Jmol tutorials

**1-butene.**

State 1: 1-butene is a linear alkene and one of four isomers of butene with the chemical formula C4H8. For 1-butene, the double bond lies between carbon atoms 1 and 2.

Ball and stick model of 1-butene here- show numbers next to atoms?

State 2: The double bond lies between carbon atoms 1 and 2.

Ball and stick model of 1-butene, highlight double bond

State 3: Carbon atom 1 (C1) has trigonal planar electron domain and molecular geometries, giving 120 degree bond angles for the H-C1-H angle and the two H-C1-C2 angles.

Ball and stick model of 1-butene with trigonal plane of C1 highlighted and 120 degree bond angles shown

State 4. Like carbon 1, carbon atom 2 (C2) has trigonal planar electron domain and molecular geometries, giving 120 degree bond angles for the C1-C2-C3, C1-C2-H, and C3-C2-H angles.

Ball and stick model of 1-butene with trigonal plane of C1 highlighted and 120 degree bond angles shown

State 5: Carbon atoms 1 and 2, the hydrogen atoms they are bonded to, and carbon atom 3 all lie in a common plane.

Show plane formed by these atoms by drawing the rectangle bounded by H, H, H and C3 around C1 and C2.

State 6: This rendition shows the plane formed by these atoms rotated so it is lying perpendicular to the screen

Rotate so looking at plane perpendicular to screenState 7: Both C3 and C4 have tetrahedral molecular geometries and are sp3-hybridized. The tetrahedral unit formed around C3 is shown here.

Tetrahedral unit around C3, show one 109.5 degree bond angle

State 8: Both C3 and C4 have tetrahedral molecular geometries and are sp3-hybridized. The tetrahedral unit formed around C4 is shown here.

Tetrahedral unit around C4, show one 109.5 degree bond angle

State 9: Carbon atoms 1 and 2 are sp2-hybridized, leaving a single unhybridized p orbital with a single electron on each of C1 and C2.

Show p orbitals on C1 and C2

State 10: The sigma bonds between C1 and C2 and their bonded atoms are represented as transparent blue lobes in this figure.

Show signal bonds on C1 and C2

State 11: State 10: The pi bond between C1 and C2 is formed from the overlap of the unhybridized p orbitals.

Show overlapping pi bond between C1 and C2

State 12: As mentioned above, C1, C2, the hydrogen atoms they are bonded to, and C3 all lie in a common plane. The atoms are constrained to this plane since the overlapping p orbitals prevents rotation occurring about the bond between C1 and C2.

As state 11, reshowing the rectangular plane present in states 5 and 6.