

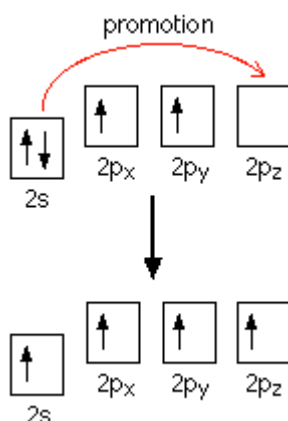
Chemguide – answers

BONDING IN BENZENE

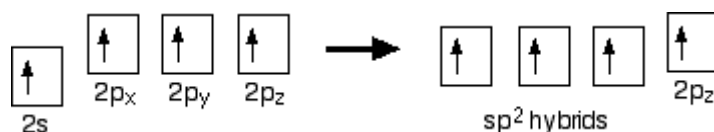
1. a) $1s^2 2s^2 2p_x^1 2p_y^1$.

b) One of the 2s electrons is promoted by moving it into the slightly higher energy $2p_z$ orbital to give the structure $1s^2 2s^1 2p_x^1 2p_y^1 2p_z^1$.

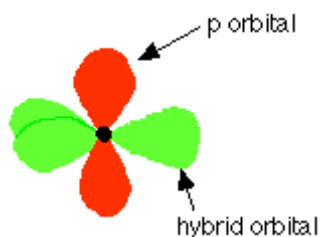
Or with a diagram:



Each carbon atom has to join to three other things (a hydrogen atom and two other carbon atoms). It reorganises 3 of its s and p electrons into 3 orbitals with the same shape and energy. These are called sp^2 hybrids. The other p orbital is left unchanged.



The sp^2 hybrids arrange themselves as far apart as possible with the remaining p orbital at right angles to them.



c) On each carbon atom, one of the sp^2 hybrid orbitals overlaps with the $1s^1$ orbital of a hydrogen atom to form a molecular orbital. The other two sp^2 orbitals overlap end-to-end with similar orbitals on the carbon atoms either side of them on the ring. All of these overlaps result in sigma bonds.

The remaining p orbitals on the carbons all overlap sideways to form a delocalised system of pi orbitals above and below the ring.

d) It shows a single pi orbital which can only hold 2 electrons. There are a total of 6 electrons involved here, and so there have to be 3 molecular orbitals to hold them.

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2. When ethene reacts with bromine, the pi part of the double bond is broken and the electrons are used to form bonds with the two bromine atoms. The pi bond no longer exists.

If you did the same thing with benzene, for every two bromine atoms you attach to the ring, you lose the contribution of two of the electrons which make up the delocalised pi system. The energetic stability of benzene relies on the complete delocalisation of the six original p electrons over the entire ring.

Breaking that delocalisation costs about 150 kJ per mole of benzene, and so it isn't energetically worthwhile for benzene to undergo addition reactions under most circumstances.