Jmol tutorials

**Trans-2-butene.**

State 1: 2-butene is a linear alkene containing 4 carbon atoms and where the double bond lies between carbon atoms 2 and 3. 2-butene exists in the form of two geometric isomers named *cis*-2-butene and *trans*-2-butene. For organic molecules, geometric isomers are isomers where functional groups are either on the same side (*cis-*) or opposite sides (*trans-*) of the molecule. For alkenes, the “sides” of the molecule are relative to the double bond. 2-butene is the simplest alkene for which *cis-* and *trans-* isomers exist. In this tutorial we will examine the structural features of the *trans* isomer.

Ball and stick models of cis and trans 2-butene shown together here.

JUSTIN-THE STATES I SHOWED FOR CIS-BUTENE ARE EXCACTLY THE SAME AS FOR THIS TUTORIAL, EXCEPT NOW WE HAVE THE METHYL GROUPS IN THE TRANS POSITION. SO USE THE CIS FIGURES TO GUIDE YOU.

State 2: Shown here is *trans*-2-butene. The two atoms containing the double bond (C2 and C3) are each bonded to a H atom and a methyl group (CH3). The methyl groups on C2 and C3 are on opposite sides of the molecule, with respect to the double bond, for *trans-*2-butene. The prefix *trans* comes from the Latin term meaning “other side of”.

Ball and stick model of trans butene with the methyl groups highlighted in green

State 3: Carbon atoms 1 and 4 have tetrahedral molecular geometries (AX4) and are sp3-hybridized. Note that the numbering of the molecule could be started at either methyl group since they will have the same priority in numbering. The geometry about C1 is highlighted here.

Show tetrahedral unit surrounding C1

State 4: Carbon atoms 1 and 2 have tetrahedral molecular geometries (AX4) and are sp3-hybridized. The geometry about C4 is highlighted here.

Show tetrahedral unit surrounding C4

State 5: Both carbon atoms 2 and 3 are sp2-hybridized and have trigonal planar electron domain and molecular geometries (AX3E0). The trigonal plane formed around C2 is shown here.

Ball and stick model of trans butene with the trigonal planar unit formed at C2 highlighted

State 6. Both carbon atoms 2 and 3 are sp2-hybridized and have trigonal planar electron domain and molecular geometries (AX3E0). The trigonal plane formed around C3 is shown here.

Ball and stick model of trans butene with the trigonal planar unit formed at C3 highlighted

State 7: Since both C2 and C3 have trigonal planar molecular geometries, C1, C2, C3, C4, and the H atoms bonded to C2 and C3 all lie in a common plane

Show trigonal planes on both C2 and C3 at the same time

State 8: State 5: Since both C2 and C3 have trigonal planar molecular geometries, C1, C2, C3, C4, and the H atoms bonded to C2 and C3 all lie in a common plane. Here the plane is shown bounded by C1, C4, and the H atoms on C2 and C3.

Show the plane defined by the rectangle formed by connecting C1, C4, H on C3, and H on C4

State 9: Carbon atoms 2 and 3 are sp2-hybridized. Carbon atom 2 forms sigma bonds to C1, C3, and H.

Show sigma bonds on C2

State 10: Carbon atoms 2 and 3 are sp2-hybridized. Carbon atom 3 forms sigma bonds to C4, C2, and H.

Show sigma bonds on C3

State 11: Carbon atoms 2 and 3 each contain an unhybridized p orbital that is perpendicular to the atoms lying in the plane formed by C1, C3, and the H atoms bonded to C2 and C3. Each of these p orbitals contains a single electron.

Show p orbitals on C2 and C3, with rectangular planar unit shown.

State 12: The pi bond between C1 and C2 is formed from the overlap of electron density in the unhybridized p orbitals as shown here.

Show overlapping pi bond between C1 and C2

State 13: The methyl groups are constrained to opposite sides of the double bond in *trans-*2-butene due to the presence of the pi bond which prevents rotation about C2 and C3.

Show overlapping pi bond between C1 and C2, along with the rectangular plane, and outline the methyl groups again. Maybe draw a two headed arrow between them if this is easily done??