Alcohols lesson

Let’s use the horizontal two column format, like the alkenes lesson I made, so I can place jpeg or gif images on the left side with the descriptions.

Log file with following optimized structures: H2O, methane, methanol, ethane, ethanol, propane, 1-propanol, 2-propanol, butane, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol.

Alkenes lesson here for reference: <http://ensignchemistry.com/jsmol%20models/lessons/alkenes/>

State 1: This tutorial consists of a sequence of interactive molecular models, with explanations, illustrating details of alcohols. Use your mouse or touch screen to rotate, zoom, and move the model on any of the states in this tutorial. Use the right arrow key to advance to the next model and accompanying explanation. Use the left arrow key to go to the previous model. Use the "reset page" button to return to the default model view, if desired, for the current model. Use the “reset tutorial” button to return to the start of the tutorial at this instruction. Click the “advance” arrow to get started!

Overview slide of a bunch of alcohols from the log file

State 2: Alcohols are organic compounds containing one or more hydroxyl functional groups (-OH) bonded to carbon. The simplest alcohols are those formed by substituting a single H atom on an alkane with a hydroxyl group. With a single hydroxyl group present, an alcohol is a **monoalcohol**. **Polyalcohols**, with more than one hydroxyl group, can be formed by substituting more than one H atom on an alkane with hydroxyl groups. In this lesson we will be focusing on the structures of representative monoalcohols, which we will refer to as “alcohols” throughout.

The simplest alcohol, methanol, will be formed by taking the simplest alkane, methane, and replacing one H atom with a hydroxyl group. This replacement is illustrated here.

Start with methane, then highlight the H (by adding translucent s orbital for example) and then switch it out for methanol. Echo text in lower left for “methane” and for “methanol” once formed. Maybe have this run as a continuous loop, like on frame 13 of the alkenes lesson (see that for what I mean).

State 3: The next simplest alcohol will be formed by replacing a H atom on ethane, C2H6, with a hydroxyl group as shown here. This alcohol is named ethanol.

Do as for methane on previous slide, but this time using ethane and switching it with ethanol. Echo text ethane and ethanol

State 4. Alcohols are named by taking the name of the alkane from which it was derived, dropping the last letter in the name (“e”) and replacing it with “ol”.

Repeating animations from previous two slides:  
Methane: echo text “Alkane name is methan**e**”  
Methanol: echo text “Alkane name is methan**ol**”  
Ethane: echo text “Alkane name is ethan**e**”  
Ethanol: echo text “Alkane name is ethan**ol**”

State 5: The position of the hydroxyl group must be indicated for alcohols formed from alkanes with chains longer than two C atoms in length. This is illustrated here with propane. If a H atom attached to a terminal C atom (at C1) is replaced by a hydroxyl group, the alcohol is named 1-propanol. The “1-“ indicates the position of the hydroxyl group in the longest continual chain, which has the root name “prop”.

Start with propane, show numbering on propane, then highlight the H (by adding translucent s orbital for example) on C1 and then switch it out for 1-propanol. Retain numbering. Echo text in lower left for “propane” and for “1-propanol” once formed. Run this as a loop too maybe.

State 6: In this rendering, a H atom on carbon atom 2 of propane is being replaced with a hydroxyl group to form the alcohol named 2-propanol. The “2-“ indicates the position where the hydroxyl group is present on the chain of C atoms. This alcohol is often referred to by the trivial name “isopropyl alcohol”, or “rubbing alcohol”.

Start with propane, show numbering on propane, then highlight the H (by adding translucent s orbital for example) on C2 and then switch it out for 2-propanol. Retain numbering. Echo text in lower left for “propane” and for “2-propanol” once formed. Run this as a loop too maybe.

State 7: Imagine we had added the hydroxyl group to carbon atom number 3 in the propane chain. The resulting alcohol would be 1-propanol, not 3-propanol. When numbering the chain of C atoms in an alcohol, always start at the end of the chain closest to where the hydroxyl group is present. Therefore, if a hydroxyl group were added to C3 of propane, the resulting alcohol is renumbered starting with “1” on the atom originally assigned as “3”.

Show same animation as in state 5, but orient and number the alkane so C3 gets swapped with an OH. Once the OH is added, change the C3 to C1 for the alcohol to illustrate the point.

State 8: Recall that the general formula for alkanes is CnH2n+2. Since monoalcohols have one H replaced by -OH, their general formula is CnH2n+2O. The chemical formulas for methanol, ethanol, and 1-propanol are CH4O, C2H6O, and C3H8O, respectively. The chemical formulas are often written by separating the H atom bonded to O in the hydroxyl group so it is present after the H, in the following fashion for the previous three examples: CH3OH, C2H5OH, C3H7OH. To provide even more information about structure, the formulas for alcohols are often written in the form of **condensed structural formulas**, where the C atoms are written in the order they are connected in a molecule, with the substituent atoms present on the C atoms written after them. By convention, the C atom to which the OH group is attached, if terminal, is usually written last in the condensed structural formula, even though the numbering starts with the C atom to which the -OH group is attached. The condensed structural formulas for methanol, ethanol, and 1-propanol are CH3OH, CH3CH2OH, and CH3CH2CH2OH, respectively.

Show methanol, ethanol, and 1-propanol on same slide, with their names and condensed structural formulas under them.

State 9: Alcohols that have the same chemical formulas, but where the positions of the hydroxyl groups differ, are structural isomers. 1-propanol and 2-propanol are structural isomers of one another.

Show 1-propanol and 2-propanol on same slide.

State 10: Adding a hydroxyl group to C1 of butane gives the alcohol 1-butanol.

Same drill…

State 11: Adding a hydroxyl group to C2 of butane gives 2-butanol.

Same drill….

State 12: Adding a hydroxyl group to C3 of butane also gives 2-butanol. This is because the numbering of the chain will change once the hydroxyl group is added. The chain is always numbered starting with the C atom closest to where the hydroxyl group will first be encountered.

Same drill, but change numbering from 1-2-3-4 when adding OH to C3 so it becomes 4-3-2-1 to illustrate the point.

State 13: Alcohols can also be formed starting with branched-chain alkanes. 2-methylpropane is an isomer of 1-butane (see branched-chain alkanes lesson). If a hydroxyl group replaces one of the H atoms on any one of the three C atoms of 2-methylpropane, an alcohol named 2-methyl-1-propanol is formed. For branched-chain alcohols, the name of the alkane is changed in the same fashion as for a linear alkane, and the resulting alcohol numbered so that lowest number is given to the C atom closest to where the -OH group is first encountered in the longest continual chain.

Show structure of 2-methylpropane with numbering changing to 2-methyl-1-propanol with numbering.

State 12: There is one additional alcohol that will have the chemical formula C4H9OH. This alcohol, shown at right, has the systematic name 2-methyl-2-propanol. This alcohol is commonly referred to by its trivial name, tert-butanol, or tert-butyl alcohol.

Show 2-methyl-2-propanol.

State 13: All four isomers of “butanol” are shown here

Show 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol.

State 14: We will now examine some general structural and electronic properties that apply to alcohols derived from alkanes. In doing so we will focus on the properties of the hydroxyl functional group. The alkyl group attached to the hydroxyl group can be represented by “R” where the group “R” is the alkyl substituent to which the hydroxyl group is attached.

Show methanol, then switch out the methyl group for a large sphere labeled R, as for frame 3 of the alkenes lesson. Easiest way is probably to hide the H atoms of the methyl group and then increase the sphere size of C and change its color to C per the alkene lesson.

State 15: The O atom of a hydroxyl group is bonded to two atoms (H, and the C of the R group) and contains two lone pairs of electrons. With two bonded and two nonbonded electron domains, the AXE designation for the O is AX2E2. With four total electron domains, the electron domain geometry surrounding the O atom is tetrahedral, as shown here.

Display generic R-OH alcohol, add sp3 orbitals to show tetrahedral electron domain geometry, then add the necessary lines to highlight the tetrahedral unit. A good way to find the end points of the lobes is to use that trick I discovered: set picking draw, draw a line, use shift click to drag the line to where it is on top of the lobe, then “show draw:.

State 16: With two bonded and two nonbonded electron domains, the molecular geometry about the O atom will be bent.

Highlight bent geometry, still showing the lone pair lobes. The bonded lobes can probably be turned off here?

State 17: The bond angles in a molecule with four electron domains, and in which all the electron domains are bonded to terminal atoms, will be exactly 109.5 degrees. For the O in alcohols, the lone pairs of electrons spread out more in space than the bonded pairs of electrons, resulting in a slight compression of the bond angle.

I got a bond angle of 107 degrees for an optimized methanol molecule in Avogadro. I think the angle is actually closer to 108-109 degrees. Anyway, it is slightly less than 109.5. just have the angle appear as what it is, as long as it is something slightly less than 109.5.

State 18: Now that we have established the molecular geometry about the O atom in an alcohol, we will look at the polarity of alcohols. Carbon and hydrogen have fairly similar electronegativity values, so each C-H bond in the alkyl portion of an alcohol is only weakly polar. O is much more electronegative than either H or C. Due to the differences in electronegativity, the O in an alcohol has a partial negative charge while the H and C atoms to which it is bonded have partial positive charges. This is highlighted here for methanol.

Show methanol, label O with delta minus and C and H with delta plus as for frame 15 in the ammonia vsepr lesson: <http://ensignchemistry.com/jsmol%20models/lessons/NH3_vsepr/>

State 19: The differences in electronegativity make the C-O and H-O bonds polar. The bond dipole moments are represented by vectors, where the arrows point in the directions of the more electronegative atoms. The length of the vector is proportional to the differences in electronegativity of the two atoms present in the bond. Shown here are the bond dipoles for the C-O and H-O bonds.

Continue using methanol. Show bond dipoles per frame 16 of VSEPR NH3 lesson. I like putting the dipole right on the bond and making the bond translucent to do this (see script for frame 16). Since C is a little more electronegative than H, you can make the O-H dipole slighty longer than the C-H dipole if you want, but this is really not necessary.

State 20: The directions and magnitudes of bond dipoles dictate whether, and to what an extent, a molecule is polar. In the case of an alcohol, the individual dipoles for the C-O and H-O bonds reinforce each other in a “vertical” direction, while they cancel one another in the “horizontal” directions. The net dipole moment due to the hydroxyl functional group, obtained by adding the individual dipole vectors, is shown, alternating with the bond dipoles. Since C and H have similar electronegativities, the C-H bonds in methanol are only slightly polar, and they are therefore disregarded here.

Reproduce frame 17 of the NH3 VSEPR lesson for methanol. Include echo text like frame 17.

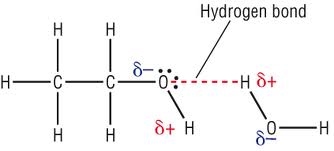
State 21: This rendering shows the electrostatic potential map for methanol. The electrostatic potential map is an isosurface which allows the visualization of partial charges within molecules due to electronegativity differences of bonded atoms. As discussed on the previous slides, since O is more electronegative than C and H, it has a partial negative charge, and there is a net dipole moment in the molecule. The colors in the electrostatic potential map allow the regions of higher and lower electron density due to bond and molecule polarity to be visualized. Red colors represent regions where electron density is being pulled towards more electronegative atom(s), while blue colors represent regions where electron density is being pulled away from electropositive atom(s). Green colors represent net electrically neutral regions. The electrostastic potential map for methanol shown here emphasizes how the electronegative O pulls electron density away from the the C and H atoms it is bonded to.

Show electrostatic potential map for methanol per frame 18 of NH3 VSEPR lesson.

select \*; if ({atomno < 10}.partialcharge == 0){calculate partialcharge};isosurface vdw map mep; isosurface translucent; spin on;

State 22: The polarity of the O-H bond in methanol allows methanol to form favorable hydrogen bonds with other methanol molecules, as well as other molecules capable of forming hydrogen bonds, like water. Methanol is miscible (soluble in all proportions) in water due to the hydrogen bonding capability.

This would be cool. Add an H2O moleculeto the log file, where they it is oriented so that a hydrogen bond can be displayed on this slide like this (but do it for methanol):



State 23: The C-O and H-O bonds in other alcohols will be polar as well. Shown here is the electrostatic potential map for ethanol, which, like methanol, is miscible in water.

Ethanol with vdw isosurface

State 24: Shown here is the electrostatic potential map for 1-propanol

1-propanol with vdw isosurface added

State 24: Due to the similarities in electronegativities of C and H, and symmetrical arrangement of atoms in alkyl groups, the alkyl portions of alcohols are largely nonpolar. As the alkyl groups of alcohols become larger, and longer in length, more London dispersion forces are formed with other alcohol molecules in the liquid and solid states of these substances. Alcohols become increasingly more nonpolar in character as the alkyl chain length attached to the hydroxyl functional group increases in length. While the OH group will always be polar, more C and H atoms in the alkyl portion will cause London dispersion forces to become increasingly more important than hydrogen bonding as an intermolecular attractive force. For this reason, the solubilities of alcohols in water decrease as the length of the alkyl chain increases. Methanol, ethanol and 1-propanol are all miscible in water, while butanol exhibits an upper solubility limit of 0.11 mol/100 g H2O. The next linear alcohol, 1-pentanol, shown here, has a solubility of only 0.030 mol/100 g H2O.

Show structure of 1-pentanol with the vdw isosurface on

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State 25: This concludes the lesson for alcohols. Click here to return to the main lessons page.

Show a bunch of different alcohols from the log file here?