Jmol tutorials

**Linear straight-chain alkanes.**

State 0. Thought it might be worth putting an instruction slide at the start for dumb people:

This tutorial consists of a sequence of interactive molecular models, with explanations below them, illustrating details of alkane structure. Use your mouse (computer) or fingers (touch screen) to rotate, zoom, and move the model on any of the pages in this tutorial. Use the large arrow key to the right of the model to advance to the next model. Use the large arrow key to the left of the model to go to the previous model. Use the “reset page” button in the upper right to return to the default page view, if desired. Use the “reset tutorial” button (upper left) to go back to the start of the tutorial. Click the “advance” arrow to get started!

Ball and stick model of n-decane where it is rotating, such that it rotates through the view looking down the chain

State 1: Hydrocarbons, containing carbon and hydrogen, are the simplest organic compounds. Alkanes are acyclic, saturated hydrocarbon for which all carbon-carbon bonds are single. All alkanes have the general formula CnH2n+2. Linear alkanes are those that have a continuous chain of carbon atoms connected together with terminal hydrogen atoms present on the carbon atoms in the chain. In this tutorial, we will look at the structures of the linear alkanes where n, the number of carbon atoms, varies from 1 to 10.

Ball and stick model of n-decane where it is rotating, such that it rotates through the view looking down the chain

State 2: The simplest alkane is methane, CH4.

Ball and stick model of methane

State 3: The molecular geometry of methane is tetrahedral. The tetrahedral unit surrounding the central C atom is highlighted here. All of the bond angles in methane are exactly 109.5 degrees.

Ball and stick model of methane with tetrahedron superimposed, and showing a bond angle

State 4. The central C atom of methane is sp3-hybridized. The four hybrid sp3 orbitals on C form sigma bonds by overlapping with the 1s atomic orbitals on the terminal H atoms.

Show sigma bonds formed by orbital overlap

State 5: Carbon and hydrogen have fairly similar electronegativity values, so each C-H bond is only weakly polar. The weak bond dipoles cancel each other out completely due to the symmetric tetrahedral arrangement of the H atoms. Methane is thus a nonpolar molecule

Show bond dipoles (arrows) on ball and stick model for methane.

State 6: Shown here is the isosurface for methane superimposed on the ball and stick model. The isosurface shows the volume of space where the electron density in the molecule may be found, and provides a more accurate representation of the actual 3-dimensional shape and size of the molecule.

Add isosurface as transparent colored surface on top of ball and stickState 7: The next simplest alkane is ethane, C2H6. It can be formed from methane by replacing one of the terminal H atoms with a methyl group (CH3).

Could we highlight a H atom on methane and show it changing into a methyl group? This would look cool if so. Show ball and stick of ethane.

State 8: Each of the two carbon atoms in ethane has a tetrahedral molecular geometry and is sp3-hybridized. Looking ahead, all carbon atoms in all alkanes share these features. Shown here is the tetrahedral unit and the sigma bonds present on C1.

Highlight tetrahedral unit on C1 and also show sigma bonds

State 9: Shown here is the tetrahedral unit and the sigma bonds present on C2.

Highlight tetrahedral unit on C2 and also show sigma bonds

State 10: There is free rotation about carbon-carbon sigma bonds, so the two methyl groups are able to freely rotate about their sigma bond. The most stable conformation for ethane will be the one in which the H atoms on the methyl groups are staggered relative to the H atoms on the other methyl group. This view looks down the axis of the C-C bond to see how the H atoms are oriented in this conformation.

Rotate so looking down C-C bond, so the H atoms on each CH3 can be seen to be staggered

State 11: Shown here is the isosurface for ethane superimposed on the ball and stick model. Ethane, as well as all alkanes, are nonpolar molecules due to the similar electronegativities of the C and H atoms and symmetry imposed by the tetrahedral geometries of the C atoms.

Add isosurface as transparent colored surface on top of ball and stick

State 12: The linear straight-chain alkane containing 3 C atoms is propane, C3H8. For propane, there are two methyl groups (CH3) at the two ends of the linear chain of carbon atoms, and a carbon atom bonded to two H atoms (CH2) between the two methyl groups. The condensed structural formula of propane (CH3-CH2-CH3) emphasizes these features.

Show ball and stick model of propane

State 13: As for all alkanes, the carbon atoms of propane all have tetrahedral molecular geometries and are sp3-hybridized. The tetrahedral unit formed around C2 is shown here. Note how for the central C there are two H atoms and two C atoms at the corners of the tetrahedron.

Show ball and stick model of propane with tetrahedral unit around C2 highlighted.

State 14: As for all alkanes, the carbon atoms of propane all have tetrahedral molecular geometries and are sp3-hybridized. The tetrahedral unit formed around C2 is shown here. Note how for the central C there are two H atoms and two C atoms at the corners of the tetrahedron.

Show ball and stick model of propane with tetrahedral unit around C2 highlighted.

State 15: Shown here is the isosurface for propane superimposed on the ball and stick model.

Add isosurface as transparent colored surface on top of ball and stick

State 16: Shown here is the isosurface for propane superimposed on the ball and stick model.

Add isosurface as transparent colored surface on top of ball and stick

State 17: The linear straight-chain alkane containing 4 C atoms is butane, C4H10. Butane has the condensed structural formula CH3-CH2-CH2-CH3.

Show ball and stick for butane side on

State 18: There is free rotation about each C-C bond of butane, allowing a large number of conformations to exist based on how adjacent CH2 and CH3 groups are rotated. The most stable conformation of butane will be the one in which the carbon chain is as fully extended as possible. By having an extended chain of carbon atoms, overlap of electron density on the different C and H atoms in the chain is minimized. This can be seen by drawing the isosurface for butane in the preferred fully extended conformational state. For more details of conformational states in hydrocarbons, see the tutoroal titled “Conformations of butane”.

Add isosurface as transparent colored surface on top of ball and stick

State 19: For each linear alkane where the value of n increases by 1, an additional “CH2” unit will be added to the linear chain of C atoms. Shown here is pentane, C5H12. Pentane has the condensed structural formula CH3-CH2-CH2- CH2-CH3.

Show pentane ball and stick

State 20: Shown here is hexane, C6H14. Hexane, like all the alkanes in this tutorial, is shown in its most stable extended conformational state. Rotate this molecule, and the subsequent ones, using your mouse or fingers to look down the long axis of the molecule formed by the chain.

Show hexane ball and stick

State 21: Shown here is heptane, C7H16.

Show heptane ball and stick

State 22: Shown here is octane, C8H18.

Show octane ball and stick

State 23: Shown here is nonane, C9H20.

Show nonane ball and stick

State 24: Shown here is decane, C9H20.

Show decane ball and stick

State 24: This final view shows the isosurface added to decane. This view is looking down the long axis formed by the extended chain.

Show decane ball and stick with isosurface