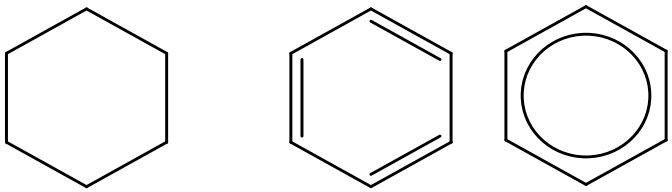
(For this worksheet you may find it helpful to read the 'How to Use the WebCSD' instruction sheet first)



Cyclohexane Benzene

1. The above diagram shows 2D pictures of cyclohexane and benzene. Using the refcodes BENZEN and CYCHEX, can you write down their molecular formulae and explain the visible differences in structures between the two molecules?

2. Why are the 2D pictures poor representations of these molecules?

3. Using the WebCSD measure the bond lengths of C-C single bonds in alkanes such as ETHANE01 and HEXANE01 and C=C double bonds in alkenes such as ETHLEN10 and COVJON.
   Now measure the bond lengths and angles between carbon atoms around the aromatic ring in BENZEN and compare them with your measured values for C=C and C-C.
   What does this suggest about the bonding in benzene?

4. The WebCSD uses real crystal structures. Due to the packing of molecules in the crystal slightly different results than expected are shown. The torsion angle is a measure of the planarity ('degree of flatness') of the selected group of atoms in the molecule. Measure the torsion angle for benzene; what should the torsion angle be?

5. Using the information from the previous questions, draw a diagram and explain the bonding in benzene.

6. Why is benzene unreactive compared to alkenes?

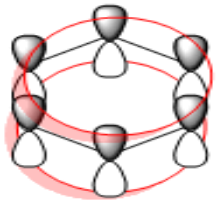
Answers

1. Cyclohexane C_6H_{12}. It is not flat and is twisted into a 'chair' conformation (this alleviates angular and torsional strain – see another worksheet for more information).
   Benzene C_6H_6. This is a flat molecule like the picture suggests.

2. The 2D representation of the molecules infers that they are both flat (planar). The 3D crystal structures show the true shapes of the molecules. Benzene is planar but cyclohexane clearly isn't.

3. Bond lengths for C-C in ethane 1.53Å & hexane 1.52Å.
   Bond lengths for C=C in ethene 1.31Å & cyclohexene 1.31-1.33Å.
   Benzene has a C-C bond length of 1.39Å and a bond angle of 119.5°. These values are longer than a C=C bond but shorter than a C-C bond, showing that it does not have the theoretical Kekule structure with conjugated single and double bonds but the delocalised ring of π-electrons which makes the C-C bonds intermediate in length. The measured bond angle is very close to the theoretical value of 120° (the interior angle of a hexagon).

4. The torsion angle measured is 1.4°. Benzene is a planar molecule so the torsion angle should be 0°.

5. 

   Each carbon has a p-orbital with a single electron in it. These orbitals overlap and the electrons become delocalised over all 6 atoms. This leads to π-bonding spread over the whole molecule.

6. The delocalisation of the π-electrons makes benzene stable. It does not undergo addition reactions as readily as an alkene.