Cyclo-hexane and -hexene

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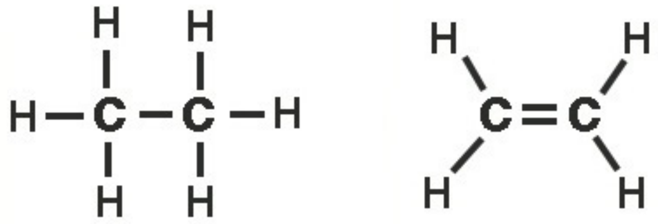
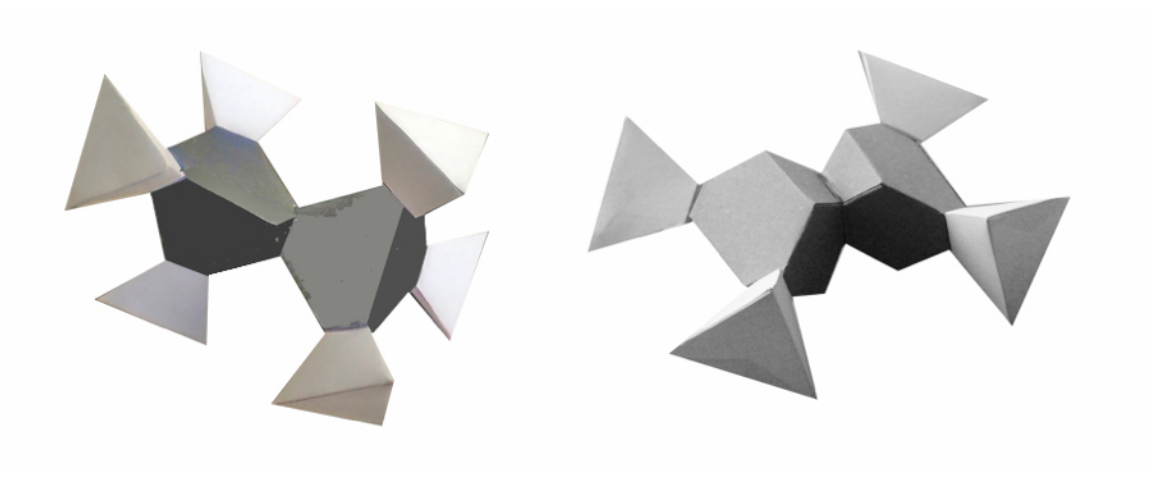
The tale of chemical bonding is the never-ending story of millions upon millions of compounds. S*ystematic naming* helps just a little.

Let's begin with ethane and ethene.

At the beginning of a name "**eth**" means two carbon atoms. **Eth**anol, **eth**anal and **eth**anoic acid each have two carbon atoms. At the end of a name "**ane**" means C—C single bonds only and "**ene**" means one C = C double bond, which is stronger and shorter than a single bond.



Ethane (left) and **ethene** (right) drawn as stick diagrams.
Ethane (left) and **ethene** (right) modelled in paper.

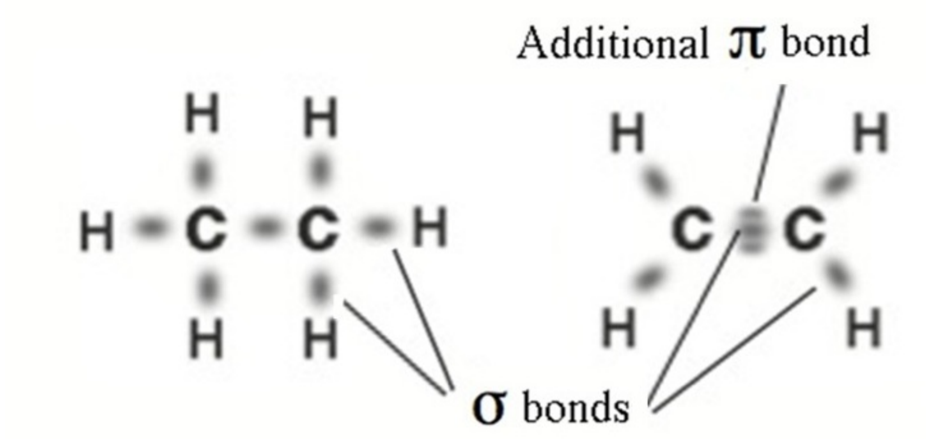


The CH_3 groups linked by the C—C single bond in the *ethane* model are glued to give the hydrogens as much space as possible. The C = C double bond in the *ethene* model is glued so that all the atoms lie in a plane.

Our paper models are fun to make: but are they useful?

To match our paper models to other people's models, and to what chemists know about the structure of these molecules, we need a result from molecular orbital theory. We need a model of bonding based on *spherical harmonics*. [To watch a mechanical spherical harmonic in action see the article linked below that shows oscillations on a water balloon.]

> *The molecular bonding model is derived from the electron shell model which is based on spherical harmonics. In this model bonds are of two types. Sigma (σ) bonds involve spherical electron shells. The spherical shells are imagined to overlap placing increased negative charge density between two positive nuclei. Pi (π) bonds concentrate negative charge density above and below a sigma bond. A Lewis double bond is a σ bond with the addition of a π bond. All multiple carbon-carbon bonds are a σ bond, plus 1 or 2 π bonds.*



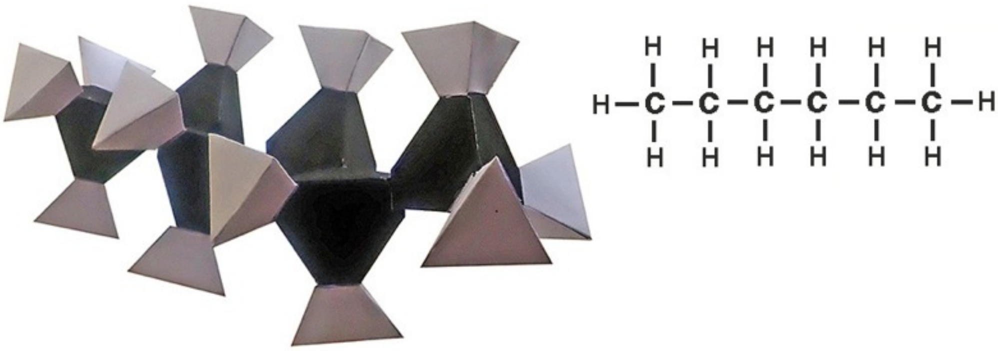
Increased negative charge density between
atoms is suggested with fuzzy diagrams.

On this model, C—C single bonds are free to rotate, but double C = C bonds involve oriented regions of increased negative charge density and do not rotate. Ethene is a flat molecule with regions of increased negative charge above and below the sigma component of the C = C bond.

> ***Please note:*** *details of the molecular orbital model of carbon-carbon bonding are to be found on the web. If you are ready for that, please do a search.*

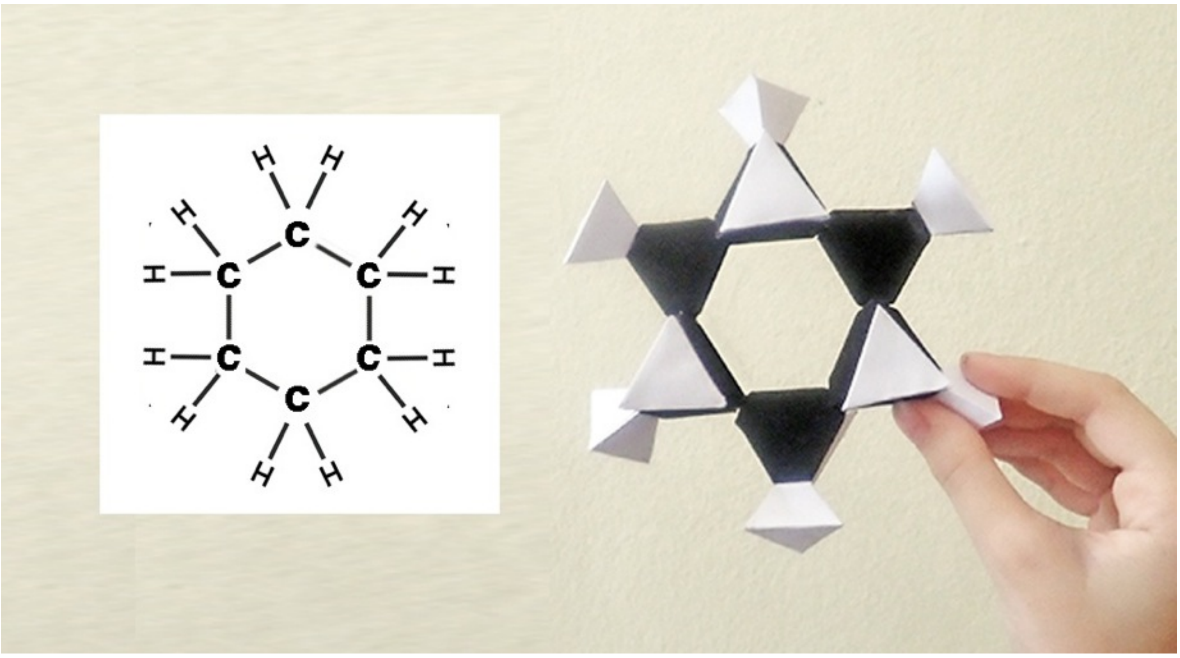
Hexane (C_6H_{14})

The prefix “**hex**” means six. **Hex**ane is a colourless liquid that smells like petrol and burns in air to form water and carbon dioxide. The molecule is a six member carbon-chain that can be linear, branched, or form a ring.



Linear n-hexane modelled in paper and as a stick diagram.

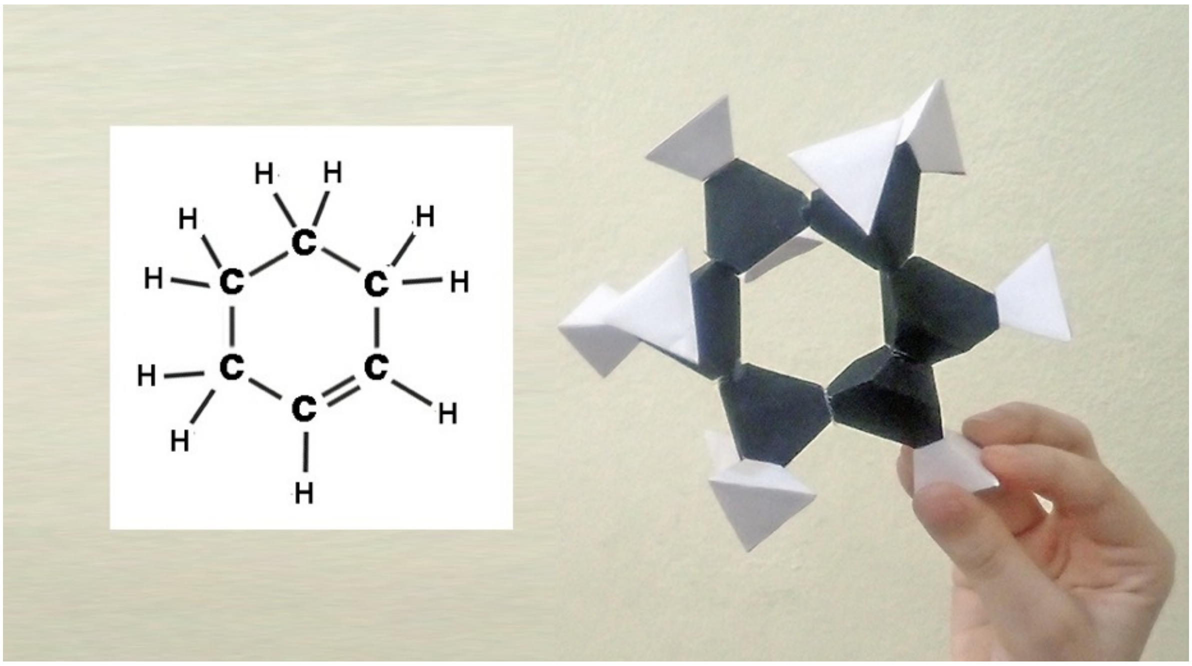
Cyclohexane (C_6H_{12})



Cyclohex**ane** as a stick diagram and modelled in paper.

Three hydrogens are hidden behind carbons in the image above. The snub points on the carbons naturally fit flat against each other to form the six carbon ring. The geometry gives a hexagonal ring without bond strain.

Cyclohexene (C_6H_{10})



Cyclohex**ene** as a stick diagram and modelled in paper.

Hex**ene** is a linear molecule with one double C = C bond. **Cyclo**hexene has six carbons arranged in a ring with one double bond and two less hydrogens than cyclohexane. The single C = C double bond is made flat in the paper model as it is in the model of ethene. The double C = C bond is shorter than a single C—C bond so there is some bond strain in the ring.

Addition and substitution reactions

We are modelling molecules, not doing lab-based Chemistry, but we report what we read.

The C = C double bond can be broken and something like bromine (Br) can be **added** into what becomes a cyclohexane ring. Any C—H bond can be broken and bromine can be *substituted* for hydrogen but *Addition* reactions are only possible with hex**ene**, not with hex**ane**.

This point eventually provided important evidence that benzene does not have three double bonds in a ring of six carbons as had been supposed in the 19th century.