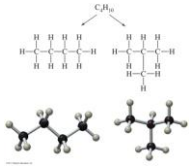
4.5 Isomerism in Organic Compounds, Part 1

Structural Isomers

- ***Structural isomers*** are compounds with the same molecular formula but a different connectivity.
- Butane, a four-carbon molecule, is the simplest alkane that has two structural isomers.

4.5 Isomerism in Organic Compounds, Part 1, Continued



- Each compound contains four carbon atoms and 10 hydrogen atoms. Each have the molecular formula, C_4H_{10}.
- The four carbons in the compound on the right are not connected in a continuous chain as they are in butane.

4.5 Isomerism in Organic Compounds, Part 1, Continued

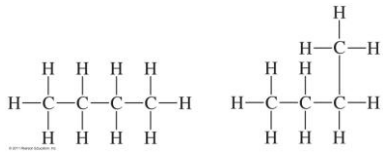
- The second structural isomer of butane forms a branched alkane and is known as ***isobutane***.
- Branched-chain alkanes do not have all their carbon atoms connected in a single continuous chain.
- Both compounds with the molecular formula of C_4H_{10} are structural isomers. That is, they have different connectivity of the atoms.

4.5 Isomerism in Organic Compounds, Part 1, Continued

Conformational Isomers

- ***Conformational isomers*** are isomers that are not different compounds because they have different arrangements of the atoms of the compound. They are also known as ***conformers***.
- Consider butane. The structure of butane can be represented as shown on the next slide.

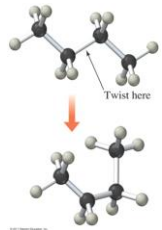
4.5 Isomerism in Organic Compounds, Part 1, Continued



- These two representations are conformational isomers of the same molecule.
- These molecules are not rigid. Since there is rotation about the single bonds of butane, the molecule can form the two conformational isomers.

4.5 Isomerism in Organic Compounds, Part 1, Continued

The three-dimensional models of the two conformational isomers of butane that demonstrate the rotation about the carbon–carbon single bond is shown as:



4.5 Isomerism in Organic Compounds, Part 1, Continued

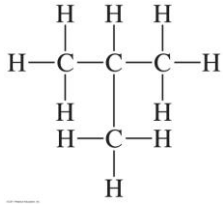
Nomenclature of Simple Organic Compounds

- Systematically naming each organic compound is a useful method to determine whether two compounds are structural or conformational isomers.
- Structural isomers will have different names, whereas conformational isomers will have the same name.
- Naming of organic compounds was developed by the International Union of Pure and Applied Chemistry, or IUPAC.

4.5 Isomerism in Organic Compounds, Part 1, Continued

Branched-Chain Alkanes

Consider the following branched-chain isomer of butane, isobutane. Naming will be done using the IUPAC system.

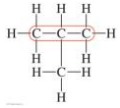


4.5 Isomerism in Organic Compounds, Part 1, Continued

Branched-Chain Alkanes, Continued

The following are rules for naming branched-chain alkanes by the IUPAC system:

Step 1. Find the longest continuous chain of carbon atoms. This is the ***parent chain***. Name the parent according to the alkane name for the appropriate number of carbon atoms. In this case, the parent chain is propane.



4.5 Isomerism in Organic Compounds, Part 1, Continued

Branched-Chain Alkanes, Continued

Step 2. Identify the groups bonded to the parent chain and not included in the main chain. These groups are called ***substituents*** and in this case, called ***alkyl groups***. The name of the alkyl group is derived from the alkane with the same number of carbon atoms by changing the *-ane* ending with *-yl*. For example, a one carbon alkyl group is named as a *methyl* group.

4.5 Isomerism in Organic Compounds, Part 1, Continued

Branched-Chain Alkanes, Continued

Step 2 (continued). This table shows the simplest alkyl substituents and their point of attachment to the parent chain.

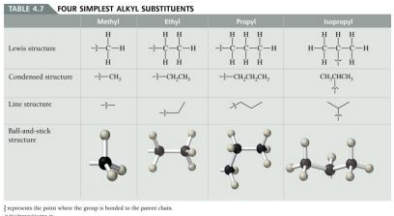


TABLE 4.7 FOUR SIMPLEST ALKYL SUBSTITUENTS

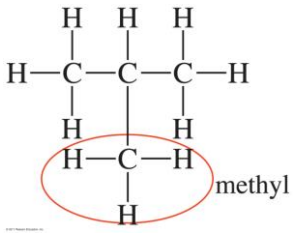
	Methyl	Ethyl	Propyl	Isopropyl
Lewis structure				
Condensed structure	$-CH_3$	$-CH_2CH_3$	$-CH_2CH_2CH_3$	CH_3CHCH_3
Line structure				
Ball-and-stick structure				

The ~ represents the point where the group is bonded to the parent chain.

4.5 Isomerism in Organic Compounds, Part 1, Continued

Branched-Chain Alkanes, Continued

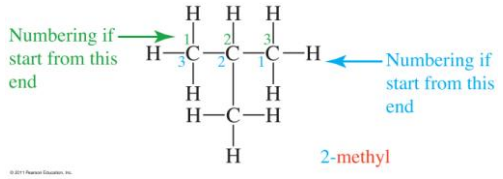
Step 2 (continued). In our case, the substituent is the methyl group.



4.5 Isomerism in Organic Compounds, Part 1, Continued

Branched-Chain Alkanes, Continued

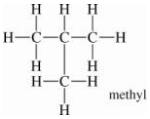
Step 3. Number the parent chain starting at the end nearer to a substituent. In our example, the substituent is on carbon 2 no matter which end you start numbering.



4.5 Isomerism in Organic Compounds, Part 1, Continued

Branched-Chain Alkanes, Continued

Step 4. Assign a number to each substituent based on location, listing the substituents in alphabetical order at the beginning of the name. Separate numbers and words in the name by a dash. Separate numbers by a comma. The IUPAC name for our example is *2-methylpropane*.



4.5 Isomerism in Organic Compounds, Part 1, Continued

Branched-Chain Alkanes, Continued

NOTE: If more than one substituent of the same type is present, indicate this by using the prefixes *di-*, *tri-*, and *tetra-,* but ignore these prefixes when alphabetizing. For example, two methyl groups on a parent chain would be named *di*methyl.

4.5 Isomerism in Organic Compounds, Part 1, Continued

Haloalkanes

- Halogens can serve as substituents on alkane chains and are known as ***haloalkanes***, or ***alkyl halides***.
- When a halogen is present, the name of the halogen is changed by replacing the *-ine* ending with an *-o*.
- Names of halogen substituents become *fluoro*, *chloro*, *bromo*, and *iodo*.
- Rules for naming haloalkanes are the same for naming branched-chain alkanes.

4.5 Isomerism in Organic Compounds, Part 1, Continued

Cycloalkanes

Rules for naming cylcoalkanes are as follows:

Step 1. The ring serves as the parent.

Step 2. As in branched-chain alkanes, identify the substituents.

Step 3. Number the carbons giving the carbon with the substituent as carbon 1.

4.5 Isomerism in Organic Compounds, Part 1, Continued

Cycloalkanes, Continued

Step 4. Assign numbers to the substituents. If only one substituent is present, it is assumed to be in position 1 and the 1 is implied and not listed. When more than one substituent is present, give all substituents the lowest possible numbers.