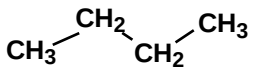
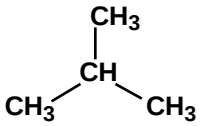
Text Related to Segment 1.04 ©2002 Claude E. Wintner

Continuing in the variation of molecular formula, propane has *two* carbon-carbon bonds about which the conformation may vary, so that the problem of representation of any single conformation in two dimensions becomes significantly greater. The next case, n-butane, contains three C—C bonds, and so on. However, already in the case of molecular formula C_4H_{10} — and in all the subsequent ones, as we shall see — a fundamentally distinct phenomenon appears: in addition to arranging four carbon atoms in the manner of normal butane, we also may do so as in isobutane:



normal butane

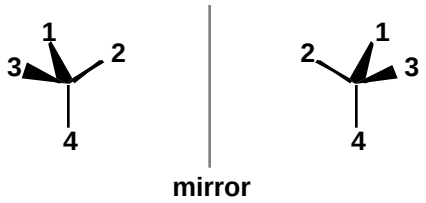


isobutane

Both molecules meet our original requirements with regard to valency; we are dealing with a difference in the "connectedness" of the carbon framework. Normal butane and isobutane possess identical molecular formulae, while differing in what is termed *constitution.* We call them constitutional *isomers*. It is crucial to note the difference between this situation and that of the conformations in ethane (or the conformations in either of the butane constitutions). The constitutional isomers cannot be made congruent by any twisting or turning about bonds. To convert one constitutional isomer into the other, one must break and remake both C—C and C—H bonds. Thus, the word "isomer" always requires a modifier, in this case "constitutional," to define the type of isomerism we are talking about.

A different kind of isomerism arises when we consider a carbon atom substituted with four different groups — for now call them simply 1, 2, 3, 4. If we

construct a single possibility for such a molecule and then construct its mirror image, the resulting two objects will not be congruent (make a model!):



Again we speak of isomers, now *configurational* isomers. Configurational isomers (as also is true of conformational isomers) do not differ in connectedness, but only in the spatial relationships among their atoms. However (in contrast to the case for conformational isomers), assuming the inviolate tetrahedrality of the carbon bonds, conformational isomers cannot be converted, one into the other, by any twist or turn. Molecules that are non-congruent mirror images of one another are termed enantiomers.

Although we will be defining all the above concepts much more closely in the sequel, already here it is important to be clear on what we mean by the word "structure." *Structure*, in its preferred present usage, most properly is invoked only in a situation where molecular formula, constitution, configuration (if relevant) and conformation *all* are defined. This is, for example, what one learns from an X-ray crystallographic analysis.