Jmol tutorials

**Acetic acid.**

State 1: Acetic acid is an organic acid (carboxylic acid) with the chemical formula C2H6O2. The chemical formula is often written in the form CH3COOH to highlight the different chemical environments of the carbon and oxygen atoms.

Ball and stick model of acetic acid here

State 2: Acetic acid is referred to as a **carboxylic acid** based on structural features of the molecule called **functional groups**. Functional groups in organic molecules are combinations of atoms with recognizable chemical structures and characteristic properties. An **alkyl group** consists of one or more C atoms bonded to H atoms through single bonds. A **methyl group** is the simplest alkyl group, consisting of three H atoms bonded to a C atom (CH3). A **carbonyl group** consists of a C atom bonded to an O atom by a double bond(C=O). A **hydroxyl group** contains an O atom bonded to a H atom (OH). When a hydroxyl group is bonded to the C atom of a carbonyl group, a new combined functional group called a **carboxyl group** is created. A carboxylic acid is an organic molecule consisting of an alkyl group bonded to the carbon atom of a carboxyl group. Acetic acid, thus, contains methyl- and carboxyl-functional groups. In this view, the methyl group is highlighted in green and the carboxyl group in red.

Ball and stick model of acetic acid with methyl atoms highlighted in green

State 3: In this view, the atoms forming the carboxyl group group are highlighted in red.

Ball and stick model of acetic acid with carboxyl group in red

State 4. The next set of structures will explore the electron domain and molecular geometries for the atoms present in acetic acid.

Reshow initial molecule

State 5: The C atom in the methyl group is bonded to four other atoms (3 H and 1 C) and has no lone pairs so it has a tetrahedral electron domain and molecular geometry (AX4). The tetrahedral unit is highlighted here.

Ball and stick model of acetic acid with methyl atoms highlighted in green and with tetrahedron overlayed

State 6: The bond angles in a molecule with geometry AX4 are all 109.5 degrees.

bond angles shown

State 7: The O atom in the hydroxyl group is bonded to two atoms (C and H) and has two lone pairs, so it has a tetrahedral electron-domain geometry and a bent molecular geometry (AX2E2). The lone pairs are represented by transparent lobes in this structure.

Ball and stick model of acetic acid with OH group highlighted, showing the lone pairs on the O

State 8: The tetrahedral electron-domain geometry surrounding the O atom of the hydroxyl group is highlighted here.

Previous State with tetrahedron shown

“The bond angle is compressed relative to that in a perfect tetrahedron due to the lonepairs spreading out more in space than bonded pairs.”

State 9: The H-O-C bond angle is compressed relative to that in a perfect tetrahedron due to the lone pairs spreading out more in space than bonded pairs.

Previous State with bond angle

State 10: The C atom in the carboxyl group is bonded to two other atoms via single bonds (the methyl C and the hydroxyl O) and one atom via a double bond (the carbonyl O) for a total of three bonded and no non-bonded electron domains (AX3). Accordingly, this C has both trigonal planar electron-domain and molecular geometries. The trigonal planar unit is highlighted here.

Trigonal plane highlighted

State 11: The O atom in the carboxyl group that is double-bonded to carbon has two lone pairs, so it has a trigonal planar electron domain geometry (AXE2). The trigonal planar unit surrounding the electron domains of O is highlighted here.

Lone pairs on O shown; Trigonal plane around O highlighted

State 12: Now that we have covered the geometries about the atoms present in acetic acid, we will explore the types of chemical bonds and orbital hybridizations responsible for these geometries.

Reset to initial acetic acid molecule to begin discussion of orbitals

State 13: The carbon atom in the methyl group of acetic acid is surrounded by four electron domains (AX4), so the orbital hybridization is sp3. This carbon atom forms sigma bonds to the terminal H atoms by overlapping the sp3 hybrid orbitals with the 1s atomic orbitals of the H atoms as shown here.

Show sigma bonds between methyl C and the three H atoms

State 14: The carbon atom in the methyl group of acetic acid also forms a sigma bond with the carbonyl carbon to which it is bonded. The sigma bond between these atoms is shown here

add sigma bond between methyl C and carbonyl C to above structure

State 15: The oxygen atom in the hydroxyl group (the hydroxyl oxygen) is surrounded by four electron domains (AX2E2), so the orbital hybridization is sp3. This carbon atom forms sigma bonds with the carbonyl oxygen and the H atom to which it is bonded.

Show sigma bonds on carbonyl C

State 16: The carbon in the carboxyl functional group (carbonyl carbon) is surrounded by three electron domains (AX3), so the orbital hybridization is sp2. This carbon atom forms sigma bonds with the methyl carbon, the carbonyl oxygen, and the hydroxyl oxygen as shown.

Show sigma bonds on carbonyl C

State 17: The carbonyl oxygen is surrounded by three electron domains (AXE2), so the orbital hybridization is sp2. This oxygen atom forms a single sigma bond with the carbonyl C (already shown above as well)

Show sigma bond on carbonyl O

State 18: Since the carbonyl C and O atoms are sp2 hybridized, they each contain a non-hybridized p orbital with a single electron in each orbital.

Show p orbitals on carbonyl O and carbonyl C

State 19: The overlap of the electrons in the p orbitals provides the pi bond between the carbonyl C and O atoms

Show p orbital overlap

State 20: There are a total of 7 sigma bonds and one pi bond in acetic acid as shown here.

Show all orbital overlaps