UNDERSTANDING BENZENE STRUCTURE

LESSON 1

Benzene is a molecule that is made from two elements.

Both elements have 3 main ***isotopes***. However, in both cases, one of the elements' isotopes has such a small abundance that it makes only a very small contribution to the A_r.

1. Define the term *isotope*
   Atoms with the same atomic number and different mass number.
   Or, Atoms with same number of protons but a different number of neutrons.
   For the lighter element the abundance data is: For the heavier element the abundance data is:

Relative Mass	Abundance (%)
1.000	99.9885
2.000	0.0115

Relative Mass	Abundance (%)
12.000	98.931
13.000	1.069

2. Define the term *relative atomic mass.*
   The average (or weighted mean) mass of atoms of an element compared to 1/12 mass of a 12C atom.
3. Calculate the relative atomic masses of the two elements and identify them. Express your answer to an appropriate number of **significant figures.**

$$\frac{(99.9885 \times 1.000) + (0.0115 \times 2.000)}{100} = 1.00 \qquad \frac{(98.931 \times 12.000) + (1.069 \times 13.000)}{100} = 12.01$$

Element A_r 1.00 Identity…Hydrogen Element A_r 12.01 Identity…Carbon

DETERMINATION OF THE EMPIRICAL FORMULA OF BENZENE.

The relative formula mass M_r of benzene was determined by mass spectrometry. The M_r is 78.0

To determine the empirical formula of benzene 1.00g of benzene was fully combusted in excess oxygen. The gaseous products were fed through powered **anhydrous copper(II)sulfate** and the remaining gas was passed through powdered **calcium oxide** (lime).

The **anhydrous copper(II)sulfate** increased in mass by **0.692g** and turned from a white solid to a mixture of some white solid and some blue solid.

The **calcium oxide** increased in mass by **3.38g**

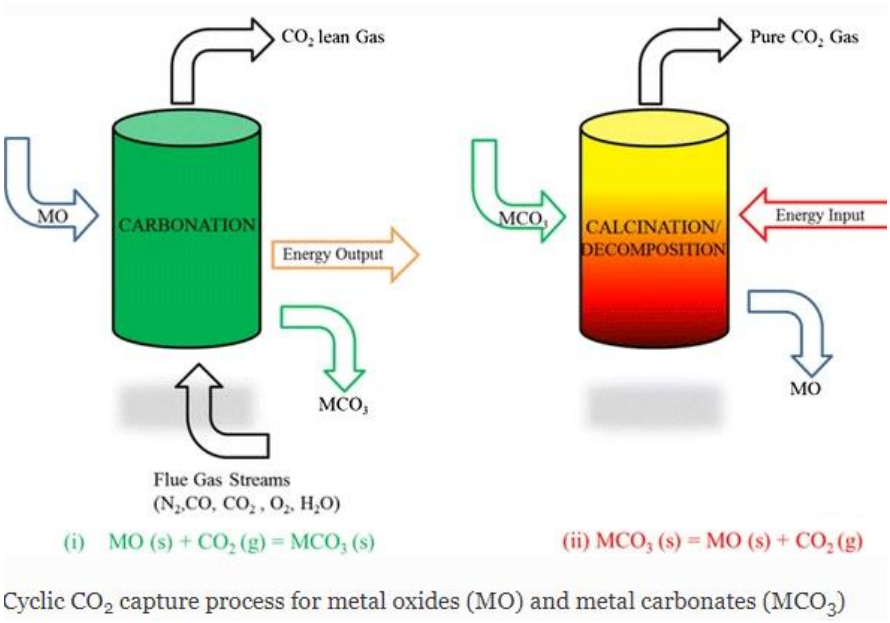
4. Define the term *empirical formula*
   The simplest whole number ratio of elements within a compound.

5. Explain why the anhydrous copper(II)sulfate gained mass.
   The anhydrous salt became hydrated/became the hydrate (by reaction with water)

6. The blue product was copper(II)sulfate pentahydrate. Write a chemical equation the represents the reaction that caused the anhydrous copper(II)sulfate to gain in mass.

   $CuSO_4 + 5\ H_2O \rightarrow CuSO_4 \bullet 5H_2O$ *(state symbols not important in this case)*

7. Explain why the calcium oxide gained mass. (clue: think about the combustion products when complete combustion takes place with a hydrocarbon. Also recall the properties of group 2 oxides).
   Calcium oxide reacted with the CO_2 gas to become calcium carbonate.
   *(Remember, CaO is the **oxide of a metal** and therefore it is **basic**. CO_2 is the **oxide of a non-metal** and therefore it is **acidic**. These react together. Metal oxides can be used to absorb CO_2 for example, from the waste gases from combustion of fossil fuels in some power stations.)*
   Here's a simple scheme of this, in action:



Cyclic CO_2 capture process for metal oxides (MO) and metal carbonates (MCO_3)

8. Write an equation for the reaction that took place when the calcium oxide gained mass.

   $CaO + CO_2 \rightarrow CaCO_3$

9. Using this data, you can now work out both the *empirical formula* and then the *molecular formula* of the benzene.
   If you are unsure what to do, look at the steps on the next page.
   See working on next page

empirical formula of benzene. **CH**

molecular formula of benzene. **C_6H_6**

a) Calculate the **moles** of water gained by the anhydrous copper(II)sulfate.
0.692g/18.0 g mol^{-1} = 0.03844mol

0.0384 mol of water

b) Calculate the total **moles** of the hydrogen present in the water. This hydrogen must have come from the benzene.
0.0384 mol x 2= 0.0769 mol (2 H atoms per H_2O molecule!)

0.0769 mol of hydrogen

c) Calculate the **moles** of carbon dioxide gained by the calcium oxide.
3.38g/44.0 g mol^{-1} = 0.0768 mol

0.0768 mol of carbon

d) Calculate the total **moles** of the carbon present. This carbon must have come from the benzene.
1 C atom per CO_2 molecule!

0.0768 mol of carbon

e) Calculate the **moles** of benzene that were combusted.
1.00g/78.0 g mol^{-1} = 0.0128 mol

0.0128 mol of benzene

f) Now, determine the **empirical formula** and **molecular formula** of benzene.

For carbon

0.0768 mol of carbon / 0.0128 mol of benzene =6.00

For hydrogen

0.0769 mol of hydrogen / 0.0128 mol of benzene = 6.01

empirical formula of benzene. **CH**

molecular formula of benzene. **C_6H_6**

10. If the combustion gases were collected at 122 ^{O}C, calculate the total volume of gases that was produced before it was passed through the copper(II)sulfate and calcium oxide. The pressure on the day that the experiment was performed was 99.7 kPa
Express your answer in cubic decimetres.

V= *n*RT/p

n=n_{H2O} + n_{CO2} = 0.0384 mol + 0.0768 mol= **0.115**mol

***R*= 8.314** *J mol^{-1} K^{-1}*

T= 122 + 273 = **395** K

***P*= 99700** Pa

V= **0.115 x 8.314 x 395/99700 = 3.79 x 10^{-3} m^3**

3.78 x 10^{-3} m^3 x 1000= 3.79dm^3 of gas produced

(or **3.80 dm^3** if you carried through the calculator values)

11. Define the term ***enthalpy of combustion, Δ_cH***

*The enthalpy change that accompanies the **full** combustion of **1 mol** of a compound.*
*Or, The enthalpy change that accompanies the combustion of **1 mol** of a compound in an **excess of oxygen***

12. Write an equation for the complete combustion of **benzene**

C_6H_6 + 7½ O_2 ➔ 6CO_2 + 3H_2O

13. Write an equation for the complete combustion of **carbon**

$$C + O_2 \rightarrow CO_2$$

14. Write an equation for the complete combustion of **hydrogen**

$$H_2 + \tfrac{1}{2} O_2 \rightarrow H_2O$$

The **enthalpies of combustion** data are presented below.

Chemical	Enthalpy of combustion / kJ mol^{-1}
hydrogen	-285.8
carbon	-393.5
benzene	-3267

15. Define ***Hess's Law***

The enthalpy change for a given process is independent of the route taken.

Or, *The sum of the enthalpy changes around a full cycle is zero.*

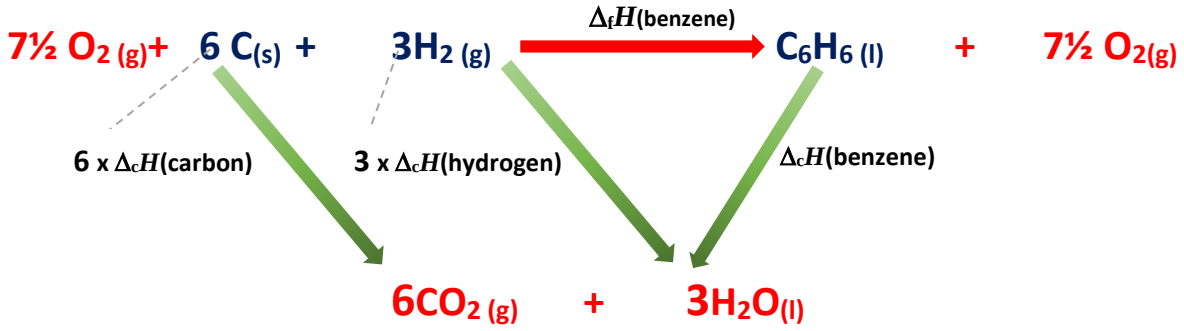
16. Define ***enthalpy of formation,*** $\Delta_f H$

*The enthalpy change that accompanies the **formation** of **1 mol** of a compound in its standard state from its elements in their standard states.*

Or, *The enthalpy change that accompanies the **formation** of **1 mol** of a compound from its elements when performed under standard conditions.*

17. Draw a Hess Cycle that would allow you to calculate the ***enthalpy of formation,*** $\Delta_f H$ of benzene using the information from the table shown above.

Use the Hess Cycle to calculate the ***enthalpy of formation,*** $\Delta_f H$ of benzene.



$\Delta_f H$(benzene) = (6 x $\Delta_c H$(carbon)) + (3 x $\Delta_c H$(hydrogen)) + (- $\Delta_c H$(benzene))

= (6 x -393.5) + (3 x -285.8) + (- - 3267) =48.60 kJ mol^{-1}

$\Delta_f H$ (benzene)= **48.60 kJ mol^{-1}**

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In conclusion, you have arrived at the **molecular formula of benzene, C_6H_6**. You may like to ponder over the possible structures of benzene that could have this molecular formula. This is what we will do in detail over the coming weeks.