

Appendix A – Mathematica Algorithm

The Mathematica algorithm only establishes the syntax so that the user can input the required equations to solve for unknowns. So this algorithm is useless unless you have used your chemistry knowledge to formulate the equations.

The algorithm is constructed in three parts: 1) Write the equations.
2) Make lists of equations and variables.
3) Solve for variables using the equations.

Part 1) Write the equations.

Name equations: \rightarrow eq1, eq2, eq3,

$$\text{eq1} = 5.6 * 10^{-4} == \frac{z^2}{x * y};$$

$$\text{eq2} = 2 * (0.10) == z + 2 x;$$

$$\text{eq3} = 2 * (0.30) == z + 2 y;$$

Single equal sign to assign equation

Double equal sign within the equation

Semicolon suppresses output

Part 2) Make lists of equations and variables.

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$$\text{equationlist} = \{\text{eq1}, \text{eq2}, \text{eq3}\};$$

$$\text{vars} = \{x, y, z\};$$

Single equal sign to assign the list

Use {curly} brackets to make a list

Part 3) Solve for all variables.

$$\text{Solve}[\text{equationlist}, \text{vars}]$$

'S' in solve must be capitalized

Use [square] brackets with 'Solve' command

Do not put a semicolon here or else the answer will not be displayed

Once the algorithm has been run:

$$\text{In}[1]= \text{eq1} = 5.6 * 10^{-4} == \frac{z^2}{x * y};$$

$$\text{eq2} = 2 * (0.10) == z + 2 x;$$

$$\text{eq3} = 2 * (0.30) == z + 2 y;$$

$$\text{In}[4]= \text{equationlist} = \{\text{eq1}, \text{eq2}, \text{eq3}\};$$

$$\text{vars} = \{x, y, z\};$$

$$\text{In}[6]= \text{Solve}[\text{equationlist}, \text{vars}]$$

$$\text{Out}[6]= \{\{x \rightarrow 0.0979783, y \rightarrow 0.297978, z \rightarrow 0.00404344\}, \\ \{x \rightarrow 0.102078, y \rightarrow 0.302078, z \rightarrow -0.00415546\}\}$$

For your answer, pick the set of values that makes sense: no imaginary numbers, and no negative numbers.