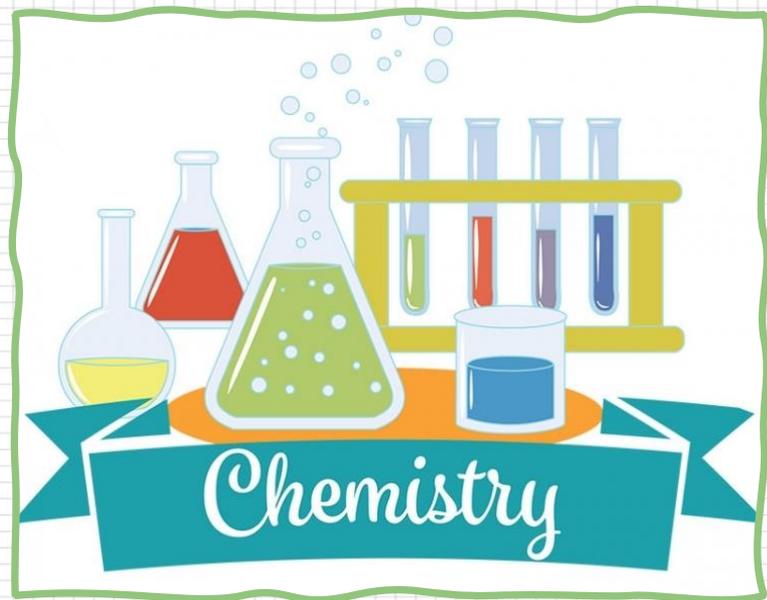


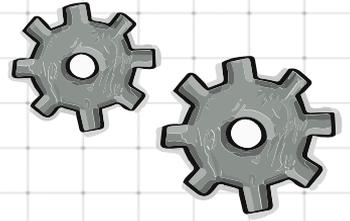
Chemistry Refresher for TUR Planning

Presented by Mel Kenerson – 6ZA
Wednesday, November 8, 2023 2:30pm-4pm

Agenda

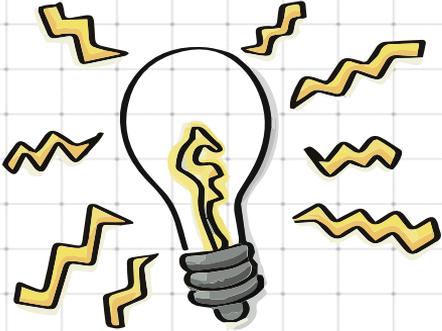
- Unit Conversion
- Solutions & Concentrations
- pH
- Volatility
- Reviewing Substitutions
- Stoichiometry





§ 1

Unit Conversions



Dimensional Analysis (review)

Gallons x Specific Gravity x Density_{H2O} = Mass

750 gal	0.96	8.34#	= 6,005 #
		gal	

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}

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

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

Used in Dimensional Analysis:

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

Temperature Conversions

Standard Temperature Scales

$$^{\circ}\text{C} = (^{\circ}\text{F} - 32) / 1.8$$

$$^{\circ}\text{F} = (1.8)^{\circ}\text{C} + 32$$

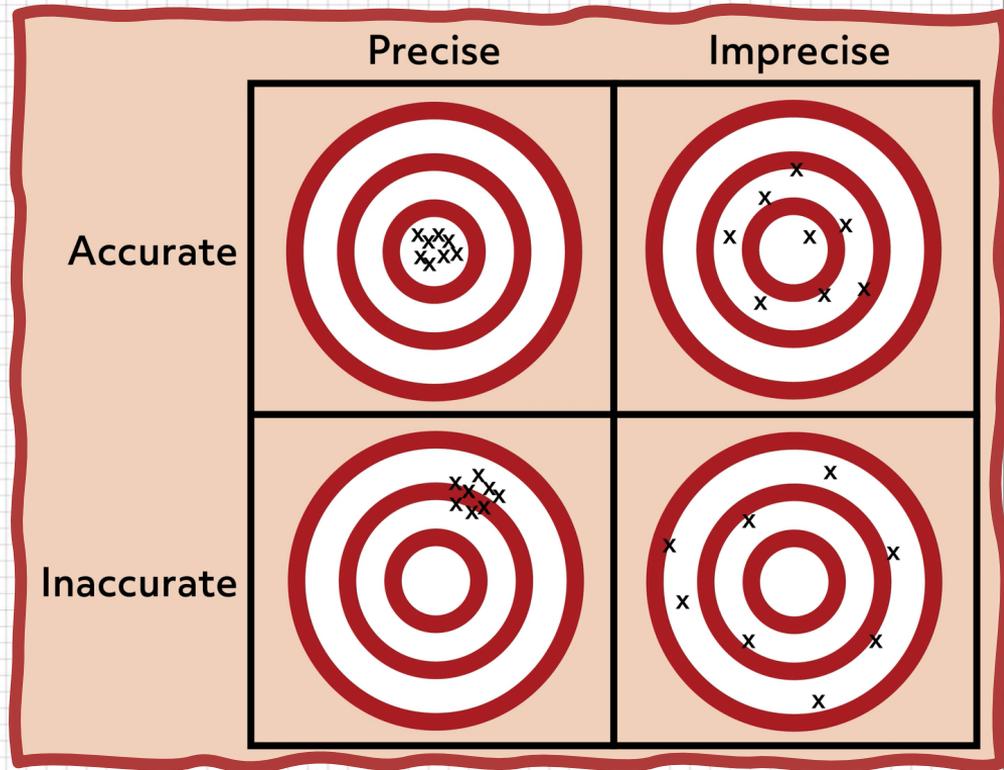
Absolute Zero Temperature Scales

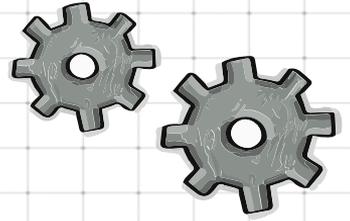
$$\text{K} = ^{\circ}\text{C} + 273.15$$

$$^{\circ}\text{R} = ^{\circ}\text{F} + 459.67$$

What about Significant Figures???

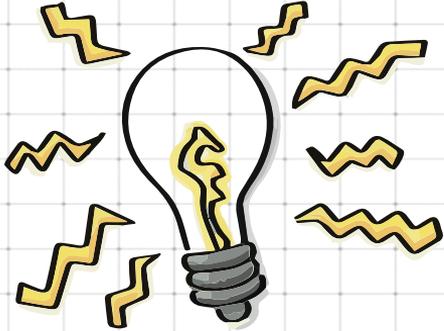
- Used to address precision and accuracy
- Your answer can not be more exact than your method to measures the inputs
- TURA asks for whole number pounds (except dioxin), so sig-fig not considered



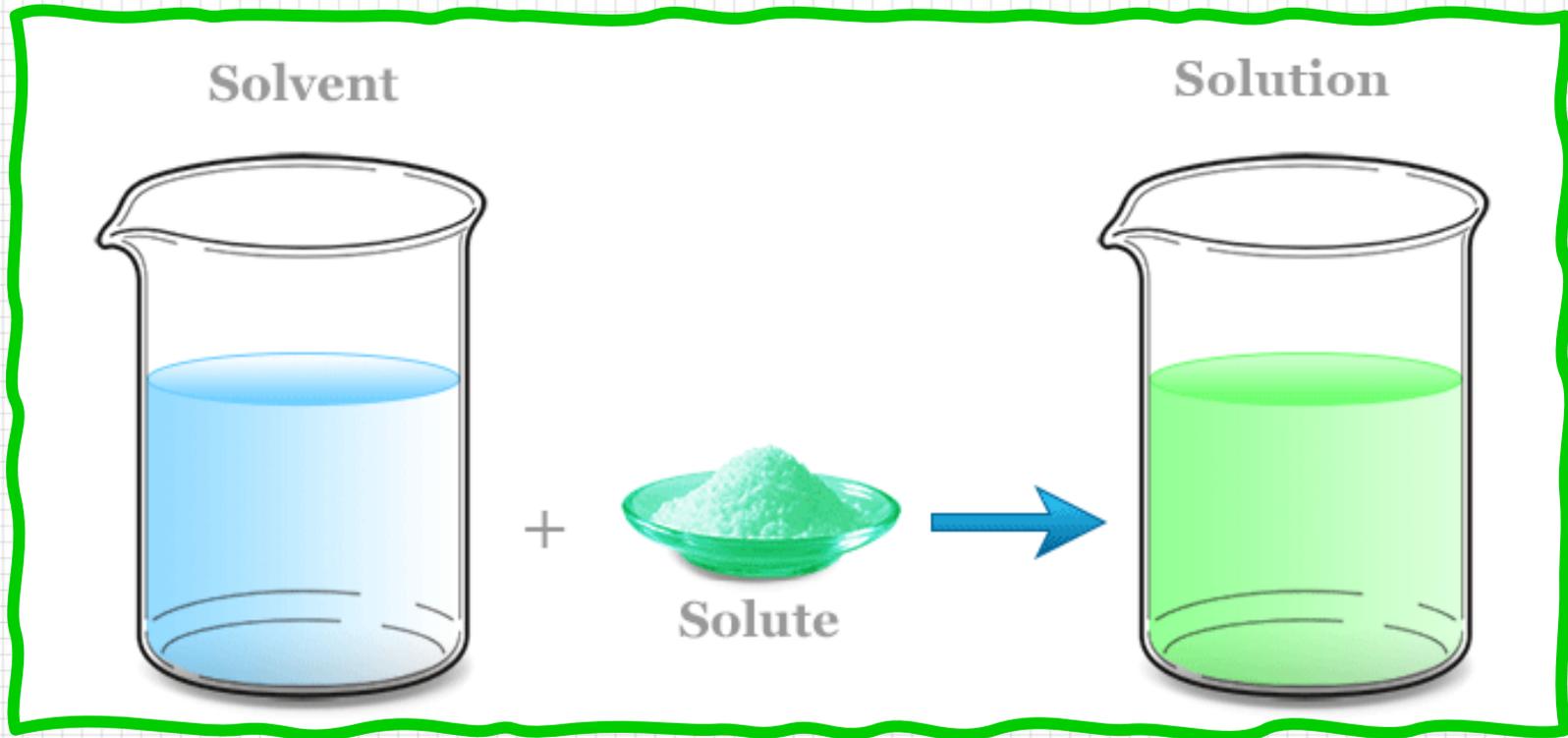


§ 2

Solutions & Concentration



Solution Terminology



So Many Units!!!

%m or %w or %w/w mass of solute x 100% **g/g #/# kg/kg**
mass of solution

%v or %v/v volume of solute x 100% **ml/ml gal/gal**
volume of solution

%m/v or %w/v mass (g) of solute x 100% **g/ml or kg/L**
volume (ml) of solution

Analytical Data in ppm

For liquid concentrations:

$$\text{ppm} \times \text{solution density} = \text{mg/L or lb/gal}$$

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

$$\text{ppm} = \text{mg/L}$$

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?

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

Our Friend the Mole

- 1 mole (abbreviated "mol") = 6.0221367×10^{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 (H₂) 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 (H₂O)?

$$\text{H: } 2 \text{ mole} * 1.008 \text{ g/mol} = 2.016 \text{ g/mol}$$

$$\text{O: } 1 \text{ mole} * 15.999 \text{ g/mol} = 15.999 \text{ g/mol}$$

$$2.016 + 15.999 = 18.015 \text{ g/mol}$$

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

1026

a. MA DEP CAS #

Lead Compounds

b. Chemical Name (Dioxin should be in grams, decimal points may be used)

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

276 regulated metal only

e. Otherwise Used

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

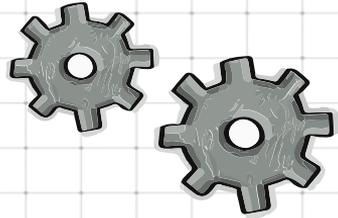
b. Chemical Was Consumed Or Transformed

21 non-metal portion of compound

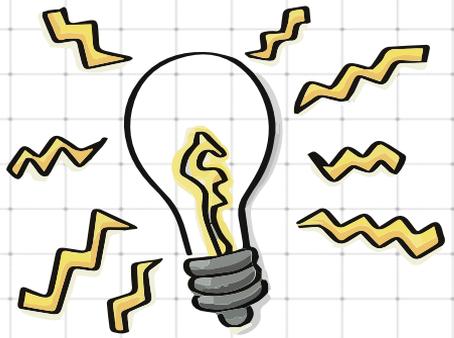
c. Chemical Was Held In Inventory

d. Chemical Is A Compound

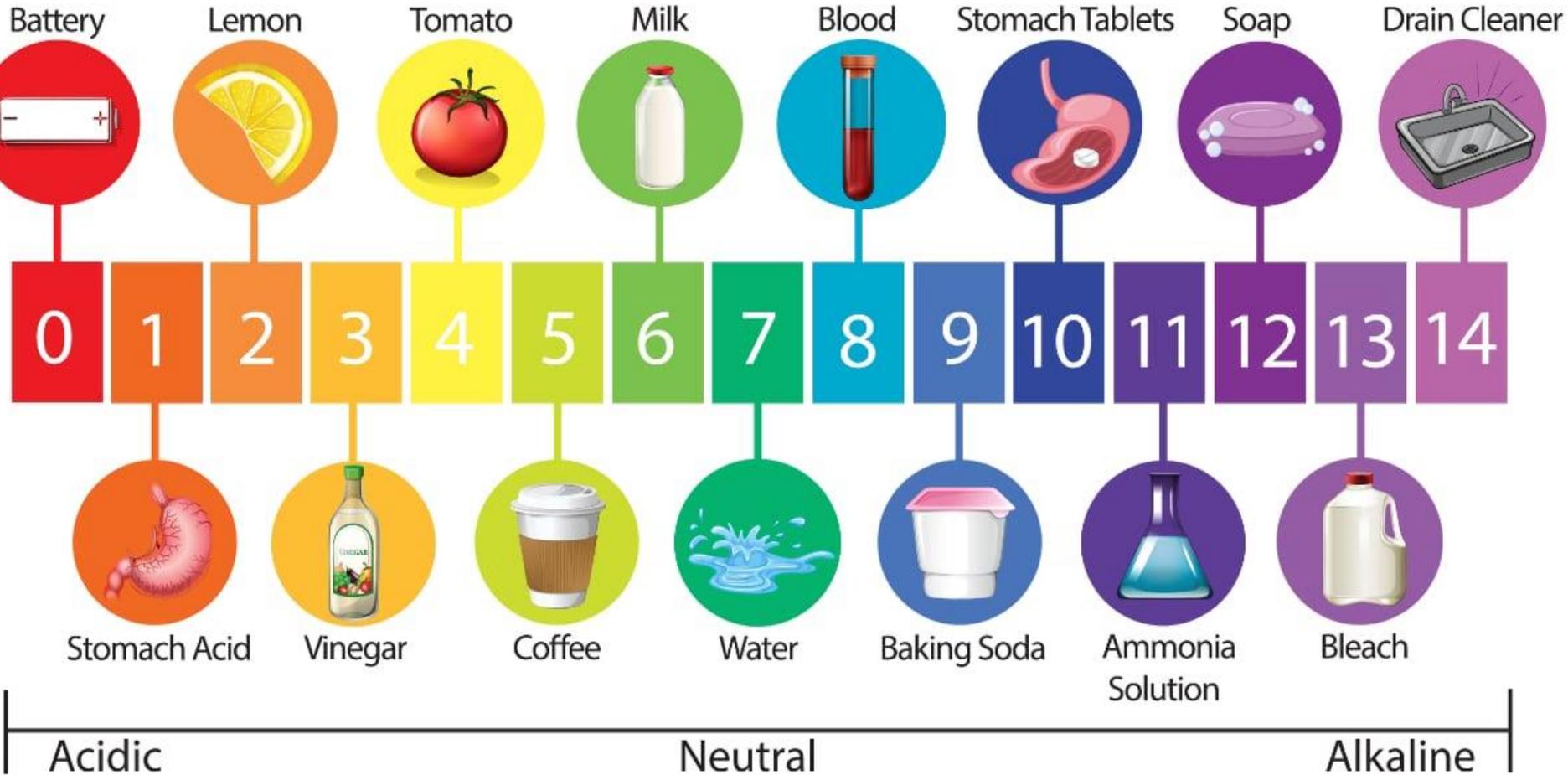
e. Other



§ 3
pt



The pH Scale



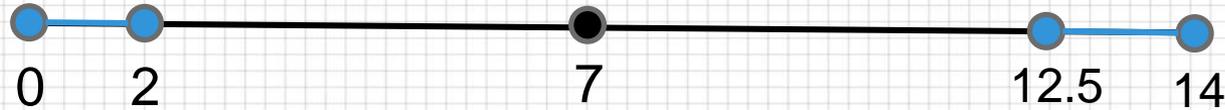
What does pH tell us?

Chemistry Test Answer:

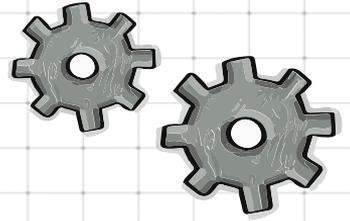
the concentration of hydronium $[H_3O^+]$ ions

Practical Answer:

if my aqueous solution is corrosive

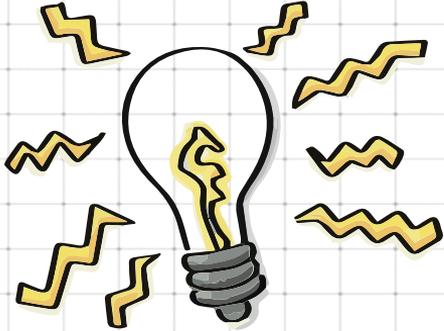


A pH less than or equal to 2 or greater than or equal to 12.5 is considered corrosive.



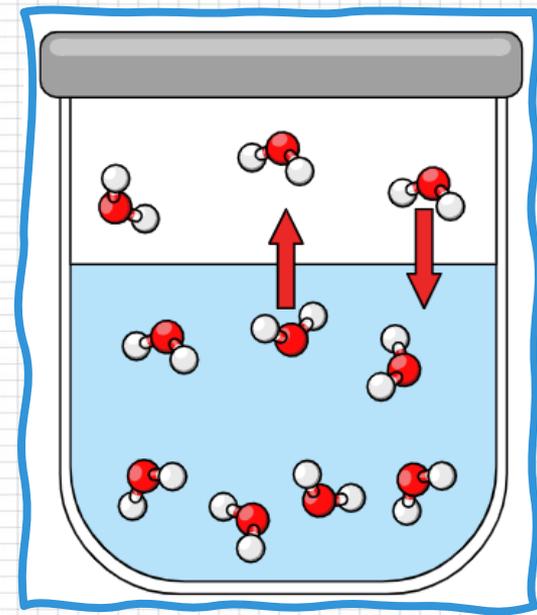
§ 4

Volatility



Vapor Pressure & Volatility

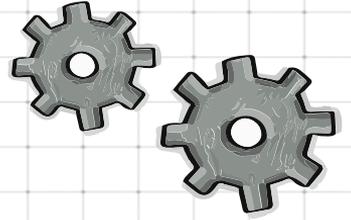
- **Vapor Pressure** is a measure of the tendency of a material to change into the gaseous or vapor state, and it increases with temperature.
- **Volatility** is the tendency or ability of a liquid to vaporize.
- Vapor pressure is a measure of a liquid's volatility. A high vapor pressure usually is an 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???

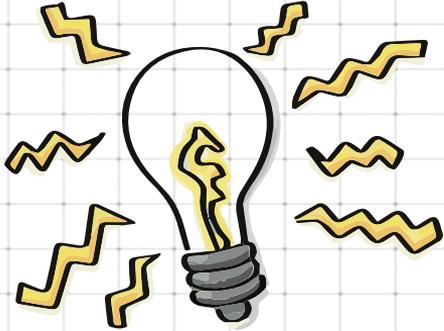
- **Volatile compounds can evaporate into air**
 - **Concern for worker safety through inhalation**
 - **Consideration for air emissions in a process**

- **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)**

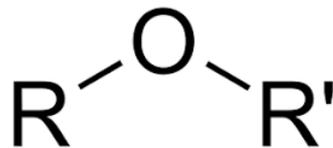
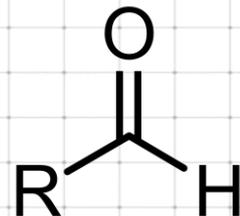
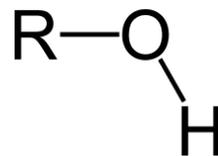
- lower volatility, combustible, but not flammable

- **-al: aldehyde**

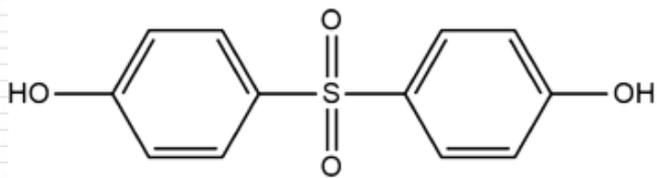
- More volatile than alcohols, Many exist as gases of volatile liquids

- **Ether (name ends in ether)**

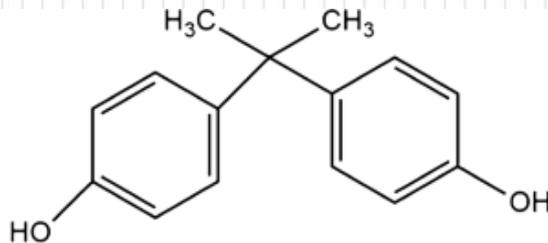
- Highly volatile



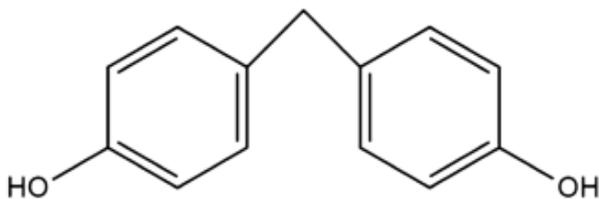
Reviewing Substitutions



Bisphenol S

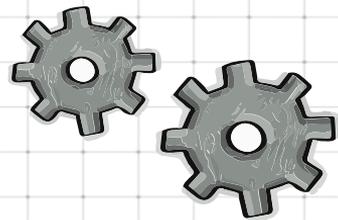


Bisphenol A



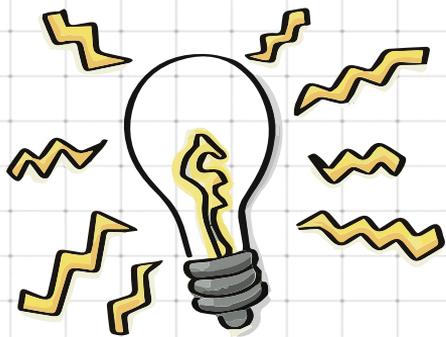
Bisphenol F

“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”)



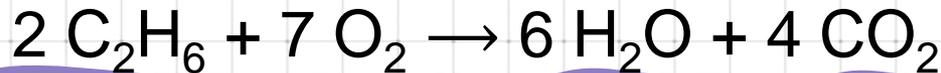
§ 6

Stoichiometry



Stoichiometry

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



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



657 lb C ₂ H ₆	454 g	mol C ₂ H ₆	4 mol CO ₂	44.01 g CO ₂	lb
	lb	30.07 g C ₂ H ₆	2 mol C ₂ H 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 ₂ H ₆	44.01 g CO ₂	4 mol CO ₂	= 1,923 lb CO ₂
	30.07 g C ₂ H ₆	2 mol C ₂ H ₆	

Questions??

1 H Hydrogen 1.008																	2 He Helium 4.003														
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180														
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948														
19 K Potassium 39.098	20 Ca Calcium 40.078											21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.630	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798				
37 Rb Rubidium 85.468	38 Sr Strontium 87.62											39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.905	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.905	54 Xe Xenon 131.294				
55 Cs Cesium 132.905	56 Ba Barium 137.327	57 La Lanthanum 138.905	58 Ce Cerium 140.12	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.054	71 Lu Lutetium 174.967	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.384	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium 209	85 At Astatine 209	86 Rn Radon 222
87 Fr Francium 223	88 Ra Radium 226	89 Ac Actinium 227	90 Th Thorium 232	91 Pa Protactinium 231	92 U Uranium 238	93 Np Neptunium 237	94 Pu Plutonium 244	95 Am Americium 243	96 Cm Curium 247	97 Bk Berkelium 247	98 Cf Californium 251	99 Es Einsteinium 252	100 Fm Fermium 257	101 Md Mendelevium 258	102 No Nobelium 259	103 Lr Lawrencium 260	104 Rf Rutherfordium 261	105 Db Dubnium 262	106 Sg Seaborgium 263	107 Bh Bohrium 264	108 Hs Hassium 265	109 Mt Meitnerium 266	110 Ds Darmstadtium 267	111 Rg Roentgenium 268	112 Cn Copernicium 269	113 Nh Nihonium 270	114 Fl Flerovium 271	115 Mc Moscovium 272	116 Lv Livermorium 273	117 Ts Tennessine 274	118 Og Oganesson 276

