CHEMICAL NOTATION AND CALCULATIONS
FOR SOIL FERTILITY

1. Molecular and formula weights –

Molecular weight is the sum of the atomic weights of the elements forming the molecule or compound in question. A mole contains $6.02 \times 10^{23}$ (Avogadro’s number) atoms or molecules of the substance in question.

Examples:

a. The molecular weight of $\text{O}_2$ is 32;

$$16 \times 2 = 32 \text{ g/mole}$$
atomic wt. of O, number of atoms present

b. The molecular weight of $\text{H}_2\text{O}$ is 18;

$$16 \times 1 = 16 \quad \text{O}$$
$$1 \times 2 = 2 \quad \text{H}$$
$$18 \text{ g/mole}$$

c. The molecular weight of $\text{CaSO}_4$ is 136.14;

$$40.08 \times 1 = 40.08 \quad \text{Ca}$$
$$32.06 \times 1 = 32.06 \quad \text{S}$$
$$16.00 \times 4 = 64.00 \quad \text{O}$$
$$136.14 \text{ g/mole}$$

Actually, the term molecular weight is not applicable to compounds such as salts, of which $\text{CaSO}_4$ is an example. For salts, the sum of the atomic weights of the elements composing the salt is termed formula weight. Molecular weight and formula weight are numerically equivalent.

1. Mole of substance on a charge basis (±) –

Information in new textbooks and research literature will express amounts and concentrations of chemicals in Standard International (SI) units. Mole by weight and equivalents are no longer used in the new system. Mole of substance on a charge basis (±) is now the accepted unit and is defined as the weight of the number of atoms or molecules necessary to give Avogadro’s number of $(6.02 \times 10^{23})$ charges. For monovalent ions, mole on a weight basis and mole on a charge basis will be numerically equal. However, if an ion is of divalent or greater charge, fewer
atoms are required to give Avogadro’s number of charges, and the weight of a mole on a charge basis is proportionally decreased.

Examples:

a. A mole of Ca\(^{++}\) on a weight basis = 40 g (from table of atomic weights).
   A mole of Ca\(^{++}\) on a charge basis (mole (+)) = weight of atoms to give \(6.02 \times 10^{23}\) charges = weight of \(3.01 \times 10^{23}\) Ca\(^{++}\) atoms = \(\frac{40}{2}\) = 20 g/mole (+)

b. Mole on a charge basis and equivalent weights are numerically equal.

c. Exchangeable cations and cation exchange capacity were previously reported in meq/100 g soil. The new SI designation is cmol (+)/kg soil.

\[\text{1 meq/100 g soil} = \text{1 cmol (+)/kg soil}\]

2. Equivalent weights –

The equivalent of an element is that weight in grams necessary to react with one gram of H\(^{+}\). The equivalent weight is calculated as the molecular weight or atomic weight divided by the number of replaceable hydrogen ions (H\(^{+}\)), hydroxyl ions (OH\(^{-}\)), or by the valence characteristic of the acidic or metallic group of the salt or compound.

<table>
<thead>
<tr>
<th>Formula of Substance</th>
<th>Replaceable Atom or Group</th>
<th>Molecular Weight (g/mole)</th>
<th>Equivalent Weight (g/eq)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{H}_2\text{O})</td>
<td>2 replaceable H(^{+})</td>
<td>18.00</td>
<td>9.00</td>
</tr>
<tr>
<td>(\text{HCl})</td>
<td>1 replaceable H(^{+})</td>
<td>36.45</td>
<td>36.45</td>
</tr>
<tr>
<td>(\text{H}_2\text{SO}_4)</td>
<td>2 replaceable H(^{+})</td>
<td>98.08</td>
<td>49.04</td>
</tr>
<tr>
<td>(\text{Ca(OH)}_2)</td>
<td>2 replaceable OH(^{-})</td>
<td>74.10</td>
<td>37.05</td>
</tr>
<tr>
<td>(\text{NaCl})</td>
<td>1 replaceable Na(^{+}) or Cl(^{-})</td>
<td>58.45</td>
<td>58.45</td>
</tr>
<tr>
<td>(\text{Ca(NO}_3)_2)</td>
<td>1 replaceable Ca(^{++}) or 2 NO(_3)(^{-})</td>
<td>164.00</td>
<td>82.00</td>
</tr>
</tbody>
</table>
3. **Percentage composition** –

The percent of a given element in a compound by weight.

Examples:

Formula weight of CaSO\(_4\) = 136.14 g

\[
\% \text{ Ca} = \frac{40.08 \text{ g}}{136.14 \text{ g}} \times 100 = 29.44\%
\]

\[
\% \text{ S} = \frac{32.06 \text{ g}}{136.14 \text{ g}} \times 100 = 23.55\%
\]

\[
\% \text{ O} = \frac{64.00 \text{ g}}{136.14 \text{ g}} \times 100 = 47.01\%
\]

4. **Valence** –

The valence of an atom is the number of hydrogen atoms (or its equivalent) that the atom in question will combine with or be replaced by.

Example:

a. The calcium atom (Ca) has a valence of two because it replaces two atoms of hydrogen from a molecule of sulfuric acid.

\[
\text{Ca}^{++} + \text{H}_2\text{SO}_4 \rightleftharpoons \text{CaSO}_4 + 2\text{H}^+
\]

5. **Radicals** –

A radical is a group of atoms which reacts as if it were a single atom and it has an overall net charge, or valence.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Radical</th>
<th>Valence of Radical</th>
</tr>
</thead>
<tbody>
<tr>
<td>KNO(_3)</td>
<td>NO(_3^-)</td>
<td>-1</td>
</tr>
<tr>
<td>K(_2)SO(_4)</td>
<td>SO(_4^{2-})</td>
<td>-2</td>
</tr>
<tr>
<td>H(_3)PO(_4)</td>
<td>PO(_4^{3-})</td>
<td>-3</td>
</tr>
<tr>
<td>Ca (OH)(_2)</td>
<td>OH(^-)</td>
<td>-1</td>
</tr>
</tbody>
</table>
### Common Ions of Familiar Chemical Elements of the Earth

<table>
<thead>
<tr>
<th>Name</th>
<th>Ion</th>
<th>Name</th>
<th>Ion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetate</td>
<td>C$_2$H$_3$O$_2^-$</td>
<td>Hydrogen</td>
<td>H$^+$</td>
</tr>
<tr>
<td>Aluminum</td>
<td>Al$^{+3}$</td>
<td>Hydroxide</td>
<td>OH$^-$</td>
</tr>
<tr>
<td>Ammonium</td>
<td>NH$_4^+$</td>
<td>Iodide</td>
<td>I$^-$</td>
</tr>
<tr>
<td>Barium</td>
<td>Ba$^{+2}$</td>
<td>Magnesium</td>
<td>Mg$^{+2}$</td>
</tr>
<tr>
<td>Bicarbonate</td>
<td>HCO$_3^-$</td>
<td>Manganous</td>
<td>Mn$^{+2}$</td>
</tr>
<tr>
<td>Bromide</td>
<td>Br$^-$</td>
<td>Nickel</td>
<td>Ni$^{+2}$</td>
</tr>
<tr>
<td>Calcium</td>
<td>Ca$^{+2}$</td>
<td>Nitrate</td>
<td>NO$_3^-$</td>
</tr>
<tr>
<td>Carbonate</td>
<td>CO$_3^{2-}$</td>
<td>Phosphate (ortho)</td>
<td>PO$_4^{3-}$</td>
</tr>
<tr>
<td>Chloride</td>
<td>Cl$^-$</td>
<td>Potassium</td>
<td>K$^+$</td>
</tr>
<tr>
<td>Cupric</td>
<td>Cu$^{+2}$</td>
<td>Sodium</td>
<td>Na$^+$</td>
</tr>
<tr>
<td>Cuprous</td>
<td>Cu$^+$</td>
<td>Sulfate</td>
<td>SO$_4^{2-}$</td>
</tr>
<tr>
<td>Ferrous (iron)</td>
<td>Fe$^{+2}$</td>
<td>Sulfide</td>
<td>S$^{2-}$</td>
</tr>
<tr>
<td>Ferric (iron)</td>
<td>Fe$^{+3}$</td>
<td>Sulfite</td>
<td>SO$_3^{2-}$</td>
</tr>
<tr>
<td>Fluoride</td>
<td>F$^-$</td>
<td>Zinc</td>
<td>Zn$^{+2}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Oxygen</td>
<td>O$^{2-}$</td>
</tr>
</tbody>
</table>

6. **Concentrations of Solutions** –

The concentrations of solutions can be expressed in several different ways.

a. **Percentage composition** – the weight of solute (salt) in 100 g of solution. Example: The solution contains 10% salt (10 g salt/100 g of solution).

b. **Molar solution** – a molar solution contains one molecular or formula weight of solute in one liter of solution. Example: A 1M solution of NaCl contains 58.46 g (1 formula weight of NaCl) in one liter of solution.

c. **Molal solution** – a solution containing one mole of solute in 1000 g of water.
d. **Normal solution** – a normal solution contains one equivalent of solute in a liter of solution. Example: a 1 N solution of CaCl₂ contains 55.49 g (1 equivalent weight of CaCl₂) in one liter of solution. A 1 N solution also contains 1 milliequivalent in one ml of solution.

7. **Units of measurement** –

<table>
<thead>
<tr>
<th>Prefixes</th>
<th>Meaning</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>micro -</td>
<td>one-millionth</td>
<td>micrometer</td>
</tr>
<tr>
<td>milli -</td>
<td>one-thousandth</td>
<td>millimeter</td>
</tr>
<tr>
<td>centi -</td>
<td>one-hundredth</td>
<td>centimeter</td>
</tr>
<tr>
<td>deci -</td>
<td>one-tenth</td>
<td>deciliter</td>
</tr>
<tr>
<td>deka -</td>
<td>ten</td>
<td>dekagram</td>
</tr>
<tr>
<td>hecto -</td>
<td>one hundred</td>
<td>hectogram</td>
</tr>
<tr>
<td>kilo -</td>
<td>one thousand</td>
<td>kilogram</td>
</tr>
</tbody>
</table>

Examples of interconversions:

1 meter (m) = 10 decimeters (dm) = 100 centimeters (cm) = 
1000 millimeters (mm) = 1,000,000 micrometers (μm)
1 kilogram = 1000 grams (g) = 10 hectograms = 100 dekagrams

Common conversions:
1 cm = 0.394 inch
1 liter = 1.057 quart
1 acre = 43,560 sq. ft.
1 cubic foot of water weighs 62.4 pounds
1 ha (10,000 sq. m) = 2.5 acres
454 g = 1 pound
1 kg = 2.2 pounds
1000 kg (1 metric ton) = 2205 pounds

8. **Common units and calculations dealing with concentrations** –

Parts per million, ppm: one part in a million parts; a ratio of one to one million.
Examples:

1 ppm = 1 lb/1×10^6 lb, 1 g/1×10^6 g, 1×10^{-6} g/g, 1μg/ml = 1μg/g

1 equivalent = 1000 milliequivalents (meq), 1 meq = 0.001 eq

Remember: A 1 normal (N) solution contains 1 equivalent of a substance dissolved in 1000 ml of solution. Therefore 1 ml of that solution contains 0.001 eq = 1 meq. Therefore, a 1N solution contains 1 meq/ml.

When working with solution concentrations, a useful relationship is:

\[ \text{ml} \times N = \text{meq} \]

If any 2 of the above 3 factors is known, then the 3rd factor can be computed.

Examples:

1. \(10 \text{ ml} \times 0.5N = 5 \text{ meq}\)

2. \(3 \text{ meq} \) of a substance is dissolved in 100 ml of solution: The normality of this solution is: \(3 \text{ meq}/100 \text{ ml} = 0.03N\)

If substance A and B will react, then 1 meq of A will react with 1 meq of B and

\[ \text{ml}_A \times N_A = \text{ml}_B \times N_B \]

9. Application of previous concepts –

a. A Ruston loamy sand from East Texas has a pH of 5.6 and a CEC of 1.5 cmol (+)/1000 g soil. The concentration of exchangeable basic cations was as follows:

<table>
<thead>
<tr>
<th>Cation</th>
<th>cmol (+)/kg soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca^{++}</td>
<td>0.41</td>
</tr>
<tr>
<td>K^{+}</td>
<td>0.12</td>
</tr>
<tr>
<td>Mg^{++}</td>
<td>0.11</td>
</tr>
<tr>
<td>Na^{+}</td>
<td>0.06</td>
</tr>
</tbody>
</table>

Calculate the lbs exchangeable Ca^{++}/A-6" present in the soil.

The atomic (or mole wt) of Ca^{++} = 40 g/mole
The mole (+) wt of Ca$^{++}$ = 40 g/2 = 20 g/mole (+)

The cmol (+) wt of Ca$^{++}$ = 20 g/mole (+) × \( \frac{1 \text{ mole (+)}}{100 \text{ cmol (+)}} \) = 0.20 g Ca$^{++}$/cmol (+)

We know the soil has an exchangeable Ca$^{++}$ concentration of 0.41 cmol (+)/1000 g.

Therefore:

\[
0.41 \text{ cmol (+) Ca/1000 g } \times 0.20 \text{ g/cmol (+)} = 0.082 \text{ g Ca}^{++}/1000 \text{ g soil} \\
= 82 \text{ g Ca}^{++}/1 \times 10^6 \text{ g soil} \\
= 82 \text{ lbs Ca}^{++}/1 \times 10^6 \text{ lbs soil}
\]

An acre - 6'' of soil weighs approximately \( 2 \times 10^6 \) lbs. Therefore, if the soil contains 82 lbs Ca$^{++}/1 \times 10^6$ lbs soil, then there are 164 (or \( 2 \times 82 \)) lbs Ca$^{++}/2 \times 10^6$ lbs of soil.

Thus, the soil contains **164 lbs exchangeable Ca$^{++}$/A-6"**.

1. 10 g of soil was saturated with Mg$^{++}$ by shaking the soil with a solution of 1 N MgCl$_2$. The Mg$^{++}$ on cation exchange sites was subsequently displaced by shaking the soil sample in a solution of 1 N CaCl$_2$. The solution containing the displaced Mg$^{++}$ was made to a final volume of 100 ml. The concentrations of Mg$^{++}$ in this solution was determined to be 122 ppm. Calculate the CEC of this soil.

The concentration of displaced Mg$^{++}$ in solution was 122 ppm.

In aqueous solutions, 1 ppm = 1μg/ml.

Therefore, 122 ppm = 122μg/ml.

Now, the displaced Mg$^{++}$ was contained in 100 ml of solution. Therefore, the total amount of Mg$^{++}$ in this 100 ml of solution was:

\[
122 \mu g \text{ Mg}^{++}/\text{ml} \times 100 \text{ ml} = 12,200 \mu g \text{ Mg}^{++} \\
= 0.0122 \text{ g Mg}^{++}
\]

This 0.0122 g Mg$^{++}$ was displaced from 10 g of soil.
Therefore, the concentration of exchangeable Mg\(^{++}\) in the soil was:

\[
0.0122 \text{ g Mg}^{++}/10 \text{ g soil}
\]

We want to calculate CEC and because the units of CEC are cmol (+)/1000 g soil, we must change the above to these units.

\[
0.0122 \text{ g Mg}^{++}/10 \text{ g soil} = 0.22 \text{ g Mg}^{++}/100 \text{ g soil} = 1.22 \text{ g Mg}^{++}/1000 \text{ g soil}
\]

Now convert 1.22 g mg\(^{++}\) to cmol (+) Mg\(^{++}\) and the CEC has been calculated.

atomic wt (or mole wt) of Mg\(^{++}\) = 24.32 g/mole
mole (+) wt of Mg\(^{++}\) = 24.32/2 = 12.16 g/mole (+)

\[
\text{cmole (+) wt of Mg}^{++} = 12.16 \text{ g/mole (+)} \times \frac{1 \text{ mole (+)}}{100 \text{ cmol (+)}} = 0.1216 \text{ g Mg}^{++} \text{ cmol (+)}
\]

Since we have 1.22 g Mg\(^{++}\), we next determine how many cmol (+)’s this is equal to by dividing by the cmol (+) wt. Thus,

\[
\frac{1.22 \text{ g Mg}^{++}}{0.122 \text{ g/cmol (+)}} = 10 \text{ cmol (+)}
\]

Therefore, the CEC of the soil is 10 cmol (+)/1000 g soil.