Branched-chain alkanes lesson

I think for this lesson it would be good to try out the two column template. We can then put the descriptions with chemdraw structures on the left side, for comparison to the jmol structures on the right side.

Log file with following structures: propane, n-butane, isobutane, n-pentane, isopentane, neopentane, n-hexane, 2-methylpentane, 3-methylpentane, 2,3-dimethylbutane, 2,2-dimethylbutane, 2-methylpentane

State 1: Structural isomers are compounds that have the same molecular formula, but different arrangements for bonded atoms. In this lesson we will look at structural isomers of alkanes called branched-chain alkanes.

Ball and stick models of n-pentane, isopentane, and neopentane

State 2: For straight-chain alkanes, all of the C atoms are connected in a continuous chain with no branching. Branched-chain alkanes are those in which one or more alkyl groups (methyl, ethyl, etc) replace one or more H atoms on a methylene group (-CH2-) in the continuous chain of a linear alkane. The shortest linear alkane for which branching can occur is propane (structural formula CH3-CH2-CH3). In this rendering, one of the methylene H atoms of propane is being replaced with the simplest alkyl group, a methyl group, to give a structural isomer of butane.

Ball and stick model of propane shown initially. Highlight one of the two H atoms, and then replace the propane structure with methylpropane in the same orientation (so it looks like the H has been replaced with CH3). Have the CH3 group highlighted as the H atom was, maybe using translucent green s orbitals on the atoms like we have done before.

State 3: The structural isomer created from propane by replacement of a methylene hydrogen with a methyl group has the same molecular formula as the linear alkane butane (C4H10). Thus, these two compounds are structural isomers. Technically, either compound can be referred to properly as “butane”. To distinguish them, straight-chain butane is called n-butane, where the “n” stands for “normal”. In this context, a “normal” alkane is one containing all C atoms in a linear chain and with no branching. The structural isomer of butane with branching may be properly referred to as “isobutane” or “2-methylpropane”. The name “isobutane” is a traditional name still used to some extent. The name “2-methylpropane” is the proper systematic name according to the nomenclature rules for naming organic compounds. When naming an alkane systematically, the longest continuous chain of C atoms serves as the base name of the compound. The C atoms in the chain are numbered starting with the first atom in the chain. The numerical position(s) on the chain of alkyl substituents are placed before the alkyl name, followed by the base name.

In this rendering, the longest continuous chains of the structural isomers n-butane and methylpropane are highlighted by changing their bond colors to yellow.

Ball and stick models of n-butane and isobutane side by side. Highlight the continuous chains by changing the bond colors for the chain to a different color, like yellow (select… color bonds yellow). Place the numbering for the C atoms on the chain (1-4 for n-butane, 1-3 for methylpropane). Systematic names written below the compounds

1. "**set echo *echoname***  **XX% YY%**", where *echoname* is the name you want to use for the echo and XX% and YY% are X and Y coordinates of the echo position from the bottom left in % of the applet size.25%
2. "**echo "your echo text"**".

State 4. If both H atoms on the methylene (-CH2-) group of propane had been replaced with methyl groups, the following compound would be formed. The longest continual chain is still propane, but now there are two methyl groups branching off of the middle C atom, and five total C atoms rather than 4. This compound is named systematically as 2,2-dimethylpropane.

Model for neopentane, with longest chain still highlighted, also numbering present. Maybe highlight both methyl groups using green s orbitals as well.

State 5: The molecular formula for 2,2-dimethylpropane is C5H12, so it is a structural isomer of the straight-chain alkane n-pentane. Henceforth, we will always place “n-“ in front of linear alkanes to conform to nomenclature rules. 2,2-dimethylpropane is often referred to by the traditional name “neopentane”.

Side by side models neopentane and n-pentane with longest chains highlighted, also numbering present.

State 6: 2,2-dimethylpropane is not the only structural isomer of n-pentane. Starting with 2,2-dimethylpropane, imagine taking one of the methyl groups from C2, and moving it to C3, at the same time moving the H from C3 to C2. These substitutions would result in a new isomer of pentane being formed where the longest continuous chain now has four C atoms rather than 3. When looking at structural formulas of alkanes, it is important to always identify the longest continual chain of C atoms to get the proper base name. The compound formed from the above substitution is 2-methylbutane. When a single substituent branches off a continual chain, the numbering of the continual chain starts with the end closest to the substituent.

dimethylpropane at left . Add arrows pointing from methyl and H atoms that are going to swap positions. Highlight these substituents. Show 2-methylbutane at right where the substituents have been swapped, still highlighted. Number both chains. State 7: Branched-chain alkanes will always have the general molecular formula CnH2n+2, the same general formula that straight-chain alkanes have. The greater the value of “n”, the more structural isomers will be present for a given alkane. There are only two structural isomers possible for alkanes with the chemical formula C4H10 (n-butane and 2-methylpropane). There are three structural isomers possible for alkanes with the chemical formula C5H12 (n-pentane, 2-methylbutane, and 2,2-dimethylpropane). All three isomers of pentane are shown here.

Show three pentane isomers. Number chains, highlight longest chain

State 8: There are five possible structural isomers possible for alkanes with the formula C6H14. Shown below is n-hexane. To identify the additional isomers, start by changing the longest continual chain from 6 to 5 carbon atoms, and then determine what possible branching could be present. These isomers are shown in the next two renderings.

Show n-hexane with numbering, and longest chain highlighted (do the same for all subsequent states: number and highlight bonds in chain)

State 9: Shown here is 2-methylpentane.

2-methylpentane

State 10: Shown here is 3-methylpentane. There are two isomers of hexane where the longest chain is 5 C atoms. There are two additional isomers where the longest chain is 4 C atoms. These will be rendered in the next two states.

3-methylpentane

State 11: 2,3-dimethylpentane

Add

State 12: 2,2-dimethylpentane

Show

State 13: Shown here are all five isomers of hexane with the formula C6H14.

Show

State 14: The number of possible structural isomers increases dramatically for each additional C atom in the reference n-alkane. There are 9 isomers of heptane (C7H16) and 18 isomers of octane (C8H18). For heptane, one structural isomers will contain an ethyl group (-CH2CH3). This isomer, 3-ethylpentane, is shown here. As the number of C atoms becomes successively greater, isomers can incorporate combinations of methyl, ethyl, propyl, and longer chain alkyl substituents. The substituents can also be branched, adding more structural complexity.

Show 3-ethylpentane with chain and numbering, highlight ethyl group.