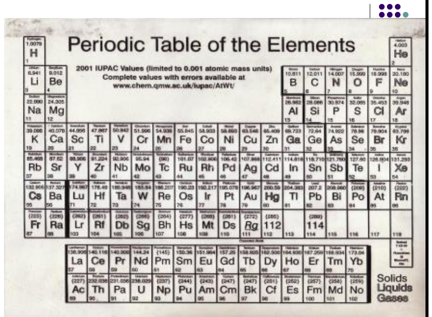
Slide 1

## Chemical Composition

Moles! Moles! Moles!

Slide 2




Slide 3

## Little Problem

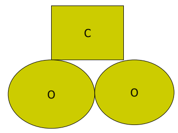
I have a sample of $CO_2$ that contains 3 moles oxygen atoms, how many grams of carbon do I have?

A. 18.0 g
B. 72.0 g
C. 48.0 g
D. 96.0 g
E. 36.0 g

Slide 4

## Building Molecules

Consider carbon dioxide – $CO_2$

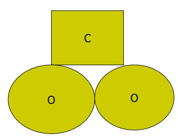



It's just like a little house made out of different size bricks

Slide 5

## Pieces of the Whole

If you look at the molecule this way, it is easy to see how the number of parts relates to the whole thing




Slide 6

## Stoichiometric Ratios

My little House of Atoms is constructed by specific ratios of each of the constituent atoms: There are always 2 oxygen atoms and 1 carbon atom in ever molecule.

$\frac{\text{2 oxygen atoms}}{\text{1 carbon atoms}}$ $\frac{\text{2 moles oxygen}}{\text{1 mole carbon}}$

$\frac{\text{2 mol O}}{\text{1 mol } CO_2}$ $\frac{\text{1 mol C}}{\text{1 mol } CO_2}$

(or the inverses)

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I have a sample of $CO_2$ that contains 3 moles oxygen atoms, how many grams of carbon do I have?

$$3 \text{ mol O} * \frac{1 \text{ mol } CO_2}{2 \text{ mol O}} * \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} * \frac{12.011 \text{ g C}}{\text{mol C}} = 18.02 \text{ g C}$$

$$3\ mol\ O \frac{1\ mol\ C}{2\ mol\ O} \frac{12.011\ g\ C}{mol\ C} = 18.02\ g\ C$$

Slide 8

## Another Little Problem

I want to make 3.00 moles of water ($H_2O$), how many grams of $O_2$ do I need to start with (assuming 100% conversion to water and sufficient $H_2$)?

A. 18.0 g
B. 72.0 g
C. 48.0 g
D. 96.0 g
E. 36.0 g

Slide 9

## Another Little Problem

I want to make 3.0 moles of water ($H_2O$), how many grams of $O_2$ do I need to start with (assuming 100% conversion to water and sufficient $H_2$)?

$$3.0 \text{ mol } H_2O * \frac{1 \text{ mol O}}{1 \text{ mol } H_2O} * \frac{1 \text{ mol } O_2}{2 \text{ mol O}} * \frac{32.0 \text{ g } O_2}{1 \text{ mol } O_2} = 48.0 \text{ g } O_2$$

$$3.0\ mol\ H2O \frac{1\ mol\ O}{1\ mol\ H2O} \frac{16\ g\ O}{1\ mol\ O} = 48.0 \text{ g O}$$

Slide 10

## Little Problem

I have a sample of $CO_2$ that contains 3.6 moles carbon, how many grams of oxygen atoms do I have?

$$3.6 \text{ mol C} * \frac{1 \text{ mol } CO_2}{1 \text{ mol C}} * \frac{2 \text{ mol O}}{1 \text{ mol } CO_2} * \frac{16.0 \text{ g O}}{\text{mol O}} = 115.2 \text{ g O}$$

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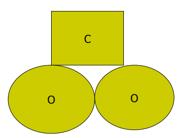
## House of Atoms

Consider the mass of the molecule - what is the total mass?




It's just the sum of the masses of the little atomic bricks.

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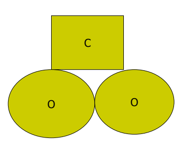
## Molar mass

Molar mass of $CO_2$ = mass of C + 2* mass of O




= 12.011 g/mol + 2*(16.00 g/mol) = 44.011 g/mol

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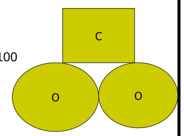
## % Composition

Because mass is conserved and the whole is simply the sum of the parts – it is possible to specify the composition as a % of the total mass!

$$\text{\% by mass Carbon} = \frac{\text{mass of carbon}}{\text{total mass } CO_2} \times 100$$

$$\text{\% C} = \frac{\text{mass of carbon}}{\text{100 g total mass } CO_2}$$

$$\text{\% by mass Oxygen} = \frac{\text{mass of oxygen}}{\text{total mass } CO_2} \times 100$$

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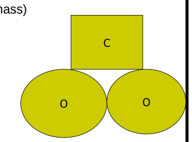
## % Composition

Because mass is conserved and the whole is simply the sum of the parts – it is possible to specify the composition as a % of the total mass!

$$\text{\% by mass Carbon} = \frac{12.011 \text{ g/mol}}{44.011 \text{ g/mol}} \times 100 = 27.29 \text{ \% C (by mass)}$$

$$\text{\% by mass Oxygen} = \frac{32.0 \text{ g/mol}}{44.011 \text{ g/mol}} \times 100 = 72.71 \text{ \% O}$$

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## Using mass % to determine composition

You can also do the reverse operation. If you know the % by mass of each constituent atom, you can determine the chemical formula.

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## A Little Problem

What is the molecular formula of a substance that is 67.1% zinc and 32.9% oxygen (by mass)?

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## Grams is good, moles is better

What is the chemical formula of a substance that is 67.1% zinc, by mass, and 32.9% oxygen?

We need molar ratios – how do we get moles from mass %?

UNITS! UNITS! UNITS!

Slide 18

## Grams is good, moles is better

What is the chemical formula of a substance that is 67.1% zinc, by mass, and 32.9% oxygen?

What are the units of mass %?

g something/100 grams total

How does this help us?

If we assume we have 100 grams total, then the % just becomes the mass!

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## Grams is good, moles is better

What is the chemical formula of a substance that is 67.1% zinc, by mass, and 32.9% oxygen?

Assume 100 grams total sample:

$\frac{67.1 \text{ g Zn}}{100 \text{ g total}}$ * 100 g total = 67.1 g Zn

$\frac{32.9 \text{ g O}}{100 \text{ g total}}$ * 100 g total = 32.9 g O

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## Grams is good, moles is better

What is the chemical formula of a substance that is 67.1% zinc, by mass, and 32.9% oxygen?

Now, I have grams: 67.1 g Zn and 32.9 g O.

How do I get moles?

MOLAR MASS!

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## Grams is good, moles is better

What is the chemical formula of a substance that is 67.1% zinc, by mass, and 32.9% oxygen?

67.1 g Zn * $\frac{1 \text{ mol Zn}}{65.409 \text{ g Zn}}$ = 1.026 mol Zn

32.9 g O * $\frac{1 \text{ mol O}}{16.0 \text{ g O}}$ = 2.056 mol O

What does this mean about the molecular formula?

$Zn_{1.026}O_{2.056}$

How does that make you feel?

Slide 22

## Numbers are good, Integers are prettier!

$Zn_{1.026}O_{2.056}$

That is the “correct” ratio, but you can't have a fraction of an atom. So, we prefer integers.

How would you turn those coefficients into integers?
Divide by the smallest one.

Slide 23

## Numbers are good, Integers are prettier!

$Zn_{1.026}O_{2.056}$

$Zn_{\frac{1.026}{1.026}}O_{\frac{2.056}{1.026}}$

$Zn_1O_{2.004}$

Close enough to round!

$ZnO_2$

Is this the actual molecular formula?
MAYBE….

Slide 24

## Empirical vs. Molecular

Suppose you had a molecule that was $Zn_2O_4$, what would the % composition, by mass, be?

$$\% \text{ mass Zn} = \frac{\text{mass Zn}}{\text{total mass}} \times 100$$

$$\% \text{ mass O} = \frac{\text{mass O}}{\text{total mass}} \times 100$$

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## Empirical vs. Molecular

Suppose you had a molecule that was $Zn_2O_4$, what would the % composition, by mass, be?

% mass Zn = $\frac{2*65.409}{(2*65.409 + 4*16.0)} \times 100$ = 67.1% Zn

% mass O = $\frac{4*16.0}{(2*65.409 + 4*16.0)} \times 100$ = 32.9% O

Same as the $ZnO_2$

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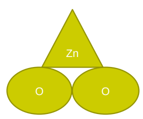
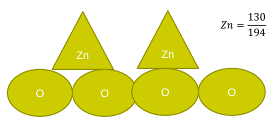



$$Zn = \frac{65.39\ g/mol}{97.39\ g/mol}$$



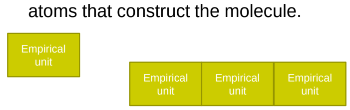

$$Zn = \frac{130.78\ g/mol}{194.78\ g/mol} = \frac{2 \times 65.39\ g/mol}{2 \times 194.78\ g/mol}$$

Slide 27

## Empirical vs. Molecular

The **empirical formula** is the smallest whole number ratio of atoms in the molecule.

The **molecular formula** is the actual ratio of atoms that construct the molecule.



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## $ZnO_2$ vs. $Zn_2O_4$

The **empirical formula** is the smallest whole number ratio of atoms in the molecule. ($ZnO_2$ – there are 2 oxygens for every zinc.)

The **molecular formula** is the actual ratio of atoms that construct the molecule. ($Zn_2O_4$ - There are actually 4 oxygen molecules and 2 zinc molecules stuck together in a single molecule!)

Slide 29

## Molecular mass

Any chemical formula determined strictly from relative amounts of the constituent atoms is an EMPIRICAL FORMULA unless you have additional information about the molecule.

You need to know the molecular mass in order to determine the actual molecular formula from the empirical formula.

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## Another example

Analysis of a compound indicates that it is 63.1% chromium, by mass, and 36.9 % oxygen. The molar mass of the compound is 167 +/- 2 g/mol. What is the empirical and molecular formula of the molecule?

What's the first thing to do?
See what you know and what you want to know! (always). Then…
Assume 100 grams!

Slide 31

## Another example

Analysis of a compound indicates that it is 63.1% chromium, by mass, and 36.9 % oxygen. The molar mass of the compound is 167 +/- 2 g/mol. What is the empirical and molecular formula of the molecule?

If I assume 100 g sample, then I have 63.1 g Cr and 36.9 g O!

Slide 32

## Molar Ratios

$63.1 \text{ g Cr} * \frac{1 \text{ mol Cr}}{51.996 \text{ g}} = 1.214 \text{ mol}$

$36.9 \text{ g O} * \frac{1 \text{ mol O}}{16.0 \text{ g O}} = 2.306 \text{ mol}$

$Cr_{1.214}\ O_{2.306}$

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## We need integers!

$Cr_{\frac{1.214}{1.214}}\ O_{\frac{2.306}{1.214}}$

$Cr_1O_{1.9}$

Close enough to round

$CrO_2$ – This is the empirical formula.

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## Molecular formula

To get the molecular formula from the empirical formula, compare the **empirical mass** to the molecular mass.

$CrO_2$ – molar mass = 51.996 + 2* 16 = 83.996 g/mol

The molecular mass is 167 +/- 2 g/mol

$\frac{167 \text{ g/mol}}{83.996 \text{ g/mol}} = 1.99$ - There must be 2 empirical units per molecule!

$Cr_2O_4$ is the molecular formula!

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## One last example

Analysis of an unknown compound determines that it is 26% nitrogen, by mass, and 74% oxygen. What is its empirical formula?

Assume 100 g: 26 g N and 74 g O

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## Molar ratios

$26 \text{ g N} * \frac{1 \text{ mol N}}{14.007 \text{ g N}} = 1.856 \text{ mol N}$

$74 \text{ g O} * \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 4.625 \text{ mol O}$

$N_{1.856}\,O_{4.625}$

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## Get integers!

$N_{\frac{1.856}{1.856}} O_{\frac{4.625}{1.856}}$

$N_1O_{2.49}$

Now, what?

It's not close enough to round – so multiply everything by 2 to get it close enough

$N_2O_5$

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## Combustion Analysis

A very common chemical technique for organic compounds is **combustion analysis**

Slide 39

## Organic Compounds

Organic compounds are chemical species made up of carbon and a few other elements (usually H, O, N, sometimes halogens, P, and S)

Despite the limited palette, there are significantly more organic compounds than any other type!

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## Combustion

When an organic compound is burned in the presence of oxygen, it creates a limited number of products:

$C_xH_yO_zN_a + O_2 \rightarrow CO_2 + H_2O + NO_2$

It is, therefore, possible to determine the composition of an organic molecule by analyzing its combustion products.

Slide 41

## Sample Problem

An unknown hydrocarbon (containing only carbon and hydrogen) is burned in the presence of oxygen. 7.5 g $CO_2$ and 3.2 g $H_2O$ are collected. What is the empirical formula of the hydrocarbon?

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## Solution

Where do we start?

MOLES! MOLES! MOLES!

Which requires a balanced equation:

$C_xH_y + O_2 \rightarrow CO_2 + H_2O$

$C_xH_y + (x+y/4)\ O_2 \rightarrow x\ CO_2 + y/2\ H_2O$

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## Predictable Products in Predictable Ratios

$C_xH_y + (x+y/4)\ O_2 \rightarrow x\ CO_2 + y/2\ H_2O$

What does this tell us?
STOICHIOMETRY!

$7.5\ g\ CO_2 * \frac{1\ mol\ CO_2}{44.011\ g\ CO_2} * \frac{1\ mol\ C}{1\ mol\ CO_2} = 0.170\ mol\ C$

$3.2\ g\ H_2O * \frac{1\ mol\ H_2O}{18.01\ g\ H_2O} * \frac{2\ mol\ H}{1\ mol\ H_2O} = 0.355\ mol\ H$

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## We have moles…now what?

0.170 mol C
0.355 mol H

$C_{0.170}H_{0.355}$

$C_{\frac{0.170}{0.170}}H_{\frac{0.355}{0.170}}$

$C_1H_{2.08}$

$CH_2$

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## Example #2

3.65 g of an organic compound containing C, H, and O is burned in the presence of oxygen. 7.43 g carbon dioxide, 2.35 g of water were quantitatively collected from the combustion. The molar mass of the compound was determined to be 170 +/- 5 g/mol. What is the molecular formula?

Slide 46

## First Step

Grams is good…moles is better!

$7.43 \text{ g } CO_2 * \frac{1 \text{ mol } CO_2}{44.011 \text{ g } CO_2} * \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 0.169 \text{ mol C}$

$2.35 \text{ g } H_2O * \frac{1 \text{ mol } H_2O}{18.01 \text{ g } H_2O} * \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} = 0.261 \text{ mol H}$

What about the oxygen?

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## The problem with oxygen

Consider the balanced equation of this reaction:

$C_xH_yO_z + (x+y/4 – z/2)\ O_2 \rightarrow x\ CO_2 + y/2\ H_2O$

Everything has oxygen! So you can't correlate the oxygen to any one product.

Slide 48

## The solution for oxygen

Mass is conserved!

The original compound is made up of C, H, and O.

So anything that isn't C or H must be O!

Slide 49

## Example #2

3.65 g of an organic compound containing C, H, and O is burned in the presence of oxygen. 7.43 g carbon dioxide, 2.35 g of water were quantitatively collected from the combustion. The molar mass of the compound was determined to be 170 +/- 5 g/mol. What is the molecular formula?

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## The mass deficit

$$0.169 \text{ mol C} * \frac{12.011 \text{ g C}}{1 \text{ mol C}} = 2.03 \text{ g C}$$

$$0.261 \text{ mol H} * \frac{1.00797 \text{ g H}}{1 \text{ mol H}} = 0.263 \text{ g H}$$

The oxygen?

g $C_xH_yO_z$ = g C + g H + g O

3.65 g $C_xH_yO_z$ = 2.03 g C + 0.263 g H + ? g O

g O = 3.65 g – 2.03 g – 0.263 g = 1.36 g O

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## Grams is good…yeah, yeah, yeah

We have the mass of oxygen originally in the sample, moles would be better!

$$1.36 \text{ g O} * \frac{1 \text{ mol O}}{16.0 \text{ g O}} = 0.085 \text{ mol O}$$

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## Putting it all together

$C_{0.169}H_{0.261}O_{0.0848}$

Divide by smallest!

$C_{\frac{0.169}{0.0848}}H_{\frac{0.261}{0.0848}}O_{\frac{0.0848}{0.0848}}$

$C_{1.99}H_{3.08}O_1$

$C_2H_3O$ – empirical formula!

Slide 53

## Example #2

3.65 g of an organic compound containing C, H, and O is burned in the presence of oxygen. 7.43 g carbon dioxide, 2.35 g of water were quantitatively collected from the combustion. The molar mass of the compound was determined to be 170 +/- 5 g/mol. What is the molecular formula?

Slide 54

## Getting Molecular Formula

$C_2H_3O$

What do we need to know to get the molecular formula from the empirical formula?

Molar Mass - 170+/-5 g/mol

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## Getting Molecular Formula

$C_2H_3O$

Empirical Mass = 2*12.011 g/mol + 3* 1.008 g/mol + 16.00 g/mol = 43.03 g/mol

Compare the empirical to molecular:

$$\frac{170 \pm 5 \text{ g/mol}}{43.03 \text{ g/mol}} = 3.95$$

$C_8H_{12}O_4$

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A. Yes
B. No
C. Maybe
D. I have no clue
E. I love you

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## Example #3

6.90 g of an organic compound containing C, H, and O is burned in the presence of oxygen. 9.52 g carbon dioxide, 4.35 g of water were quantitatively collected from the combustion. The molar mass of the compound was determined to be 361 +/- 5 g/mol. What is the molecular formula?

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## First Step

Grams is good…moles is better!

$$9.52\text{ g }CO_2 * \frac{1\text{ mol }CO_2}{44.011\text{ g }CO_2} * \frac{1\text{ mol C}}{1\text{ mol }CO_2} = 0.216\text{ mol C}$$

$$4.35\text{ g }H_2O * \frac{1\text{ mol }H_2O}{18.01\text{ g }H_2O} * \frac{2\text{ mol H}}{1\text{ mol }H_2O} = 0.483\text{ mol H}$$

What about the oxygen?

Slide 59

## The mass deficit

$$0.216\text{ mol C} * \frac{12.011\text{ g C}}{1\text{ mol C}} = 2.59\text{ g C}$$

$$0.483\text{ mol H} * \frac{1.00797\text{ g H}}{1\text{ mol H}} = 0.487\text{ g H}$$

The oxygen?

g $C_xH_yO_z$ = g C + g H + g O

6.90 g $C_xH_yO_z$ = 2.59 g C + 0.487 g H + ? g O

g O = 6.90 g – 2.59 g – 0.487 g = 3.82 g O

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## Grams is good…yeah, yeah, yeah

We have the mass of oxygen originally in the sample, moles would be better!

$$3.82\text{ g O} * \frac{1\text{ mol O}}{16.0\text{ g O}} = 0.238\text{ mol O}$$

Slide 61

## Putting it all together

$C_{0.216}H_{0.483}O_{0.239}$

Divide by smallest!

$C_{\frac{0.216}{0.216}}H_{\frac{0.483}{0.216}}O_{\frac{0.239}{0.216}}$

$C_1H_{2.24}O_{1.10}$

$C_4H_9O_4$ – empirical formula!

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## Putting it all together

$C_4H_9O_4$ – empirical formula!

Formula mass = 4x12.011 g/mol + 9*1 g/mol + 4*16 g/mol = 121 g/mol

$\frac{361 \text{ g/mol}}{121 \text{ g/mol}} = 2.98$

$C_{12}H_{27}O_{12}$

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## Your turn

Estrone is a C, H, O containing female sexual hormone. Combustion analysis of a 1.893 g sample of strone produced 5.545 g of $CO_2$ and 1.388 g of $H_2O$. The molar mass of estrone is 270.36 g/mol. What is the empirical formula for estrone?

A. $C_9H_{11}O$
B. $C_{10}H_{13}$
C. $C_5H_6O$
D. $C_{10}H_{12}O$
E. $C_8H_{11}O_2$