Formula Calculations

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Chemical Calculations

The first definitions,
conversions,
memorized periodic elements
and polyanions
provide the foundation for the rest of the class

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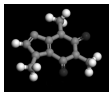
Chemical Formula

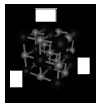
Represents the particulate (molecular) species

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 (Formula Units)
NaCl KBr $Mg(NO_3)_2$



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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 a formula
typically used for ionic compounds
Molecular Mass = average mass of atoms in a molecule
typically used for molecular compounds

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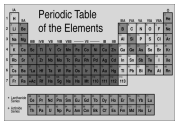
Determining Formula / Molecular Mass

Obtain Correct Chemical Formula
Given
From Memory
Create From Name
For each element in Formula:
Count atoms
Find atomic mass in Periodic Table
Multiply # atoms x atomic mass
Sum & Round



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Calculating Molecular Mass (Weight)

Count atoms

For: H_2O	CO_2
2 H	1 C
1 O	2 O

Multiply # atoms x atomic mass

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

Mass = 18.016 ➔ 18.02 amu **= 44.01 amu**

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Calculating Formula Mass (Weight)

Count Atoms

$CaSO_4 \cdot 2\ H_2O$

1 Ca 4 H

1 S 2 O

4 O

Water - part of formula

Multiply # atoms x atomic mass; 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) = 32.06 amu 2 O (2 x 16.00) = 32.00 amu

4 O (4 x 16.00) = 64.00 amu

Dry Mass = 136. 14 amu 36.032 ➔ 36.03 amu

Hydrate Mass = 172.17 amu

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Calculating Formula Mass (Weight)

Multiply everything inside a parenthesis by the subscript

$Ba_3(PO_4)_2$

Count atoms, multiply # atoms x atomic mass

3 Ba (3 x 137.3) amu = 411.9 amu

2 P (2 x 30.97) amu = 61.94 amu

8 O (8 x 16.00) amu = 128.00 amu

Sum & round

Mass = 601.84 ➔ 601.8 amu

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Calculating Formula Mass (Weight)

Multiply everything inside a parenthesis by the subscript

$Fe_2(SO_4)_3$

Count atoms, multiply # atoms x atomic mass

2 Fe (2 x 55.85) = 111.60 amu

3 S (3 x 32.07) = 96.21 amu

12 O (12 x 16.00) = 192.00 amu

Sum & round

Mass = 399. 81 amu

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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

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Calculate the formula mass of:

Iron (III) nitrate

Write formula

$Fe(NO_3)_3$

Count atoms, multiply # atoms x atomic mass

1 Fe = (1 x 55.85) amu = 55.85 amu

3 N = (3 x 14.01) amu = 42.03 amu

9 O = (9 x 16 .00) amu = 144.0 amu

Sum & round

Mass = 241.88 ➔ 241.9 amu

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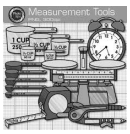
Science is "about measurement"

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

Chemistry is science of measuring:
matter
and
interactions of matter



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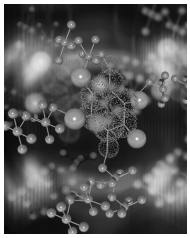
Molecules Are Too Small To See

We must "deduce" number of molecules involved in reactions



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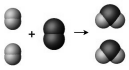
Reactions occur at the particulate level:

$2H_2 + O_2 \rightarrow 2H_2O$



Molecules "collide" to form new products
(Collision Theory)

Need way to determine number of reacting atoms

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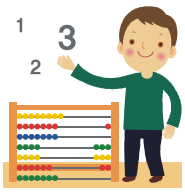
The Mole is a Chemist's Way of Counting Atoms & Molecules



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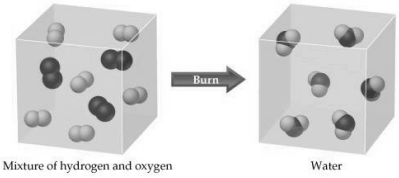
Historical Problem

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



Not consistent with 1800's understanding:
2 atomos hydrogen + 1 atomos oxygen ➔ 2 atomos water

Atomos = invisible smallest unit

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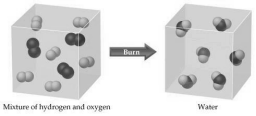
Avogadro's Hypothesis

Lawyer, turned chemist
1811- Proposed:
All gases at same temperature and pressure conditions contain the same number (value unknown) of molecules

formation of water explained by interactions of molecules, not atoms



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

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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 on pure Titanium (1930)

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

Common (class) use: 6.02 x 10^{23} (3 sig figs)

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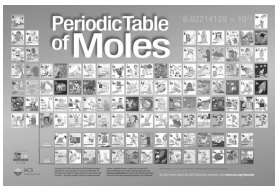
The "Mole"

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



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The "Mole"

Mole always contains the same number of atomic units:
6.02 x 10^{23} (*Avogadro's Number*)
Rigorously: exactly 6.02214076×10^{23} elementary entities.

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

So, the "per" expressions:
1 mole = 6.02x10^{23} atoms
1 mole = 6.02x10^{23} molecules
1 mole = 6.02x10^{23} formula units

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Elemental & Compound Masses

12.01 g C
1.008 g H
2.016 g H_2
16.00 g O
32.00 g O_2
22.99 g Na
35.45 g Cl
18.02 g H_2O
58.44 g NaCl
159.7 g Fe_2O_3
108.0 g N_2O_5
~68,000 g Hemoglobin

= Avogadro's number of atoms or molecules

Do you have mole problems?
If so, call Avogadro at 602-1023

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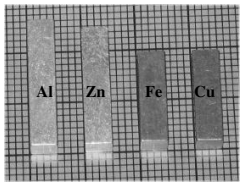
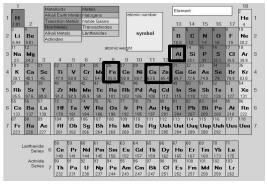
Each metal bar contains 1 mole

The more dense the solid element, the less volume 1mole occupies





Element	Atomic Mass (amu)	Density (g/mL)
Al	29.68	2.70
Zn	65.37	7.14
Fe	55.85	7.86
Cu	63.55	8.96

Density (g/mL) determined by: atomic mass + atomic geometry

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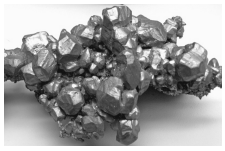
Molar Calculations (Atoms to Moles)

Calculate the number of moles in 4.88×10^{25} atoms of Cu

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



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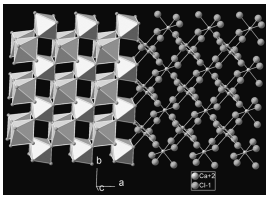
Molar Calculations (Moles to Formula Units)

Calculate the number of formula units in 5.331 moles of $CaCl_2$

$$5.331 \text{ moles} \times \frac{6.02 \times 10^{23} \text{ fu}}{1 \text{ mole}} = 3.21 \times 10^{24} \text{ fu}$$



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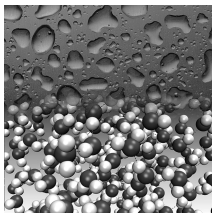
Molar Calculations (Molecules to Moles)

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

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



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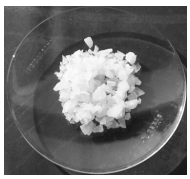
Molar Calculations (Molecules to Moles)

How many moles are in 7.892×10^{24} molecules of $Al_2(SO_4)_3$?

$$7.892 \times 10^{24} \text{ molecules } Al_2(SO_4)_3 \times \frac{1 \text{ mole } Al_2(SO_4)_3}{6.02 \times 10^{23} \text{ molecules } Al_2(SO_4)_3} = 13.1 \text{ moles}$$



Let the units drive the solution

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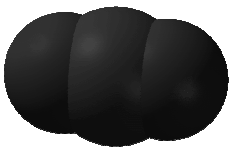
Molar Calculations (Moles to Molecules)

Calculate the number of molecules in 13.7 moles of CO_2

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



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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 mass; Sum

1 C = 1 x 12.01 = 12.01

2 O = 2 x 16.00 = 32.00

Mass = 44.01 g/mole

Calculate mass in grams based on formula mass

$$\frac{44.01\ g}{1\ mole} \times 13.7\ moles = 602.937 \rightarrow 603\ g$$

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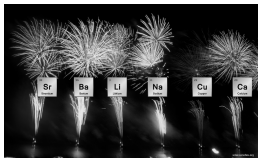
Molar Calculations (Moles to Grams)

How many grams of the barium chloride in 0.0360 mole?

$$0.0360\ moles\ BaCl_2 \times \frac{208.2\ g\ BaCl_2}{1\ moles\ BaCl_2} = 7.70\ g$$



Let the units drive the solution

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Molar Calculations (Grams to Moles)

Calculate the number of moles in 88.0 grams of carbon dioxide

Write formula

CO_2

Count atoms, multiply # atoms x atomic mass; Sum

1 C = 1 x 12.01 = 12.01

2 O = 2 x 16.00 = 32.00

Mass = 44.01 g/mole

Calculate moles based on formula mass

$$88.0\ g \times \frac{1\ mole}{44.01\ g} = 1.9996\ mol \rightarrow 2.00\ mole$$

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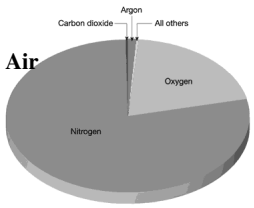
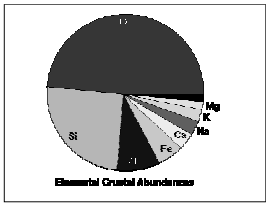
% Composition Calculations

Percent (%) = parts per hundred

$$\% A = \frac{\text{amount A}}{\text{total A}} \times 100$$

Chemists ASSUME molar % unless otherwise specific





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% Composition Calculations

Determine % calcium in calcium fluoride

Write the formula

CaF_2

Count atoms, multiply # atoms x atomic mass; 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 mass x 100

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

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% Composition Calculations

Determine % fluorine in calcium fluoride

Write the formula

CaF_2

Count atoms, multiply # atoms x atomic mass; Sum

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

Mass of 1 mole = 78.08

% fluoride = amount F / total compound mass x 100

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

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Q: How many guacs are in a bowl of guacamole?
A: Avocados number.


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