WELCOME TO QUANTITATIVE ANALYSIS

also known as Analytical Chemistry

CHAPTERS 0 AND 1

The Analytical Process and Measurements
What is Analytical Chemistry?

IT’s NOT what you see on TV!

Identifying an Unknown Is Not As Easy as Portrayed by the CSI TV Show.

Typically Requires More Than One Experiment and > 45 Minutes of Analysis with corresponding high cost (single DNA analysis ~$10,000)

OK… SO What is Analytical Chemistry?

**ANALYTICAL CHEMISTRY**: The Science of Chemical Measurements.

Types of Questions Asked in Analytical Chemistry
a.) What is in the sample? (qualitative analysis)
   b.) How much is in the sample? (quantitative analysis)
Introduction to Analytical Chemistry

**Techniques used in Analytical Chemistry:**

a.) **Wet Chemical Methods:** titrations, color-forming reactions, precipitations, etc.
b.) **Instrumental Methods:** spectrometry, chromatography, etc.

What is it?  
How much is there?  
How pure is it?  
What are the impurities?

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**The Analytical Process**

1.) **Formulating the Question:**
   
   *Translate General Question into Specific Question*
   
   *Is this water safe to Drink? → What is the concentration of Arsenic in the water sample?*

2.) **Selecting Analytical Procedures:**
   
   a.) Choose procedure to measure Arsenic in water
      
      (i) Uncertainty in measurement  
      (ii) Limit of detection  
      (iii) Destroy sample  
      (iv) Availability, time, cost  
   
   b.) If necessary, develop new procedure

3.) **Sampling:**
   
   a.) Select representative material to analyze
      
      (i) don’t use the entire sample  
      (ii) consistency in sample collection

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<table>
<thead>
<tr>
<th>Source</th>
<th>Caffeine (mg per serving)</th>
<th>Serving size (oz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regular coffee</td>
<td>106-164</td>
<td>5</td>
</tr>
<tr>
<td>Decaffeinated coffee</td>
<td>2-5</td>
<td>5</td>
</tr>
<tr>
<td>Tea</td>
<td>21-50</td>
<td>5</td>
</tr>
<tr>
<td>Cocoa beverage</td>
<td>2-8</td>
<td>6</td>
</tr>
<tr>
<td>Baking chocolate</td>
<td>35</td>
<td>1</td>
</tr>
<tr>
<td>Sweet chocolate</td>
<td>20</td>
<td>1</td>
</tr>
<tr>
<td>Milk chocolate</td>
<td>6</td>
<td>1</td>
</tr>
<tr>
<td>soft drinks</td>
<td>36-57</td>
<td>12</td>
</tr>
</tbody>
</table>
The Analytical Process

4.) Sample Preparation:
   a.) convert sample into form suitable for chemical analysis
      (i) Dissolve sample
      (ii) Concentrate sample
      (iii) Remove species that interfere with analysis

The Analytical Process

4.) Sample Preparation:
   a.) Example:

How do you prepare samples for Drug Discovery?

What we want to know:

- Is the drug active? Does it cure the disease/illness?
- How is the drug taken? (Pill, injection)
- How often does the drug need to be taken?
- Does the drug have side-effects?

How these Questions are Typically Addressed:

- Treat animal (rat, mice, etc) with drug
- Monitor drug duration in animal
- Monitor location of drug accumulation
- Monitor animal health

How do you treat the animal with the drug?
How do you monitor the drug concentration in the Animal?
How do you determine the drug location?
How do you determine the animals health?

Tumor size is measured by fluorescence through the mouse skin using quantum dots as a function drug dosage
The Analytical Process

4.) Sample Preparation:
   a.) Example:

   How do you prepare samples for Drug Discovery?

![Cross-section of sacrificed mouse showing tissue removal](image)

Inject mouse with drug

Tissue plug from mouse kidney

Chromatography indicates presence of drug and metabolites in tissue sample

Determine drug quantity and distribution


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The Analytical Process

5.) Analysis:
   a.) measure concentration of analyte in several identical aliquots (portions)
      (i) Replicate measurements \(\rightarrow\) uncertainty in the analysis
          ➢ Avoid large errors
          ➢ Reliability of measurement
      (ii) Calibration Curve
          ➢ Measure response for known samples

6.) Report and Interpretation of Results

7.) Drawing Conclusions
   a) How the Report is used
Units and Concentrations

To a large extent, analytical chemistry is a science of measurement and measurements require minimizing errors.

Sugar Consumption

Units of Measurement

1.) SI Units:
   a.) international units of measurement (metric units)
   b.) ALL SI units are based on certain fundamental quantities

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Unit (Symbol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>Meter (m)</td>
</tr>
<tr>
<td>Mass</td>
<td>Kilogram (kg)</td>
</tr>
<tr>
<td>Time</td>
<td>Second (s)</td>
</tr>
<tr>
<td>Electric current</td>
<td>Ampere (A)</td>
</tr>
<tr>
<td>Temperature</td>
<td>Kelvin (K)</td>
</tr>
<tr>
<td>Luminous intensity</td>
<td>Candela (cd)</td>
</tr>
<tr>
<td>Amount of substance</td>
<td>Mole (mol)</td>
</tr>
<tr>
<td>Plane angle</td>
<td>Radian (rad)</td>
</tr>
<tr>
<td>Solid angle</td>
<td>Steradian (sr)</td>
</tr>
</tbody>
</table>
Units of Measurement

Standards of length were once represented by the distance between two marks on a solid metal bar. Copies of these standards were displayed in public places so that people could check the accuracy of the rules they were using.

Standards Of Length (1876) Trafalgar Square

In 1588, Elizabeth I issued a new standard yard which remained the legal British yard for over 300 years.

History of the meter

Origins of the meter go back to at least the 18th century

- Two competing approaches to the definition of a standard unit of length.
  - define the meter as the length of a pendulum having a half-period of one second
  - define the meter as one ten-millionth of the length of the earth's meridian along a quadrant

- (1791) French Academy of Sciences chose the meridian
  - force of gravity varies slightly over the surface of the earth, affecting the period of the pendulum.
  - meter equal $10^7$ of the length of the meridian through Paris from pole to the equator.
  - prototype was short by 0.2 millimeters because researchers miscalculated the flattening of the earth due to its rotation.

- (1960) used a definition based upon a wavelength of krypton-86 radiation

- (1983) meter replaced by the following definition:
  - The meter is the length of the path traveled by light in vacuum during a time interval of $1/299,792,458$ of a second.
Units of Measurement

1.) SI Units:

   d.) To indicate multiples or fractions of units, various prefixes are used

Example:

3.2\times10^{-11} \text{ s} = 32 \times10^{-12} \text{ s} = 32 \text{ ps}

<table>
<thead>
<tr>
<th>Prefix</th>
<th>Symbol</th>
<th>Factor</th>
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<tr>
<td>Mega</td>
<td>M</td>
<td>10^6</td>
</tr>
<tr>
<td>Kilo</td>
<td>k</td>
<td>10^3</td>
</tr>
<tr>
<td>Hecto</td>
<td>h</td>
<td>10^2</td>
</tr>
<tr>
<td>Deca</td>
<td>da</td>
<td>10^1</td>
</tr>
<tr>
<td>Deci</td>
<td>d</td>
<td>10^{-1}</td>
</tr>
<tr>
<td>Centi</td>
<td>c</td>
<td>10^{-2}</td>
</tr>
<tr>
<td>Milli</td>
<td>m</td>
<td>10^{-3}</td>
</tr>
<tr>
<td>Micro</td>
<td>µ</td>
<td>10^{-6}</td>
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<tr>
<td>Nano</td>
<td>n</td>
<td>10^{-9}</td>
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<tr>
<td>Pico</td>
<td>p</td>
<td>10^{-12}</td>
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<tr>
<td>Femto</td>
<td>f</td>
<td>10^{-15}</td>
</tr>
<tr>
<td>Atto</td>
<td>a</td>
<td>10^{-18}</td>
</tr>
</tbody>
</table>

Units of Measurement

1.) SI Units:

   e.) Conversions to SI units

   f.) Liter is commonly used for volume instead of m^3

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Unit</th>
<th>Symbol</th>
<th>SI equivalent</th>
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</thead>
<tbody>
<tr>
<td>Volume</td>
<td>liter</td>
<td>L</td>
<td>*10^{-3} m^3</td>
</tr>
<tr>
<td></td>
<td>milliliter</td>
<td>mL</td>
<td>*10^{-6} m^3</td>
</tr>
<tr>
<td>Length</td>
<td>angstrom</td>
<td>Å</td>
<td>*10^{-10} m</td>
</tr>
<tr>
<td></td>
<td>inch</td>
<td>in.</td>
<td>*0.0254 m</td>
</tr>
<tr>
<td>Mass</td>
<td>pound</td>
<td>lb</td>
<td>*0.45359237 kg</td>
</tr>
<tr>
<td></td>
<td>metric ton</td>
<td></td>
<td>*1000 kg</td>
</tr>
<tr>
<td>Force</td>
<td>dyn</td>
<td>dyn</td>
<td>*10^{-5} N</td>
</tr>
<tr>
<td>Pressure</td>
<td>bar</td>
<td>bar</td>
<td>*10^5 Pa</td>
</tr>
<tr>
<td></td>
<td>atmosphere</td>
<td>atm</td>
<td>*101,325 Pa</td>
</tr>
<tr>
<td></td>
<td>torr</td>
<td>Torr</td>
<td>133.322 Pa</td>
</tr>
<tr>
<td></td>
<td>pound/in^2</td>
<td>psi</td>
<td>6894.76 Pa</td>
</tr>
<tr>
<td>Energy</td>
<td>erg</td>
<td>erg</td>
<td>*10^{-7} J</td>
</tr>
<tr>
<td></td>
<td>electron volt</td>
<td>eV</td>
<td>1.6021764626\times10^{-19} J</td>
</tr>
<tr>
<td></td>
<td>calorie, thermochemical</td>
<td>cal</td>
<td>*4.184 J</td>
</tr>
<tr>
<td></td>
<td>Calorie (British)</td>
<td>Cal</td>
<td>*1000 cal = 4.184 kJ</td>
</tr>
<tr>
<td>British thermal unit</td>
<td>Btu</td>
<td></td>
<td>1055.06 J</td>
</tr>
<tr>
<td>Power</td>
<td>horsepower</td>
<td></td>
<td>745.700 W</td>
</tr>
<tr>
<td>Temperature</td>
<td>Centigrade (= Celsius)</td>
<td>°C</td>
<td>*K - 273.15</td>
</tr>
<tr>
<td></td>
<td>Fahrenheit</td>
<td>°F</td>
<td>*1.8°C + 32</td>
</tr>
</tbody>
</table>

CHM 212
M. Prushan
Units of Measurement

2.) **Expressions of Concentration:**
   a.) **Molarity (moles/L, or M):**
      (i) Most common unit of concentration
      - Gives number of moles of a substance in 1 liter of the given solvent.
      - Recall: 1 mole (mol) of a substance = \(6.022 \times 10^{23}\) units (atoms, molecules, ions, etc).
      - Molecular weight (MW): the mass of a substance that contains 1 mole.
      - Example:

      Find the concentration in Molarity (M) of 12.00g of benzene \((\text{C}_6\text{H}_6)\) dissolved up to a total volume of 250.00 ml in hexane.

      \[
      \text{MW benzene} = 6 \times (12.011) + 6 \times (1.008) = 78.114 \text{ g/mol}
      \]

      \[
      \text{Conc. C}_6\text{H}_6 = \frac{1 \text{ mol}}{78.114 \text{ g}} \times \frac{12.00 \text{ g}}{0.2500 \text{ L}} = 0.6144 \text{ M}
      \]

      **Make Sure Units Cancel!!**

b.) **Formality (F):**
   (i) Concentrations expressed in M describe the actual concentration of a given chemical species in solution.
   - Some chemicals when placed in solution will dissociate or converted to multiple forms
   - Example:

   Acetic Acid: \(\text{CH}_3\text{CO}_2\text{H} \rightleftharpoons \text{CH}_3\text{CO}_2^- + \text{H}^+\)

   (ii) Not convenient to refer to the concentrations of each individual form.
   (iv) Instead, concentration of total substance originally added to the solution is used.
   - Formal concentration or Formality given in (mol/L)
   - **Note:** For compounds with a single form in solution, \(M = F\)
Units of Measurement

2.) **Expressions of Concentration:**
   b.) **Percent Composition:**
      (i) **Weight Percent (wt/wt or w/w):** Concentration expressed in terms of **mass of substance** versus the total mass of the sample.
      
      \[
      \text{Weight percent} = \frac{\text{mass of substance}}{\text{mass of total solution or total sample}} \times 100 \%
      \]

      (ii) **Volume Percent (vol/vol or v/v):** Concentration expressed in terms of **volume of substance** versus the total volume of the sample.
      
      \[
      \text{Volume percent} = \frac{\text{volume of substance}}{\text{volume of total solution or total sample}} \times 100 \%
      \]

      (iii) **Weight-Volume Percent (wt/vol or w/v):** Concentration expressed in terms of **mass of substance** versus the total volume of the sample.
      
      \[
      \text{Weight-volume percent} = \frac{\text{mass of substance}}{\text{volume of total solution or total sample}} \times 100 \%
      \]

   

   3.) **Solution Preparation:**
   a.) **Dilution of a Solution:**
      
      \[
      M_c V_c = M_d V_d
      \]
      
      where:
      
      \[
      \begin{align*}
      M_c & = \text{Molarity of substance in the concentrated solution} \\
      V_c & = \text{volume of concentrated solution used} \\
      M_d & = \text{desired Molarity of the diluted solution} \\
      V_d & = \text{total volume of final diluted solution}
      \end{align*}
      \]
What are the ways I can make a solution?

(a) From dry, pure material
Prepare 500 mL of 0.9% (w/v) NaCl

(b) By dilution
Prepare 2.0 L of 1.0 M HNO₃ from conc. HNO₃ (70 % w/w); ρ of conc. HNO₃ = 1.42 g/mL
What are the ways I can make a solution?

(c) Serial Dilutions

Why do you need serial dilutions?

Prepare 100 mL of a 1 ppm Pb solution from a stock solution of 10,000 ppm Pb.

How many grams of perchloric acid, $\text{HClO}_4$, are contained in 37.6 g of 70.5 wt% aqueous perchloric acid? How many grams of water are in the same solution?

$$\text{Weight percent} = \frac{\text{mass of substance}}{\text{mass of total solution or total sample}} \times 100$$
What is the maximum volume of 0.25M sodium hypochlorite solution (NaOCl, laundry bleach) that can be prepared by dilution of 1.00 L of 0.80 M NaOCl?

AND NOW FOR THE HOMEWORK

Chapter 0 : 0-1, 0-2, 0-3, 0-4, 0-5a

Chapter 1 : 1-5, 1-6, 1-7, 1-22, 1-24, 1-26
BUT REMEMBER!

PLEASE

SHOW YOUR WORK

First, I looked in the back of the book, but it wasn’t an odd-numbered problem.

Then I asked my little brother, but he wanted me to pay him $5.

Finally, I found it on the Internet with Google.

AH!

MY MATH TEACHER WANTS US TO SHOW HOW WE GET OUR ANSWERS.

BUT REMEMBER!

AND

DON’T OVER COMPLICATE THE PROBLEM!

\[
\int_{0}^{\pi} \sin^2 \frac{x}{2} \, dx = \int_{0}^{\pi} \frac{1}{2} (\sin x + 1) \, dx = \frac{\pi}{2} - \frac{1}{2}
\]

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