Hydrocarbon structures and isomers

Hydrocarbon structures and types of isomerism (structural isomers, cis / trans isomers, and enantiomers).

Introduction

If you put gasoline into a car, what does it look like? To the naked eye, gasoline is a pretty uninteresting yellowish-brown liquid. If you could zoom in to the molecular level, though, you'd see that gasoline is actually made up of a striking range of different molecules, most of them hydrocarbons (molecules containing just hydrogen and carbon).

Some would be small, with just four carbon atoms, while others would be larger, with up to twelve carbons. Some would form straight lines, while others would branch; some would have only single bonds, while others would have double bonds; and still others would have rings, including aromatic rings (flat rings with alternating double bonds). The different hydrocarbons in gasoline have different properties, such as melting point and boiling point, and the mixture of hydrocarbons (together with some non-hydrocarbon molecules) gives gasoline properties that allow it to combust well in an engine.

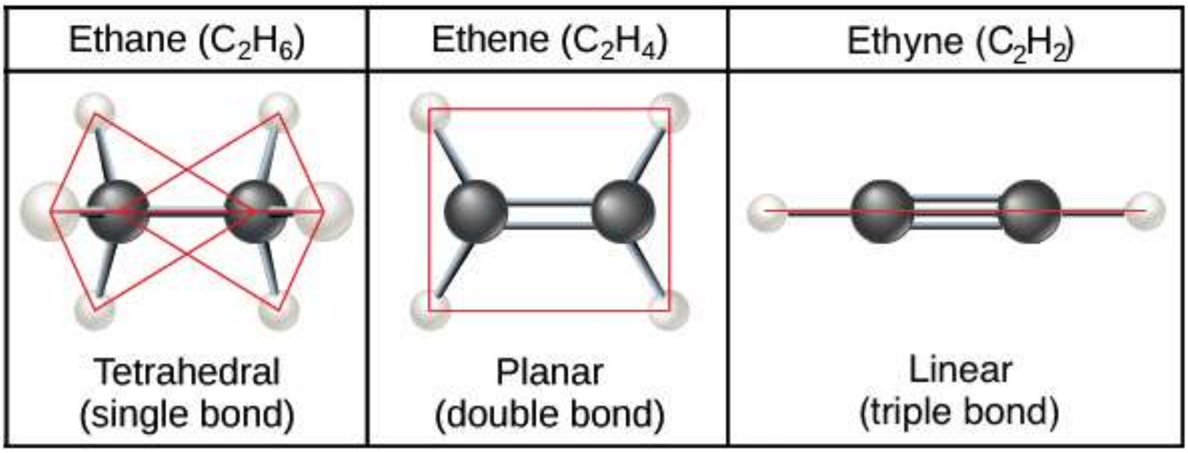
Hydrocarbons are diverse!

As this example shows, hydrocarbons come in many different structures. They may differ in length, be branched or unbranched, form linear or ring shapes (or a combination), and include various combinations of single, double and triple carbon-carbon bonds. Even if two hydrocarbons have the same chemical formula, their atoms may be connected or arranged in space in different ways, making them isomers of one another (and sometimes giving them very different properties).

All of these types of structural differences influence the three-dimensional shape, or **conformation**, of a hydrocarbon molecule. In the context of macromolecules (large biological molecules such as DNA, proteins, and carbohydrates), structural differences in the carbon skeleton often affect how the molecule functions.

Branching, multiple bonds, and rings in hydrocarbons

Hydrocarbon chains are formed by a series of bonds between carbon atoms. They may be long or short: for instance, ethane has just two carbons, while decane has ten. Chains with larger numbers of carbons may also be linear or branched. For instance, decane's ten carbon atoms line up in a row, but other hydrocarbons with the same formula ($C_{10}H_{22}$) have a shorter primary chain with side branches. (In fact, there are 75 slightly different branching structures for $C_{10}H_{22}$) In addition, hydrocarbons may contain varying numbers of single, double, and triple bonds. The hydrocarbons ethane, ethene, and ethyne provide an example of how different types of bonds affect the geometry of a molecule.



Ethane: tetrahedral organization of bond substituents about the carbon atoms.

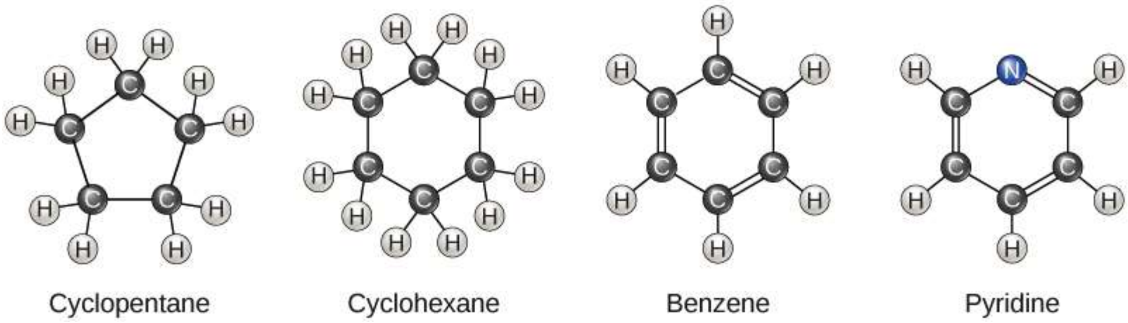
Ethene: planar structure due to the presence of the double bond.

Ethyne: linear structure due to the presence of the triple bond.

Image credit: image modified from "Carbon: Figure 2," by OpenStax College, Biology (CC BY 3.0).

- Ethane (C_2H_6), with a single bond between carbons, forms a two-tetrahedron shape (one tetrahedron about each carbon), and can rotate freely around the carbon-carbon bond.
- In contrast, the double bond of ethene (C_2H_4) gives it a flat (planar) configuration and prevents rotation about the carbon-carbon bond. This is a general feature of carbon-carbon double bonds, so anytime you see one of these in a molecule, remember that the portion of the molecule with a double bond will be planar (and unable to rotate).
- Finally, the triple bond of ethyne (C_2H_2) results in not just a planar, but actually a linear, shape for the molecule.

An additional feature that adds diversity to hydrocarbon structures is the possibility of ring formation. Rings of various sizes may be found in hydrocarbons, and these rings may also bear branches or include double bonds. Rings with certain patterns of double bonds, like the benzene ring shown below, are exceptionally stable and take on a flat, planar shape. These rings, called aromatic rings, are found in some amino acids, as well as in hormones like testosterone and estrogens (the primary male and female sex hormones, respectively).



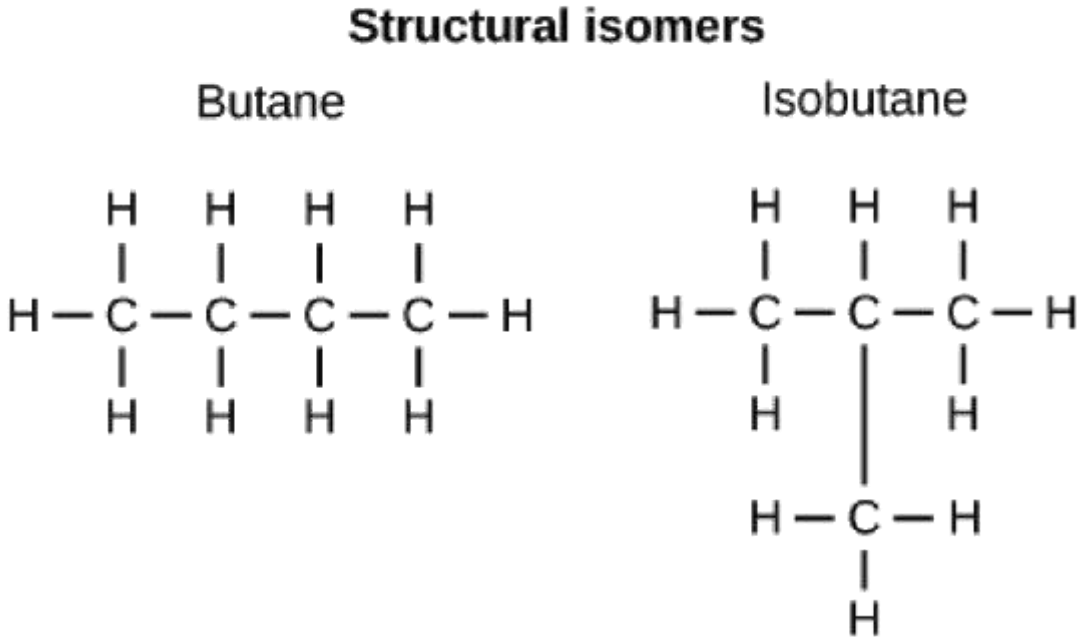
Organic molecules with ring structures: cyclopentane, cyclohexane, benzene, and pyridine. *Image credit: OpenStax Biology.*

Some aromatic rings contain atoms other than carbon and hydrogen, such as the pyridine ring shown above. Due to their additional atoms, these rings are not considered to be hydrocarbons. You can learn more about aromatic compounds in the aromatic compounds chemistry topic.

Isomers

The three-dimensional placement of atoms and chemical bonds within organic molecules is central to understanding their chemistry. Molecules that share the same chemical formula but have their atoms connected differently, or arranged differently in space, are known as **isomers**.

Structural isomers



Example of structural isomers: butane and isobutane.

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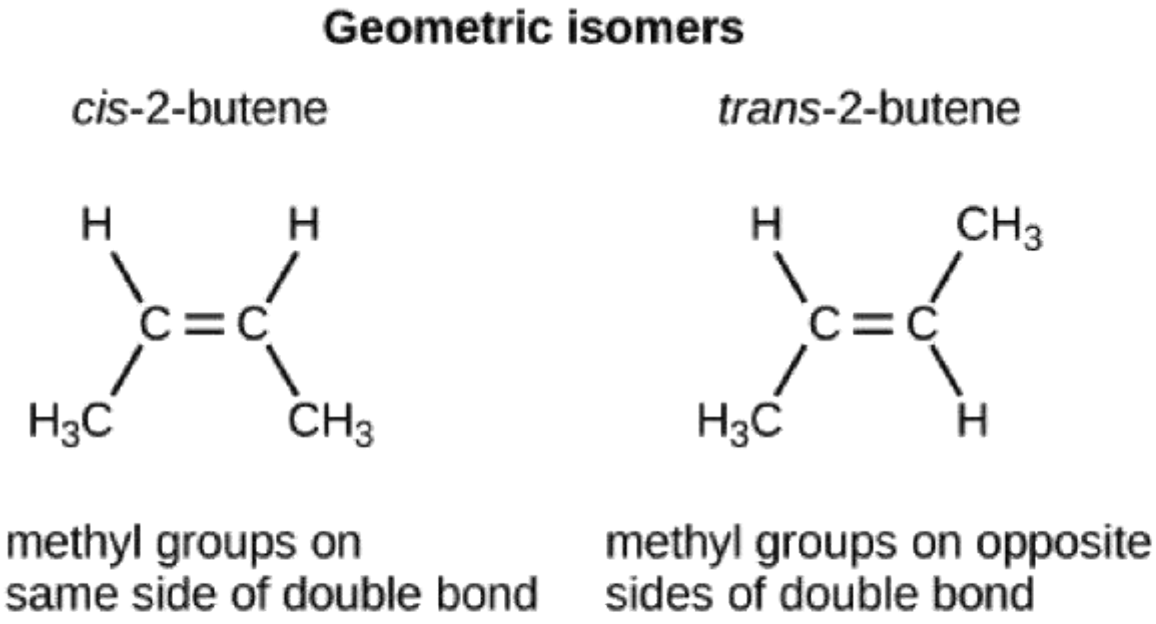
Structural isomers (like butane and isobutane, shown at right) actually have their atoms bonded together in different orders: both molecules have four carbons and ten hydrogens (C_4H_{10}), but the atoms are connected differently within the two molecules, leading to differences in their chemical properties (such as a lower melting point and boiling point for isobutane). Because of these differences, butane is suited for use as a fuel for cigarette lighters and torches, whereas isobutane is best used as a refrigerant and a propellant in spray cans.

Cis-trans (geometric) isomers

Cis-trans (**geometric**) **isomers**, on the other hand, have their atoms connected in the same order, but differ in the configuration of atoms around these bonds. *Cis-trans* isomerism does not apply to linear molecules that have only single carbon-carbon bonds, as these bonds can rotate freely. In molecules that have double bonds, however, the double bonds' inability to rotate means that the atoms attached to the two bond carbons will get stuck in one of two possible configurations. If all of the attached atoms are the same, this won't make any difference; however, if each carbon has two different atoms or groups attached to it, two different arrangements are possible.



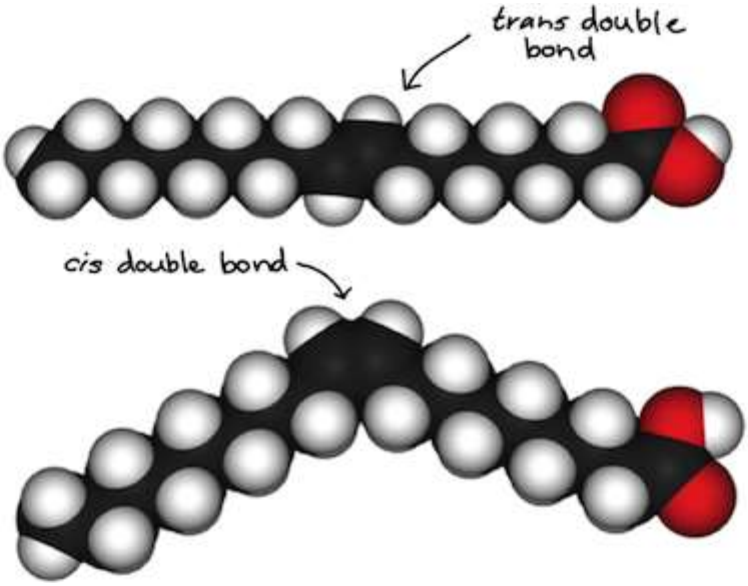
Example of geometric isomers: cis-2-butene and trans-2-butene.

Image modified from "Carbon: Figure 4," by OpenStax College, Biology (CC BY 3.0).
For example, in 2-butene (C_4H_8), the two methyl groups (CH_3) can occupy different positions in relation to the double covalent bond central to the molecule. butene (C_4H_8), the two methyl groups (CH_3) can occupy different positions in relation to the double covalent bond central to the molecule. If both methyl groups are on the same side of the double bond, this is called the *cis* configuration; if they are on opposite sides, this is the *trans* configuration.

In the *trans* configuration, the carbons form a more or less linear structure, whereas the *cis* configuration causes a bend in the carbon backbone. (Some ring-shaped molecules can also have *cis* and *trans* configurations, in which attached atoms are trapped on the same or on opposite sides of the ring.)

In fats and oils, long carbon chains known as fatty acids may contain double bonds, which can be in either the *cis* or *trans* configuration (as shown at right). When some of these bonds are in the *cis* configuration, the resulting bend in the carbon backbone of the chain keeps the molecules from packing tightly, so they remain liquid (oil) at room temperature. On the other hand, molecules with *trans* double bonds (popularly called *trans* fats), have relatively linear fatty acids that can pack tightly together at room temperature and form solid fats.

Trans fats are linked to an increased risk of cardiovascular disease, so many food manufacturers have eliminated their use in recent years. Fats with *trans* double bonds are found in some types of shortening and margarine, while fats with *cis* double bonds may be found in oils, such as olive oil. See the article on lipids to learn more about the different types of fats.



Space-filling molecular models of fatty acids, showing an example of a fatty acid with a trans double bond (with a straight structure) and an example of a fatty acid with a cis double bond (with a bent structure).

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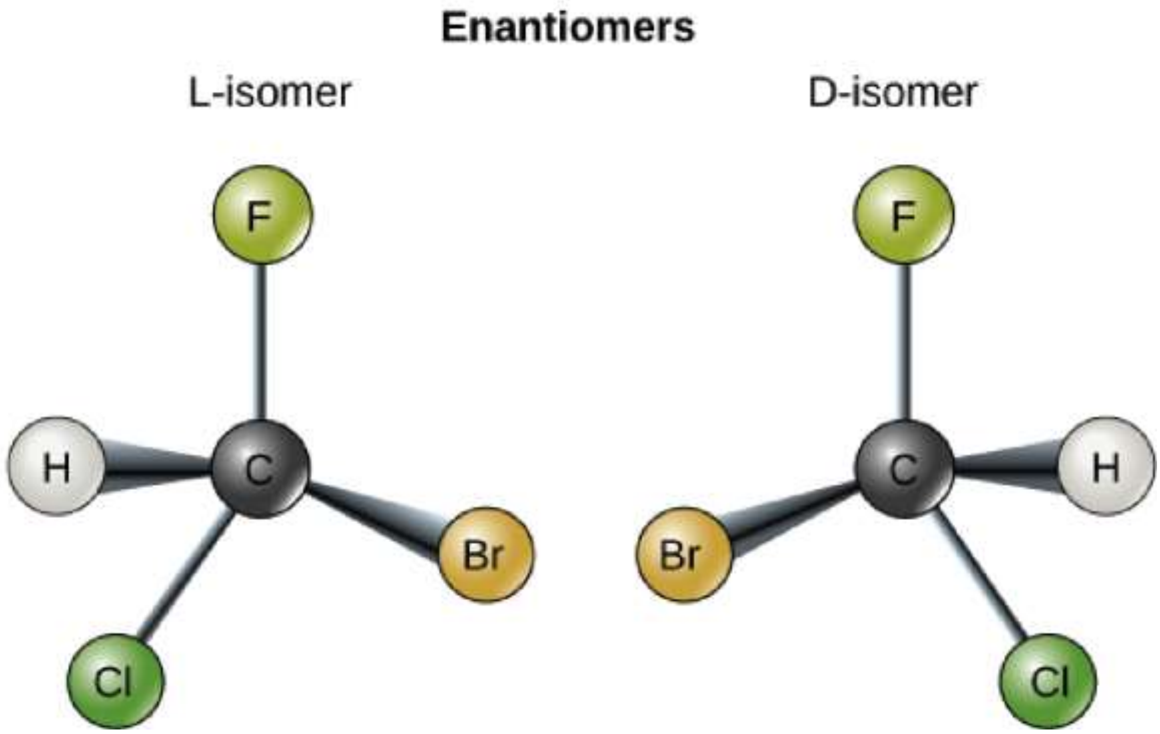
Enantiomers

Enantiomers have the same chemical structure but differ in their three-dimensional placement of atoms, such that they are mirror images of one another and cannot be superimposed (made to align perfectly). Enantiomerism is only seen for molecules with asymmetric carbons, which are carbon atoms with four different atoms or groups attached.



Examples of enantiomers: two forms of CHFClBr (with hydrogen and the halogens bonded to a central asymmetric carbon). The two are nonsuperimposable mirror images of one another.

Image modified from "Carbon: Figure 4," by OpenStax College, Biology (CC BY 3.0).
The molecules above are an example of an enantiomer pair. Both have the same chemical formula and are made up of chlorine, fluorine, bromine and hydrogen atoms bonded to a central carbon atom. However, the two molecules are mirror images of one another, and if you try to place them on top of each other, you'll find that there's no way to make them fully match up. Enantiomers are often compared to a person's right and left hands, which are also mirror images that cannot be superimposed (aligned one atop the other in space).

Amino acids, the building blocks of proteins, also contain an asymmetric carbon. In the image below, you can see space-filling models of the two enantiomers of the amino acid alanine. Amino acid (and other) enantiomers have historically been given the prefixes L and D, and biologists often still use this terminology for amino acids and sugars. However, in the wider world of chemistry, the D/L system has been replaced by another naming system (the *R/S* system), which is more flexible and broadly usable. You can learn more about enantiomers and the *R/S* naming system in the organic chemistry section.

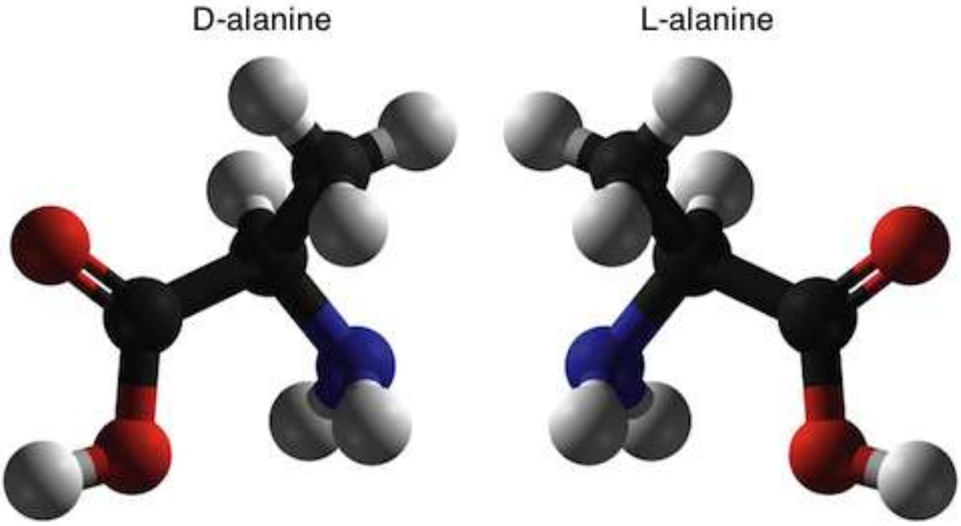


Image of the L and D isomers of alanine. The two are made up of the same atoms, but are non-superimposable mirror images of one another.

Image modified from "Carbon: Figure 6," by OpenStax College, Biology (CC BY 3.0).

The difference between a pair of enantiomers may seem very small. In some cases, though, only one isomer may be produced by the body, or the two isomers may have very different biological effects. For example, in nature, only the L forms of amino acids are typically used to make proteins, although the D forms of amino acids are occasionally found in the cell walls of bacteria. Similarly, the D enantiomer of the sugar glucose is the main product of photosynthesis, while the L form is rarely seen in nature. Drugs may also come in different enantiomer forms with different effects: for instance, the D form of the drug ethambutol is used to treat tuberculosis, while the L form actually causes blindness.