Chemical Formulas & Calculations

Working with grams, moles and formulas

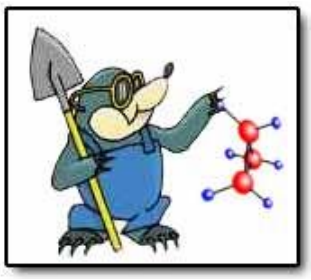
Chemical Formula

Represents the particulate (molecular) species

Can be Atoms (elements)
H He Na Cu Hg

Can be Molecules (Compounds)
CO_2 N_2 Cl_2 H_2SO_4

Can be Ionic
NaCl KBr $Mg(NO_3)_2$



Masses

Atomic Number = Z ==> number protons in nucleus
Mass Number = protons + neutrons

Atomic Mass = in AMU's, based on Carbon-12
= average weight of atoms in element
1 amu **=** 1/12 of mass of carbon-12 atom

Formula Mass = average mass of atoms in formula

Calculating Molecular Mass

Count atoms

H_2O	**CO_2**
2 H	1 C
1 O	2 O

H_2O		**CO_2**	
2 H (2 x 1.008)	= 2.016 amu	1 C (1 x 12.01)	= 12.01 amu
1 O (1 x 16.00)	= 16.00 amu	2 O (2 x 16.00)	= 32.00 amu

Sum & round

Molecular Mass = 18.016 ==> 18.02 amu 44.01 amu

Calculating Formula Mass - Hydrate
$CaSO_4 \cdot 2\ H_2O$

Count Atoms

1 Ca	4 H
1 S	2 O
4 O	

Water - part of formula

Multiply # atoms x atomic weight; then sum & round

$CaSO_4$	**$2\ H_2O$**
1 Ca (1 x 40.08) = 40.08 amu	4 H (4 x 1.008) = 4.032 amu
1 S (1 x 32.06) = 32.064 amu	2 O (2 x 16.00) = 32.00 amu
4 O (4 x 16.00) = 64.00 amu	

Dry Mass = 136. 144 ==> 136.14 amu 36.032 ==> 36.03
Hydrate Mass = 172.17 amu

Calculating Formula Mass – Polyatomic Anion
$Ba_3(PO_4)_2$

Multiply everything inside a parenthesis by the subscript
Count atoms, multiply # atoms x atomic weight

3 Ba (3 x 137.3) = 411.9 amu
2 P (2 x 30.97) = 61.94 amu
8 O (8 x 16.00) = 128.0 amu

Sum & round
Mass = 601.84 ➔ 601.8 amu

Calculating Formula Mass
$Fe_2(SO_4)_3$

Multiply everything inside a parenthesis by the subscript
Count atoms, multiply # atoms x atomic weight

2 Fe (2 x 55.85) = 111.60
3 S (3 x 32.07) = 96.21
12 O (12 x 16.00) = 192.0

Sum & round

Weight = 399. 81 ➔ 399.8 amu

Calculate the formula mass of:
ammonium carbonate

Write formula

$(NH_4)_2 CO_3$

Count atoms, multiply # atoms x atomic mass

2 N = 2 x 14.01) amu = 28.02 amu
8 H = 8 x 1.008) amu = 8.064 amu
1 C = 1 x 12.01) amu = 12.01 amu
3 O = 3 x 16.00) amu = 48.00 amu

Sum & round

Mass = 96.094 ➔ 96.09 amu

Calculate the formula mass of: iron(III) nitrate

Write formula

$Fe(NO_3)_3$

Multiply everything inside a parenthesis by the subscript
Count atoms, multiply # atoms x atomic weight

1 Fe = 1 x 55.85 = 55.85 amu
3 N = 3 x 14.01 = 42.03 amu
9 O = 9 x 16 .0 = 144.0 amu

Sum & round

Weight = 241.88 ➔ 241.9 amu

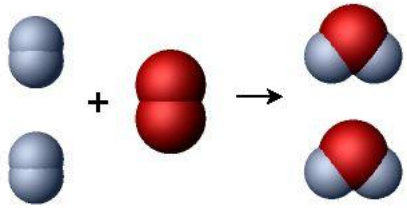
Science is "about measurement"

"If you can't measure it, it ain't science!"

Chemistry is science of measuring matter & interactions of matter

Reactions occur at the particulate level:

$2H_2 + O_2 \rightarrow 2H_2O$

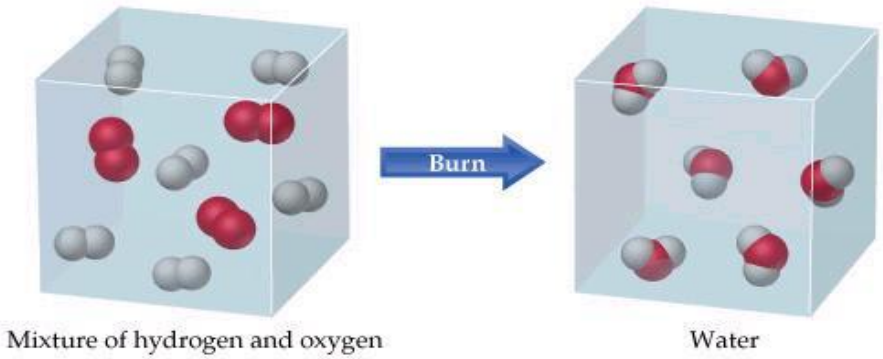


Need to have a measurement of quantity

Simple weight does not account for atomic masses

Historical Problem

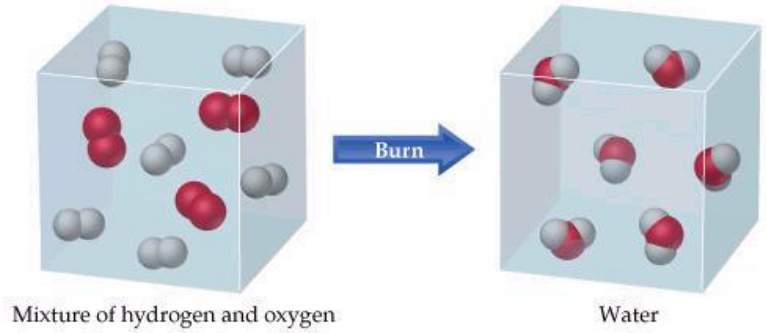
Observation:
2 volumes of hydrogen + 1 volume oxygen ➔ 2 volumes water



Not consistent with 1800's understanding:
2 atomos + 1 atomos oxygen ➔ 2 atomos water
Atomos = invisible particle responsible for identity

Avogadro's Hypothesis

Lawyer, turned chemist
1811- Proposed
All gases at same temperature and pressure conditions contain the same (unknown) number of molecules
And
the formation of water explained by interactions of molecules, not atomos



2 molecules hydrogen plus 1 molecule oxygen ➔ 2 molecules of water

$2\ H_2 + O_2 \rightarrow 2\ H_2O$

Avogadro's Number (N_A, an experimental value)

Not determined by Avogadro

Loschmidt, gas kinetics 1885: ~2.6567772 x 10^{25}
Planck, black body radiation 1900: 6.175×10^{23}
Rutherford, radium radioactive decay 1903: 6.1 x 10^{23}
Einstein, Brownian Movement 1905: 2.1 x 10^{23}
Baptiste, 1909: coined term, "Avogadro's Number"
Millikan, electron charge 1911: 6.064 x 10^{23}
NIST, mass Carbon-12 1998: 6.0221415 ± 0.0000010 x 10^{23}

Using x-ray diffraction and a pure Titanium crystal (1930)

$$\text{Avogadro's Number} = \frac{2\,\text{Ti atoms}}{1\,\text{unit cell}} \cdot \frac{1\,\text{unit cell}}{(3.306 \times 10^{-8})^3\,\text{cm}^3} \cdot \frac{47.88\,\text{g Ti}}{1\,\text{g-mol Ti}} \cdot \frac{1\,\text{cm}^3}{4.401\,\text{g Ti}} = 6.02 \times 10^{23}\ \text{atoms Ti}/\text{g-mol Ti}$$

Typically (in class) N_A = 6.02 x 10^{23} (3 sig figs)

The "Mole"

English equivalent of German "Mol"
Short form of "Molekulargewicht" (molecular weight)
Gram-Molecular Weight
Molecular Weight Expressed in grams
Contains Avogadro's Number (6.02 x 10^{23} molecules or atoms)

Elemental & Compound Masses

12.01 g C
1.008 g H
16.00 g O
22.99 g Na
35.45 g Cl **= Avogadro's number of atoms**
18.02 g H_2O
58.44 g NaCl
159.7 g Fe_2O_3
108.0 g N_2O_5

Mole always contains the same number of formula units: 6.02 x 10^{23} (*Avogadro's Number*)

1 mol element = 6.02x10^{23} atoms
1 mol diatomic element = 6.02x10^{23} molecules
1 mol molecular compound = 6.02x10^{23} molecules
1 mol ionic compound = 6.02x10^{23} formula units

So, the "per" expression is 1 mol = 6.02x10^{23} atoms

Molar Calculations

Calculate the number of moles in 4.88 x 10^{25} formula units (atoms) of copper

$$4.88 \times 10^{25} \text{ atoms} \times \frac{1 \text{ mole}}{6.02 \times 10^{23} \text{ atoms}} = 81.1 \text{ mol}$$

Calculate the number of formula units in 5.33 moles of $CaCl_2$

$$5.33 \text{ moles} \times \frac{6.02 \times 10^{23} \text{ atoms}}{1 \text{ mole}} = 3.21 \times 10^{24} \text{ atoms}$$

Calculate the number of moles in 1.74 x 10^{21} molecules of H_2O

$$1.74 \times 10^{21} \text{ molecules} \times \frac{1 \text{ mole}}{6.02 \times 10^{23} \text{ molecules}} = 2.89 \times 10^{-3} \text{ mol}$$

Calculate the number of molecules in 13.7 moles of CO_2

$$13.7 \text{ moles} \times \frac{6.02 \times 10^{23} \text{ molecules}}{1 \text{ mole}} = 8.25 \times 10^{24} \text{ molecules}$$

Molar Calculations (Moles to Grams)

Calculate the number of grams of CO_2 in 13.7 moles of CO_2

Write formula

CO_2

Count atoms, multiply # atoms x atomic weight, sum & round

1 C = 1 x 12.01 = 12.01
2 O = 2 x 16.00 = 32.00

Mass = 44.01

Calculate weight based on formula mass

$$\frac{44.01 \text{ g}}{\text{mole}} \times 13.7 \text{ moles} = 602.937 \rightarrow 603 \text{ g}$$

Molar Calculations (Gram to Mole)

Calculate the number of moles in 88.0 grams of carbon dioxide

Write formula

CO_2

Count atoms, multiply # atoms x atomic weight; Sum

1 C = 1 x 12.01 = 12.01
2 O = 2 x 16.00 = 32.00

Mass = 44.01

Calculate moles based on formula mass

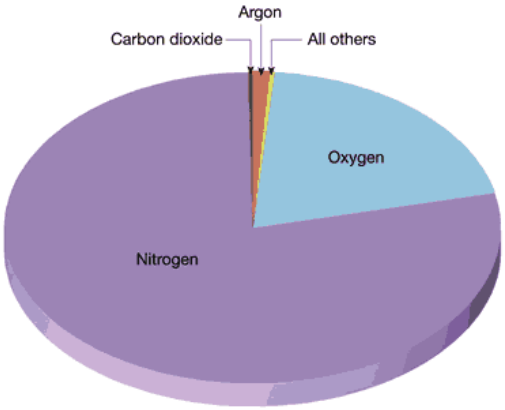
$$88.0\ g \times \frac{1\ mole}{44.01\ g} = 1.9996\ mol \rightarrow 2\ mol$$

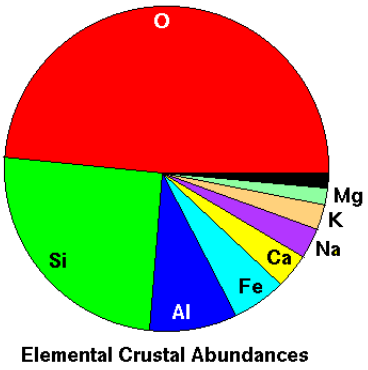
% Composition Calculations

Percent (%) = parts per hundred

$$\%\ A = \frac{\text{amount A}}{\text{total A}} \times 100 \quad \text{or} \quad \%\ A = \frac{\text{One Component (A)}}{\text{All Components}} \times 100$$

% Calculations Often Represented As "Pie Charts"





% Composition Calculations

Determine % calcium in calcium fluoride

Write the formula

CaF_2

Count atoms, multiply # atoms x atomic weight; Sum

1 Ca 1 x 40.08 = 40.08
2 F 2 x 19.00 = 38.00

Mass of 1 mole = 78.08

% calcium = amount Ca / total compound weight x 100

$$\% \text{ calcium} = \frac{40.08 \text{ g}}{78.08 \text{ g}} \times 100 = 51.33$$

% fluoride = amount F / total compound weight x 100

$$\% \text{ fluorine} = \frac{38.00 \text{ g}}{78.08 \text{ g}} \times 100 = 48.67$$

Assignment

Continue Taking Unit 5 Practice Test
Blackboard only records highest score
Take until multiple 100's have been scored (questions are variable)
(Gives sense of test exam format and content)

The Practice Quiz is very similar to the Unit Exam
Success on Unit exam is directly related to practice exam experiences

By now, the elements, the diatomic molecules, and polyatomic ions should have been memorized.