Atoms and Molecules

Chemistry 35

Fall 2000

How Big is an Atom?

Not too hard to calculate:

-use *molar mass (M)* and *density (d)* to obtain ***Molar Volume (V_m):*** **V_m = molar mass/density**

$cm^3/mol = (g/mol)/(g/cm^3)$

EXAMPLE: **Copper** (d= 8.96 g/cm^3, M = 63.55 g/mol)

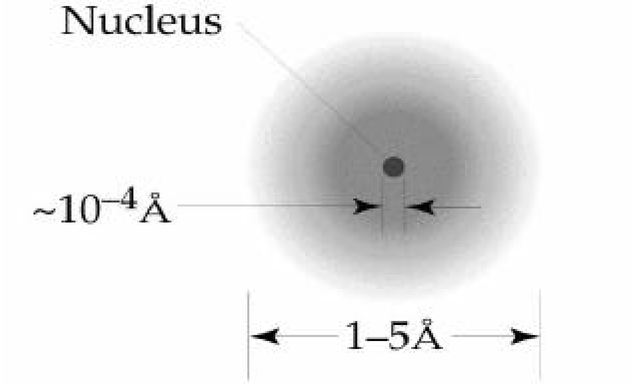
$V_m = 63.55/8.96 = 7.1$ cm^3/mol

So, for ONE atom of Cu:

$(7.1\ cm^3/mol)/(6.022 \times 10^{23}\ atoms/mol) = 1.18 \times 10^{-23}\ cm^3/atom$

Constrained to a cube: ≈ 2.25×10^{-8} cm (= ***2.25 Å***)

Atomic Size

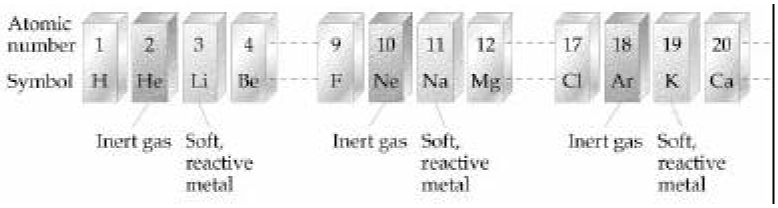


They sure are small!

Organizing the Elements

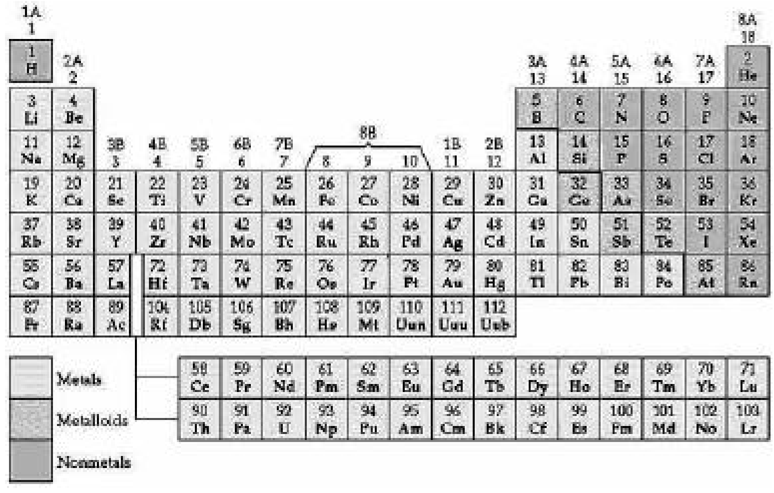
- Late 1800's: *Mendeleyev* arranges elements in order of **increasing atomic mass**

  -finds ***periodic trends in reactivity:***



- arranges so that *elements with similar reactivity* are **grouped**

The Periodic Table



1A 1	2A 2	3B 3	4B 4	5B 5	6B 6	7B 7	8B 8	9	10	1B 11	2B 12	3A 13	4A 14	5A 15	6A 16	7A 17	8A 18
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Uun	111 Uuu	112 Uub						

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Metals
Metalloids
Nonmetals

Groups on the Periodic Table

- Group 8A (far right): ***Noble Gases***
  -***VERY*** unreactive
- Group 1A (far left): ***Alkali Metals***
  -Soft, low m.p. metals
  -***VERY*** reactive (they react with water to give off H_2)
- Group 2A: ***Alkaline Earth Metals***
- Group 7A: ***Halogens***
  -NON-metals (insulators, brittle, gaseous)
- Group 6A: ***Chalcogens***

Molecules

- Definition: *Two or more atoms bound together*
- Identified by a ***Formula***:

Molecular Formula – gives the *actual* numbers and types of atoms in molecule

Empirical Formula – gives the *relative numbers* of atoms in molecule (smallest whole-number ratio)

Mole-Based Calculations

- How many grams of Phosphorous are there in 0.010 mol P_2O_5?

Strategy: *mol P_2O_5 -> mol P -> g P*

$$0.010 \text{ mol } P_2O_5 \times \frac{2 \text{ mol P}}{1 \text{ mol } P_2O_5} \times \frac{30.974 \text{ g P}}{1 \text{ mol P}} = \mathbf{0.61948 \text{ g P}}$$

Round to: ***0.62 g Phosphorous***

Empirical Formula from %-Composition

- **What is the empirical formula for a binary compound which is found to be:**

56.4% Oxygen (by mass)
43.6% Phosphorous (by mass)?

Strategy: *% -> grams -> mol*

(% is a *relative* measure, so DEFINE a sample size (100 g))

In a 100-g sample:

$$56.4\text{ g O} \times \frac{1\text{ mol O}}{15.999\text{ g O}} = \underline{3.525\text{ mol O}}$$

$$43.6\text{ g P} \times \frac{1\text{ mol P}}{30.974\text{ g P}} = \underline{1.4076\text{ mol P}}$$

Emp. Form. - continued

This gives: $P_{1.4076}O_{3.525}$

Dividing: $\mathbf{PO_{2.50}}$ **->** P_2O_5

- ***What about a MOLECULAR formula?***

-need a molecular mass of the compound

Example: MW of P_2O_5 cmpd is 284 g/mol

Empirical Formula Mass ≈ 2x31 + 5x16 = 142

MW/Emp Form Mass = 284/142 = 2

So: 2 X P_2O_5 = $\mathbf{P_4O_{10}}$

%-Composition from a Formula

Calculate the *%-P, %-O* in P_2O_3:

1) Calculate grams P & O per mol P_2O_3

$$1\text{ mol }P_2O_3 \times \frac{2\text{ mol P}}{1\text{ mol }P_2O_3} \times \frac{30.974\text{ g P}}{1\text{ mol P}} = \mathit{61.948\ g\ P}$$

$$1\text{ mol }P_2O_3 \times \frac{3\text{ mol O}}{1\text{ mol }P_2O_3} \times \frac{15.999\text{ g O}}{1\text{ mol O}} = \mathit{47.997\ g\ O}$$

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2) Calc grams per mole P_2O_3

2 P = 2 x 30.974 = 61.948

3 O = 3 x 15.999 = 47.997

109.945 g/mol P_2O_3

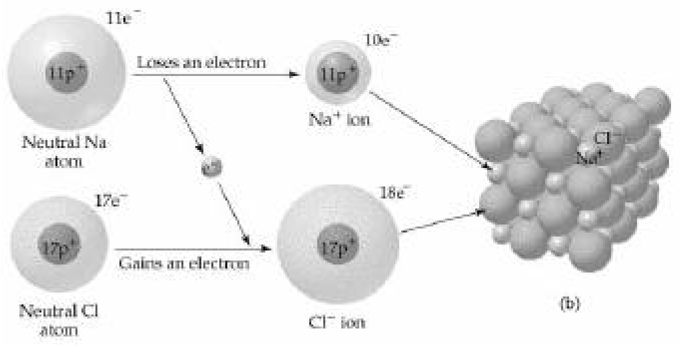
3) Divide to get %-composition

P: $$\frac{61.948\text{ g P}}{109.945\text{ g }P_2O_3} \times 100 = \mathbf{56.34\ \%\ P}$$

O: $$\frac{47.997\text{ g O}}{109.945\text{ g }P_2O_3} \times 100 = \mathbf{43.66\ \%\ O}$$

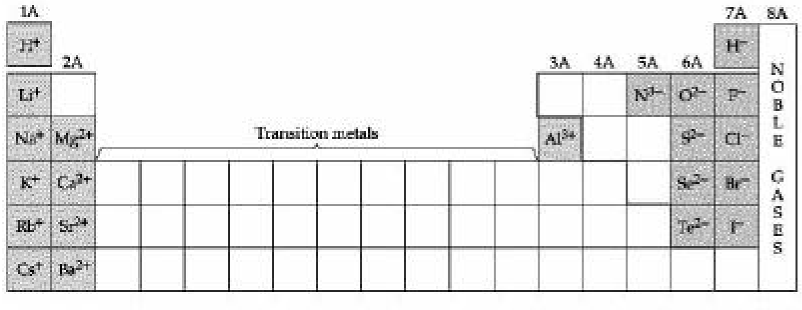
Not all Compounds are Molecules

Let's look at the reaction of an *Alkali Metal (Na)* and a *Halogen (Cl)*:



Ionic Compounds

Formed by reaction of a metal with a non-metal:



Chemical Reactivity

- Why do elements in a *group* have similar reactivity?

  *-have the same # of **valence** electrons*

  -<u>The Octet Rule</u>: elements react so as to attain a Noble Gas configuration (8 e^- in “valence shell”

  HOW? *Share e^-* -> **Covalent Bond**
  Transfer e^- -> **Ionic Bond**

Bonding/Reactivity Examples

- <u>NaCl – ionic bond</u>

  Na – Group 1A – 1 valence e^-
  Cl - Group 7A – 7 valence e^-
  Na $Na^+ + e^-$ (gives Na a full shell)
  Cl + e- Cl^- (gives Cl a full shell)

- <u>O_2 – covalent bond</u>

  O – Group 6A – 6 valence e^-
  O + $2e^-$ O^{2-} (oxide anion)
  -> Where will *EACH O* get 2 e^-? **SHARE**

  O + O   O=O (double bond – share 4 e^-)

Bonding: Ionization Energies

- Ionization Energy (IE)

  -quantifies the tendency of an electron to leave an atom in the gas phase:

$$X\ (g) \qquad X^+\ (g) + e^- \qquad \Delta E = IE$$

IE: -***always*** positive (energy ADDED)

-INCR across row

-DECR down a group

Bonding: Electron Affinity

- Electron Affinity (EA)

  -quantifies ability of an atom to *attract* an e^- in the gas phase

$$X\ (g) + e^- \rightarrow X^-\ (g) \qquad -\Delta E = EA$$

EA: -it's the energy *released* upon addition of an electron to an atom

-can be *positive* or *negative*

(**pos**: atom *wants* the e^-

neg: atom happy as an atom)

Bonding: Electronegativity

- Electronegativity (EN)

  -combines IE and EA terms to give the relative ability of an atom to attract e^-'s to itself ***when bonded*** to another atom

EN:
- -INCR across a row
- -DECR down a group
- -Best to consider ΔEN for a bond

EN: Examples

NaCl:	Na	EN = 0.93	
			ΔEN = 2.23 (ionic)
	Cl	EN = 3.16	
O_2:	O	EN = 3.44	ΔEN = 0 (covalent)
HCl:	H	EN = 2.2	
			ΔEN = 0.96 (?)
	Cl	EN = 3.16	(polar covalent)

Bond Polarity: Dipole Momement

- HCl $\delta+$ $\delta-$ ← partial charges

  H – Cl

  2.2 3.2

Polar Covalent bond*:* share e^-, but not equally

-Quantify via: DIPOLE MOMENT (μ)

$\mu = \delta$ x d ← Bond length (m)

1 Debye (D)
= 3.34×10^{-30} C-m

Amt of displaced charge (C)

Dipole Moment Examples

- H_2O O EN = 3.44

  H EN = 2.2 ΔEN = 1.24

-*each H-O bond* is polar, but does the MOLECULE have a *net* dipole moment?

- CH_4 C EN = 2.55

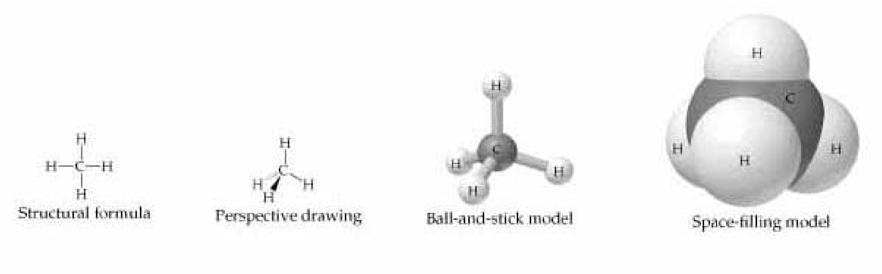
  H EN = 2.2 ΔEN = 0.35

-*each C-H bond* has a dipole moment, but does the entire MOLECULE have a *net dipole moment?*

We need to know the STRUCTURE!

Visualizing Molecules

CH_4



How do we figure out the structure?

Lewis Bonding Theory

- **Based on some simple assumptions**:

  -*valence electrons* are the major players in chemical bonding

  -**ionic bonds** form when electrons are transferred between atoms

  -**covalent bonds** form when electrons are shared by atoms

  -the extent of electron transfer/sharing is so as to give each atom a stable electron configuration (usually an **octet**)

Lewis Symbols

- Place *valence electrons* around element symbol:

:X: <- element X (4 e^-)

- pair electrons, when possible

- bonds represented by dashes (-)

<u>Example:</u>

.. ..
:F - F:
.. ..

Drawing Lewis Structures

- **<u>The Quick and Dirty Method:</u>**
  1. Add up the **<u>total</u>** number of valence electrons (from Group #)
  2. Draw *skeleton structure* with only single bonds
  3. <u>Distribute</u> remaining electrons around atoms as *non-bonding* electrons
  4. *<u>Redistribute</u>* non-bonded electrons into *multiple bonds* so that each atom has an **octet**

Example

Sulfur Dioxide (SO_2):

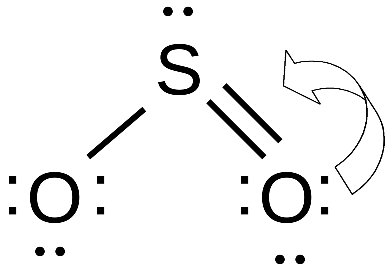
S & O: Group 6A -> *6 x 3 = 18 e^-*

-Draw Skeleton structure

2 e^-/bond, leaves **14 e^-**

-Move e^- to make multiple bonds and octets

Done!



Getting Structures

- Once we have the Lewis diagram, we can determine the *structure* by looking at the distribution of bonded and non-bonded electron pairs about a central atom, using:

  Valence **S**hell **E**lectron **P**air **R**epulsion Theory

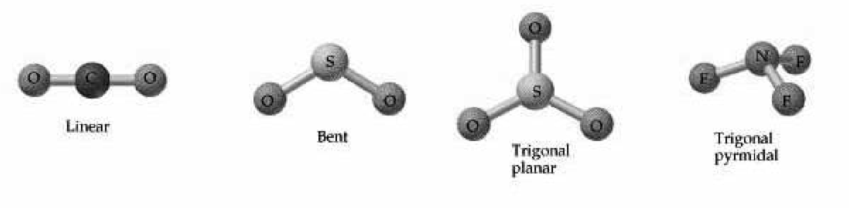
- ➢ *electron pairs* will ***repel*** each other and will distribute themselves about a central atom so as to maximize their separation in 3-dimensional space

VSEPR Theory

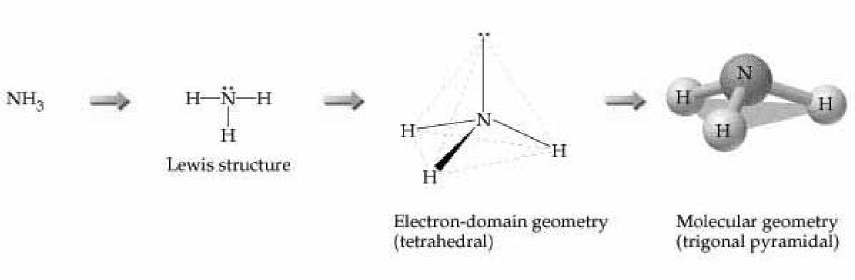
- Count electron pairs (include non-bonded!)

2 -> **Linear** (180^o bond angle)
3 -> Trigonal Planar (120^o bond angle)
4 -> Tetrahedral (109.5^o bond angle)
5 -> Trigonal Bipyramidal
6 -> Octahedral

VSEPR Structures



An Example: NH_3

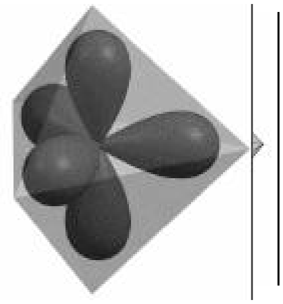


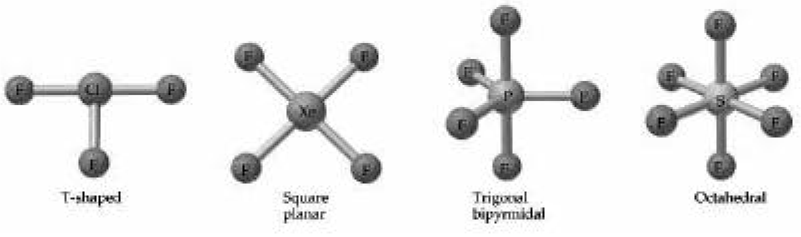
Exceptions to the Octet Rule

- Sometimes it’s not filled
  -incomplete octet (BeF_2, BF_3)
- Sometimes it’s OVER filled
  -”expanded” octet (SF_4, PCl_5, SF_6)
- Sometimes it *can’t* be filled
  -odd # of electrons (NO)

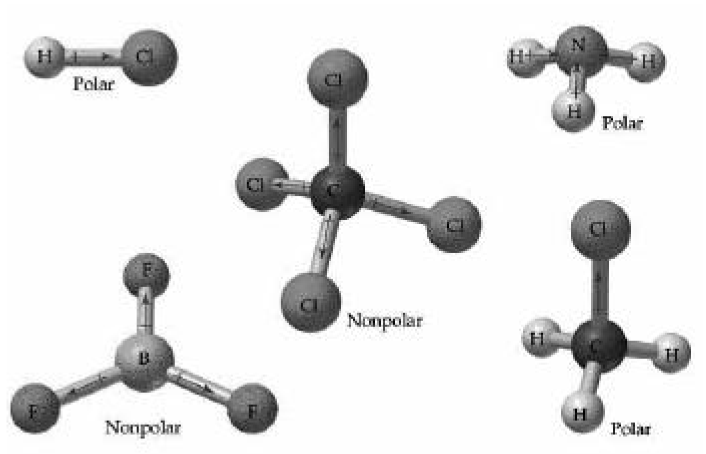
Expanded Octets

- <u>The Trigonal Bipyramid</u>:





Back to Dipoles



Writing and Balancing Chemical Equations: An Example

- *One type of rocket fuel reacts hydrazine and dinitrogen tetroxide and produces nitrogen gas and water*

1. hydrazine + dinitrogen tetroxide → nitrogen + water
2. $N_2H_4 + N_2O_4 \rightarrow N_2 + H_2O$ **Formulas**
3. $\boldsymbol{2}N_2H_4 + N_2O_4 \rightarrow \boldsymbol{3}N_2 + \boldsymbol{4}H_2O$ **Balanced**
4. $\boldsymbol{2}N_2H_4\ (l) + N_2O_4\ (l) \rightarrow \boldsymbol{3}N_2\ (g) + \boldsymbol{4}H_2O\ (l)$ **Done!**

Another Example

- *A solution of sodium chloride was added to a solution of silver nitrate, forming a precipitate of silver chloride*

1. sodium choride + silver nitrate → silver chloride + sodium nitrate
2. $NaCl + AgNO_3 \rightarrow AgCl + NaNO_3$ **Formulas**
3. $NaCl + AgNO_3 \rightarrow AgCl + NaNO_3$ **Balanced**
4. $NaCl\ (aq) + AgNO_3\ (aq) \rightarrow AgCl\ (s) + NaNO_3\ (aq)$

$$Na^+\ (aq) + Cl^-\ (aq) + Ag^+\ (aq) + NO_3^-\ (aq) \rightarrow AgCl\ (s) + Na^+\ (aq) + NO_3^-\ (aq)$$

$Ag^+\ (aq) + Cl^-\ (aq) \rightarrow AgCl\ (s)$ **Net Ionic Equation**

Quantifying Reaction Chemistry

- How many *grams of* O_2 can be produced via the following reaction from *3.0 grams of* $KClO_3$?

$$KClO_3\ (s) \xrightarrow{\Delta} KCl\ (s) + O_2\ (g) \uparrow$$

-First, need a balanced equation:

$$\mathbf{2}KClO_3\ (s) \xrightarrow{\Delta} \mathbf{2}KCl\ (s) + \mathbf{3}O_2\ (g) \uparrow$$

More QRC

- Next: remember that only MOLES can be used to quantify chemical changes:

g $KClO_3$ ®*mol* $KClO_3$ ®*mol* O_2 ®*g* O_2

$$3.0\ g\ KClO_3 \times \frac{1\ mol\ KClO_3}{122.548\ g\ KClO_3} \times \frac{3\ mol\ O_2}{2\ mol\ KClO_3} \times \frac{31.998\ g\ O_2}{1\ mol\ O_2} =$$

= 1.17498 g O_2

= **1.2 g O_2**

Reaction Reality:
Percent Yield

- Previous example gave the *theoretical* yield for the reaction . . . more realistically:

-Suppose the reaction of 3.0 g $KClO_3$ produced 0.55 g O_2; calculate the *percent yield* of the reaction

$$\%\text{-yield} = \frac{\text{Actual (exptl) Yield}}{\text{Theoretical Yield}} \times 100$$

$$= \frac{0.55 \text{ g } O_2}{1.175 \text{ g } O_2} \times 100 = \underline{\boldsymbol{47\%}}$$

Limiting Reagent

- We don't always react a *stoichiometric* amount of reactants:

-How many *g P_2O_5* will be produced by the reaction of *2.00 g P* with *5.00 g O_2*?

<u>Reaction:</u> $P + O_2 \rightarrow P_2O_5$

<u>Balance:</u> $\mathbf{4}P + \mathbf{5}O_2 \rightarrow \mathbf{2}P_2O_5$

<u>Moles:</u> $2.00 \text{ g P} \times \frac{1 \text{ mol P}}{30.974 \text{ g P}} = 0.06457 \text{ mol P}$

$5.00 \text{ g } O_2 \times \frac{1 \text{ mol } O_2}{31.998 \text{ g } O_2} = 0.1563 \text{ mol } O_2$

Limiting Reagent: Cont’d

- Compare *actual* mol to mol *required*:

$$0.06457 \text{ mol P} \times \frac{5 \text{ mol } O_2}{4 \text{ mol P}} = 0.08071 \text{ mol } O_2$$

\# mol O_2 needed to react
with actual amt of P

So, there will be *O_2 leftover* after all of the P is consumed:

$$\begin{array}{rl} 0.1503 \text{ mol } O_2 & \text{- actual} \\ \underline{-0.08071 \text{ mol } O_2} & \text{- reacted} \\ \mathbf{0.0756 \text{ mol } O_2} & \textit{unreacted} \text{ (excess)} \end{array}$$

The reaction is limited by the amount of **P**, so it is the ***Limiting Reagent.***

Limiting Reagent:
The Final Straw

- Since **P** is the limiting reagent, we use *its amount* for the final calculation:

g P ® mol P ®mol P_2O_5 ®g P_2O_5

$$2.00 \text{ g P} \times \frac{1 \text{ mol P}}{30.974 \text{ g P}} \times \frac{2 \text{ mol } P_2O_5}{4 \text{ mol P}} \times \frac{141.943 \text{ g } P_2O_5}{1 \text{ mol } P_2O_5} =$$

$= 4.58265 \text{ g } P_2O_5$

$= \underline{\mathbf{4.58 \text{ g } P_2O_5}}$