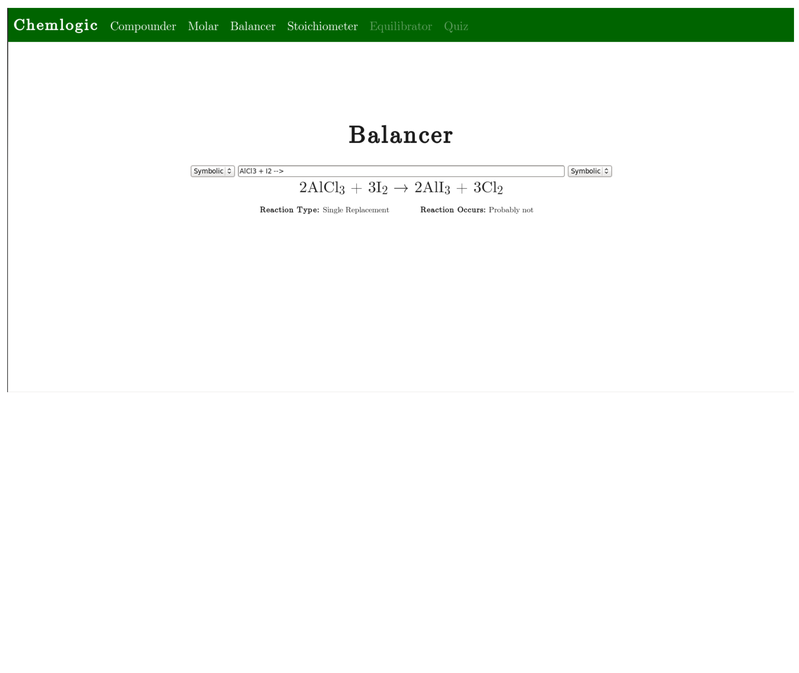
$$W = 15.0,\ \mathrm{X} = 0.0,\ \mathrm{Y} = 5.0,\ Z = 8.0375$$

Reverse Parsing

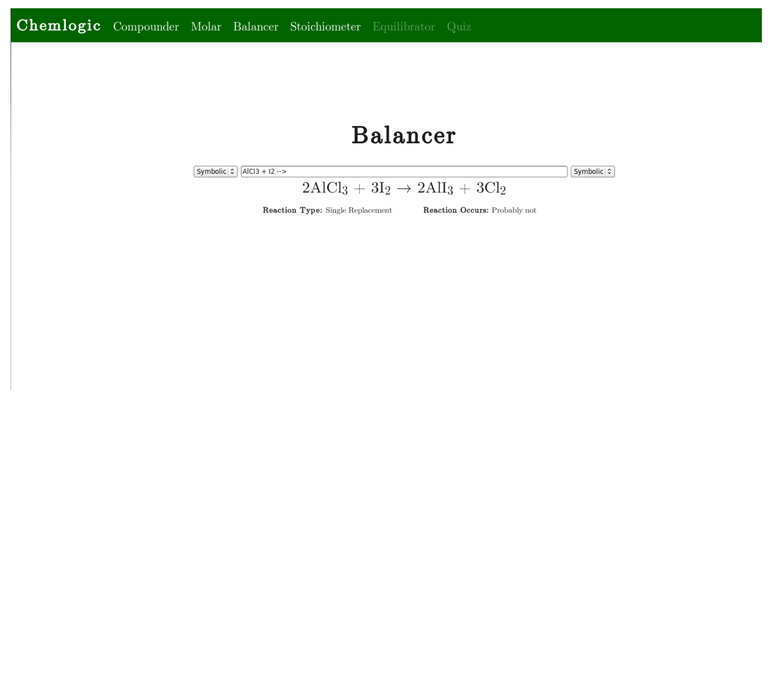
$$\mathrm{20\,\mathit{L}\,\mathit{CH_4} + 10\,L\,\mathit{2}O_2 \rightarrow CO_2 + \mathit{2}H_2O}$$

Results: $=15\ L\ excess$ $=0\ L\ excess$ $=5\ L\ produced$ $=8\ g\ produced$

Solving Stoichiometry Problems



An Example of a Complex Stoichiometry Problem



Reaction Type Analysis

Procedure for Completing Equations

(Example of Double Replacement Reaction)

$$\mathrm{ZnBr_2 + NaCl \rightarrow}$$

Parsing

```
Equation = [[[["Zn", 1], ["Br", 2]], [["Na", 1], ["Cl", 1]]], _]
```

Pattern Matching

```
[[[Metal1,_],[NonMetal1,_]],[[Metal2,_],[NonMetal2,_]]],
[[[Metal1,_],[NonMetal2,_]],[[Metal2,_],[NonMetal1,_]]]
```

Determine Formulas

$$\begin{aligned} (\text{Metal, ChargeM, NonMetal, ChargeNM}) &\Rightarrow [[\text{Metal, ChargeNM}], [\text{NonMetal, ChargeM}]] \\ (\text{"Na"}, 1, \text{"Br"}, -1) &\Rightarrow [[\text{"Na"}, 1], [\text{"Br"}, 1]] \\ (\text{"Zn"}, 2, \text{"Cl"}, -1) &\Rightarrow [[\text{"Zn"}, 1], [\text{"Cl"}, 2]] \end{aligned}$$

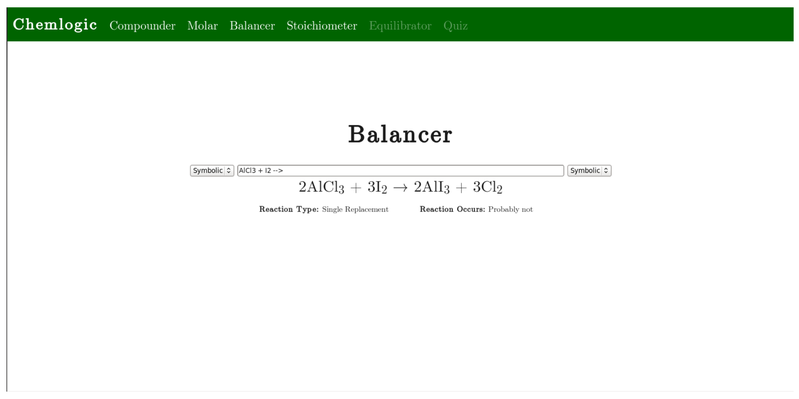
Insert Products

```
Equation = [[[["Zn", 1], ["Br", 2]], [["Na", 1], ["Cl", 1]]], [[["Na",1],["Br",1]],[["Zn",1],["Cl",2]]]]
```

Reverse Parsing

$$\mathrm{ZnBr_2 + NaCl \rightarrow \mathit{ZnCl_2} + \mathit{NaBr}}$$

Identifying, Completing and Predicting Occurence of Reaction



Using the Android App to Complete an Equation