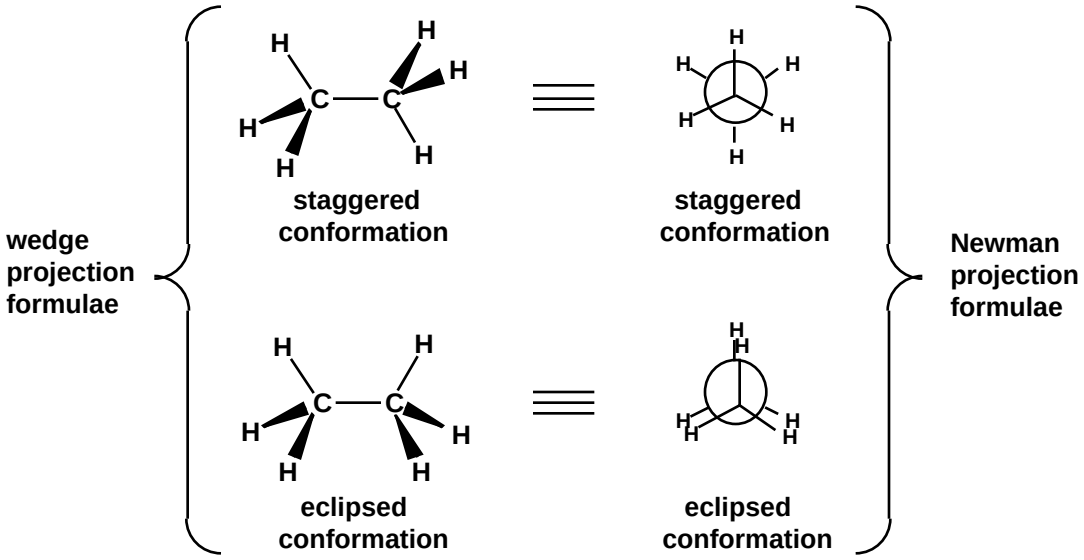
Text Related to Segment 2.01 ©2002 Claude E. Wintner

A model of ethane implies the existence of an infinite series of structures for ethane, differing in rotational angle about the carbon-carbon bond. Two extremes, called *staggered* and *eclipsed,* are shown below, employing alternative common notations: as before, wedge projection formulae; and also, what are termed Newman projection formulae.



three-dimensional conformational formulae for ethane

In fact, the model is quite faithful to the observed state of affairs. The two extreme structures — and all others with intermediate dihedral angle — do exist, if one considers an instantaneous time scale. These structures are said to differ among each other in conformation. *Differing conformations of a molecule have different spatial arrangements of its atoms, obtained by torsion about one or more single bonds.*

There is a most important point to be kept in mind here: in fact, *only one* ethane is isolated. The energy barrier opposing the rotation in ethane is small — about 3 kilocalories per mole — when compared with the thermal energy supplied at

room temperature by the collisions of the surrounding molecules — about 20 kilocalories per mole. Hence, the ethane gas which one has in a container at room temperature is a single substance, although it can exist in an infinite number of conformations, and thus is capable of infinite structural variety. Constant rotation about the carbon-carbon bond is taking place, at a rate of about a billion revolutions per second. (That there is a quantitative relationship between the height of the energy barrier opposing rotation and the rate of rotation will be discussed later.) It is necessary to remember that the phenomenon of conformational difference ordinarily is associated with small differences in energy, and that a change in the conformation of a molecule generally can be achieved rapidly at room temperature. Conformations that lie at energy minima, such as the staggered conformation of ethane, are termed conformational isomers, or conformers. In the case of ethane, then, there exist three conformational isomers or conformers, which are degenerate because they are congruent, have the same energy, and are, in all respects, indistinguishable. The energy gap of 3 kilocalories per mole between the two extreme forms translates into a population difference: at any given instant at room temperature there will be on average 100 ethane molecules in the staggered form for each one in the eclipsed form. (Again, this quantitative relationship will be discussed later.) Thus, it is reasonable to say that from the point of view of its properties ethane exists in the staggered conformation.