12 Chemistry

In society

Mark Dewar

16 O bjectives

1. MANUFACTURING
2. % YIELD
3. ATOM ECONOMY
4. LIMITING REACTANT

CHEMISTRY IN SOCIETY

Chemists constantly design new products in order to benefit society

CHEMISTRY IN SOCIETY

This has to be done with minimal waste and maximum profit

New Product Creation

There are many factors to be considered:

- **Availability, sustainability and cost of feedstock**
- **Recycling**
- **Energy requirement**
- **By-products**
- **Product yield**

What is a feedstock?

A **feedstock** is a reactant from which other chemicals can be extracted or synthesised.

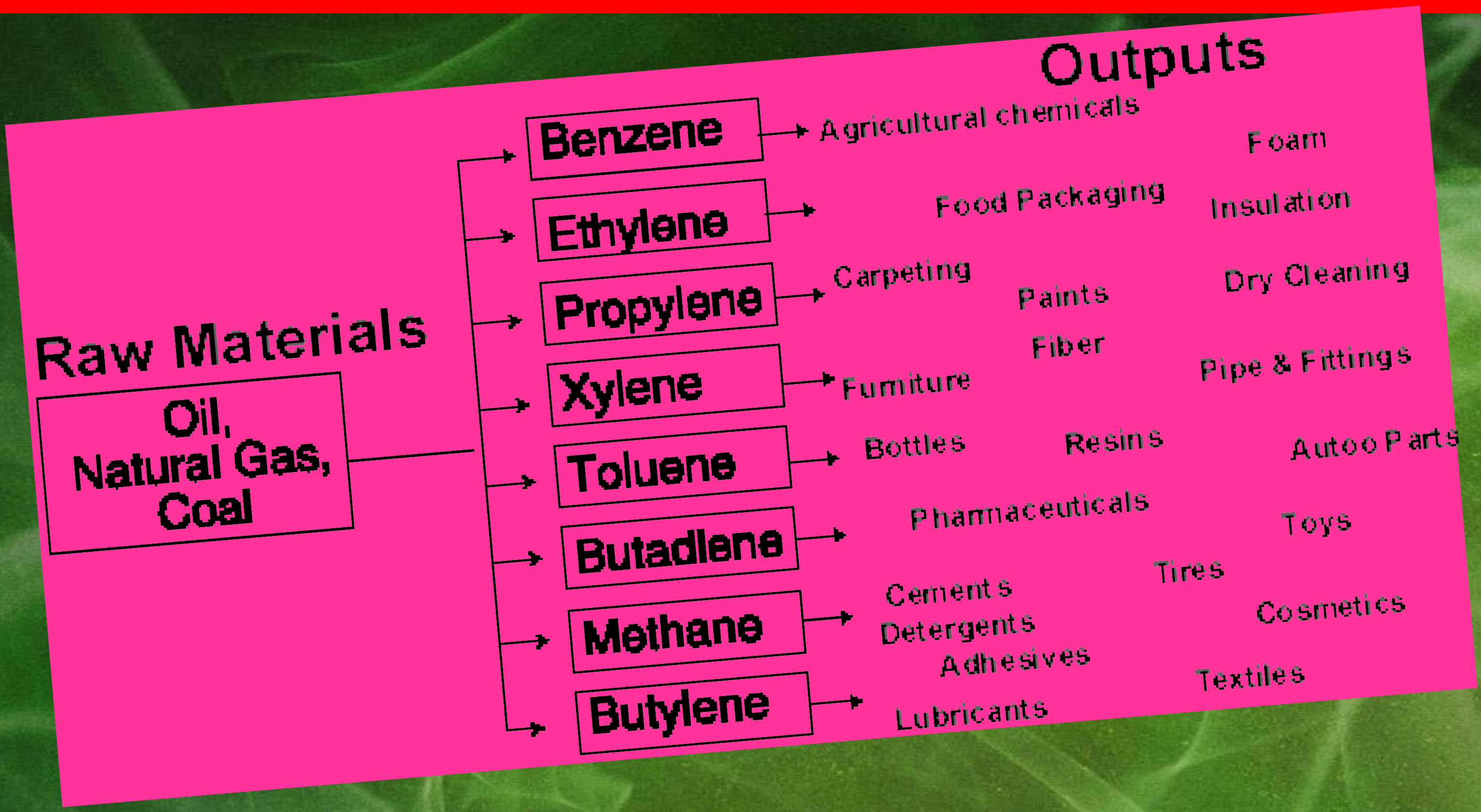
What is a feedstock?

Feedstocks are derived from raw materials such as: water, crude oil and air.

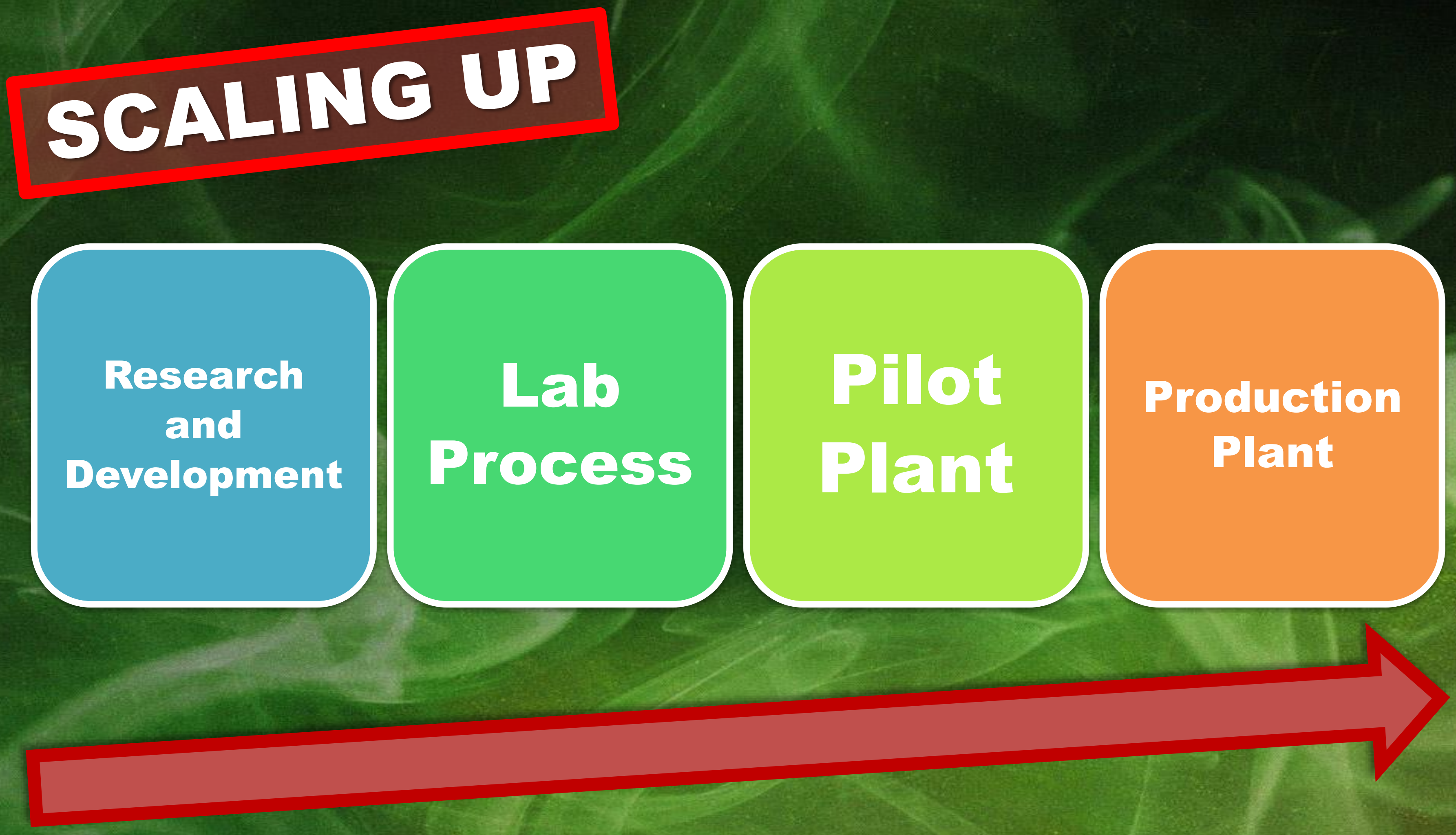
E.g. NITROGEN and OXYGEN (feedstocks) can be extracted from air (raw material).

What is a raw material?

A raw material is a substance that is naturally occurring



New Product Creation

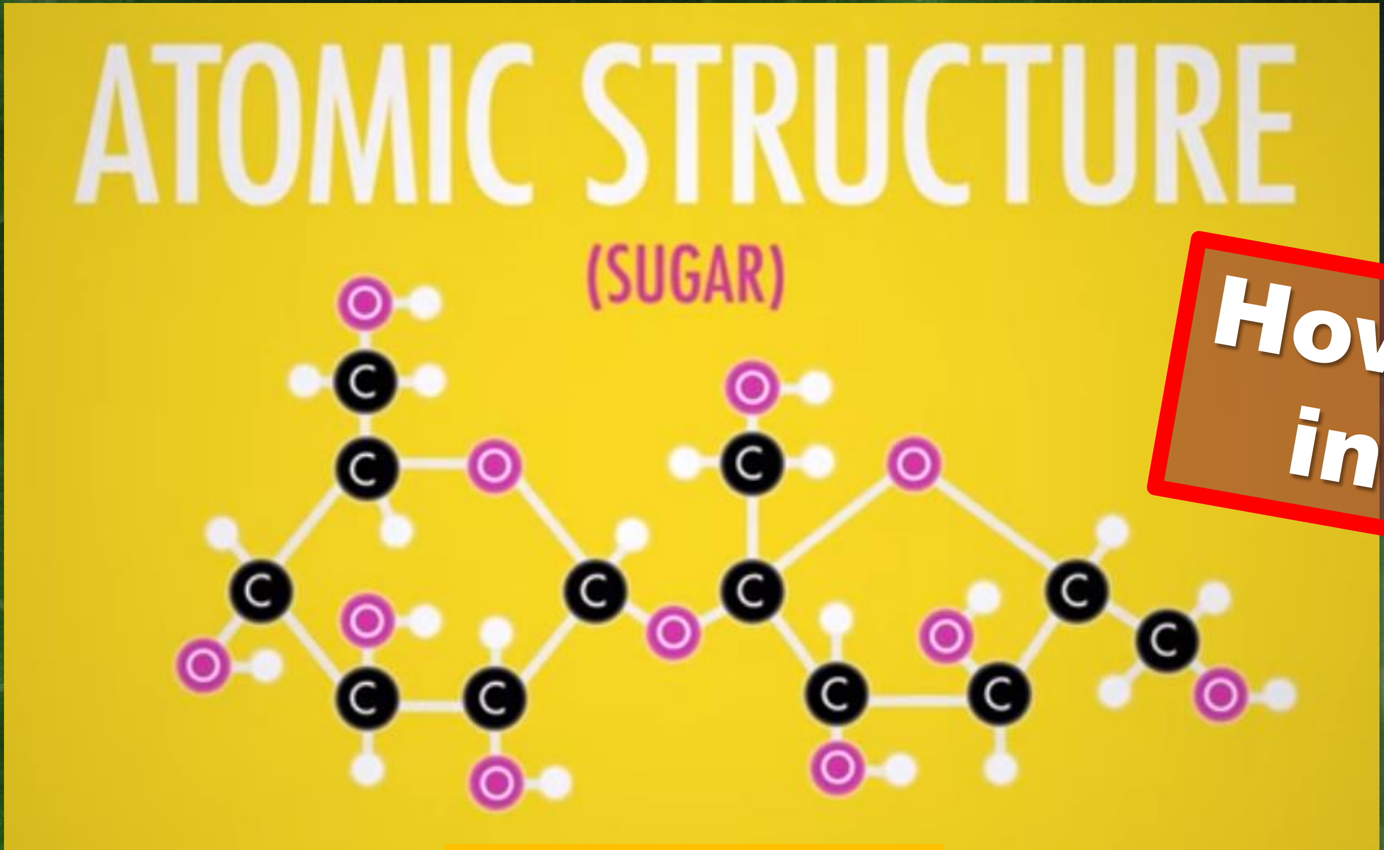


CALCULATIONS

STOICHIOMETRY

1. MEASURING CHEMICALS THAT GO INTO, AND COME OUT OF, ANY GIVEN REACTION.
2. IN GREEK, MEANS "MEASURING ELEMENTS"
3. ALLOWS US TO COUNT ATOMS AND MOLECULES BY WEIGHING THEM.

CALCULATIONS



$C_{12}H_{22}O_{12}$

How much in tea?

CALCULATIONS

MASS

MOLES

ATOMIC MASS

CALCULATIONS

MOLES

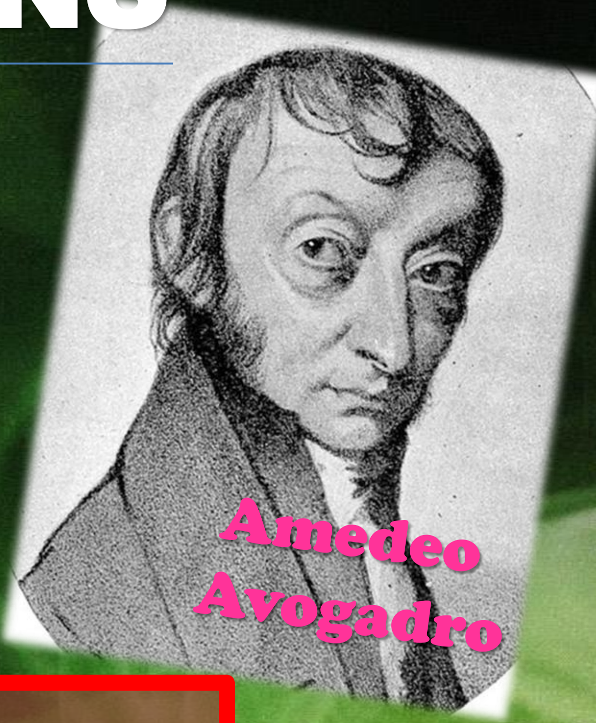
Link between CHEMICAL FORMULAE and CAKE

One mole of a substance is its gram formula mass (GFM).

CALCULATIONS

MOLES

Avogadro's Constant



One mole of a substance contains 6.02×10^{23} formula units

CALCULATIONS

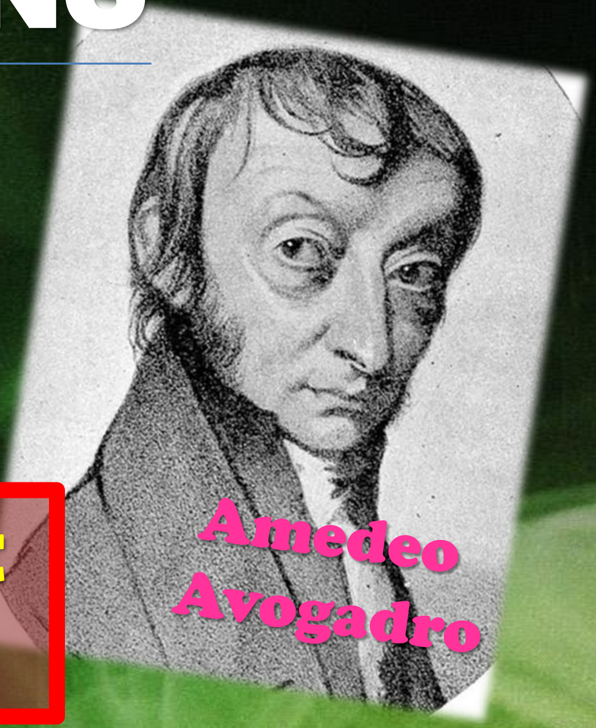
MOLES

Avogadro's Constant
$= 6.02 \times 10^{23}$

<u>molecules</u> in 2moles of H_2 gas?

CALCULATIONS

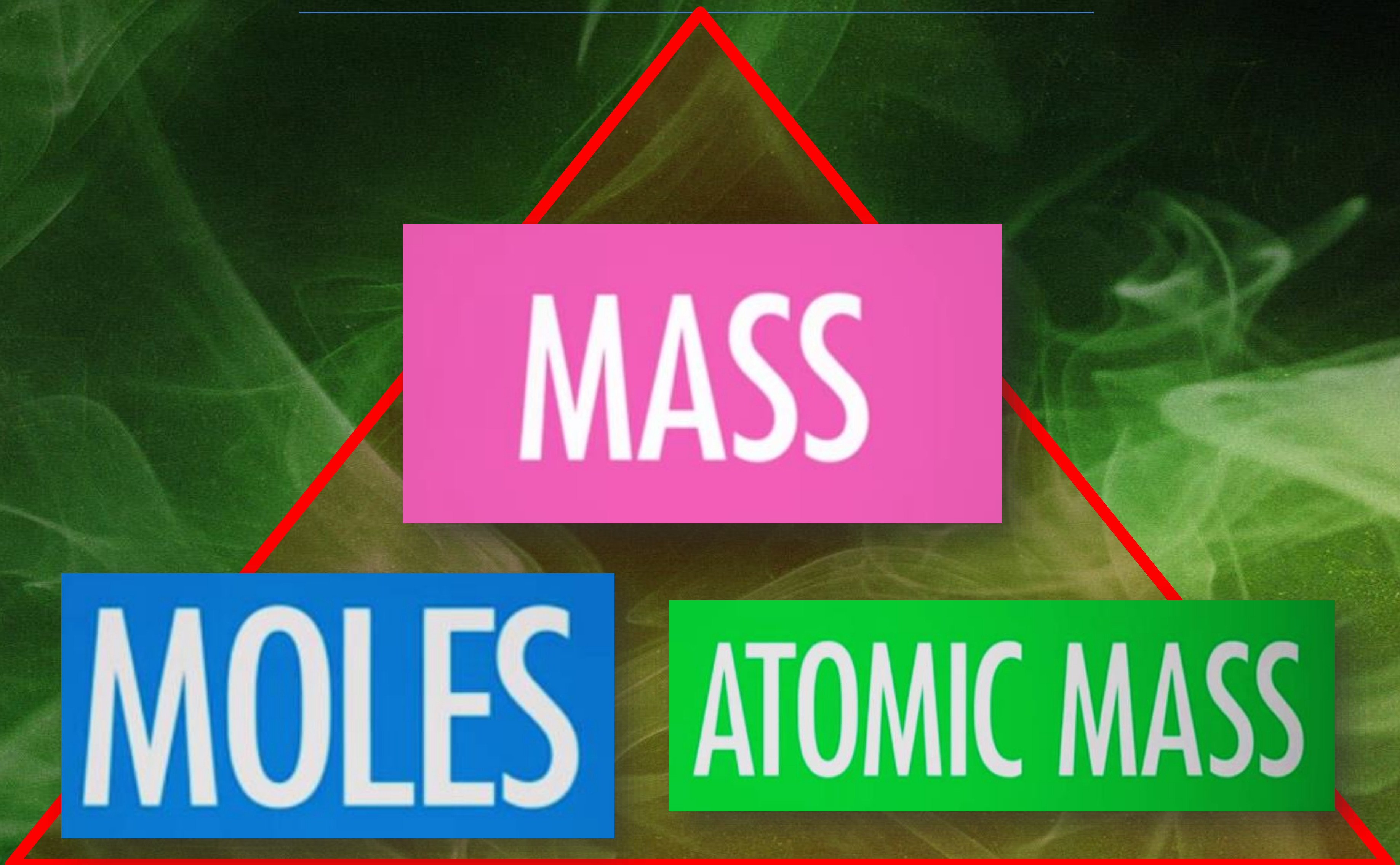
MOLES



Avogadro's Constant
$= 6.02 \times 10^{23}$

1.204×10^{24} molecules

CALCULATIONS



CALCULATIONS

$$\text{MOLES} = \frac{\text{MASS}}{\text{ATOMIC MASS}}$$

CALCULATIONS

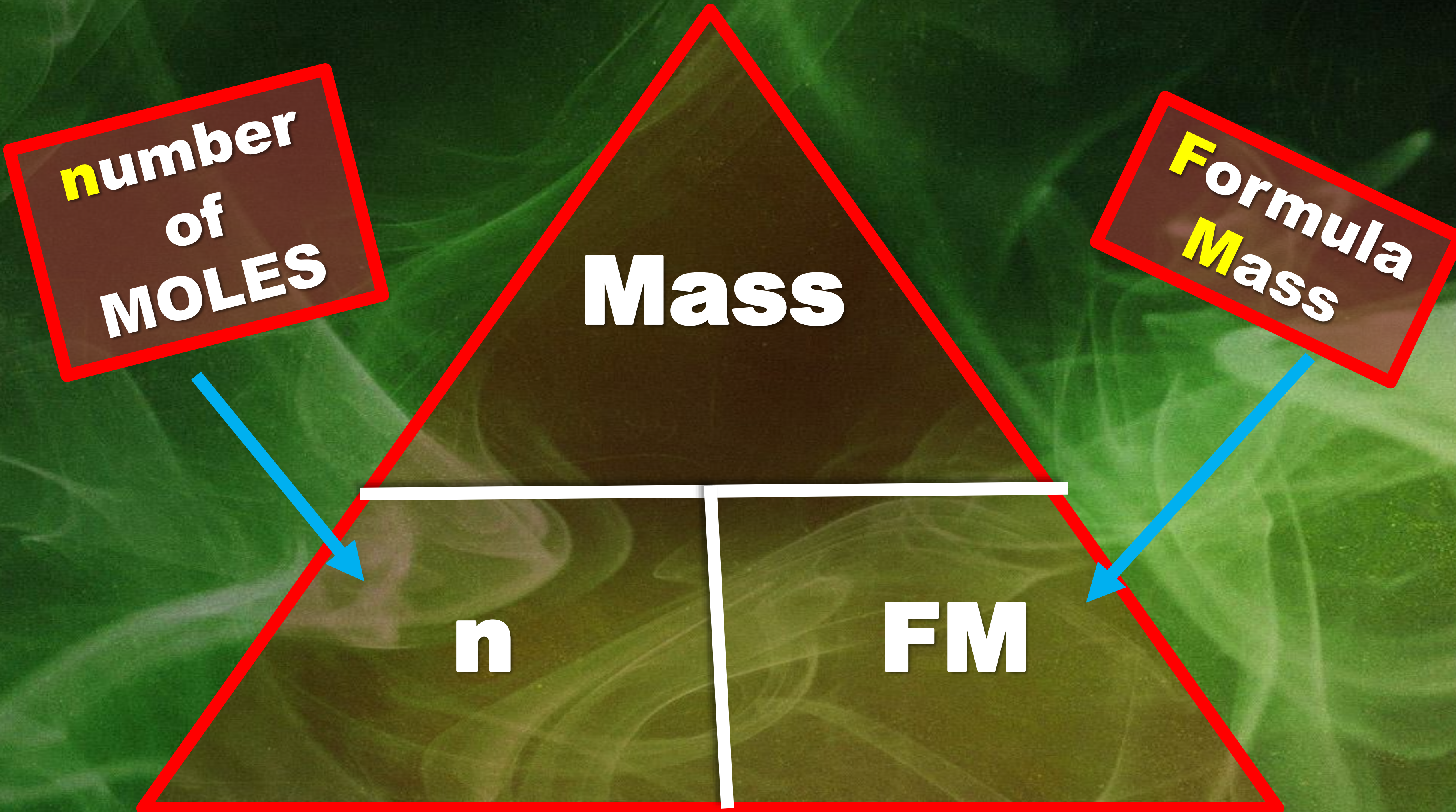
$$\text{ATOMIC MASS} = \frac{\text{MASS}}{\text{MOLES}}$$

CALCULATIONS

MASS = MOLES x ATOMIC MASS

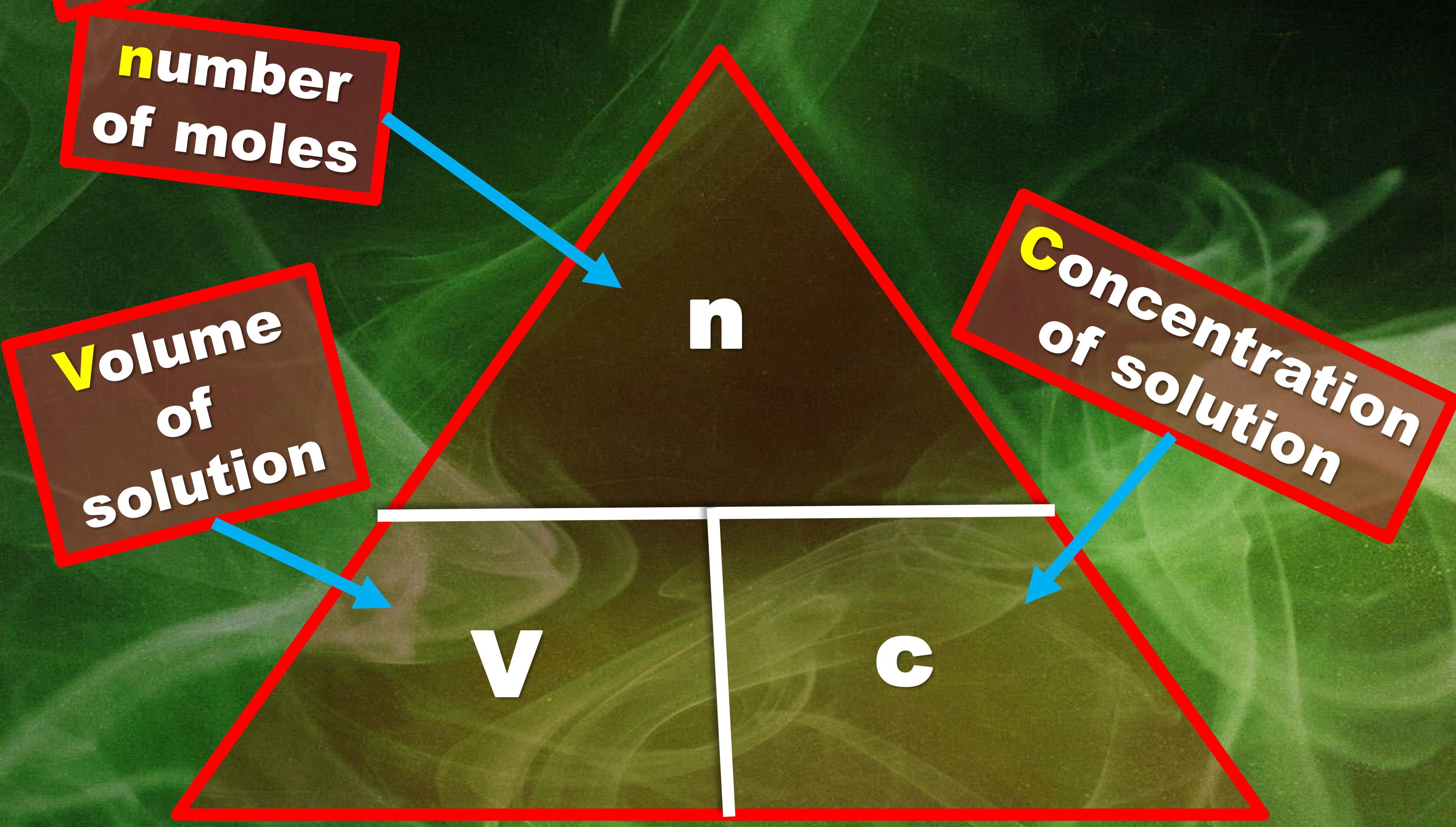
SOLIDS!

CALCULATIONS



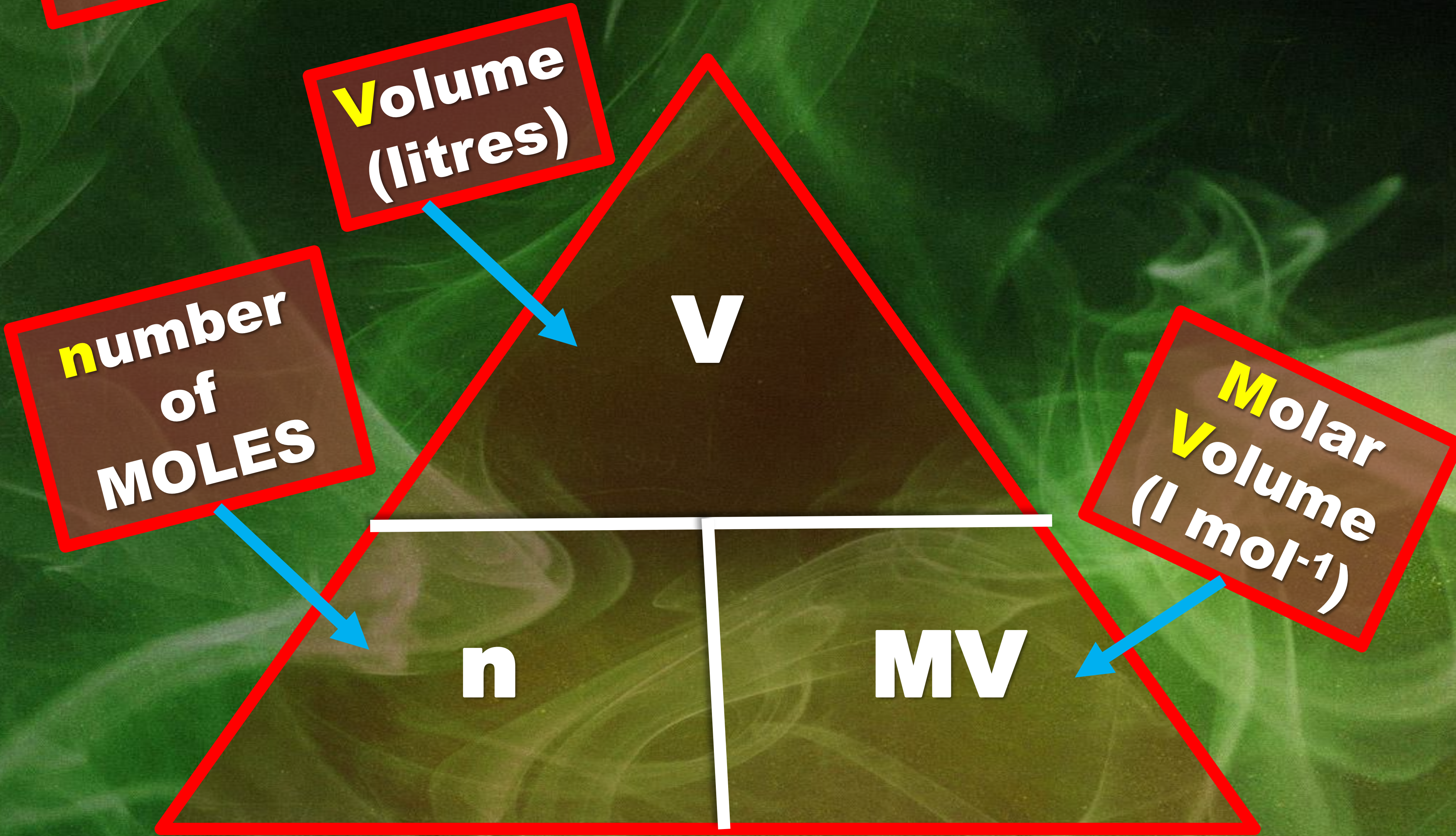
LIQUID!

CALCULATIONS



GAS!

CALCULATIONS



CALCULATIONS

STOICHIOMETRY

$2NaOH + H_2SO_4 \longrightarrow Na_2SO_4 + 2H_20$

How much mass do we need of each?

CALCULATIONS

STOICHIOMETRY

$2NaOH + H_2SO_4 \longrightarrow Na_2SO_4 + 2H_2O$

MOLES

2moles + 1mole ----------------► 1mole + 2moles

CALCULATIONS

STOICHIOMETRY

$2NaOH + H_2SO_4 \text{ ---------------}\blacktriangleright Na_2SO_4 + 2H_20$

MOLES

2moles + 1mole -------------▶ 1mole + 2moles

ATOMIC MASS

40 + 98 ------------▶ 142 + 18

CALCULATIONS

STOICHIOMETRY

$2NaOH + H_2SO_4$ ----------------► $Na_2SO_4 + 2H_20$

MOLES

2moles + 1mole ----------------► 1mole + 2moles

ATOMIC MASS

2x(40) + 1x(98) ----------------► 1x(142) + 2x(18)

MASS

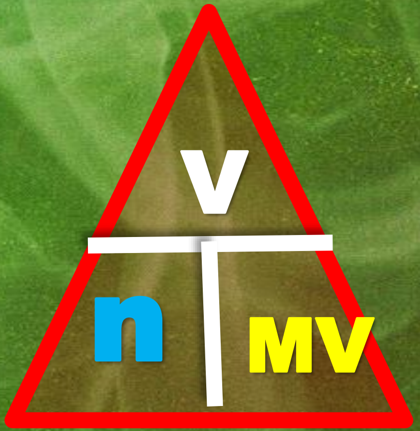
80g + 98g ----------------► 142g + 36g

CALCULATIONS

GAS!

What is the volume occupied by 2moles of hydrogen gas, (assume molar volume of 24 litres/mol)

?

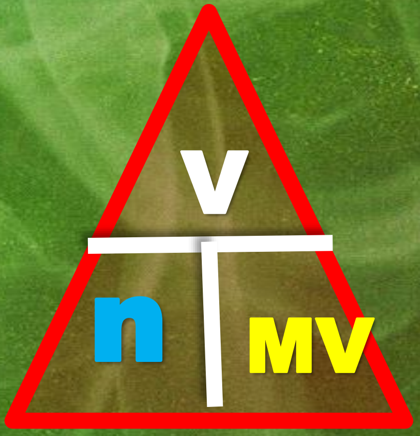


CALCULATIONS

GAS!

The volume occupied by 2moles of hydrogen gas, (assume molar volume of 24 litres)

48 litres



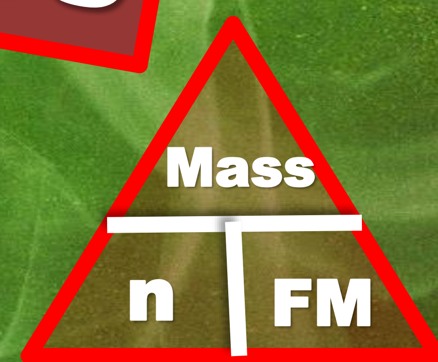
CALCULATIONS

GAS!

The volume occupied by 2moles of hydrogen gas, (assume molar volume of 24 litres)

48 litres

Mass?



CALCULATIONS

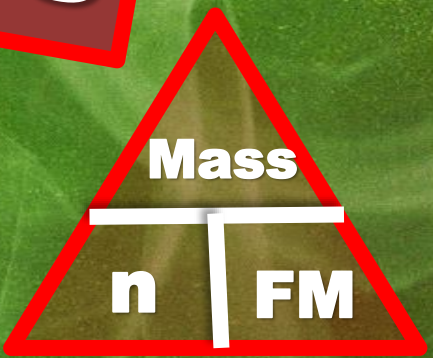
GAS!

The volume occupied by 2moles of hydrogen gas, (assume molar volume of 24 litres)

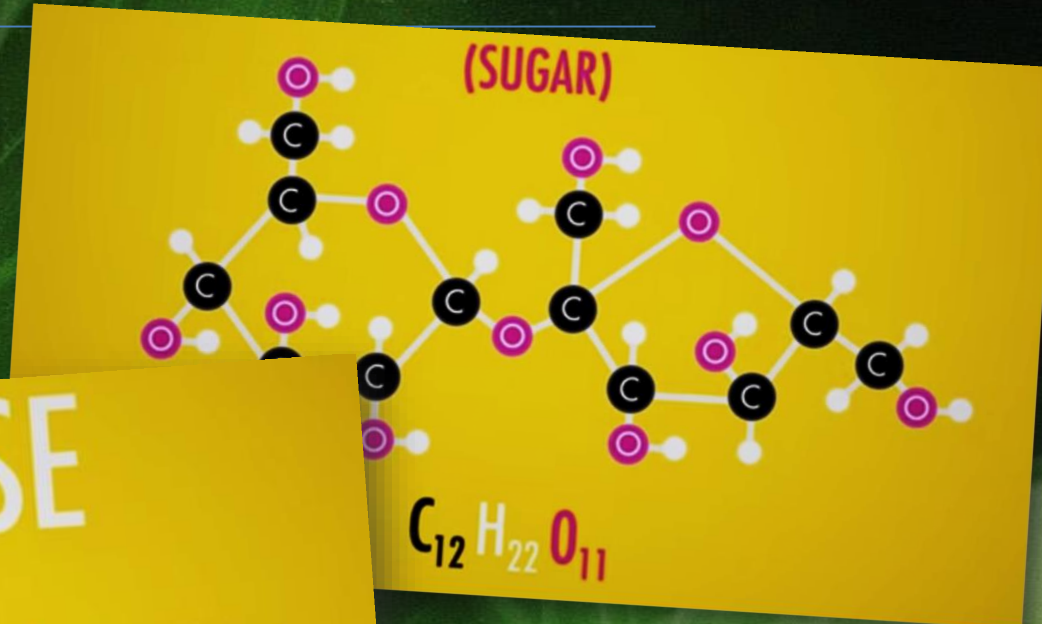
H_2

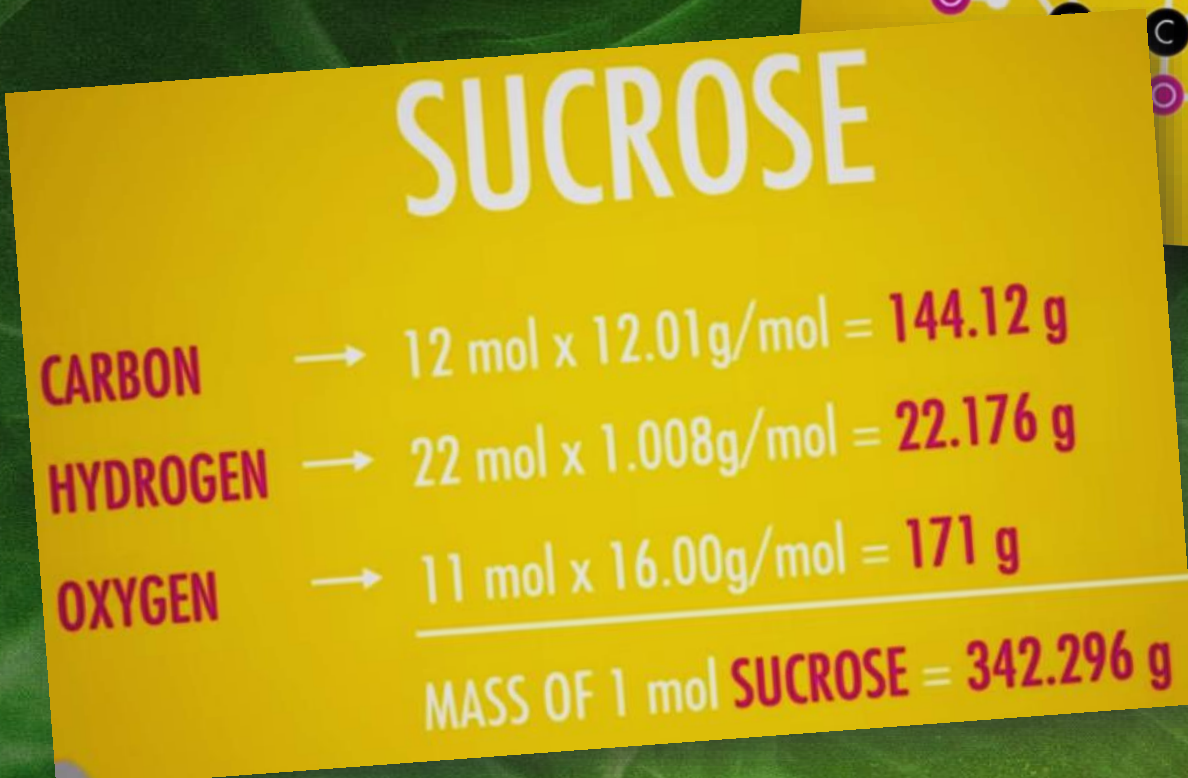
48 litres

4g



CALCULATIONS





CALCULATIONS

REACTANTS AND PRODUCTS

$$C_{12}H_{22}O_{11} + O_2 = CO_2 + H_2O$$

REACTANTS

PRODUCTS

Digesting sugar!

CALCULATIONS

EQUATION BALANCING

$$C_{12}H_{22}O_{11} + 12\ O_2 = 12\ CO_2 + 11\ H_2O$$

Digesting sugar!

CALCULATIONS

$$C_{12}H_{22}O_{11} + 12\ O_2 = 12\ CO_2 + 11\ H_2O$$

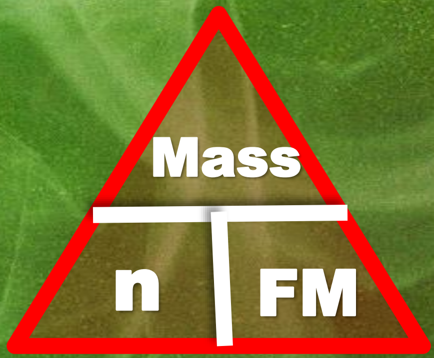
Only 5g of sucrose in cake

How much oxygen do I need to burn off the 5g of sugar?

CALCULATIONS

$$C_{12}H_{22}O_{11} + 12\ O_2 = 12\ CO_2 + 11\ H_2O$$

1mole of sucrose
12moles of oxygen



CALCULATIONS

$$C_{12}H_{22}O_{11} + 12\ O_2 = 12\ CO_2 + 11\ H_2O$$

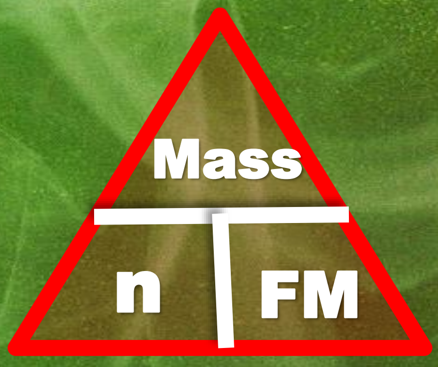
SUCROSE

CARBON → 12 mol x 12.01g/mol = **144.12 g**

HYDROGEN → 22 mol x 1.008g/mol = **22.176 g**

OXYGEN → 11 mol x 16.00g/mol = **171 g**

MASS OF 1 mol **SUCROSE** = **342.296 g**

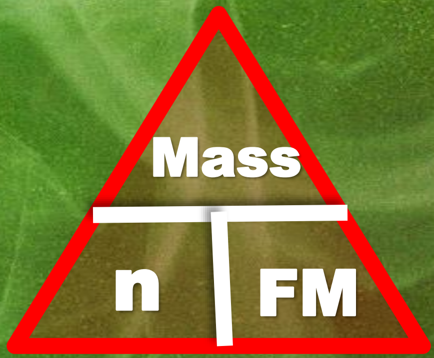


CALCULATIONS

$$C_{12}H_{22}O_{11} + 12\ O_2 = 12\ CO_2 + 11\ H_2O$$

SUCROSE = 342.296 g

12 MOLES OF O_2
= (12 x 32) = 384g



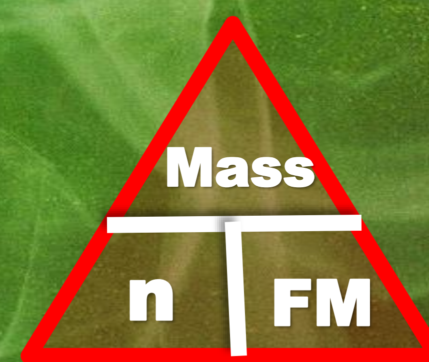
CALCULATIONS

$$C_{12}H_{22}O_{11} + 12\ O_2 = 12\ CO_2 + 11\ H_2O$$

SUCROSE = 342.296 g

12 MOLES OF O_2 = (12 x 32) = 384g

Only 5g of sucrose in cake



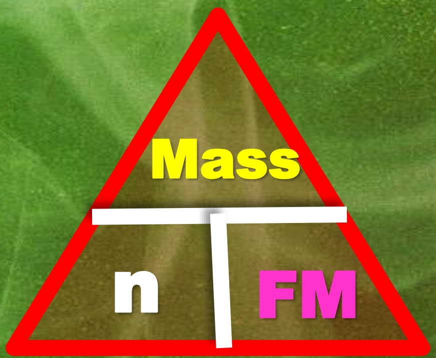
CALCULATIONS

$$C_{12}H_{22}O_{11} + 12\ O_2 = 12\ CO_2 + 11\ H_2O$$

SUCROSE = 342.296 g

12 MOLES OF O_2
= (12 x 32) = 384g

n = 5g/342.296
= 0.015 moles of sucrose



CALCULATIONS

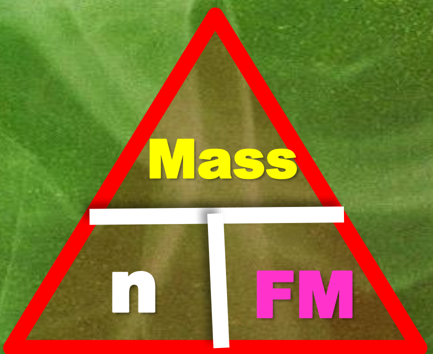
$$C_{12}H_{22}O_{11} + 12\ O_2 = 12\ CO_2 + 11\ H_2O$$

0.015 moles of sucrose

(12 x 0.015) moles of oxygen

mass = (12 x 0.015) x 32

= 5.76g



CALCULATIONS

LIMITING REACTANT

4 Tires

+

2 Headlights

=

1 Car

Say We Have:

14 headlights	Enough headlights to make 7 cars
20 tires	Enough tires to make 5 cars ← Limiting "Reactant"

CALCULATIONS

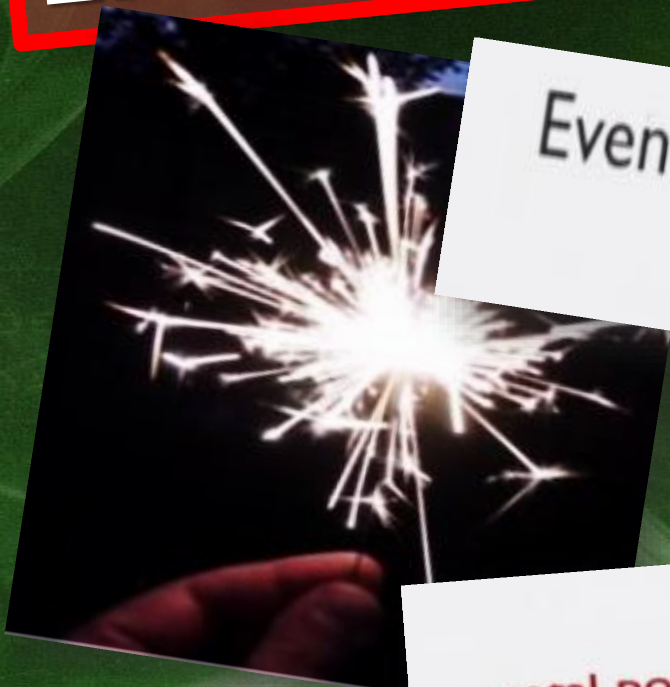
LIMITING REACTANT

metal powder — "air" — Aluminum Oxide

$$4\,Al + 3O_2 \rightarrow 2Al_2O_3$$

CALCULATIONS

LIMITING REACTANT



Eventually, you will run out of aluminum as the reaction proceeds forward

metal powder		"air"		Aluminum Oxide
$4\,Al$	$+$	$3O_2$	$\rightarrow$	$2Al_2O_3$

CALCULATIONS

LIMITING REACTANT

$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$

34g

32g

LIMITING REACTANT ?

CALCULATIONS

LIMITING REACTANT

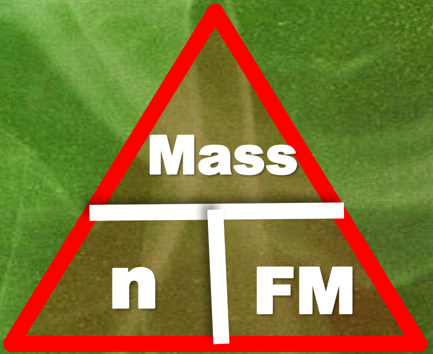
$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$

34g

FM = 17

32g

FM = 32



CALCULATIONS

LIMITING REACTANT

$$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$$

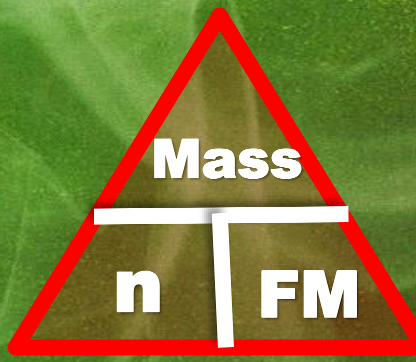
34g

32g

FM = 17

FM = 32

n = mass/FM = 34/17
= 2



CALCULATIONS

LIMITING REACTANT

$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$

34g

32g

FM = 17

FM = 32

n = mass/FM = 34/17 = 2

n = 32/32 = 1

CALCULATIONS

LIMITING REACTANT

$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$

2mole

1mole

NOT ENOUGH O_2

CALCULATIONS

LIMITING REACTANT

$$C_6H_8O_6 + I_2 \rightarrow C_6H_6O_6 + 2H^+ + 2I^-$$

25 cm^3
0.1 mol l^{-1}

0.27 g

LIMITING REACTANT ?

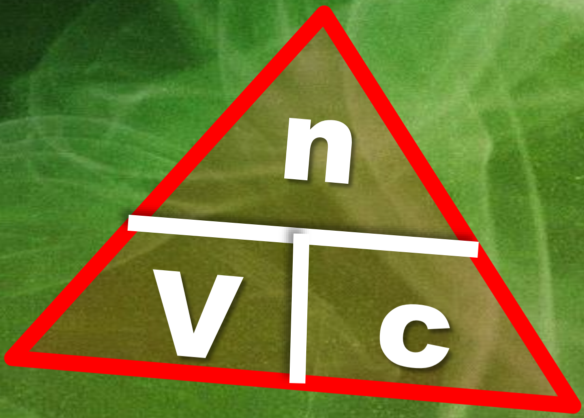
CALCULATIONS

LIMITING REACTANT

$$C_6H_8O_6 + I_2 \rightarrow C_6H_6O_6 + 2H^+ + 2I^-$$

25 cm^3
0.1 mol l^{-1}

0.27 g



CALCULATIONS

LIMITING REACTANT

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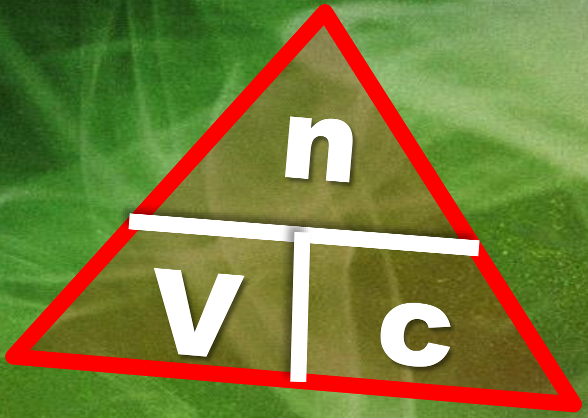


$n = 0.025\ l \times 0.1\ mol\ l^{-1} = \underline{0.0025\ moles}$

CALCULATIONS

LIMITING REACTANT

$$C_6H_8O_6 + I_2 \rightarrow C_6H_6O_6 + 2H^+ + 2I^-$$

25 cm^3
0.1 mol l^{-1}
0.0025 moles

0.27 g

$$n = \frac{0.27\text{g}}{253.8\text{ g/mol}} = \underline{0.001\text{ moles}}$$

Mass
n | FM

CALCULATIONS

LIMITING REACTANT

$$C_6H_8O_6 + I_2 \rightarrow C_6H_6O_6 + 2H^+ + 2I^-$$

25 cm^3
0.1 mol l^{-1}
0.0025 moles

0.27 g
0.001 moles

Ratio of reactants required = $\dfrac{1mol}{1mol}$

CALCULATIONS

LIMITING REACTANT

$C_6H_8O_6 + I_2 \rightarrow C_6H_6O_6 + 2H^+ + 2I^-$

25 cm^3
0.1 mol l^{-1}

0.27 g

Ratio of reactants available = $\frac{0.0025mol}{0.001mol}$

CALCULATIONS

LIMITING REACTANT

$C_6H_8O_6 + I_2 \rightarrow C_6H_6O_6 + 2H^+ + 2I^-$

0.0025mol

0.001mol

NOT ENOUGH I_2

I need a ratio of 1 to 1 to make reaction happen.

Percentage Yield

Percentage yield → efficiency of a reaction

% → mass of the theoretical product

Percentage Yield

EXAMPLE

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

- If we burned 16g of methane (CH_4), we would expect there to be 44g of carbon dioxide (CO_2) produced.

- This is because 1 mole of methane (gfm=16g) ought to produce 1 mole of carbon dioxide (gfm=44g)

Percentage Yield

EXAMPLE

BUT!

Sometimes less than the expected is actually synthesised.

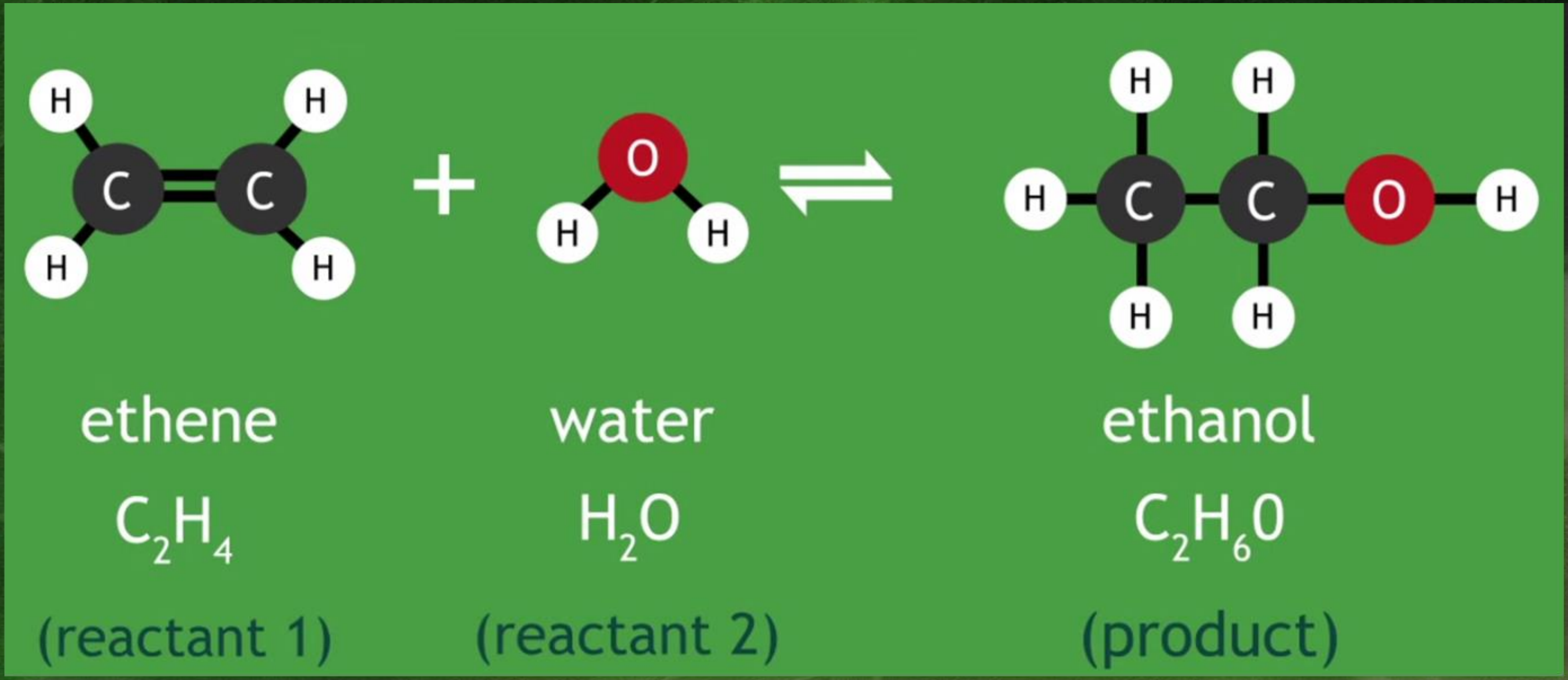
If only 17g of the expected 44g of carbon dioxide was produced from the methane burned, what would the PERCENTAGE YIELD be?

Percentage Yield

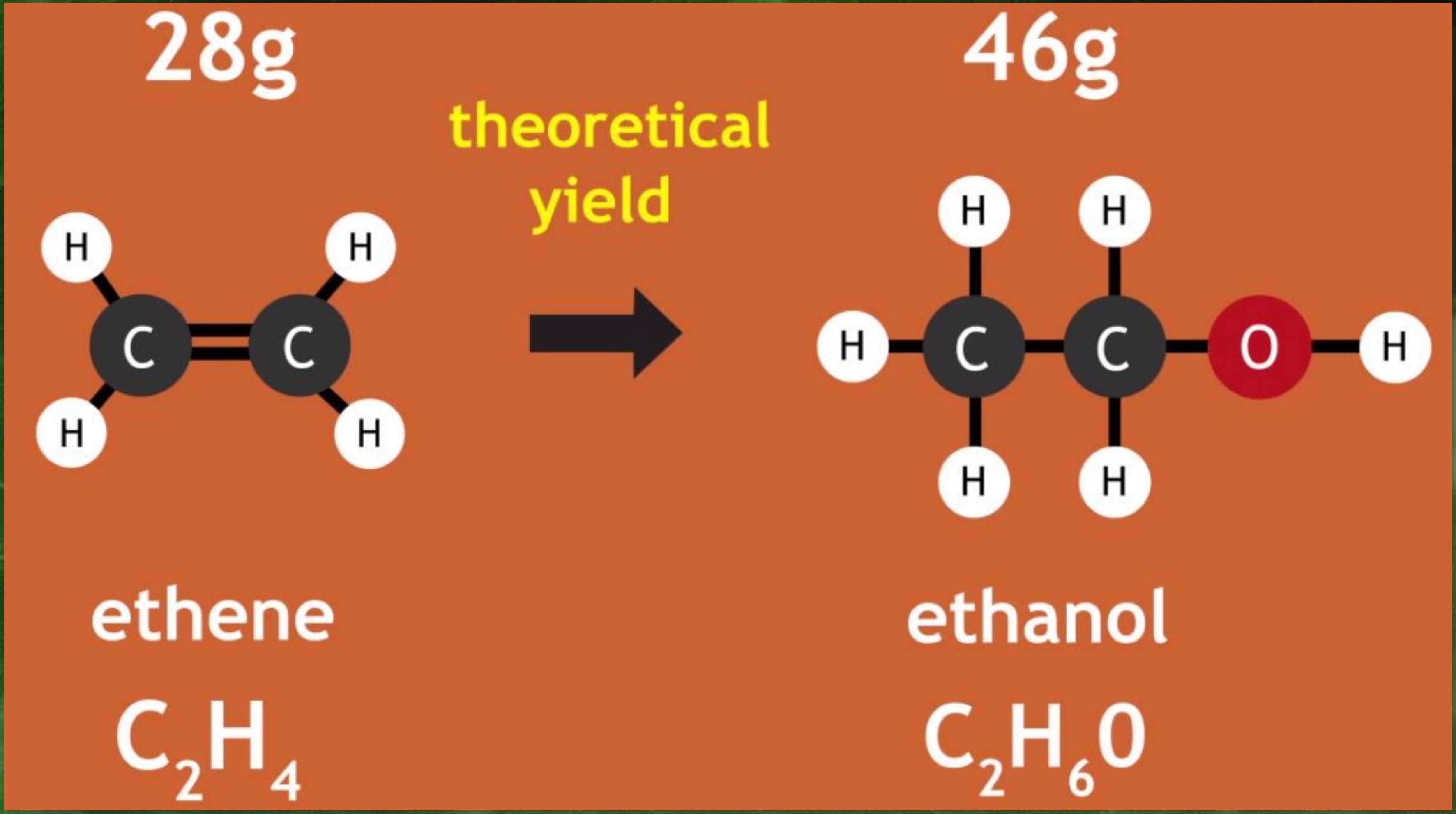
formula of percentage yield

$$\frac{\text{actual yield of products formed}}{\text{theoretical yield of products formed}} \times 100$$

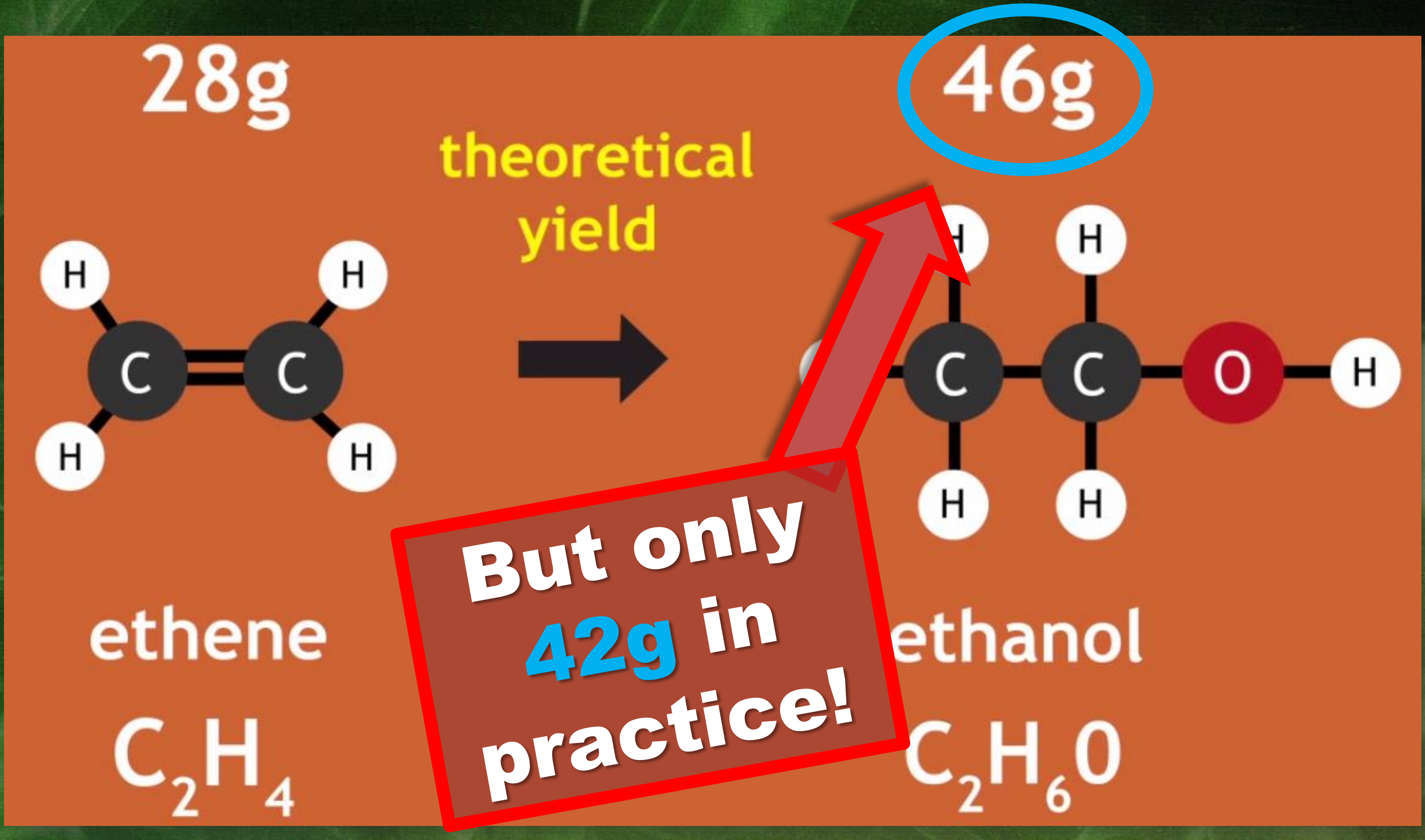
Percentage Yield



Percentage Yield



Percentage Yield



Percentage Yield

practical yield
42

→ percentage (%) →

theoretical yield
46

formula of percentage yield

$$\frac{\text{practical yield of products formed}}{\text{theoretical yield of products formed}} \times 100 = \text{percentage yield}$$

?

Percentage Yield

practical yield 42 → percentage (%) → theoretical yield 46

formula of percentage yield

0.913 X 100 = 91.3%

Percentage Yield

actual yield

0.740 moles

theoretical yield

0.755 moles

formula

$$\frac{\text{actual yield}}{\text{theoretical yield}} \times 100 = \text{Percentage yield}$$

?

Percentage Yield

actual yield	theoretical yield
0.740 moles	0.755 moles

formula | 0.987 x 100 = 98%

Why is the yield not 100%?

There are a variety of reasons why each reaction does not produce a 100% yield of the product:

- not all the reactants being used up
- products escaping the reaction vessel
- physical loss of products during transfer

HOW to increase % yield?

Alter the reaction conditions:

- Temperature
- Pressure
- Catalyst
- Use a reactant in excess

OR

Use a different chemical reaction

Atom Economy

reactant A + reactant B → product (+ waste)

Usually only interested in product.

Atom Economy

reactant A + reactant B → product (+ waste)

Usually only interested in product.

Atom economy = % of useful product

Atom Economy

reactant A + reactant B → product (+ waste)

the atom economy ↑ ↓ less waste is produced

Atom Economy

1) Reaction

2) Equation

3) Molecular masses

Atom Economy

$$\text{atom economy} = \frac{\text{the mass of the desired products}}{\text{mass of all products}} \times 100$$

Atom Economy

$$\frac{\text{the mass of the useful product}}{\text{mass of all products}} \times 100 = \text{atom economy}$$

(reactant)		(reactant)		(product)		(product)		(product)
$2NH_3$	+	$NaOCl$	$\rightarrow$	N_2H_4	+	$NaCl$	+	H_2O
ammonia		sodium hypochlorite		hydrazine		sodium chloride		water
(34)		(74.5)		(32)		(58.5)		(18)

?

Atom Economy

$$\frac{32}{108.5} \times 100 = 29.5\%$$

(reactant)		(reactant)		(product)		(product)		(product)
$2NH_3$	+	$NaOCl$	$\rightarrow$	N_2H_4	+	$NaCl$	+	H_2O
ammonia		sodium hypochlorite		hydrazine		sodium chloride		water
(34)		(74.5)		(32)		(58.5)		(18)

Atom Economy

Example

Calculate the atom economy for this reaction where hydrogen is the desired product.

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

Step 1: Calculate mass of desired product
Step 2: Calculate total mass of products/reactants
Step 3: Divide the answer from Step 1 by the answer from Step 2 and multiply by 100.

Answer: [redacted] ?

Atom Economy

Example

Calculate the atom economy for this reaction where hydrogen is the desired product.

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

Step 1: Calculate mass of desired product
Step 2: Calculate total mass of products/reactants
Step 3: Divide the answer from Step 1 by the answer from Step 2 and multiply by 100.

Answer: 6/34 x 100 = 17.65%

QUESTIONS

- Calculate the atom economy for:

- $CaCO_3 + 2HCl \rightarrow CaCl_2 + CO_2 + H_2O$

?

QUESTIONS

- Calculate the atom economy for:
- $CaCO_3 + 2HCl \rightarrow CaCl_2 + CO_2 + H_2O$

64.18%

QUESTIONS

- Calculate the atom economy for:

- $4NH_3 + 6NO \rightarrow 5N_2 + 6H_2O$

?

QUESTIONS

- **Calculate the atom economy for:**

- **$4NH_3 + 6NO \rightarrow 5N_2 + 6H_2O$**

56.45%

QUESTIONS

- **Calculate the atom economy for:**

  - $C_2H_4 + CH_3CO_2H + \frac{1}{2}O_2 \rightarrow$ $C_2H_3O_2CCH_3 + H_2O$

?

QUESTIONS

- Calculate the atom economy for:

- $C_2H_4 + CH_3CO_2H + ½O_2 \rightarrow$ $C_2H_3O_2CCH_3 + H_2O$

82.69%

QUESTIONS

Propanol, C_3H_7OH, can be dehydrated to produce propene, C_3H_6, using excess sulfuric acid. Propoxypropane, $C_3H_7OC_3H_7$, and water are also produced.

$$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$$

Mass of one mole= 60g

Mass of one mole = 42g

?

QUESTIONS

$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$

Mass of
one mole= 60g

Mass of
one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?

?

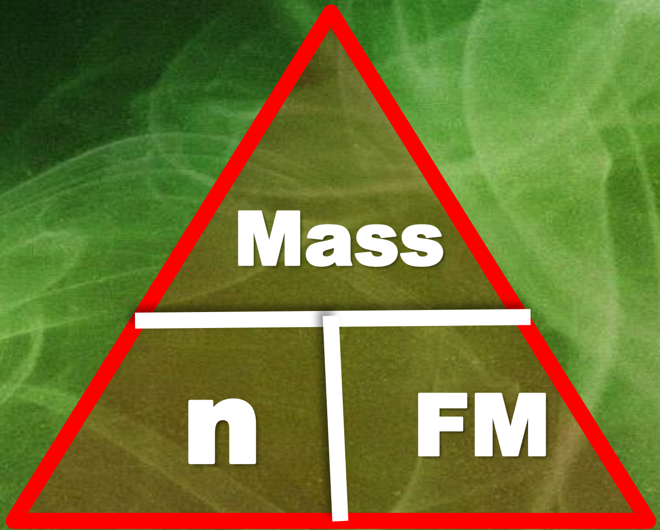
QUESTIONS

$$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$$

Mass of one mole= 60g

Mass of one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?



QUESTIONS

$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$

Mass of one mole= 60g

Mass of one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?

$$n = \frac{\text{Mass}}{\text{FM}}$$

QUESTIONS

$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$

Mass of one mole= 60g

Mass of one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?

$$n = \frac{270}{60}$$

QUESTIONS

$$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$$

Mass of one mole= 60g

Mass of one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?

n = 4.5

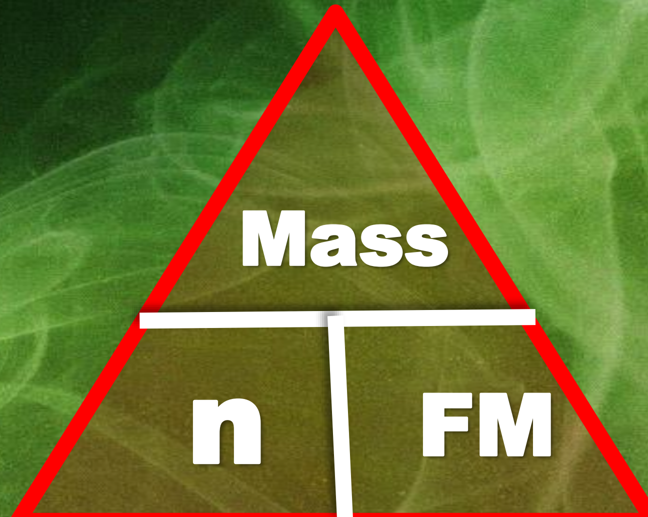
QUESTIONS

$$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$$

Mass of one mole= 60g

Mass of one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?



QUESTIONS

$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$

Mass of one mole= 60g

Mass of one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?

Mass =

n x FM

QUESTIONS

$$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$$

Mass of one mole= 60g

Mass of one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?

$$4.5\ C_3H_7OH \rightarrow 2.25\ C_3H_6$$

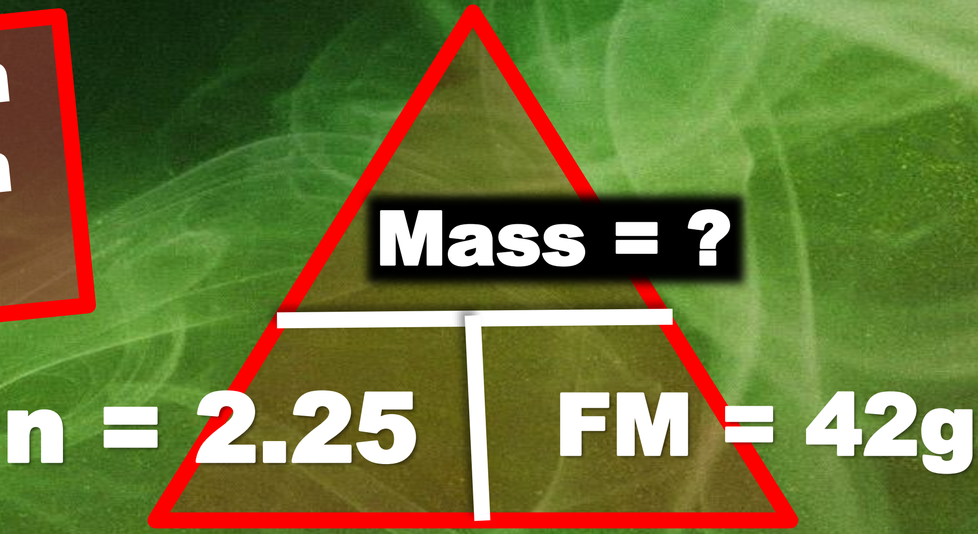
QUESTIONS

$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$

Mass of one mole= 60g

Mass of one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?



QUESTIONS

$$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$$

Mass of one mole= 60g

Mass of one mole = 42g

Theoretical yield, in kg, of propene from 270 kg propanol?

mass = 94.5kg

QUESTIONS

$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$

Mass of one mole= 60g

Mass of one mole = 42g

an actual yield of propene = 21kg

%Yield?

?

QUESTIONS

$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$

Mass of one mole= 60g

Mass of one mole = 42g

an actual yield of propene = 21kg

%Yield?

$$\frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

QUESTIONS

$4C_3H_7OH \rightarrow 2C_3H_6 + C_3H_7OC_3H_7 + 3H_2O$

Mass of one mole= 60g

Mass of one mole = 42g

an actual yield of propene = 21kg

%Yield?

%Yield = 22.2%