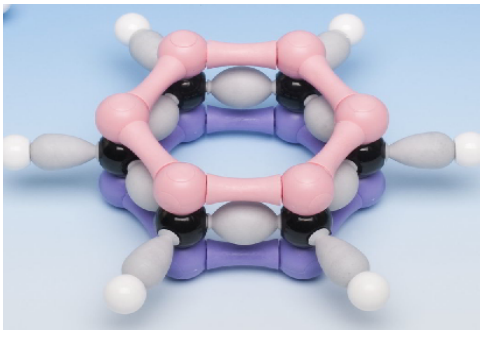
HL Answers to Electrophilic substitution questions

1. Each carbon atom is sp^2 hybridized with each sp^2 hybrid orbital containing one electron. One of these hybrid orbitals combines with the single electron in the 1s atomic orbital of a hydrogen atom forming a sigma bond. The other two sp^2 hybrid orbitals each combine with one of the hybrid sp^2 orbitals of two other carbon atoms to form sigma bonds. This results in a planar hexagonal ring with bond angles of 120°. The six remaining outer electrons (one on each carbon atom occupying a p orbital) form a delocalized pi bond spread equally above and below the plane of all six carbon atoms.



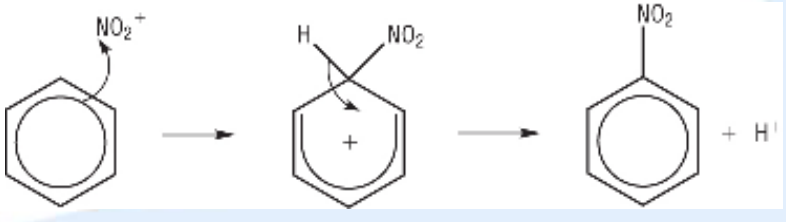
2. i. $C_6H_6 + HNO_3 \xrightarrow{H_2SO_4} C_6H_5NO_2 + H_2O$

ii. It is a catalyst. It functions as an acid, protonating the nitric acid to form $H_2NO_3^+$ which then breaks down to form water and the nitronium ion.
$H_2SO_4 + HNO_3 \rightarrow H_2NO_3^+ + HSO_4^-$ then $H_2NO_3^+ \rightarrow NO_2^+ + H_2O$

iii. The nitronium ion, NO_2^+.

iv. Substitution, unlike addition, does not involve the extra energy required to overcome the delocalization energy of the benzene ring.

v.



iv. Further nitration of the benzene ring will occur (to form 1,3-dinitrobenzene).

3. i. $C_6H_6 + Cl_2 \xrightarrow{AlCl_3} C_6H_5Cl + HCl$

ii. Cl^+.
The $AlCl_3$ acts as a Lewis acid, accepting a pair of electrons from Cl_2 to form $AlCl_4^-$ and Cl^+.

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