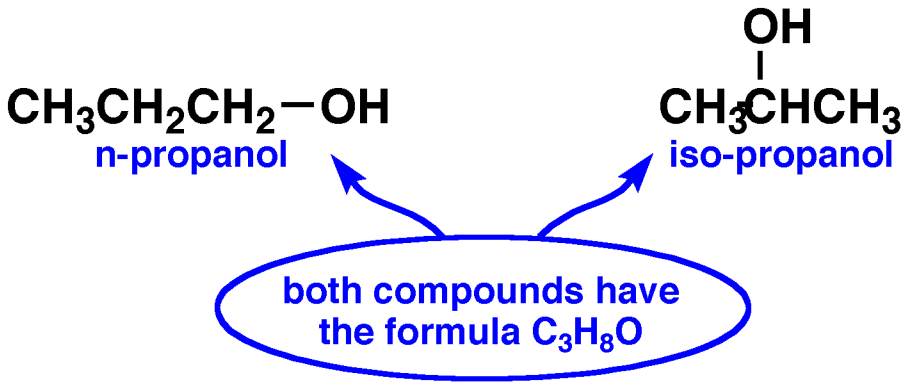
Stereochemistry:
There's More to Structure Than Connectivity

Stereochemistry has to do with the spatial arrangement of atoms within a molecule. It is an aspect of structure that goes beyond bonding connectivity. At the heart of the matter is a comparison between two structures. There are two questions of prime importance: (1) are the two structures the same or not the same and (2) if they are not the same, then how do they differ?

Isomers are two different structures that have the same molecular formula. **Constitutional isomers** are isomers that differ according to the way the bonds are connected. An example of two different structures that are related as constitutional isomers is n-propanol and iso-propanol. Both have the same molecular formula so they are isomers. Yet, they are obviously not the same. They differ in the way the atoms are connected together.



constitutional isomers have the same molecular formula but different bonding connectivity

Stereoisomers

Isomers with the same bonding connectivity but which differ according to how the atoms are arranged in space are called **stereoisomers**. Consider the two cyclohexane structures below. Both have the same molecular formula and both have the their atoms connected in the same way. For example, in both structures the bonding pathway from chlorine to oxygen involves four bonds. All other bonding pathways are the same in both structures. The way they differ is in how the atoms are arranged in space. For the structure on the left, the Cl and OH are oriented in opposite directions with respect to the cyclohexane plane of reference. In the structure on the right, both the Cl and the OH are oriented above the plane of reference. **The different spatial relationship among their atoms is what makes this a pair of stereoisomers.**

***trans*-3-chloro-cyclohexanol** ***cis*-3-chloro-cyclohexanol**

both compounds have the formula $C_6H_{11}ClO$ and both have the same bonding connectivity

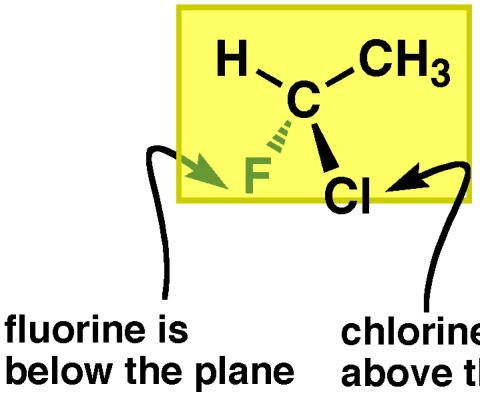
stereoisomers differ by the way their atoms are arranged in space

cis means "on the same side"
trans means "on opposite sides"

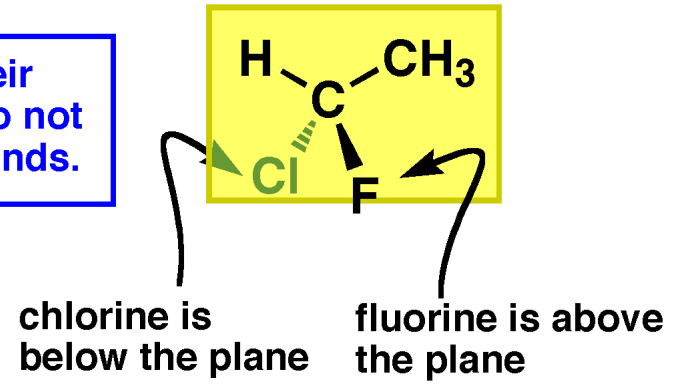
Convention

- Wedge - toward viewer
- Dash - away from viewer
- Wiggly - toward or away

The Same or Not the Same?



These stereoisomers differ in their configuration at carbon. They do not interconvert without breaking bonds.

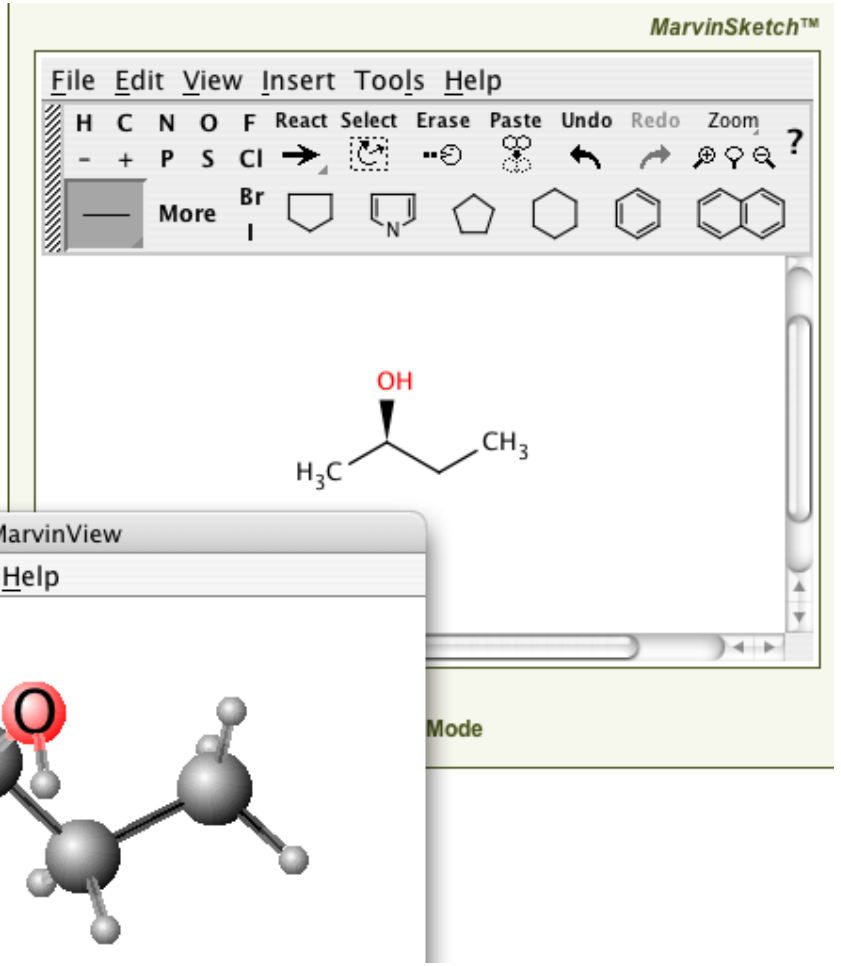


At this point it is best to build a model of each 1-chloro-1-fluoroethane stereoisomer shown above (computer models in ACE Organic work well for this purpose). Build them exactly as they are shown. Can you superimpose one on the other, atom-for-atom? If not, then they are not the same.

Be warned!! ACE can be a picky butt when it comes to stereochemical representations using wedges and dashes. ACE is picky because it wants to avoid ambiguities. Rest assured that if ACE cannot reliably assign a stereochemical configuration, than neither could a human.

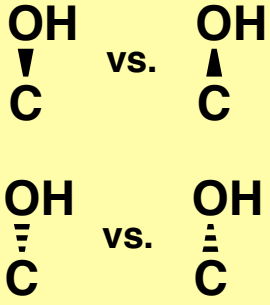
Make Friends with MarvinSketch & MarvinView

This is a good time to familiarize yourself with the way that ACE Organic interprets stereochemistry. Practice going back and forth from 2D line-angle drawings to 3D representations. Rotate the structure. Study the views. **Be inquisitive!**



Some things to play around with:

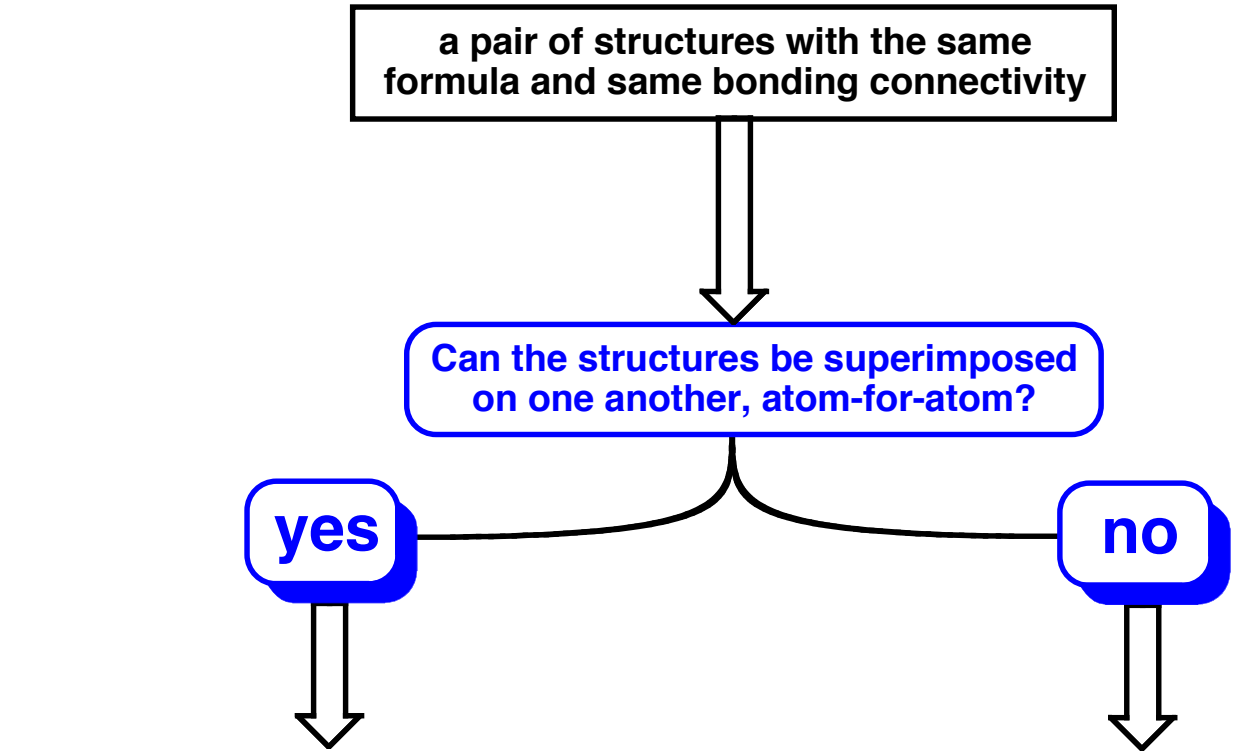
1. Position of substituents
2. Showing / not showing implied hydrogen
3. Wedge orientation



vs.

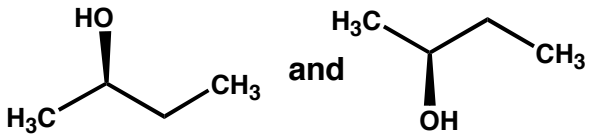
vs.

A Flowchart to Determine if a Pair of Structures Are Stereoisomers



Now try these two problems

Problem #1



Problem #2