Task 1

In 1825 benzene gas was discovered by Michael Faraday. He determined the empirical formula for the compound using elemental analysis (burning the benzene and determining the amount of carbon dioxide and water produced).

Draw as many structures with an empirical formula CH as you can in three minutes.

[Your structures must obey all of the usual rules for molecular structures, e.g. each carbon atom must have four chemical bonds or a positive/negative charge.]

Task 2

In 1834 Eilhard Mitscherlich determined the M_r of benzene to be 78.

Eliminate all of the possible structures which do not have an M_r of 78. Add further possibilities if you can think of any.

[Your structures must obey all of the usual rules for molecular structures, e.g. each carbon atom must have four chemical bonds or a positive/negative charge.]

Task 3

Many of the possible structures for benzene are unsaturated hydrocarbons due to the low ratio of hydrogen atoms to carbon atoms.

Describe the test for unsaturation and draw a mechanism to explain why unsaturated molecules behave in this way.

Task 4

A number of experiments were carried out on benzene in order to try to narrow down the possible structures. When bromine water was added to benzene the bromine water was not decolourised. However, benzene did decolourise bromine water when it was heated in the presence of a catalyst, such as $FeBr_3$.

What does this suggest about the structure of benzene? Explain your answer.

Do any of your potential structures account for this behaviour? Eliminate any structures which would decolourise bromine water.

Task 5

In 1865 a German chemist had one of the most famous dreams in the history of science. It is known as 'Kekulé's dream'.

Watch the following clip on YouTube from 0:30 to 1:02.

http://www.youtube.com/watch?v=dmqcnlaRA68

What was the dream about? Draw the structure of benzene that Kekulé predicted.

Task 6

Although Kelulé's structure represented a big step forwards in terms of understanding the behaviour of benzene, the structure does not fully explain why benzene does not decolourise bromine water. Kekulé proposed a 'fluxional' structure in which the double and single bonds were continually swapping over in a dynamic equilibrium.

Draw a diagram to illustrate the fluxional nature of Kekulé's benzene. To what extent do you think that this modification deals with the unusual reactivity of benzene?

Task 7

Some historical structures for benzene are shown below:

From left to right: Claus (1867), Dewar (1867), Ladenburg (1869), Armstrong (1887), Thiele (1899) and Kekulé (1865).

Which of these structures do you find the most plausible for explaining the unusual reactivity of benzene? Explain your answer.

Task 8

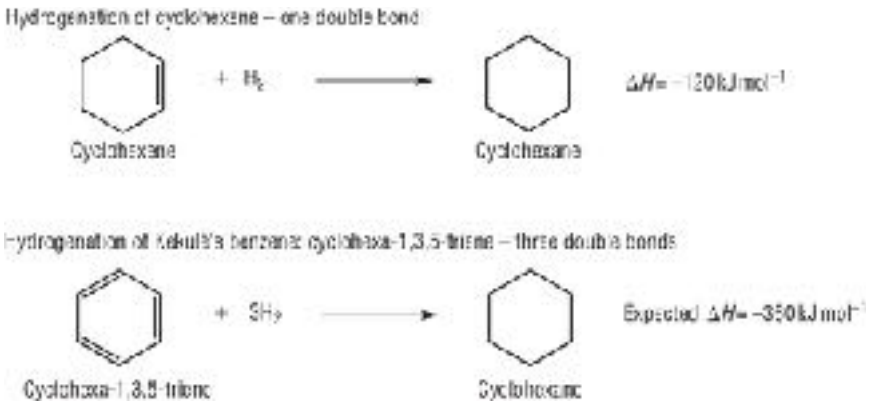
In 1929 Kathleen Lonsdale produced the crystal structure of benzene while working under Sir William Henry Bragg. X-ray crystallography was a new technique which involved firing X-rays at a crystal and monitoring how the X-rays were scattered from the individual atoms in the crystal structure.

Complete the worksheet: K1-Benzene/Aromaticity Worksheet/Tutorial using WebCSD.

http://webcsd.ccdc.cam.ac.uk/teaching_database_demo.php

Task 9

Another way of determining how many double bonds a structure has is to measure the enthalpy of hydrogenation.



Predict the true value of the enthalpy of hydrogenation for benzene.

Task 10

The actual enthalpy of hydrogenation for benzene is ΔH = -208 $kJmol^{-1}$.

How much more stable is benzene than Kekulé predicted?

The increased stability of benzene is due to delocalisation energy, or resonance stability. This means that the sharing of electrons in the π-bonding system makes the whole molecule less reactive.

Draw an energy level diagram to show the enthalpy of hydrogenation for Kekulé's structure, benzene and the resonance stability.