ARENES: INTRODUCTION

1. a) In each case there is a carbon atom at each corner of the hexagon with a hydrogen atom attached to it.

   In the Kekulé structure there are alternating double and single bonds around the ring.

   The circle in the modern structure represents the delocalised electrons. In this case, all the carbon-carbon bonds in the ring are identical.

   b) Double carbon-carbon bonds are shorter than single ones, and that would produce an irregular hexagon. In benzene, the carbon-carbon bonds are all exactly the same length, and the hexagon is regular with the bond lengths being between the usual single and double carbon-carbon bond lengths.

   c) The Kekulé structure containing the double bonds would suggest that benzene would have reactions rather like ethene and other alkenes – undergoing addition reactions. In fact, benzene is very reluctant to undergo addition reactions, and instead undergoes substitution reactions, replacing one or more hydrogen atoms by something new.

   d) The delocalisation of the electrons in benzene makes benzene more energetically stable than it would otherwise be by about 150 kJ mol^{-1}. If something was added to the ring, that would use up some of the delocalised electrons and the delocalisation would be broken, costing lots of energy. So addition to benzene is difficult.

   If benzene undergoes substitution, the delocalisation is broken temporarily, but comes back again when the reaction is completed. That increases the activation energy for the reactions, and so they are relatively slow but, overall, substitution is energetically possible.

2. a) Methyl groups tend to "push" electrons away from themselves towards whatever they are attached to. That leaves the methyl group very slightly positive and the ring very slightly negative.

   b) Methylbenzene is a bigger molecule than benzene and so has greater dispersion forces. It also has a small amount of dipole-dipole attractions on top of this. In the liquid, more energy has to be put in to break these forces than in benzene and so the boiling point is greater.

   In the solid, how the molecules pack is also important. If the molecules don't pack as efficiently, the intermolecular forces won't work as well. In the methylbenzene case, the methyl groups get in the way of really close packing.

   c) For the arene to dissolve, you have to break the quite strong dispersion forces in the arene and the hydrogen bonds between water molecules. If the arene molecules get between the water molecules, lots of hydrogen bonds are broken as well as the dispersion forces between the arene molecules. These are only replaced by smaller dispersion between the small water molecules and the arene molecules. So you don't get enough energy back to compensate for the energy used to break the original attractions, and solution isn't energetically profitable.