Titrators

Demystifying the titrators – how to calculate out a sample concentration

Titrations can sometimes seem like a mystery, with how they function and how they calculate the final concentration. This procedure will help to demystify the process bit and show step by step how Thermo Scientific™ Orion Star™ T900 Series Automated Titrators use the data found from the titration to calculate the final concentration. This is also very helpful for troubleshooting purposes if there is a discrepancy in results, or possibly something doesn't quite line up.

What you will need and where to find it

- Reaction ratio of the analyte in the sample to the titrant. Reaction ratio = moles of analyte in sample ÷ moles of titrant. Found from the chemical equation for the reaction of the sample with the titrant.

- Volume of titrant in mL dispensed to reach the endpoint. If using the automatic titrator, the endpoint volume (mL) data can be found on the titration report or in the titration log on the titrator.

- Titrant concentration in molarity (M, mol/L). Can be found on the bottle of titrant. If the concentration is stated in normality (N, equivalents/L), convert to M. (See appendix for how to do that).

- Amount of sample titrated as a volume or weight.

- The molecular weight of the analyte. Needed if results will be reported by weight instead of moles, for example, results as mg/L vs. M.

How to manually calculate out results:

1. Calculate the moles of titrant dispensed. Use the molarity (M) of the titrant (moles/L) and the volume (V) of the titrant dispensed (endpoint volume in mL).

   Moles of titrant = $M_{titrant}$ (mol/L) x $V_{titrant}$ (mL) ÷ 1000 mL/L

2. Determine the reaction ratio for the titration. Look at the balanced equation for the titration. Below is an example of titrating sulfuric acid (analyte, H_2SO_4) with sodium hydroxide (titrant, NaOH).

   $H_2SO_4 + 2\ NaOH = Na_2SO_4 + 2\ H_2O$

   Based on the reaction, it takes 1 mole of H_2SO_4 (analyte) to react with 2 moles of NaOH (titrant). That means the reaction ratio (RR) is

   RR = (moles analyte) / (moles titrant) =
   (1 mole H2SO4) / (2 mole NaOH) = 0.5

3. Calculate the moles of analyte in the sample. The reaction ratio is used to convert the moles of titrant to the moles of analyte.

   Moles of analyte = moles of titrant x RR

4. Calculate the final concentration (Conc) results of the analyte in the sample based on the results units desired.

   Examples for liquid samples:
   Conc in M = (moles analyte ÷ Vs) x 1000 mL/L
   Conc in mg/L = (moles analyte ÷ Vs) x 1000 mL/L x MW x 1000 mg/g

Where:

Vs = volume of sample titrated, mL

MW = molecular weight of the analyte, grams/mole

Examples for solid samples:

Conc in mg/kg = (moles analyte ÷ Ws) x MW x 1,000,000 mg/kg

Conc in wt % (w/w) = (moles analyte ÷ Ws) x MW x 100

Where:

Ws = weight of sample titrated, grams

MW = molecular weight of the analyte, grams/mole

What is Molarity?

Molarity is perhaps the most common unit of concentration used by chemists. It is expressed as the number of moles of solute (analyte) dissolved in exactly 1 liter of solution.

$$\text{Molarity (M)} = \frac{\text{number of moles of solute}}{\text{1 liter of solution}}$$

The unit for molarity is mole/L or mol/L and is abbreviated as "M." For example, to prepare a solution of 0.1M sodium hydroxide (NaOH), dissolve 0.1 mole of NaOH into 1 L of water. Then find the weight of 0.1 mole of NaOH, multiply the molecular weight of NaOH (40.0 g/mol) by the desired molarity of the solution. 0.1M NaOH solution = 40.0 g/mol x 0.1 mol/L = 4.0 g NaOH/L solution.

What is Normality?

Another unit of concentration that is commonly used is normality. It is expressed as the number of equivalents of a solute (analyte) dissolved in exactly 1 liter of solution.

$$\text{Normality (N)} = \frac{\text{number of equivalents of solute}}{\text{1 liter of solution}}$$

The unit for normality is equivalents/L or eq/L and is abbreviated as "N." An equivalent is the number of protons, electrons, or ions exchanged per mole in a chemical reaction, like a titration.

Converting Molarity to Normality

To convert a concentration in normality (N) to molarity (M), the following equation can be used:

$$M = N \div n$$

Where n = number of protons, electrons, or ions exchanged per mole in a chemical reaction

For example, to determine the M of a solution of 0.1N NaOH, divide the N of the solution by the number of protons exchanged. For NaOH, n = 1 because each mole of NaOH is capable of neutralizing one mole of protons (H+). The M of a 0.1 N NaOH solution is N/1 = 0.1/1 = 0.1 M. For sulfuric acid (H_2SO_4), n = 2 because each mole of H_2SO_4 is capable of providing 2 moles of protons (H+). The M of a 0.1 N H_2SO_4 solution is N/2 = 0.1/2 = 0.05 M.

Below is a chart of some common titrants with normality, molarity, and the molar equivalent factor.

Common titrants

Titrant	Chemical name	Titration type	Normality (N)	Equiv/mole	Molarity (M)
HCl	hydrochloric acid	acid/base	1	1	1
H_2SO_4	sulfuric acid	acid/base	1	2	0.5
NaOH	sodium hydroxide	acid/base	1	1	1
$Ca(OH)_2$	calcium hydroxide	acid/base	1	2	0.5
I_2	iodine	redox	1	2	0.5
KI-KIO_3	iodide/iodate (iodine)	redox	1	2	0.5
KIO_3	potassium iodate in moderate acid	redox	1	6	0.167
KIO_3	potassium iodate in strong acid	redox	1	4	0.25
$Na_2S_2O_3$	sodium thiosulfate	redox	1	1	1
$C_2H_3NaO_2$	sodium acetate	acid/base	1	1	1
$HClO_4$	perchloric acid	acid/base	1	1	1
$AgNO_3$	silver nitrate	precipitation	1	1	1
NH_4SCN	ammonium thiocynanate	precipitation or complexation	1	1	1
KSCN	potassium thiocyanate	precipitation	1	1	1
EDTA	ethylenediaminetetraacetic acid	complexation	1	1	1
TBAH	tetrabutylammonium hydroxide	acid/base	1	1	1
FAS	ferrous ammonium sulfate	redox	1	1	1
$KMnO_4$	potassium permanganate	redox	1	5	0.2

Appendix – Sample Calculations

The following calculations are shown to further illustrate the above explained process. Each calculation is done using a common application for the Orion Star T900 series titrators. Each shows a separate set of titration conditions and a result in a different concentration unit. The chosen application notes are “Total alkalinity in water by automatic titration,” “Determination of salt content in prepared food by automatic titration” and “Titratable acidity in wine by automatic titration.”

Total alkalinity in water sample calculation

Information Needed	
Molecular weight	100.09 g/mol $CaCO_3$
Reaction ratio	1.000
Titrant molarity	0.05132 M
Volume of titrant dispensed	0.742 mL
Amount of sample	100.0 mL

1. The information needed (above) can be found in the Titration Report (pdf).

2. Calculate the moles of titrant dispensed. Use the molarity (M) of the titrant (moles/L) and the volume (V) of the titrant dispensed (endpoint volume in mL).

   Moles of titrant = 0.05132 mol/L x 0.742 mL ÷ 1000 mL/L = 0.00003808 mol titrant

3. Calculate the moles of analyte in the sample. The reaction ratio is used to convert the moles of titrant to the moles of analyte.

   Moles of analyte = 0.00003808 moles titrant x 1 RR = 0.00003808 mol analyte

4. Calculate the final concentration (Conc) results of the analyte in the sample based on the results units desired.

$$Conc, \frac{mg}{L} = \frac{0.00003808 \text{ } mol\ analyte}{100.0 \text{ } mL} \times 1000 \frac{mL}{L} \times$$

$$100.09 \frac{g}{mol} \times 1000 \frac{mg}{g} = 38.11 \frac{mg}{L} \text{ } as\ CaCO_3$$

Salt in Prepared Food Sample Calculation

Information Needed	
Molecular weight	58.44 g/mol NaCl (salt)
Reaction ratio	1.000
Titrant molarity	0.1127 M
Volume of titrant dispensed	2.421 mL
Amount of sample	0.5675 g

1. The information needed (above) can be found in the Titration Report (pdf).

2. Calculate the moles of titrant dispensed. Use the molarity (M) of the titrant (moles/L) and the volume (V) of the titrant dispensed (endpoint volume in mL).

   Moles of titrant = 0.1127 mol/L x 2.421 mL ÷ 1000 mL/L = 0.0002728 mol titrant

3. Calculate the moles of analyte in the sample. The reaction ratio is used to convert the moles of titrant to the moles of analyte.

   Moles of analyte = 0.0002728 mol titrant x 1 RR = 0.0002728 mol analyte

4. Calculate the final concentration (Conc) results of the analyte in the sample based on the results units desired.

   Conc in weight % (w/w) = (mol analyte ÷ Ws) x MW x 100

$$Conc\%, w/w = \frac{0.0002728 \text{ } mol\ analyte}{0.5675 \text{ } g} \times 58.44 \frac{g}{mol} \times$$

$$100 = 2.810\% \text{ } w/w\ NaCl\ (salt)$$

Titratable acidity in wine sample calculation

Information Needed	
Molecular weight	150.09 g/mol tartaric acid
Reaction ratio	0.500
Titrant molarity	0.1015 M
Volume of titrant dispensed	3.851 mL
Amount of sample	5.0 mL

1. The information needed (above) can be found in the Titration Report (pdf).

2. Calculate the moles of titrant dispensed. Use the molarity (M) of the titrant (moles/L) and the volume (V) of the titrant dispensed (endpoint volume in mL).

   Moles of titrant = 0.1015 mol/L x 3.851 mL ÷ 1000 mL/L = 0.0003909 mol titrant

3. Calculate the moles of analyte in the sample. The reaction ratio is used to convert the moles of titrant to the moles of analyte.

   Moles of analyte = 0.0003909 mol titrant x 0.5 RR = 0.0001954 mol analyte

4. Calculate the final concentration (Conc) results of the analyte in the sample based on the results units desired.

$$\textit{Conc}, \frac{g}{L} = \frac{0.0001954 \textit{ mol analyte}}{5.0 \textit{ mL}} \times 1000 \frac{mL}{L} \times 150.09 \frac{g}{mol} = 5.866 \frac{g}{L} \textit{ as a tartaric acid}$$

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