

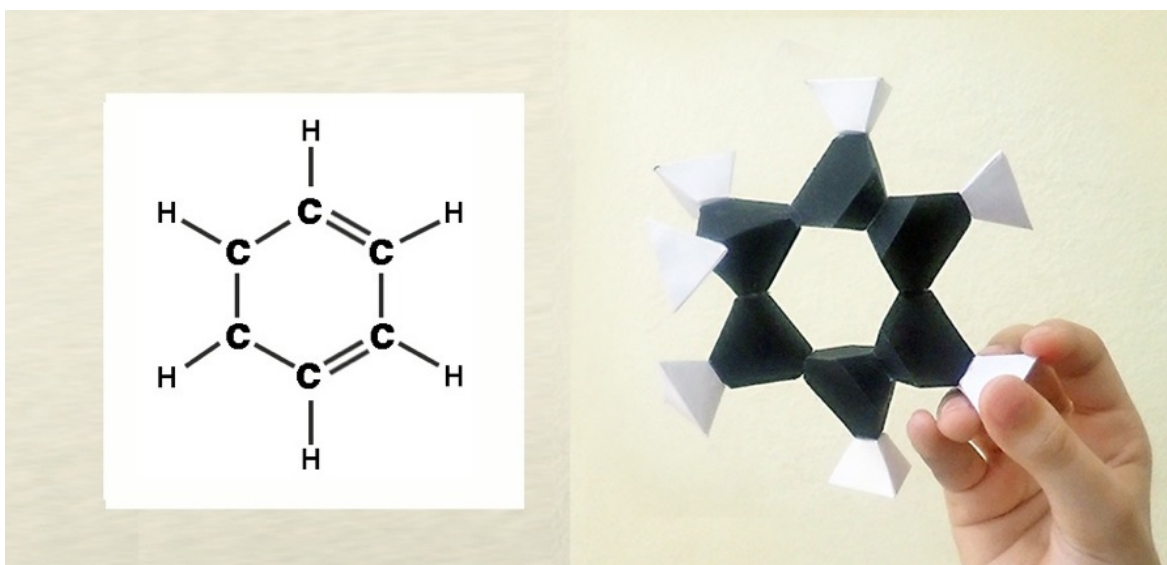
Benzene bonding

Shannon and Ian Jacobs

Benzene was isolated by Michael Faraday in England in 1825. The clear liquid at room temperature smells like petrol and floats on water. What we now know to be a carbon ring surrounded by six hydrogens is a more stable molecule than expected and occurs as a unit in many organic compounds. Faraday knew in 1825 that the empirical formula of his new compound was CH, with equal numbers of carbon and hydrogen atoms, but the structure with so few hydrogens was a puzzle at the time. The German Chemist, August Kekulé, got it almost right in 1865 when he proposed a ring structure that would have been named in modern terms as **cyclohexatriene**. That benzene does have a ring structure was confirmed in the 1930's, but the details remained obscure until later in the 20th century.

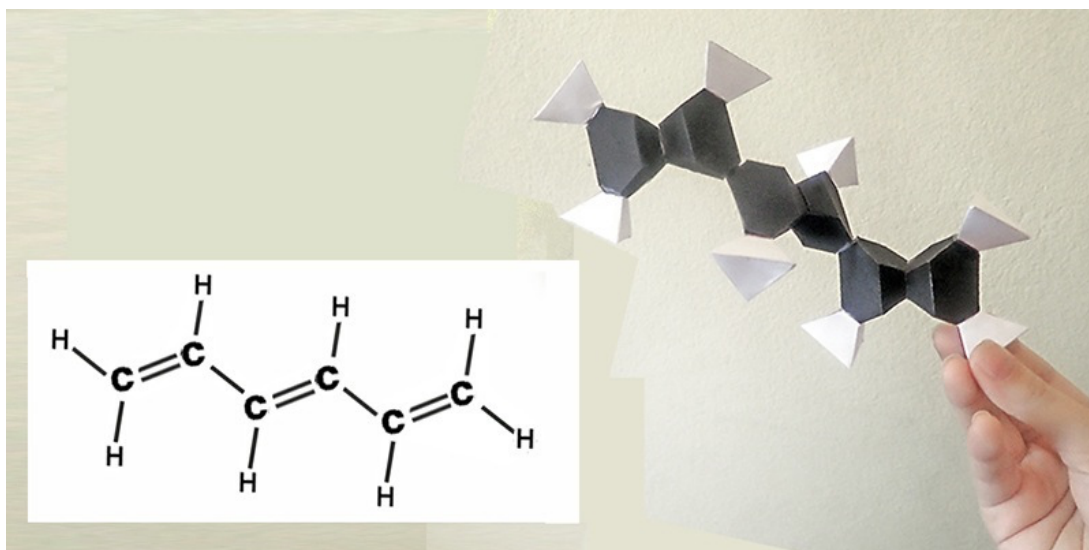
Modelling the structure of benzene

Hexene and hexadiene are linear six carbon molecules with one double bond (hexene) and two double bonds (hexadiene). Like hexane both hexene and hexadiene form stable cyclic molecules.

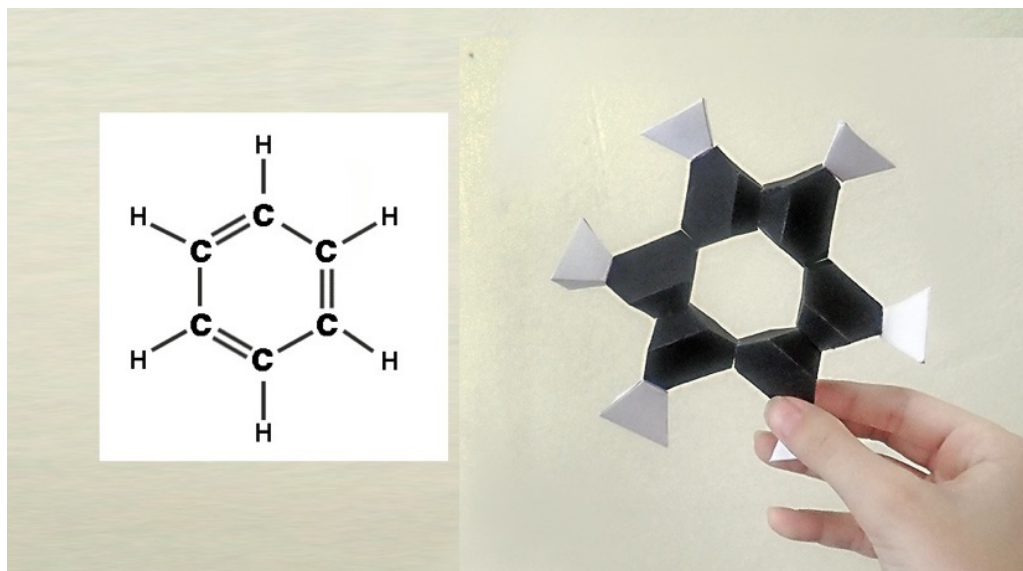


Cyclohexadiene with two double bonds is modelled as a diagram and in paper.

Linear **Hexatriene** is modelled below as a diagram and in paper.

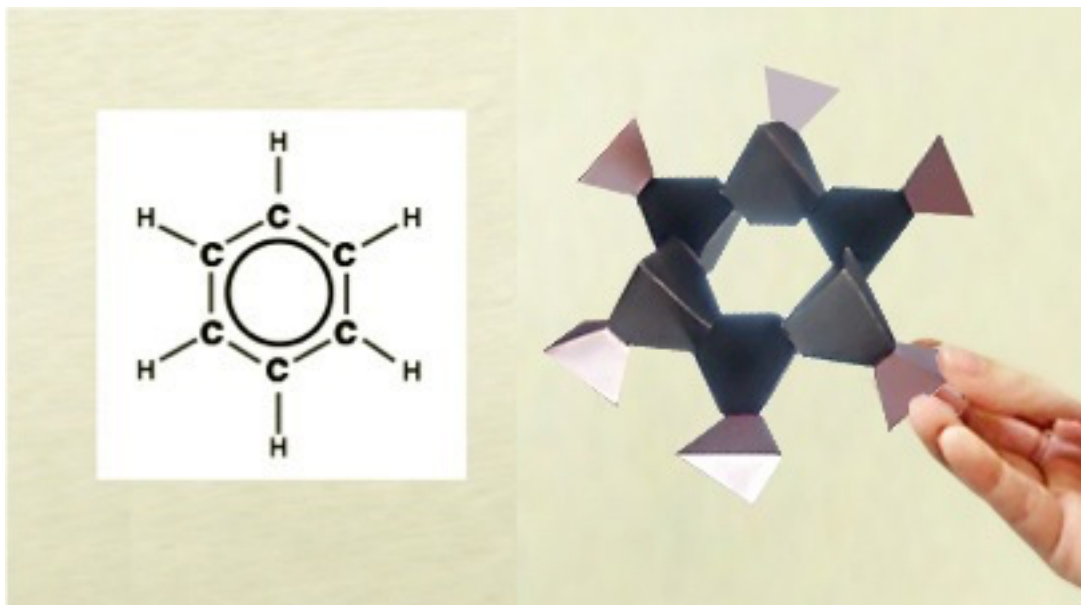


The linear hexatriene molecule with three double C = C bonds in the chain of six carbons is stable. Kekulé assumed, like everyone else, that cyclohexatriene below would be stable like cyclohexane, cyclohexene and cyclohexadiene.

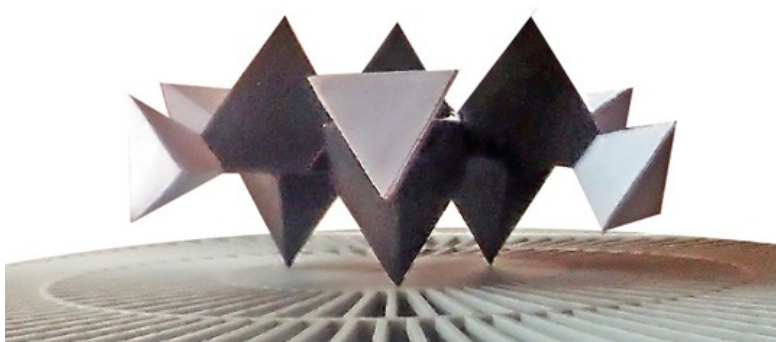


But ... it became clear in the 20th century that benzene is a *regular* hexagon with C-C bonds of the *same length and strength* (between that of single and double bonds). Benzene is not cyclohexatriene, which is *not stable*. Bonding electrons must somehow be distributed around the ring to form six equivalent bonds!

To model that, we redraw the diagram with an inner circle to suggest distributed bonding electrons and modify the tetrahedron with two larger triangular snub points for shorter stronger bonds and leave one sharp point.



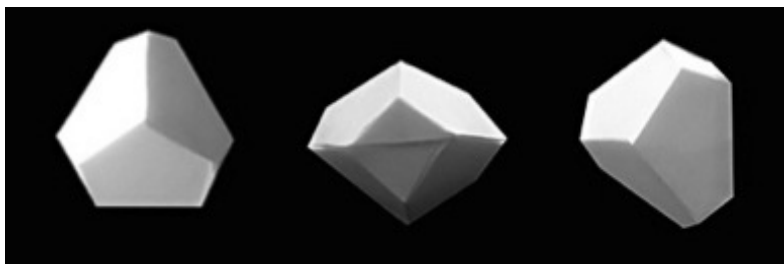
A benzene model made in this way has some suggestive features. The hexagon is regular when viewed from above, and the equal length bonds around the ring are shorter than in cyclohexane. The hydrogens are more or less in the same plane.



The three black points above and below the ring suggest rings of electron charge above and below the ring and naked benzene rings fit together naturally to model graphene. To avoid bond strain the benzene ring as we have it above must be in the chair form and is not flat. We could perhaps overlook this but it's not right.

Modern studies show that the benzene ring in nature is flat like a dinner plate, not spikey like a hedgehog.

To better model the benzene structure, following the practice of constructing molecular bonding orbitals by combining spherical harmonics *in the ratios required to give us what we want*, we further modify carbon nets to model the bonding electrons of the carbon atoms in what is called the sp^2 configuration.

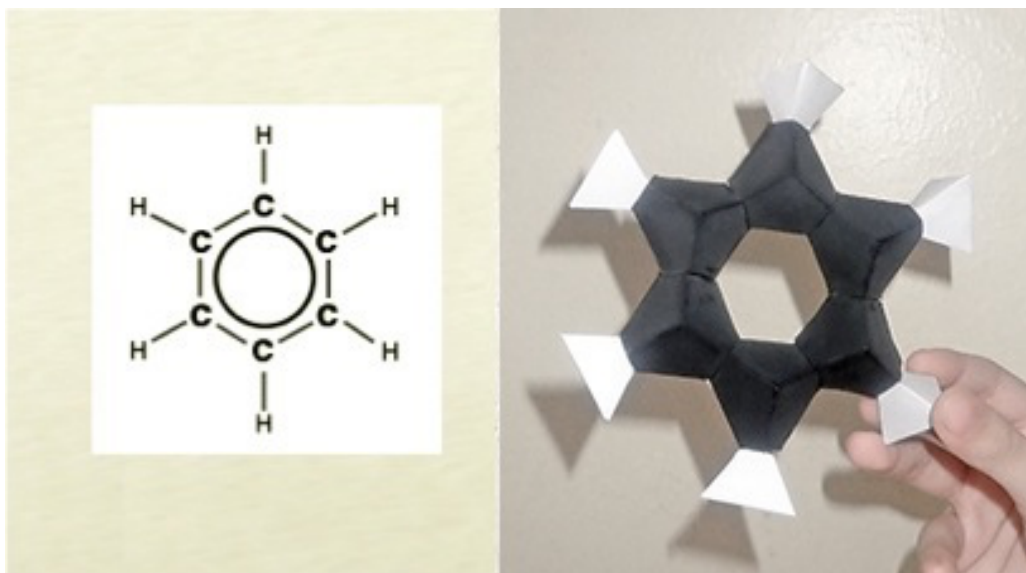


Modified nets are linked below and the models are in two symmetrical halves glued together.

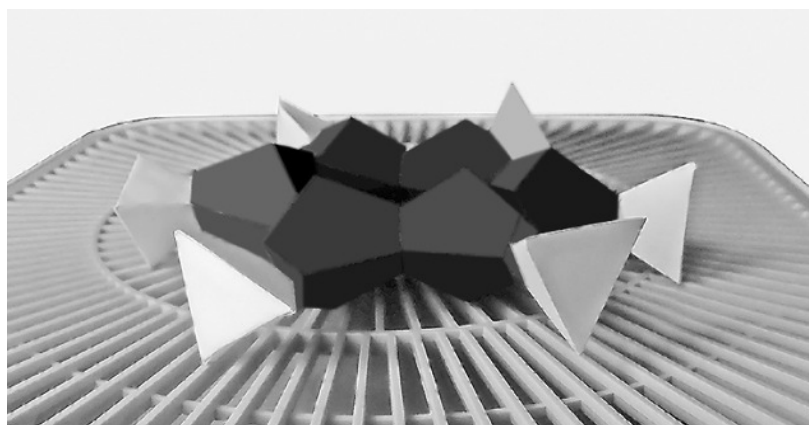


Six carbon models form a regular hexagonal ring with snub points of equal size at 120 degrees.

Benzene modelled with a diagram and with a revised symmetrical paper ring.



The hexagon is now regular with each carbon atom represented by an identical model. That the ring is now flat is seen in the image below.



The size of these models and the bond lengths may be changed by modifying the nets. Note that the improved two-part models take more time to make than the previous single net benzene models.

Look up *Kekulé* on the web and read the *History of Benzene* and look for discussions of sp , sp^2 and sp^3 hybridisation of carbon bonding electron orbitals.