Topic 5: Stoichiometry - Chemical Arithmetic

Masses of some atoms:

\[ ^1\text{H} = 1.6736 \times 10^{-24}\text{ g} \quad ^{16}\text{O} = 2.6788 \times 10^{-23}\text{ g} \quad ^{238}\text{U} = 3.9851 \times 10^{-22}\text{ g} \]

Introducing . . . . . . the Atomic Mass Unit (amu)

1 amu = 1.66054 \times 10^{-24} g

5.1: Atomic Mass Unit

Atomic Mass is defined relative to Carbon -12 isotope

12 amu is the mass of the $^{12}\text{C}$ isotope of carbon

Carbon -12 atom = 12.000 amu
Hydrogen -1 atom = 1.008 amu
Oxygen -16 atom = 15.995 amu
Chlorine -35 atom = 34.969 amu

5.1: Atomic Mass - Natural Abundance

We deal with the naturally occurring mix of isotopes, rather than pure isotopes

Carbon has three natural isotopes

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Mass (amu)</th>
<th>Abundance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}\text{C}$</td>
<td>12.000</td>
<td>98.892</td>
</tr>
<tr>
<td>$^{13}\text{C}$</td>
<td>13.00335</td>
<td>1.108</td>
</tr>
<tr>
<td>$^{14}\text{C}$</td>
<td>14.00317</td>
<td>$1 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Any shovelful of Carbon from living material will have a Naturally Occurring Abundance of 98.892% $^{12}\text{C}$, 1.108% $^{13}\text{C}$ and 0.0001% $^{14}\text{C}$
5.1: Atomic Mass - Relative Abundance

How do we take into account the naturally occurring Abundances?

Take the average mass of the various isotopes weighted according to their Relative Abundances.

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</tr>
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<td>$^{13}\text{C}$</td>
<td>13.00335</td>
<td>1.108</td>
<td>0.0108</td>
</tr>
<tr>
<td>$^{14}\text{C}$</td>
<td>14.00317</td>
<td>$1 \times 10^{-4}$</td>
<td>$1 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

N.B. The % Abundance adds up to 100
The Relative Abundance adds up to 1

5.1: Average Atomic Mass

The Average Atomic Mass is given by:

$$(0.98892 \times 12.000 \text{ amu}) + (0.01108 \times 13.00335 \text{ amu}) + (1 \times 10^{-6} \times 14.00317 \text{ amu}) = 12.011 \text{ amu}$$

5.1: Atomic and Molecular Mass

You can calculate the mass of any compound from the sum of the atomic masses from the periodic table.

Example: Molecular Mass of $\text{H}_2\text{SO}_4$

$\text{H}_2\text{SO}_4$

2 Hydrogen atoms

1 Sulfur atom

4 Oxygen atoms
5.1: Molecular Mass

\[ \text{H}_2\text{SO}_4 \]

2 Hydrogen atoms  
4 Oxygen atoms  
1 Sulfur atom  

\[(2 \times 1.01 \text{ amu}) + (1 \times 32.07 \text{ amu}) + (4 \times 16.00 \text{ amu}) \]

\[= 2.02 \text{ amu} + 32.07 \text{ amu} + 64.00 \text{ amu} \]

\[= 98.09 \text{ amu} \]

5.1: Formula Mass

What is the formula mass of:

(Calcium nitrate tetrahydrate)  
\[\text{Ca(NO}_3\text{)_2}\cdot4\text{H}_2\text{O} \]

1 Calcium  
2 Nitrogens  
8 Hydrogens  
10 Oxygens  

\[(1 \times 40.08 \text{ amu}) + (2 \times 14.01 \text{ amu}) + (8 \times 1.01 \text{ amu}) + (10 \times 16.00 \text{ amu}) \]

\[= 236.18 \text{ amu} \]

5.1: Formula Mass vs. Molecular Mass

Use **MOLECULAR MASS** when talking about MOLECULES  

\[\text{e.g. } \text{CO}_2 \quad \text{H}_2\text{O} \quad \text{C}_6\text{H}_{12}\text{O}_6 \]

Use **FORMULA MASS** when talking about IONIC COMPOUNDS  

\[\text{e.g. } \text{NaCl} \quad \text{Cu(NO}_3\text{)_2} \quad \text{CaO} \]

BUT the two terms are basically interchangeable
5.2: How to Avoid Huge Numbers

Recall the introduction of Atomic Mass Units

1 \text{ amu} = 1.66054 \times 10^{-24} \text{ g}

This avoids working with ridiculously small masses

How to avoid the problem of counting huge numbers of molecules / atoms?

5.2: How to Avoid Huge Numbers - Use moles!

How does a chemist say how many ATOMS or MOLECULES she reacted?

She talks of \textit{moles} of Atoms or Molecules reacted

1 mole = 6.022142 \times 10^{23}

Avogadro’s Number (\(N_A\))

5.2: A mole is 6.02 \times 10^{23} of anything

1 mole = 6.02 \times 10^{23}

\begin{align*}
\text{PEANUTS} & \quad \text{PEANUTS} \\
\text{K MnO}_4 & \quad \text{K MnO}_4 \\
\text{ANTS} & = 6.02 \times 10^{23} \quad \text{ANTS} \\
\text{Br}_2 \text{ molecules} & \quad \text{Br}_2 \text{ molecules} \\
\text{BEERS} & \quad \text{BEERS} \\
\text{CH}_3\text{COOH} & \quad \text{CH}_3\text{COOH}
\end{align*}

The NUMBER is constant, NOT the MASS
5.2: The mole: Where does it come from?

Definition:

1 mole is the number of Carbon atoms found in EXACTLY 12.00 g of $^{12}$C

\[
12 \text{ amu} \times 6.02 \times 10^{23} = 12 \text{ g}
\]

\[
12 \text{ amu} = \frac{12 \text{ g}}{6.02 \times 10^{23}} = 12 \text{ g mole}^{-1}
\]

5.2: Molar mass

How to calculate the mass of 1 mole of a compound?

= the molecular mass in grams

\[
\begin{align*}
\text{H}_2\text{SO}_4 & \quad 2 \text{ Hydrogen atoms} \\
& \quad 1 \text{ Sulfur atom} \\
& \quad 4 \text{ Oxygen atoms}
\end{align*}
\]

\[
(2 \times 1.0079 \text{ g mol}^{-1}) + (1 \times 32.065 \text{ g mol}^{-1}) + (4 \times 15.999 \text{ g mol}^{-1}) = 98.077 \text{ g mol}^{-1}
\]

5.2: Molar mass

Examples:

1 molecule of KCl has molecular mass of 74.55 amu.,

1 mol of KCl has a mass of 74.55 g.,
and contains $6.02 \times 10^{23}$ molecules of KCl.

1 mole of H$_2$O has a mass of ? g
5.2: Calculations of molar amounts

How many moles of ethanol (C₆H₅OH) are there in a schooner of beer?
(The average schooner contains 20.8 g ethanol)

Mass of ethanol = 20.8 g
Molar mass of ethanol = 46.08 g.mol⁻¹

\[
\text{no. of moles of ethanol} = \frac{\text{mass (g)}}{\text{molar mass (g.mol⁻¹)}}
\]

\[
= \frac{20.8 \text{ g}}{46.08 \text{ g/mol}} = 0.451 \text{ mol}
\]

5.2: Calculations of molar amounts

How many moles of caffeine (C₈H₁₀N₄O₂) are there in a tin of Red Bull?
(1 tin contains 80 mg of caffeine)

Mass of C₈H₁₀N₄O₂ = 80 mg = 0.08 g
Molar mass of C₈H₁₀N₄O₂ = 194.22 g.mol⁻¹

\[
\text{no. of moles of caffeine} = \frac{\text{mass (g)}}{\text{molar mass (g.mol⁻¹)}}
\]

\[
= \frac{0.08 \text{ g}}{194.22 \text{ g/mol}} = 4 \times 10^{-4} \text{ mol caffeine}
\]

5.2: Calculations of molecular amounts

How many MOLECULES of ethanol (C₂H₅OH) are there in a schooner of beer?
(The average schooner contains 20.8 g ethanol)

Mass of ethanol = 20.8 g
Molar mass of ethanol = 46.08 g.mol⁻¹
No. of molecules 1 mole = 6.02 × 10²³ molecules.mol⁻¹

\[
\text{no. of molecules of ethanol} = \frac{\text{no. of moles of ethanol} \times \text{no. of molecules 1 mole}}{	ext{mol}}
\]

\[
= 0.451 \text{ mol} \times 6.02 \times 10^{23} \text{ molecules/mol} = 2.72 \times 10^{23} \text{ molecules of ethanol}
\]
5.2: Calculations of molecular amounts

How many MOLECULES of nicotine (C_{10}H_{14}N_{2}) are there in an average cigarette (1.2 mg)?

Mass of nicotine = 1.2 mg = 1.2 \times 10^{-3} g
Molar mass of nicotine = 162.26 g.mol^{-1}
No. of molecules 1 mole = 6.02 \times 10^{23} molecules.mol^{-1}

Step 1: Convert mass to moles using molar mass

no. of moles of nicotine
\[= \frac{1.2 \times 10^{-3} \text{ g}}{162.26 \text{ g.mol}^{-1}}\]
\[= 7.4 \times 10^{-6} \text{ moles of nicotine}\]

Step 2: Convert moles to molecules using Avogadro’s number

no. of molecules of nicotine
\[= 7.4 \times 10^{-6} \text{ mol} \times 6.02 \times 10^{23} \text{ molecules.mol}^{-1}\]
\[= 4.4 \times 10^{18} \text{ molecules of nicotine}\]

1 mole = 6.022142 \times 10^{23} things