

Answer all the questions below as fully as you can then check your answers

1. What type of reaction would you expect unsaturated molecules such as alkenes to undergo?
2. Is benzene an unsaturated molecule?
3. What is resonance?
4. How does Kekulé model of benzene differ from the modern idea of the structure of benzene?
5. The following all relate to evidence that Kekulé proposed to help validate his model for the structure of benzene.
 - a. Kekulé's model of benzene proposed one isomer of bromobenzene when bromine and benzene reacted. Draw the structure of this isomer.
 - b. Kekulé's model of benzene proposed four isomer of dibromobenzene; draw the structure of these four isomers.
 - c. Only 3 isomers of dibromobenzene could be isolated and not the 4 predicted from Kekulé model. Explain how Kekulé explained this.
6. Explain why cyclo-hexa-1,3,5-triene, an early name for benzene is a not a suitable name for benzene today.
7. Write an equation to show represent the enthalpy of hydrogenation of cyclohexane and give the approximate enthalpy change for this reaction.

- b. Predict the enthalpy change for:
- i. cyclohexa-1,4-diene and cyclo-hexa-1,3,5-triene.
- c. Explain why the enthalpy of hydrogenation is much less than expected. You should mention delocalisation energy in your answer.
8. Describe the carbon carbon bond lengths in benzene when compared to C-C and C=C bonds. Offer an explanation for your answer.

Answers

1. What type of reaction would you expect unsaturated molecules such as alkenes to undergo?

Unsaturated molecules such as alkenes would be expected to undergo electrophilic addition reactions.

2. Is benzene an unsaturated molecule?

The molecular formula of benzene suggests it is unsaturated but its chemical reactions would suggest otherwise. Benzene does not undergo electrophilic addition reactions that would be expected of an unsaturated molecule. Benzene does not contain carbon carbon double bonds ($C=C$) so it is not an unsaturated molecule.

3. What is resonance?

Resonance is the theory that electrons within molecules/ions are able to move while the nuclei stay in place. Molecules which are able to undergo resonance are generally more stable than might otherwise be predicted.

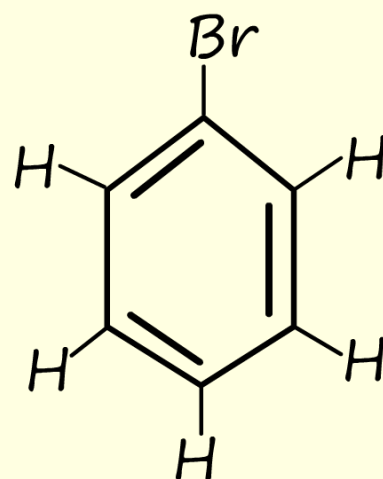
4. How does Kekulé model of benzene differ from the modern idea of the structure of benzene?

- Kekulé suggested a structure with alternate $C-C$ and $C=C$ bonds. Modern theory shows all the $C-C$ bond lengths in benzene are intermediate between $C-C$ and $C=C$ and all the bonds are the same length.
- Modern theory suggests that the structure of benzene is resonance stabilised with the 6 pi electrons all delocalised in areas of electron density above and below a flat planar molecule. Kekulé imagined benzene as an unsaturated molecule with $C-C$ and $C=C$ bonds.
- All the $C-C$ bond lengths in modern structure of benzene are the same, Kekulé's model had long $C-C$ and short $C=C$.
- Kekulé's model had the $C=C$ bonds alternating in position within the molecule. Modern structure has delocalised electrons.

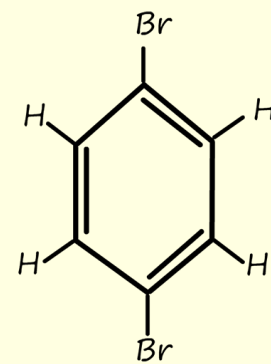
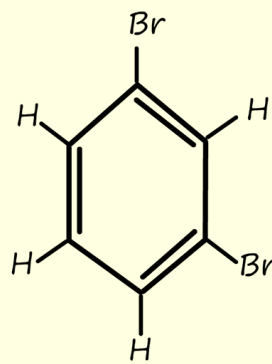
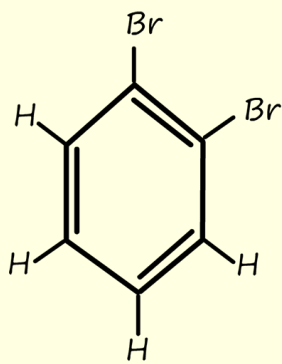
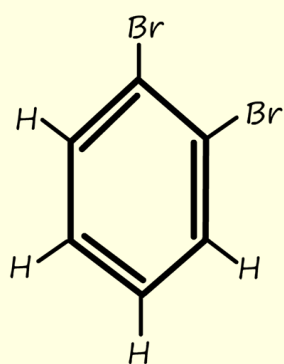
5. The following all relate to evidence that Kekulé proposed to help validate his model for the structure of benzene.

- a. Kekulé's model of benzene proposed one isomer of bromobenzene when bromine and benzene reacted. Draw the structure of this isomer.

Shown opposite is the structure of bromobenzene. Only one isomer of this is possible as it makes no difference where the bromine atom is placed, all structures will be identical.



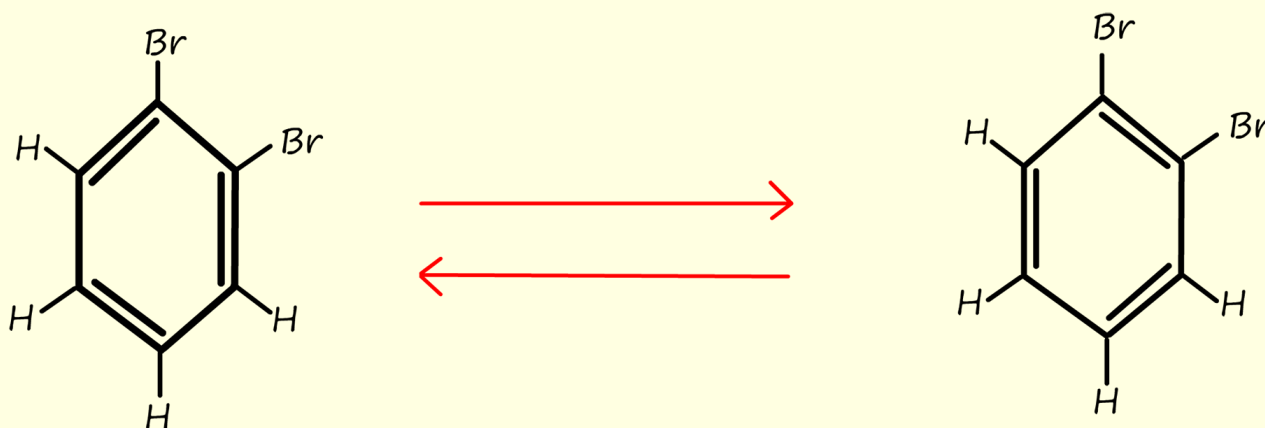
- b. Kekulé's model of benzene proposed four isomers of dibromobenzene; draw the structure of these four isomers.



1,2-dibromobenzene two isomers are possible. 1,3-dibromobenzene 1,4-dibromobenzene

- c. Only 3 isomers of dibromobenzene could be isolated and not the 4 predicted from Kekulé model. Explain how Kekulé explained this.

Kekulé suggested that the two isomers of 1,2-dibromobenzene interconvert rapidly, this meant that it was not possible to separate them out.



6. Explain why cyclo-hexa-1,3,5-triene, an early name for benzene is a not a suitable name for benzene today.

All the C-C bond lengths in benzene are similar, not the case with cyclo-hexa-1,3,5-triene, alkenes such as cyclo-hexa-1,3,5-triene would be expected to undergo electrophilic addition reactions, benzene does not.

7. Write an equation to show represent the enthalpy of hydrogenation of cyclohexane and give the approximate enthalpy change for this reaction.



- b. Predict the enthalpy change for:

- i. cyclohexa-1,4-diene and cyclo-hexa-1,3,5-triene.

The diene should have an enthalpy change of around $\Delta H = -240 \text{ kJ mol}^{-1}$ and the triene should have an enthalpy change of approximately $\Delta H = -360 \text{ kJ mol}^{-1}$

- c. Explain why the enthalpy of hydrogenation is much less than expected. You should mention delocalisation energy in your answer.

The pi(π) electrons are delocalised within the benzene molecule, this delocalisation created stability within the molecule. This delocalisation is the same as resonance. In the case of a benzene molecule the delocalisation energy is the difference in energy within a benzene molecule and a cyclohexa-1,3,5-triene molecule.

8. Describe the carbon carbon bond lengths in benzene when compared to C-C and C=C bonds. Offer an explanation for your answer.

C-C bond length 147pm (1pm = 1×10^{-12} m)

C=C bond length 135pm (1pm = 1×10^{-12} m)

C-C bond length in benzene 140pm (1pm = 1×10^{-12} m)

The carbon carbon length in benzene is intermediate between a single and a double bond, it is as if we have 1.5 electrons in each carbon carbon bond!