Lecture 5, The Mole

What is a mole?
Moles
Atomic mass unit and the mole

- amu definition: $^{12}\text{C} = 12$ amu.
- The atomic mass unit is defined this way.
- $1$ amu $= 1.6605 \times 10^{-24}$ g
- How many $^{12}\text{C}$ atoms weigh 12 g?
  - $6.02 \times 10^{23}$ $^{12}\text{C}$ weigh 12 g.
- Avogadro’s number
- The mole
Atomic mass unit and the mole

- amu definition: $^{12}\text{C} = 12$ amu.
- $1$ amu $= 1.6605 \times 10^{-24}$ g
- How many $^{12}\text{C}$ atoms weigh $12$ g?
- $6.02 \times 10^{23}^{12}\text{C}$ weigh $12$ g.
- Avogadro’s number
- The mole

- $\text{#atoms} = \frac{1 \text{ atom}}{12 \text{ amu}} \cdot \frac{1 \text{ amu}}{1.66 \times 10^{-24} \text{ g}} \cdot (12 \text{ g})$
  $= 6.02 \times 10^{23}^{12}\text{C}$ weigh $12$ g
Therefore:

- $6.02 \times 10^{23}$
- 1 mole of $^{12}$C has a mass of 12 g
The mole

- The mole is just a number of things
- 1 dozen = 12 things
- 1 pair = 2 things
- 1 mole = $6.022141 \times 10^{23}$ things
Molar Mass
The trick:
• By definition, this is the mass of 1 mol of a substance (i.e., g/mol)
  – The molar mass of an element is the mass number for the element that we find on the periodic table
  – The formula weight (in amu’s) will be the same number as the molar mass (in g/mol)
Using Moles

Moles provide a bridge from the molecular scale to the real-world scale.

The number of moles correspond to the number of molecules. 1 mole of any substance has the same number of molecules.
Mole Relationships

<table>
<thead>
<tr>
<th>Name of substance</th>
<th>Formula</th>
<th>Formula Weight (amu)</th>
<th>Molar Mass (g/mol)</th>
<th>Number and Kind of Particles in One Mole</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic nitrogen</td>
<td>N</td>
<td>14.0</td>
<td>14.0</td>
<td>$6.022 \times 10^{23} \text{ N atoms}$</td>
</tr>
<tr>
<td>Molecular nitrogen</td>
<td>N$_2$</td>
<td>28.0</td>
<td>28.0</td>
<td>$6.022 \times 10^{23} \text{ N}_2 \text{ molecules}$</td>
</tr>
<tr>
<td>Silver</td>
<td>Ag</td>
<td>107.9</td>
<td>107.9</td>
<td>$6.022 \times 10^{23} \text{ Ag atoms}$</td>
</tr>
<tr>
<td>Silver ions</td>
<td>Ag$^+$</td>
<td>107.9$^a$</td>
<td>107.9</td>
<td>$6.022 \times 10^{23} \text{ Ag}^+ \text{ ions}$</td>
</tr>
<tr>
<td>Barium chloride</td>
<td>BaCl$_2$</td>
<td>208.2</td>
<td>208.2</td>
<td>$6.022 \times 10^{23} \text{ BaCl}_2 \text{ units}$</td>
</tr>
</tbody>
</table>

$^a$Recall that the electron has negligible mass; thus, ions and atoms have essentially the same mass.

- One mole of atoms, ions, or molecules contains Avogadro’s number of those particles
- One mole of molecules or formula units contains Avogadro’s number times the number of atoms or ions of each element in the compound
Molar mass examples

- Molecular compound
- Molar mass of water H$_2$O
  \[
  \begin{align*}
  2H &= 2 \times 1.008 = 2.016 \\
  1O &= 16.00 = 16.00 \\
  \text{Molar mass} &= 18.016
  \end{align*}
  \]

- Ionic compound, NaCl
- Na = 22.99
- Cl = 35.45
- Molar mass = 58.44
Examples

• What is the mass of 3 moles of water
  18.016 g/mole(3 moles) = 54.048 g

• How many moles in 64 g methane CH₄?
  4H = 1.008*4 = 4.032
  1C = 12.01
  16.033 g/mole
  64 g (1mole/16.033g) = 3.991 moles
Stoichiometry is the measurement of elements.
Finding Empirical Formulas
Combustion Analysis gives % composition

Compounds containing C, H and O are routinely analyzed through combustion in a chamber like this:

- %C is determined from the mass of CO\(_2\) produced
- %H is determined from the mass of H\(_2\)O produced
- %O is determined by difference after the C and H have been determined

\[
\text{C}_n\text{H}_n\text{O}_n + \text{O}_2 \rightarrow n\text{CO}_2 + \frac{1}{2}n\text{H}_2\text{O}
\]
Calculating Empirical Formulas

One can calculate the empirical formula from the percent composition
Example

• An oxide of copper contains 88.82% Cu. What is the formula of the oxide?

\[
\begin{align*}
\text{Cu: } (88.82\%) &= 88.82 \text{ g} \\
\text{O: } 100-88.82 &= 11.18\% = 11.18 \text{ g}
\end{align*}
\]

\[
\begin{align*}
\text{Calculate moles} & \quad \frac{88.82 \text{ g}}{63.546 \text{ gmol}^{-1}} = 1.348 \text{ mole} \\
\text{Get mole ratio} & \quad \frac{1.348 \text{ mol}}{0.699 \text{ mol}} = 2 \\
\end{align*}
\]

\[
\begin{align*}
\text{Cu}_2\text{O} & \quad \text{copper (I) oxide}
\end{align*}
\]
• A compound of boron and hydrogen contains 78.14% B. What is the empirical formula of the compound? If the molar mass is 27.7 gmol⁻¹, what is the molecular formula?

B: 78.14% = 78.14 g
H: 100-78.14 = 21.86 g

\[
\frac{78.14 \text{ g}}{10.811 \text{ gmol}^{-1}} = 7.228 \quad \frac{21.86}{1.008 \text{ gmol}^{-1}} = 21.686
\]

1

\[
\frac{21.6863.00}{7.228} = 3
\]

BH₃ mass = 10.811 + 1.008*3 = 13.825 g/mol
27.77 gmol⁻¹/13.824 gmol⁻¹ = 2
Molecular weight: (BH₃)*2=B₂H₆
• What is the percent by mass of nitrogen in ammonium nitrate?

• $\text{NH}_4\text{NO}_3$  2N:  $14.0067 \times 2 = 28.134$

• 3O  $16.00 \times 3 = 48.00$

• 4H  $1.008 \times 4 = 4.032$

• 80.166 g/mole

• $28.134/80.166 = 0.3509$
Calculating Empirical Formulas

The compound *para*-aminobenzoic acid (you may have seen it listed as PABA on your bottle of sunscreen) is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula of PABA.
Calculating Empirical Formulas

Assuming 100.00 g of para-aminobenzoic acid,

- **C:** $61.31 \text{ g} \times \frac{5.105 \text{ mol} \text{ C}}{12.01 \text{ g}} = 5.105 \text{ mol C}

- **H:** $5.14 \text{ g} \times \frac{5.09 \text{ mol} \text{ H}}{1 \text{ mol}} = 5.09 \text{ mol H}

- **N:** $10.21 \text{ g} \times \frac{0.7288 \text{ mol} \text{ N}}{14.01 \text{ g}} = 0.7288 \text{ mol N}

- **O:** $23.33 \text{ g} \times \frac{1.456 \text{ mol} \text{ O}}{16.00 \text{ g}} = 1.456 \text{ mol O}
Calculating Empirical Formulas

Calculate the mole ratio by dividing by the smallest number of moles:

C: \[ \frac{5.105 \text{ mol}}{0.7288 \text{ mol}} = 7.005 \approx 7 \]

H: \[ \frac{5.096 \text{ mol}}{0.7288 \text{ mol}} = 6.984 \approx 7 \]

N: \[ \frac{1.000}{0.7288 \text{ mol}} = 1.000 \]

O: \[ \frac{2.001}{0.7288 \text{ mol}} = 2.679 \approx 2 \]

1.458 mol

\[ \frac{1.458 \text{ mol}}{0.7288 \text{ mol}} = 1.998 \approx 2 \]
Calculating Empirical Formulas

These are the subscripts for the empirical formula:

\[ \text{C}_7\text{H}_7\text{NO}_2 \]
More examples for your pedagogical pleasure

What is the average mass of a single molecule of ethanol, CH₃CH₂OH (C₂H₆O)?
Mol. Mass = 2(12.01 amu/C) + 6(1.008 amu/H) + 1(16.00 amu/O) = 46.068

Does every molecule of ethanol weigh the same?

1.256 g of Sulfur reacts with excess fluorine gas (F₂) to produce 5.722 g of a substance SFₓ. What is the substance?

\[
\begin{align*}
S & \quad + \quad F_2 \quad \rightarrow \quad SF_x \\
1.256g & \quad 5.722-1.256=4.466 g \quad \quad 5.722 g \\
(1.256 g)/32.06 \text{ gmol}^{-1} & \quad 4.466 g/18.998 \text{ gmol}^{-1} \\
3.918 \times 10^{-2} \text{ mole S} & \quad 0.2351 \text{ mole F} \\
3.918 \times 10^{-2} /3.918 \times 10^{-2} =1 & \quad 0.2351/3.918 \times 10^{-2} = 6.00 \quad SF_6
\end{align*}
\]
A compound was analyzed and found to contain 53.30% carbon, 11.19% hydrogen and 35.51% oxygen by mass. The molar mass was determined to be about 90 g/mol. What is the empirical formula and what is the molecular formula of the compound?

<table>
<thead>
<tr>
<th>Element</th>
<th>Mass (g)</th>
<th>Molar Mass (g/mol)</th>
<th>Moles</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>53.3</td>
<td>12.01</td>
<td>4.438</td>
<td>2</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>11.19</td>
<td>1.008</td>
<td>11.012</td>
<td>5</td>
</tr>
<tr>
<td>Oxygen</td>
<td>35.51</td>
<td>16.00</td>
<td>2.22</td>
<td>1</td>
</tr>
</tbody>
</table>

Mass of Empirical formula: \(2(12.01 \text{ g/mol C}) + 5(1.008 \text{ g/mol H}) + 16.00 \text{ g/mol O} = 45.06 \text{ g/mole Empirical formula}\)

\(90 \text{ g/mol} /45.06 \text{ g/mol} \text{ empirical mass} = 2\). So the compound is: \(2(C_2H_5O)\ C_4H_{10}O_2\)
Even More examples for your pedagogical pleasure

Suppose a hydrocarbon (compound containing only C and H) is burned in air, producing CO$_2$ and H$_2$O. This is called a **combustion reaction**. The number of moles of CO$_2$ produced is 1.5 times the number of moles of water produced. What is the empirical formula of the original molecule you burned? If the molecular mass of the compound is 120 gmol$^{-1}$, what is the molecular formula of the compound?

Assume 3 moles of CO$_2$, therefore 2 moles water.

1. Write down the reaction:

   $$C_NH_M + O_2 \rightarrow CO_2 + H_2O$$

   3 moles C: 3 moles H: 4 Therefore C$_3$H$_4$

   Empirical mass: $3(12.01 \text{ gmol}^{-1} \text{ C}) + 4(1.008 \text{ gmol}^{-1} \text{ H}) = 40.0 \text{ gmol}^{-1}$

   $120 \text{ gmol}^{-1}/40 \text{ gmol}^{-1} = 3$

   $3(C_3H_4) = C_9H_{12}$ molecular formula
Even More examples for your pedagogical pleasure

A 15.67 g sample of a hydrate of magnesium carbonate was carefully heated in an oven to drive off the water. The mass reduced to 7.58 g. What is the formula of the hydrate?

Molar mass of MgCO₃ = 84.31 g mol⁻¹
Molar mass of H₂O = 18.016 g mol⁻¹

MgCO₃·(H₂O)_n ----→ MgCO₃ + nH₂O

15.67 g 7.58 g 15.67 g – 7.58 g = 8.09 g
15.67 g 7.58 g/84.31 g mol⁻¹ = .08990 mole 8.09 g/18.016 g mol⁻¹ = .4490 mol

.08990/.08990=1 .4490/.08990=4.995

N=5 MgCO₃·(H₂O)_5
A compound of carbon, hydrogen, and nitrogen was analyzed and found to contain 45.92% C, 12.20% H and 42.38% N. What is the empirical formula of the compound?

Assume 100g:

<table>
<thead>
<tr>
<th>Element</th>
<th>Mass (g)</th>
<th>Mass (g)/Molar Mass</th>
<th>Molar Mass</th>
<th>Molar Mass/Molar Mass</th>
<th>Molar Mass/Molar Mass x 100g</th>
<th>Empirical Formula</th>
<th>Total Mole</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>45.42</td>
<td>45.42 g/12.01=3.782 mole</td>
<td>12.01</td>
<td>3.782/3.025=1.250 mole</td>
<td>1.25*4=5.00</td>
<td>C_5</td>
<td>5</td>
</tr>
<tr>
<td>H</td>
<td>12.20</td>
<td>12.20 g/1.008gmol^{-1}=12.103 mole</td>
<td>1.008</td>
<td>12.103/3.025=4.00 mole</td>
<td>4*4=16</td>
<td>H_16</td>
<td>16</td>
</tr>
<tr>
<td>N</td>
<td>42.38</td>
<td>42.38 g/14.01gmol^{-1}=3.025 mole</td>
<td>14.01</td>
<td>3.025/3.025=1 mole</td>
<td>1*4=4</td>
<td>N_4</td>
<td>4</td>
</tr>
</tbody>
</table>

\( \text{C}_5\text{H}_{16}\text{N}_4 \)
Stoichiometry:

Calculations with Chemical Formulas and Equations
Anatomy of a Chemical Equation

$\text{CH}_4(\text{g}) + 2\text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2\text{H}_2\text{O}(\text{g})$
Anatomy of a Chemical Equation

\[
\text{Reactants appear on the left side of the equation.}
\]

\[
\text{CH}_4(g) + 2 \text{O}_2(g) \rightarrow \text{CO}_2(g) + 2 \text{H}_2\text{O}(g)
\]
Anatomy of a Chemical Equation

Products appear on the right side of the equation.

\[ \text{CH}_4(g) + 2 \text{O}_2(g) \rightarrow \text{CO}_2(g) + 2 \text{H}_2\text{O}(g) \]
Anatomy of a Chemical Equation

The states of the reactants and products are written in parentheses to the right of each compound.

$$\text{CH}_4(g) + 2 \text{O}_2(g) \rightarrow \text{CO}_2(g) + 2 \text{H}_2\text{O}(g)$$

The **states** of the reactants and products are written in parentheses to the right of each compound.
Coefficients are inserted to balance the equation.
Subscripts and Coefficients Give Different Information

<table>
<thead>
<tr>
<th>Chemical symbol</th>
<th>Meaning</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2O$</td>
<td>One molecule of water:</td>
<td>Two H atoms and one O atom</td>
</tr>
<tr>
<td>$2H_2O$</td>
<td>Two molecules of water:</td>
<td>Four H atoms and two O atoms</td>
</tr>
<tr>
<td>$H_2O_2$</td>
<td>One molecule of hydrogen peroxide:</td>
<td>Two H atoms and two O atoms</td>
</tr>
</tbody>
</table>

- Subscripts tell the number of atoms of each element in a molecule
Subscripts and Coefficients Give Different Information

- Subscripts tell the number of atoms of each element in a molecule
- Coefficients tell the number of molecules (compounds).
Stoichiometry of Chemical Reactions
Balancing an equation

1. Write the correct formula for all the participants
2. Select the most complicated formula and balance those atoms first
3. Start with those atoms that occur in only one formula on each side
4. Leave simple molecules such as $H_2$ and $O_2$ until the end.

Examples:

$\text{Al}_4\text{C}_3 + \text{H}_2\text{O} \rightarrow \text{Al(OH)}_3 + \text{CH}_4$

$\text{NH}_3 + \text{O}_2 \rightarrow \text{NO} + \text{H}_2\text{O}$

$\text{C}_3\text{H}_8 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O}$
Stoichiometry of Chemical Reactions
Balancing an equation

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2. Select the most complicated formula and balance those atoms first
3. Start with those atoms that occur in only one formula on each side
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Examples:

\[
\begin{align*}
\text{Al}_4\text{C}_3 & \quad + \quad 12\text{H}_2\text{O} & \quad \rightarrow & \quad 4\text{Al(OH)}_3 & \quad + \quad 3\text{CH}_4 \\
2\text{NH}_3 & \quad + \quad 5/2\text{O}_2 & \quad \rightarrow & \quad 2\text{NO} & \quad + \quad 3\text{H}_2\text{O} \\
4\text{NH}_3 & \quad + \quad 5\text{O}_2 & \quad \rightarrow & \quad 4\text{NO} & \quad + \quad 6\text{H}_2\text{O} \\
\text{C}_3\text{H}_8 & \quad + \quad 5\text{O}_2 & \quad \rightarrow & \quad 3\text{CO}_2 & \quad + \quad 4\text{H}_2\text{O}
\end{align*}
\]
Stoichiometry of Chemical Reactions

When doing stoichiometric calculations you must always work in moles? Because moles tell you how many molecules/atoms you have.

\[ \text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} \]

1 mole of propane requires _____ moles of \( \text{O}_2 \)
1 mole of propane produces _____ moles of \( \text{CO}_2 \)

What mass of carbon dioxide is produced from 110 g of propane?
How many moles of water are produced?
What mass of oxygen is required?
What happens if there is not enough oxygen?

\[ \text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} \]

110 g
110/44=2.5 mole
110/44=2.5 mole
2.5\times3=7.5 \text{ mole}
2.5\times4=10 \text{ moles}
7.5\times44\text{mol}^{-1}=330 g

What happens if there is not enough oxygen?

The reaction goes, but not all of the 110 g of propane can react, so some is left over
This is the case of the \textit{limiting reactant}. 