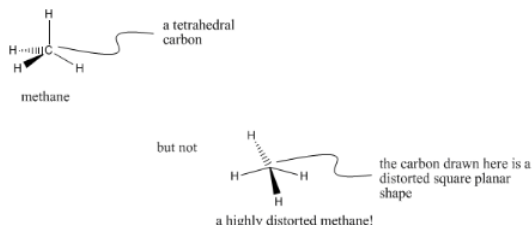


4.9: Three Dimensional Drawings

Our purpose in this chapter is to be able to represent the structure of a molecule. When we draw the Lewis structure for methane, it is only a 2-dimensional representation, but really the compound has a three-dimensional shape. The central carbon in methane is tetrahedral, with the four hydrogens at the alternate corners of a cube.

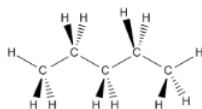
We can draw a tetrahedron by making a vertex between two lines, then attaching a wedged line and a hatched line to the outside of the corner. The black, wedged line is read as "this atom is towards us". The hatched line is read as "this atom is farther away from us". Although the drawing is flat, the hatched and wedged lines is a shorthand notation for 3-dimensionality.



Representing the three-dimensional shape of a molecule can be done on paper, but only if we are very careful about drawing conventions such as wedge-dash drawings.

Carbons that have bonds to four *different* neighbors are always tetrahedral. The neighbors arranged around a tetrahedral carbon are around 109° apart. Sometimes, for reasons we won't go into here, tetrahedral carbons are called sp^3 carbons.

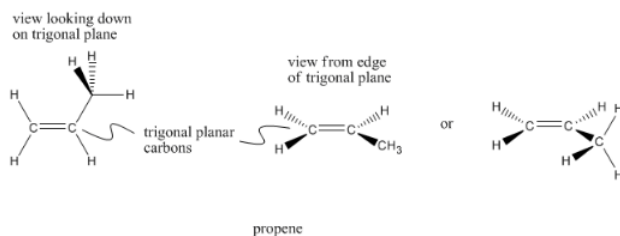
Pentane is a compound that contains four tetrahedral carbons in a row. Each tetrahedral carbon could be shown with wedge - dash projections.



It is also very common to use computer drawing programs to show the shapes of molecules. You can view the three-dimensional structure of pentane in many different ways. Three of the most common ways are shown here. Ball & Stick is an easy way to see where all the atoms are and how they are connected. Wireframe allows you to see connections without having your view obscured by atoms. Space-filling models are meant to most closely show you the shape of the molecule, although the atoms involved get obscured in this view.

[Go to Animation IM9.1. A three-dimensional model of pentane.](#)

Carbons double bonded to one neighbor, and consequently bonded to three different neighbors overall, are trigonal planar. The neighbors are all in the same plane and are about 120° apart. Trigonal planar carbons are sometimes described as sp^2 carbons.

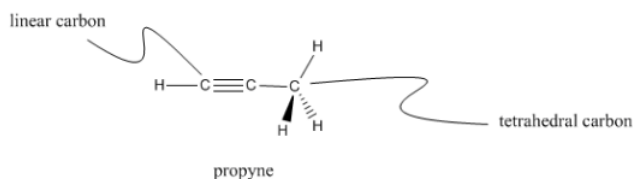


Propene has two trigonal planar carbons as well as one tetrahedral carbon. Notice that a trigonal planar carbon is flat if viewed from one direction, but not if viewed from the other. Sometimes you will see trigonal carbons drawn differently, if the drawer wants you to look at the molecule from one direction or the other.

See if you can find both kinds of carbon on the model below.

[Go to Animation IM9.2. A three-dimensional model of propene.](#)

Carbons that have only two different neighbors are linear; each neighbor is 180° apart from the other. Linear carbons are sometimes called sp carbons.



Kekule structure of propyne, showing linear arrangement of triple bond and tetrahedral arrangement of hydrogens around the terminal, single-bonded carbon.

Propyne has two linear carbons as well as one tetrahedral carbon. See if you can find both kinds of carbon on the model below.

[Go to Animation IM9.3. A three-dimensional model of propyne.](#)

Saying a carbon is sp or sp^2 is only giving the shape of one atom within a molecule. The molecule itself may have a particular shape which is determined by the geometries of its constituent atoms, but which can't be described simply in words as "tetrahedral" or "linear".

Pentane is roughly a zig-zag shape. In a space-filling model, it resembles a fat caterpillar inching along. Propene is almost boomerang-shaped. Propyne is shaped like a dart; it has a pointed end and a feathered end.

Other molecules have more complicated shapes. The shape of ginkgolide B (a natural product isolated from the medicinally interesting *ginkgo biloba* tree) is hard to describe. However, it is clear that individual carbons in ginkgolide B are mostly tetrahedral, with just a couple of trigonal planar ones.

[Go to Animation IM9.4. A three-dimensional model of ginkgolide B.](#)

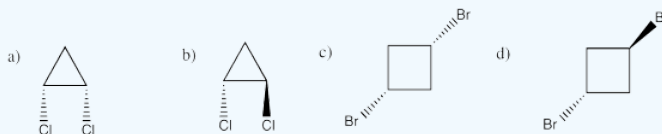
Understanding the overall shape of a molecule is particularly important in various aspects of biochemistry. For example, the effect of any drug in the body is strongly influenced by the shape of the drug and how that shape can interact with specific receptors.

? Exercise 4.9.1

Cis and trans cyclic isomers have two substituents attached to a ring. The cis isomer has both substituents on the same face of the ring. The trans isomer has substituents on opposite faces of the ring. Use wedge-dash projections to draw the shapes of the following molecules:

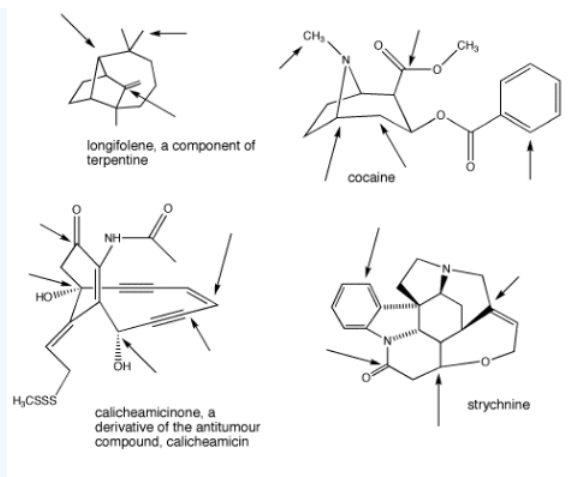
- cis-1,2-dichlorocyclopropane, $C_3H_4Cl_2$ (the numbers mean there is a chlorine on the first carbon and a chlorine on the second carbon)
- trans-1,2-dichlorocyclopropane, $C_3H_4Cl_2$
- cis-1,3-dibromocyclobutane, $C_4H_6Br_2$
- trans-1,3-dibromocyclobutane, $C_4H_6Br_2$

Answer

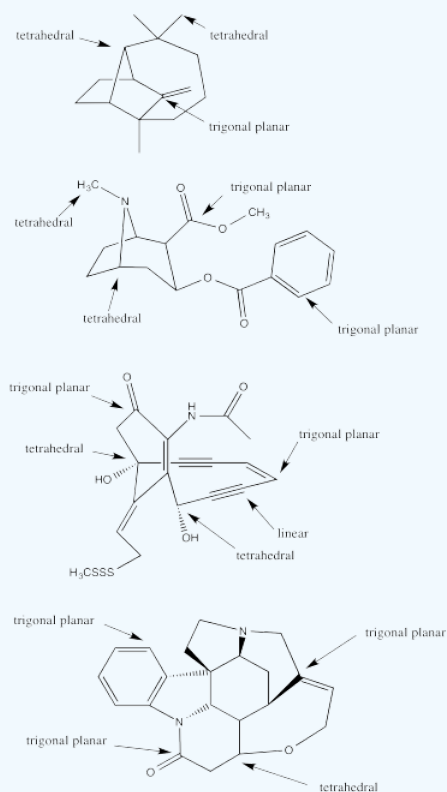


? Exercise 4.9.2

Identify the geometry at the indicated carbons in the following molecules:



Answer



AnswerExercise 4.9.2, showing structural formulas for longifolene, cocaine, calicheamicinone, and strychnine.

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