UNITS OF CONCENTRATION

There are a number of different ways of expressing solute concentration that are commonly used. Some of these are listed below.

Molarity, M = moles solute/liter of solution

Normality, N =equivalents of solute/liter of solution

Weight %, Wt % = mass ratio x 100% = mass of solute/mass of solution x 100%

Parts per million, ppm = mass ration x 10^6 = mass of solute/mass of solution x 10^6

Mass per volume, mg/L = mass of solute/liter of solution

molality, m = moles of solute/mass of solvent

mole fraction, χ = moles of solute/total moles

Concentrations expressed as ppm and N are less familiar to most students at this stage.

Parts per million:

Parts per million concentrations are essentially mass ratios (solute to solution) x a million (10^6). In this sense, they are similar to wt %, which could be thought of as parts per hundred (although nobody uses this term). Since 10^6 milligrams = 1 kg, 1 mg/kg is equivalent to 1 ppm. Similarly, 1 μ g/g and 1 ng/mg are equivalent to 1 ppm.

Given that the density of dilute aqueous solutions is ~ 1.00 kg/L, 1 mg/L of solute in freshwater ≈ 1 ppm. This is true for most freshwater and other dilute aqueous solutions, but not for seawater and concentrated wastewater solutions.

Other variations on this theme include:

ppt – parts per thousand (used for common ions in sea water)

ppb – parts per billion (used for heavy metals and organics)

pptr – parts per trillion (used for trace metals and trace organics)

The following table summarizes common mass ratios for solutions and solids.

Unit	In General		Dilute Aqueous Solutions	
ppm	mg/kg	μg/g	mg/L	μg/mL
ppb	μg/kg	ng/g	μg/L	ng/mL
pptr	ng/kg	pg/g	ng/L	pg/mL

To convert concentrations in mg/L (or ppm in dilute aqueous solution) to molarity, divide by the molar mass of the analyte to convert mass in mg into a corresponding number of moles.

Example: What is the molarity of a 6.2 mg/L solution of $O_2(aq)$?

$$\frac{6.2 \text{ mg O}_2}{L} \times \frac{1 \text{ mol O}_2}{32.09} \times \frac{19}{10^3 \text{ mg}} = 1.9_4 \times 10^{-4} \text{ M}$$

To convert from molarity to mg/L (or ppm in dilute aqueous solution), multiply by the molar mass of the analyte to convert moles into corresponding number of moles.

Example: The Maximum Acceptable Concentration (MAC) of Pb in drinking water is 10 ppb. If a sample has concentration of 55 nM, does it exceed the MAC?

$$55 \times 10^{-9} \frac{\text{mols Pb}}{L} \times \frac{207.29 \, \text{Pb}}{|mol|} \times \frac{10^6 \text{ug}}{|g|} \times \frac{1L}{|kg|}$$

$$= 1/.4 \, \frac{\text{ug}}{kg} = 1/.4 \, \text{ppb}$$

Note 1: In seawater, $1.00 \text{ mg/L} \neq 1.00 \text{ ppm}$ since the density of seawater is 1.035 kg/L.

Hence, $1.00 \text{ mg/L}_{sewater} = 1.00 \text{ mg/L} \times 1 \text{ L/1.035 kg} = 0.966 \text{ mg/kg}$ or 0.966 ppm

Example: The concentration of K⁺ in seawater is reported as 10.6 mM. Convert this conc to ppm.

$$10.6 \times 10^{-3} \frac{\text{mols } K^{+}}{L} \times \frac{39.1 \text{ g } K^{+}}{1 \text{ mol}} \times \frac{1L}{1.035 \text{ kg}} \times \frac{10^{3} \text{ mg}}{9}$$

$$= 400. \frac{mg}{kg} = 400. \text{ ppm}$$

Note 2: Some concentrations are expressed in terms the species actually measured e.g., mg/L of NO₃ (mass of nitrate ions per liter)

Or in terms of a particular element in a species that was measured. e.g., mg/L of NO₃ - N (mass of nitrogen in the form of nitrate ions per liter)

To convert from one to the other of these, use the molar mass ratio of the element to that of the chemical species measured. In the example above use, $14 \text{ mg N/}62 \text{ mg NO}_3$. It is important to clearly report unit values to avoid serious error in interpretation of results. Similar situations arise in reporting the concentrations of ammonia-nitrogen, phosphate-phosphorous and others.

Example: A water sample has a measured phosphate concentration of 6.8 μ M. Express this as μ g/L PO_4^{3-} and ppb PO_4^{3-} P.

6.8 × 10-6 mols P043-
$$\frac{95.0 \text{ g P04}^{3-}}{1 \text{ mol}} \times \frac{10^6 \text{ ug}}{1 \text{ g}} = 650 \text{ ug P04}^{3-}$$
6.46 ug P04 × $\frac{1 \text{ mol P04}^{3-}}{95.0 \text{ g P03}^{3-}} \times \frac{31.0 \text{ g P}}{1 \text{ mol P}} \times \frac{12}{1 \text{ kg}} = 210 \text{ ug P}$
kg

Note 3: Some aggregate parameters are reported in terms of a single surrogate species.

e.g., total hardness is usually reported as the mass of CaCO₃ that would be required to provide the same number of moles of calcium ions.

Example: A groundwater sample has been determined to contain 100. ppm Ca and 80. ppm Mg by flame atomic absorption spectrophotometry. Express the total hardness as ppm CaCO₃.

$$[Ca^{2+}] = 100 \text{ mg Ca} \times \frac{1 \text{ mol}}{40.1 \text{ g Ca}} \times \frac{19}{10^3 \text{ mg}} = 2.49 \times 10^{-3} \text{ mol Ca}$$

$$[Mg^{2+}] = 80 \text{ mg Mg} \times \frac{1 \text{ mol}}{34.3 \text{ g Mg}} \times \frac{19}{10^3 \text{ mg}} = 3.29 \times 10^{-3} \text{ mol Mg}$$

$$[M^{2+}] = [Ca^{2+}] + [Mg^{2+}] = 5.78 \times 10^{-3} \text{ mols } M^{2+}$$

$$5.78 \times 10^{-3} \frac{\text{mols}}{L} \times \frac{100.9 \text{ CaCO}_3}{1.\text{mol}} \times \frac{10^3 \text{ mg}}{9} = 578 \text{ mg CaCO}_3$$

$$578 \text{ mg CaCO}_3 \times \frac{1L}{L} = 578 \text{ mg CaCO}_3 = 578 \text{ ppm CaCO}_3$$

$$\frac{1}{L} \times \frac{1}{L} = 578 \text{ mg CaCO}_3 = 578 \text{ ppm CaCO}_3$$

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Example: A water sample has been found to contain 0.6 mM of As, F and NO₃. The drinking water guidelines for arsenic, fluoride and nitrate-nitrogen are 10 ppb, 1.5 ppm and 10 ppm, respectively. Does this sample exceed the drinking water guidelines for arsenic, fluoride or nitrate - nitrogen?

$$0.6 \times 10^{-3} \frac{\text{mols As}}{\text{L}} \times \frac{74.9 \text{ g As}}{|\text{Imol}|} \times \frac{10^6 \text{ug}}{|\text{Ig}|} \times \frac{1L}{|\text{lkg}|} = \frac{45,000 \text{ ug}}{|\text{kg}|} \text{ As}$$

$$0.6 \times 10^{-3} \frac{\text{mols } F}{\text{L}} \times \frac{19.0 \text{ g } F}{|\text{Imol}|} \times \frac{10^3 \text{ mg}}{|\text{Ig}|} \times \frac{1L}{|\text{lkg}|} = 11.4 \frac{\text{mg } F}{|\text{kg}|}$$

$$0.6 \times 10^{-3} \frac{\text{mol } N0_3^-}{\text{L}} \times \frac{62.0 \text{ g } N0_3^-}{|\text{Imol}|} \times \frac{10^3 \text{ mg}}{|\text{Ig}|} \times \frac{1L}{|\text{lkg}|} = 37 \frac{\text{mg } N0_3^-}{|\text{kg}|}$$

$$37 \frac{\text{mg } N0_3^-}{|\text{kg}|} \times \frac{14.0 \frac{\text{g/mol } N}{|\text{No}_3^-|} = 8.4 \frac{\text{mg } N}{|\text{kg}|}$$

Example: A commercial bleach solution NaOCl(aq) is reported to be 12.5% (weight). If the density is 1.05 g/mL, calculate the molar concentration.

Example: A standard solution is prepared by dissolving 225 mg of sodium thiosulfate pentahydrate in a one litre volumetric flask. After thoroughly mixing, 5.00 mL was transferred to a 250. volumetric flask and diluted to the mark. What is the concentration of molar of thiosulfate in the final solution?

$$Na_2S_2O_3 \cdot 5 H_2O$$
 $MW = 2/2.0 g/mol$
 $\frac{225 \text{ mg}}{1 \text{ L}} \times \frac{1 \text{ mol}}{2/2g} \times \frac{5.00 \text{ mL}}{250. \text{ mL}} \times \frac{/g}{10^3 \text{ mg}} = 2.12 \times 10^{-5} \text{ M}$

Normality is a concentration unit that is still encountered in many texts and lab manuals. It has particular advantages when carrying out acid/base and redox titration calculations, however it can be confusing for the uninitiated. Normality is defined as the number of equivalents of solute per liter, where an equivalent is defined as a mole of reacting species (H⁺ or e-). Normality is always a multiple of Molarity.

$$N = K \times M$$

where K = #equivalents per mole, K is an integer constant ≥ 1

Hence:

Equiv. Weight = M.W./K

and

equivalents of solute = mass of solute/equiv. weight

K for a particular species is defined by the context of the chemical reaction (acid/base vs redox) and the number of moles of H⁺ or e- exchanged per mole of reacting substance.

For acid/base rxn's: K is the number of moles of H⁺ ions produced or neutralized per mole of acid or base supplied. Thus,

Acid/base	K	M.W.	E.W.
	(equiv/mol)	(g/mol)	(g/equiv)
HC1	1	36.5	36.5
H ₂ SO ₄	2	98.1	49.0
CaCO ₃	2	100	50.0
Al(OH) ₃	3	78.0	26.0

Thus, for the reaction;

$$CaCO_3 + 2H^+ \rightarrow Ca^{2+} + H_2CO_3$$

there are 2 moles of H⁺ transferred per each mole of CaCO₃ reacted, so K for CaCO₃ (in this context) is equal to 2 equiv/mol and the equivalent weight of CaCO₃ is equal to 50 g/equiv.

For oxidation/reduction reactions, K is the number of moles of e- transferred per mole of oxidant or reductant in the balanced half-reaction.

Balanced half reaction	K (equiv/mol)	
Fe ³⁺ → Fe	3	
$I_2 \rightarrow 2 \Gamma$	2	
$2 S_2 O_3^{2-} \rightarrow S_4 O_6^{2-}$	1	

Thus, for the reaction;

$$I_2 + 2 S_2 O_3^{2-} \rightarrow 2 I^- + S_4 O_6^{2-}$$

there are 2 moles of electrons transferred per mole of I₂ reacted, so K for I₂ (in this context) is 2 equiv/mol.

Working with Normality in titration calculations

Method 1: Use the appropriate conversion factor (K = #equiv/mol) to convert Normality to Molarity, (i.e., $0.250 \text{ N } \text{H}_2\text{SO}_4 = 0.125 \text{ M } \text{H}_2\text{SO}_4$) and use the coefficients in the balanced chemical equations to solve for the number of moles of analyte in given sample volume.

Method 2: Use the Normal concentrations directly and convert your final analyte concentration from #equiv/L to moles/L or mg/L using K or E.W., respectively. Although you will need to know the chemical form of the analyte in the final product, you do not need the balanced chemical equations.

of equiv. of analyte = # equiv. titrant

This is particularly useful in volumetric determinations, where we can always write;

 $\mathbf{N}_{analyte} \times \mathbf{V}_{analyte} = \mathbf{N}_{titrant} \times \mathbf{V}_{titrant}$ regardless of the complexity of the reaction chemistry involved.

EXAMPLES

1. When 25.00 mL of **NaOH** solution was titrated with 0.572 N **H₂SO₄**, 23.40 mL of was required to reach the end point. Find the molarity of the **NaOH**.

Method 1 convert 0.572
$$\frac{eq}{L} \times \frac{1}{2} \frac{mol}{eq} = 0.286 \frac{mol}{L} H_2 SO_4$$
 $M_{NaOH} = \frac{M_{H_2 SO_4} \times \frac{2 mol}{1 mol} \frac{NaOH}{1 mol} H_2 SO_4}{26.0 \times (0^{-3} L)}$
 $= \frac{M_{H_2 SO_4} \cdot V_{H_2 SO_4} \cdot \frac{2 mol}{1 mol} \frac{NaOH}{1 mol} H_2 SO_4}{25.0 \times (0^{-3} L)}$

Method 2 $= 0.534 M$
 $N_{NaOH} = \frac{N_{H_2 SO_4} \cdot V_{H_2 SO_4}}{V_{NaOH}} = \frac{(0.572 \frac{eq}{L})(23.40 mL)}{(25.0 mL)}$
 $= 0.534 \frac{eq}{L}$
 $K = \frac{1}{1 mol} \text{ for } NaOH, \text{ thus } 0.534 \frac{mol}{L} NaOH$

2. The Winkler titration for the determination of dissolved oxygen involves the treatment of the sample with iodide ion (Γ) in the presence of manganese ion catalyst (\mathbf{Mn}^{2+}) as follows.

$$O_2 + 2 Mn^{2+} + 4 OH^- \rightarrow 2 MnO_2(s) + 2 H_2O$$

 $MnO_2(s) + 4 H^+ + 2 I^- \rightarrow Mn^{2+} + I_2 + 2 H_2O$

The liberated iodine is then titrated with a standard thiosulfate solution.

$$I_2 + 2S_2O_3^2 \rightarrow 2I + S_4O_6^2$$

A 50.00 mL sample of water was treated as above and the I_2 liberated was titrated with 8.11 mL of 0.01136 N $Na_2S_2O_3$ to reach the end point. Determine the concentration of the dissolved O_2 in equiv./L, moles/L and mg/L.

#equiv. analyte = #equiv. titrant

$$No_2 \cdot Vo_2 = Ns_2o_3^2 \cdot Vs_2o_3^2$$
 $\therefore No_2 = \frac{Ns_2o_2^2 \cdot Vs_2o_3^2}{Vo_2} = \frac{(0.01136 \cdot \frac{eq}{2})(8.11 \cdot mL)}{(50.00 \cdot mL)}$

= 0.001843 \frac{eq}{L}

Converting.

$$0.00184_3 \stackrel{eq}{=} \times \frac{1 mol O_2}{4 eq. O_2} = 4.608 \times 10^{-4} \frac{mol O_2}{L}$$
 $0.00184_3 \stackrel{eq}{=} \times \frac{8,000 \text{ mg}}{1 eq} = 14.74 \frac{mg O_2}{L}$
Where $K = \frac{4 \text{ equiv}}{1 \text{ mol}} \text{ for } O_2$, Since there are $4 \text{ mols } g = t \text{ transferred}$
per mole $g = \frac{1}{2} \text{ veacted}$.