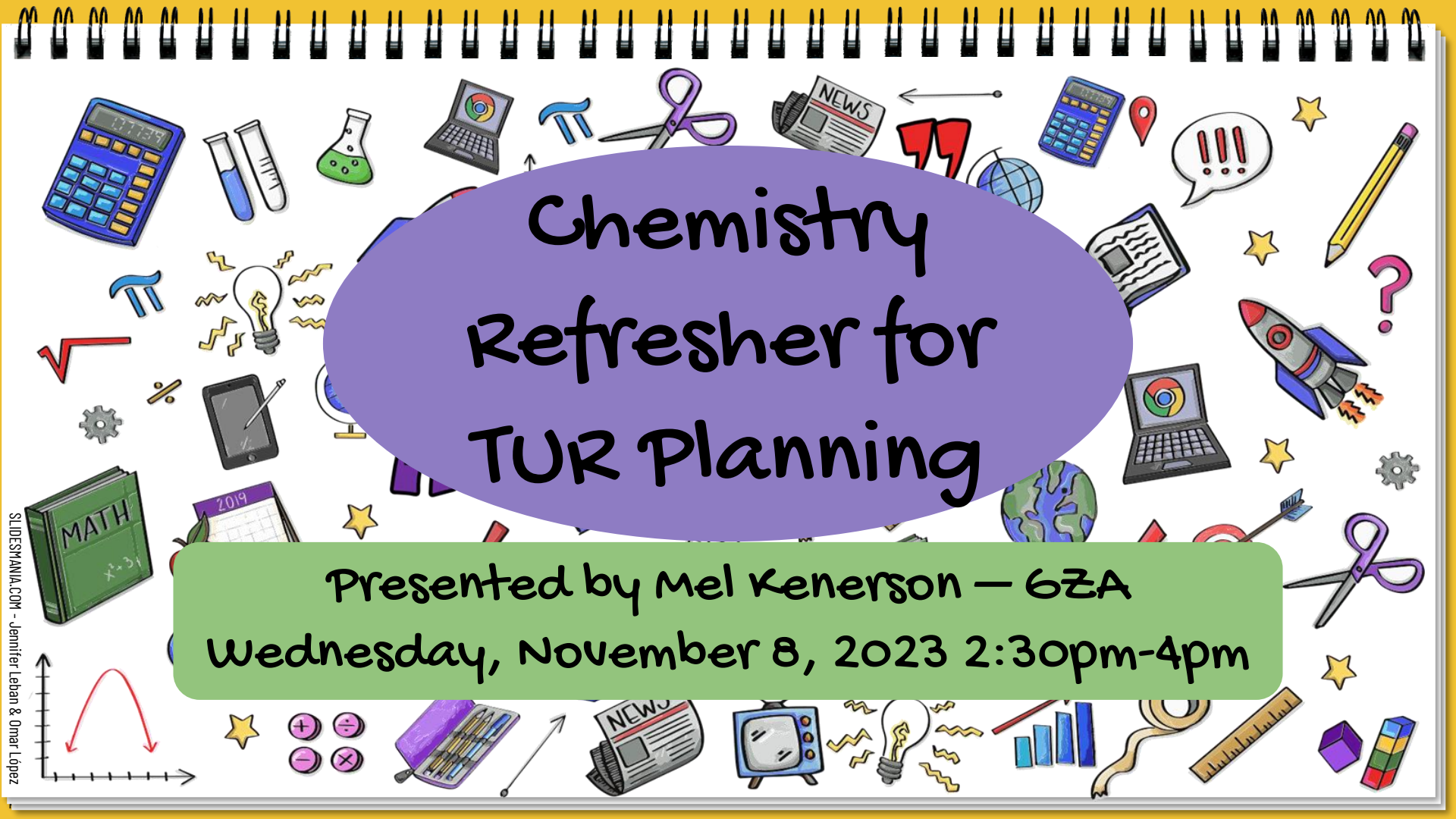
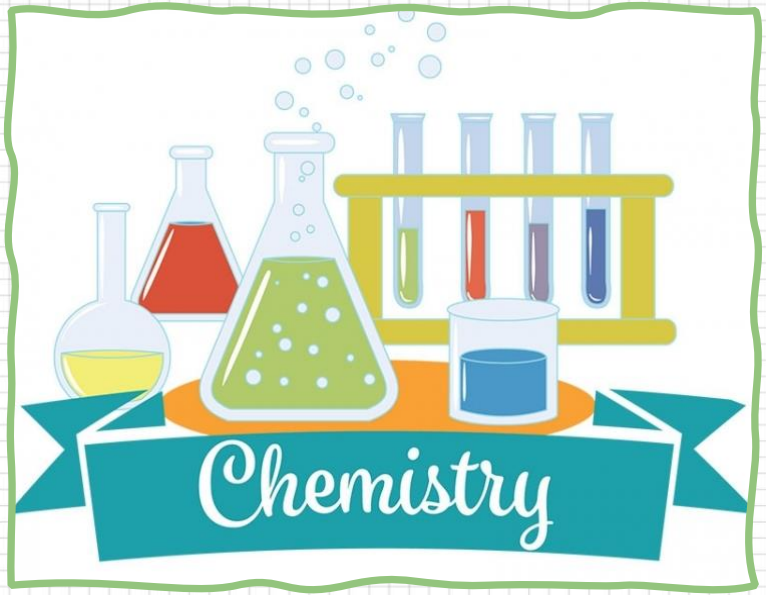
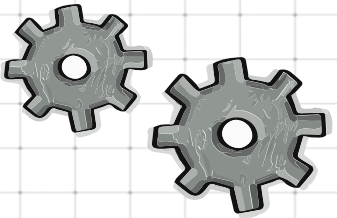

Chemistry Refresher for TUR Planning
Presented by Mel Kenerson — GZA
Wednesday, November 8, 2023 2:30pm-4pm
MATH
NEWS
2019
SLIDESMANIA.COM - Jennifer Leban & Omar López

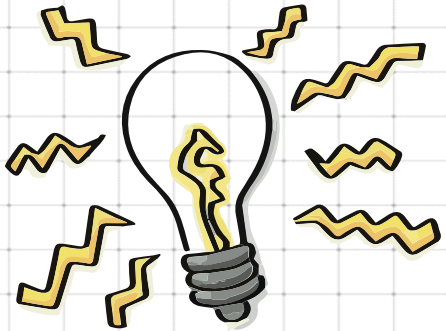
Agenda

- Unit Conversion
- Solutions & Concentrations
- pH
- Volatility
- Reviewing Substitutions
- Stoichiometry





§ 1
Unit Conversions



Dimensional Analysis (review)

Gallons x Specific Gravity x Density$_{H_2O}$ = Mass

750 gal	0.96	8.34#
		gal

= 6,005 #

Used when:

- Converting between units, such as metric to empirical
- Using provided data, such as density or analytical data, to determine a specific quantity, such as pounds of material used

Metric Conversions

PREFIX	SYMBOL	UNIT EQUIVALENT
tera	T	10^{12}
giga	G	10^{9}
mega	M	10^{6}
kilo	k	10^{3}
deci	d	10^{-1}
centi	c	10^{-2}
milli	m	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}
pico	p	10^{-12}

$1\ kg = 10^{3}\ g$

$1\ \mu g = 10^{-6}\ g$

Used in Dimensional Analysis:

$$\frac{124\ mg}{L} \left| \frac{10^{-3}\ g}{mg} \right. = 0.124\ g/L$$

Temperature Conversions

Standard Temperature Scales

$$°C = (°F - 32)/1.8$$

$$°F = (1.8)°C + 32$$

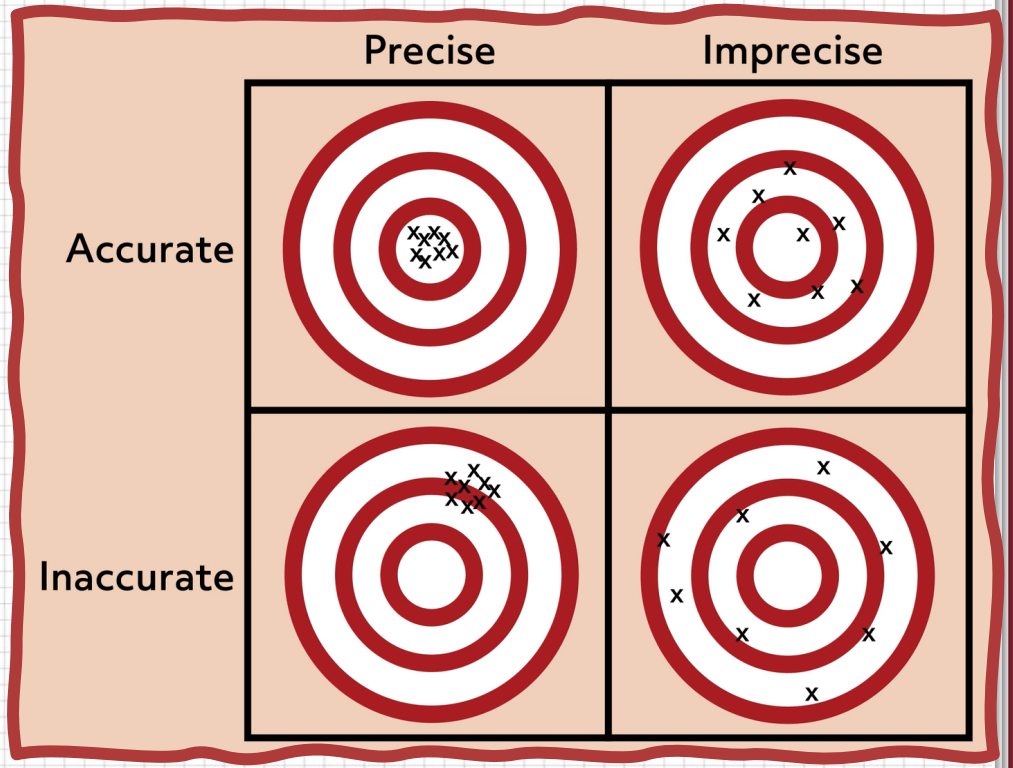
Absolute Zero Temperature Scales

$$K = °C + 273.15$$

$$°R = °F + 459.67$$

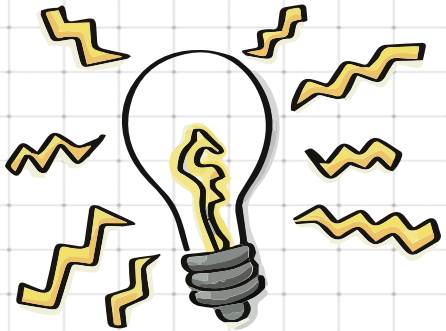
What about Significant Figures???

- Used to address precision and accuracy
- Your answer can not be more exact than your method to measures the inputs
- TURA asks for whole number pounds (except dioxin), so sig-fig not considered

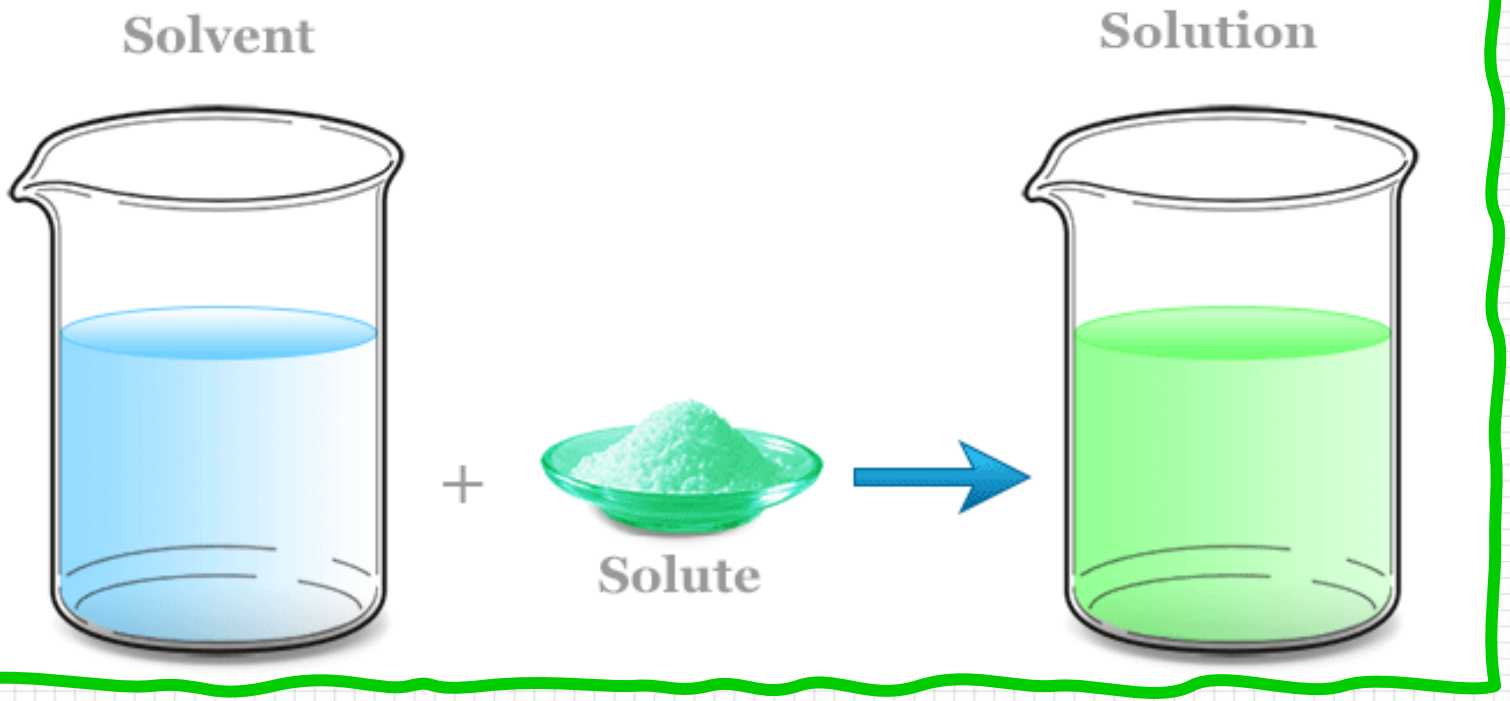


§ 2

Solutions & Concentration



Solution Terminology



So Many Units!!!

%m or **%w** or **%w/w**

$$\frac{\text{mass of solute}}{\text{mass of solution}} \times 100\%$$

g/g #/# kg/kg

%v or **%v/v**

$$\frac{\text{volume of solute}}{\text{volume of solution}} \times 100\%$$

ml/ml gal/gal

%m/v or **%w/v**

$$\frac{\text{mass (g) of solute}}{\text{volume (ml) of solution}} \times 100\%$$

g/ml or kg/L

Analytical Data in ppm

For liquid concentrations:

ppm x solution density = mg/L or lb/gal

When density of solution is close to 1 mg/L (such as a dilute aqueous solution):

ppm = mg/L

Analytical Data in ppm

For airborne concentrations, convert ppm parts into moles

conversion factor: **1 mole of gas = 24.45 L @SATP**

(25°C and 1atm)

485 ppm styrene in stack test. How many pounds per cubic foot is this?

$$\frac{485 \text{ mol styrene}}{10^6 \text{ mol air}} \times \frac{104.15 \text{ g}}{\text{mol}} \times \frac{1 \text{ mol}}{24.45 \text{ L}} \times \frac{\text{lb}}{454 \text{ g}} \times \frac{28.32 \text{ L}}{\text{ft}^3} = 1.3 \times 10^{-4} \text{ lb/ft}^3$$

Our Friend the Mole

- **1 mole (abbreviated "mol") = 6.0221367 x 10^{23} particles**
- **particles = atoms, ions, electrons, molecules, ionic compounds (formula units)**

Image source: American Chemical Society

"Mole Day": October 23 from 6:02 a.m. to 6:02 p.m.
The theme of this past year was "molEvengers".

Image source: DeviantArt

Molar Mass (aka mass of 1 mole)

- **Molar mass** is the mass in grams of one mole of any pure substance.

- **The molar mass of any element is numerically equivalent to its atomic mass and has the units g/mol.**

1 mole of iron (Fe) 55.845 g/mol

Watch out for diatomic elements:

1 mole of Hydrogen gas (H_2) 2(1.008) = 2.016 g/mol

The molar mass of a compound equals the molar mass of each element, multiplied by the moles of that element in the chemical formula, added together.

What is the molar mass of water (H_2O)?

H: 2 mole * 1.008 g/mol = 2.016 g/mol

O: 1 mole * 15.999 g/mol = 15.999 g/mol

2.016 + 15.999 = 18.015 g/mol

Reporting Metal Compounds for TURA

For metals reported as compounds, the total weight of the compound in the amount manufactured, processed or otherwise used is counted. However, only the weight of the parent metal being reported is counted in calculating byproducts. (TURA Reporting Instructions)

- **297 pounds of lead oxide manufactured – report as pounds of lead oxide**
- **297 pounds in waste scrap (by-product) – report as pounds of lead (base metal)**

Use molar mass ratio to create conversion: _____#Pb/# PbO

$$\frac{207.2 \text{ g/mol (Pb)}}{223.2 \text{ g/mol (PbO)}} = 0.928 \text{ \#Pb/\#PbO}$$

297 # PbO (0.928 #Pb/#PbO) = 276 pounds Pb (By-Product)
297 # PbO – 275 # Pb = 21 # O (Chemical is a Compound)

Section 1: Facility-Wide Use of Listed Chemical

a. MA DEP CAS #	b. Chemical Name (Dioxin should be in grams, decimal points may be used)
1026	Lead Compounds

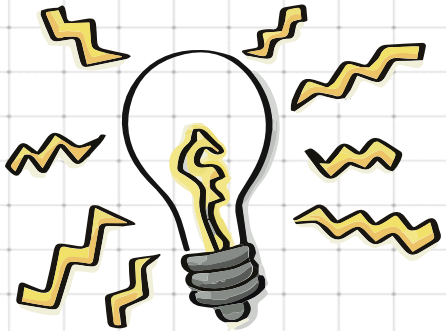
Facility-wide use of chemical identified in a. Enter the total amount (in POUNDS, except for dioxin) for each applicable category. **NOTE:** 'Generated as byproduct' (item f.) means all waste containing the listed chemical before the waste is handled, transferred, treated, recycled or released. Please refer to the reporting instructions before completing this section.

297 Entire Compound c. Manufactured	d. Processed
e. Otherwise Used	**276** regulated metal only f. Generated As Byproduct
g. Shipped In Or As Product	h. Production or Activity Ratio

Section 2: Materials Balance

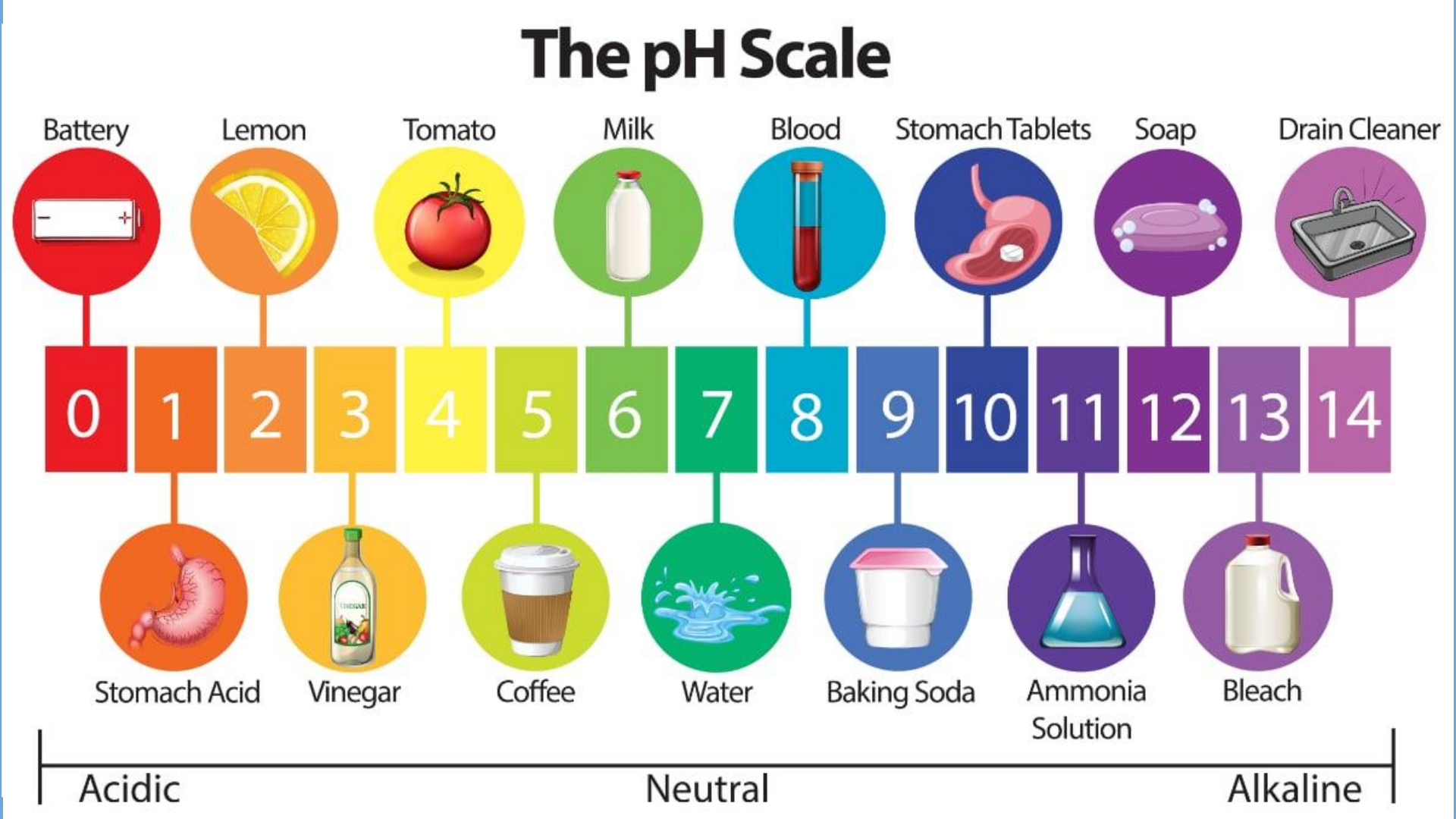
When the amounts reported in c, d and e in Section 1 are added together, the sum will in many cases equal the sum of f and g. In other words, lines c, d and e will often form a "materials balance." If lines c, d and e are not in approximate balance, you must use this section to explain why. Indicate all the reasons that apply by entering the number of pounds on the appropriate line below (e.g., 4,000 Chemical was held in inventory).

a. Chemical Was Recycled On Site	b. Chemical Was Consumed Or Transformed
c. Chemical Was Held In Inventory	**21** non-metal portion of compound d. Chemical Is A Compound
e. Other	



§ 3
pH

The pH Scale


Battery
Lemon
Tomato
Milk
Blood
Stomach Tablets
Soap
Drain Cleaner
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
Stomach Acid
Vinegar
Coffee
Water
Baking Soda
Ammonia Solution
Bleach
Acidic
Neutral
Alkaline

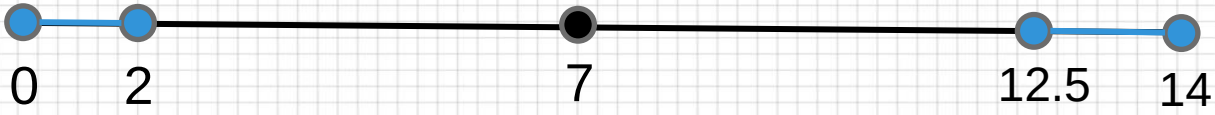
What does pH tell us?

Chemistry Test Answer:

the concentration of hydronium [H_3O+] ions

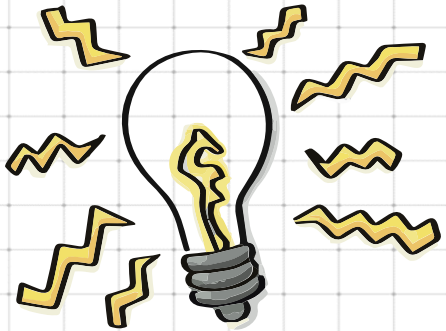
Practical Answer:

if my aqueous solution is corrosive

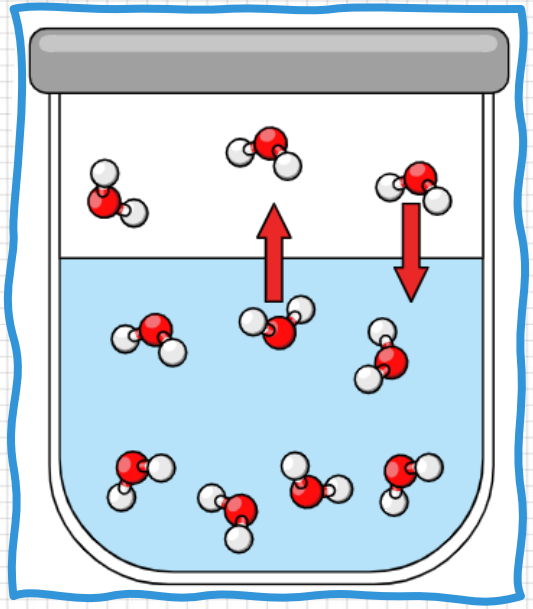


A pH less than or equal to 2 or greater than or equal to 12.5 is considered corrosive.

§ 4
Volatility



Vapor Pressure & Volatility

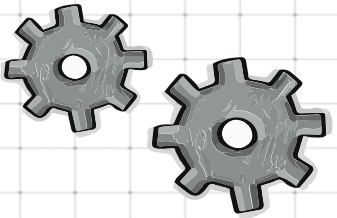


- **Vapor Pressure** is a measure of the tendency of a material to change into the gaseous or vapor state, and it increases with temperature.
- **Volatility** is the tendency or ability of a liquid to vaporize.
- Vapor pressure is a measure of a liquid's volatility. A high vapor pressure usually is an indication of a volatile liquid, or one that readily vaporizes.
- Council Directive 1999/13/EC of 11 March 1999 - any organic compound is considered to be a volatile organic compound (VOC) if it has a **vapor pressure of 10 Pa or more at 20°C**

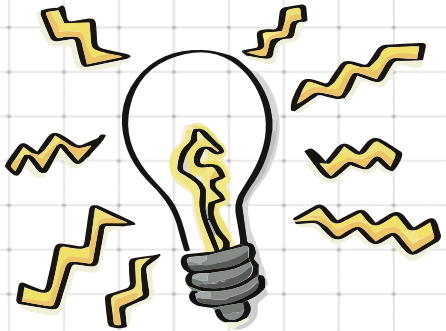
Why Include Volatility???

- Volatile compounds can evaporate into air
  - Concern for worker safety through inhalation
  - Consideration for air emissions in a process

- Usually expressed as “% volatile” on an SDS
  - If 20% volatile, can expect under normal, open conditions, 20% of the amount used becomes a vapor
  - More detailed analysis may be needed at each process step to determine the amount of chemical lost to evaporation → air emissions (by-product)

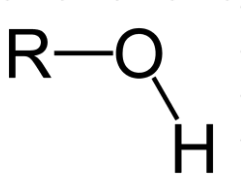


§ 5
Reviewing Substitutions

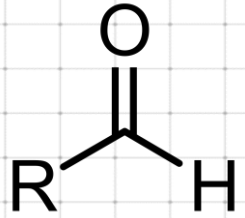


Chemical Groups

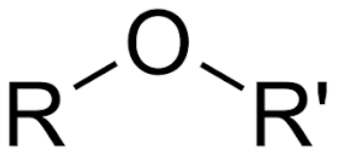
- -ol: alcohol (-OH on a carbon chain)
  - Flammable, volatile



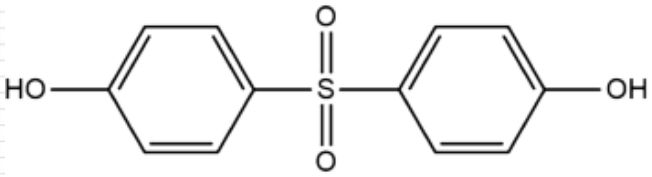
- Phenol subgroup (-OH on benzene ring)
  - Volatile and soluble in water
  - May produce flammable vapor when heated
- Polyol: (multiple –OH groups on organic structure)
  - lower volatility, combustible, but not flammable



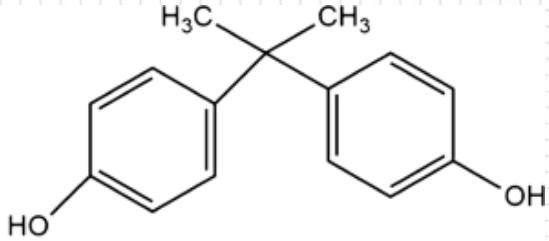
- -al: aldehyde
  - More volatile than alcohols, Many exist as gases of volatile liquids
- Ether (name ends in ether)
  - Highly volatile



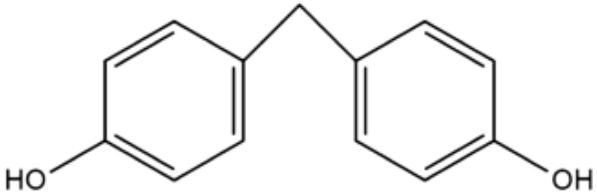
Reviewing Substitutions



Bisphenol S

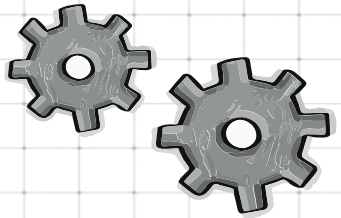


Bisphenol A

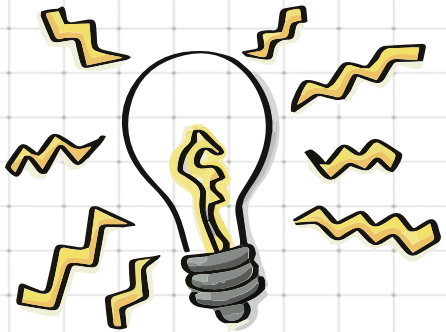


Bisphenol F

"Because BPA substitutes such as BPS and BPF have similar structures to BPA, they appear to have similar metabolism, potencies, and action to BPA. In addition, they may pose similar potential health hazards as BPA." (National Center for Biotechnology Information – "Concern about the Safety of Bisphenol A substitutes")



§ 6
Stoichiometry



Stoichiometry

- **Calculations based on balanced stoichiometric equations**
- **Can using starting values and stoichiometry, along with molar mass to calculate products of the reaction**

$$2\ C_2H_6 + 7\ O_2 \longrightarrow 6\ H_2O + 4\ CO_2$$

If our process uses 657 pounds of ethane, how much carbon dioxide is theoretically produced?

$$2\ C_2H_6 + 7\ O_2 \longrightarrow 6\ H_2O + 4\ CO_2$$

657 lb C_2H_6	454 g	mol C_2H_6	4 mol CO_2	44.01 g CO_2	lb
	lb	30.07 g C_2H_6	2 mol C_2H_6	mol CO_2	454 g

Calculations reduce to ratio of molar mass and ratio of stoichiometric coefficients. Each ratio has end point over starting point.

657 lb C_2H_6	44.01 g CO_2	4 mol CO_2
	30.07 g C_2H_6	2 mol C_2H_6

= 1,923 lb CO_2

Questions??