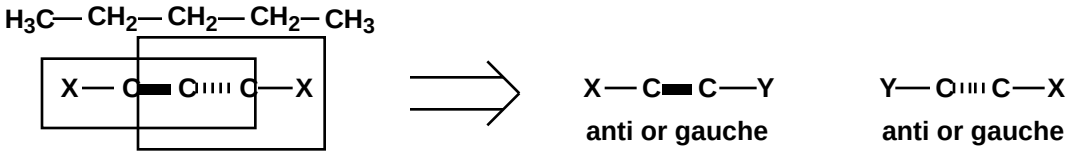
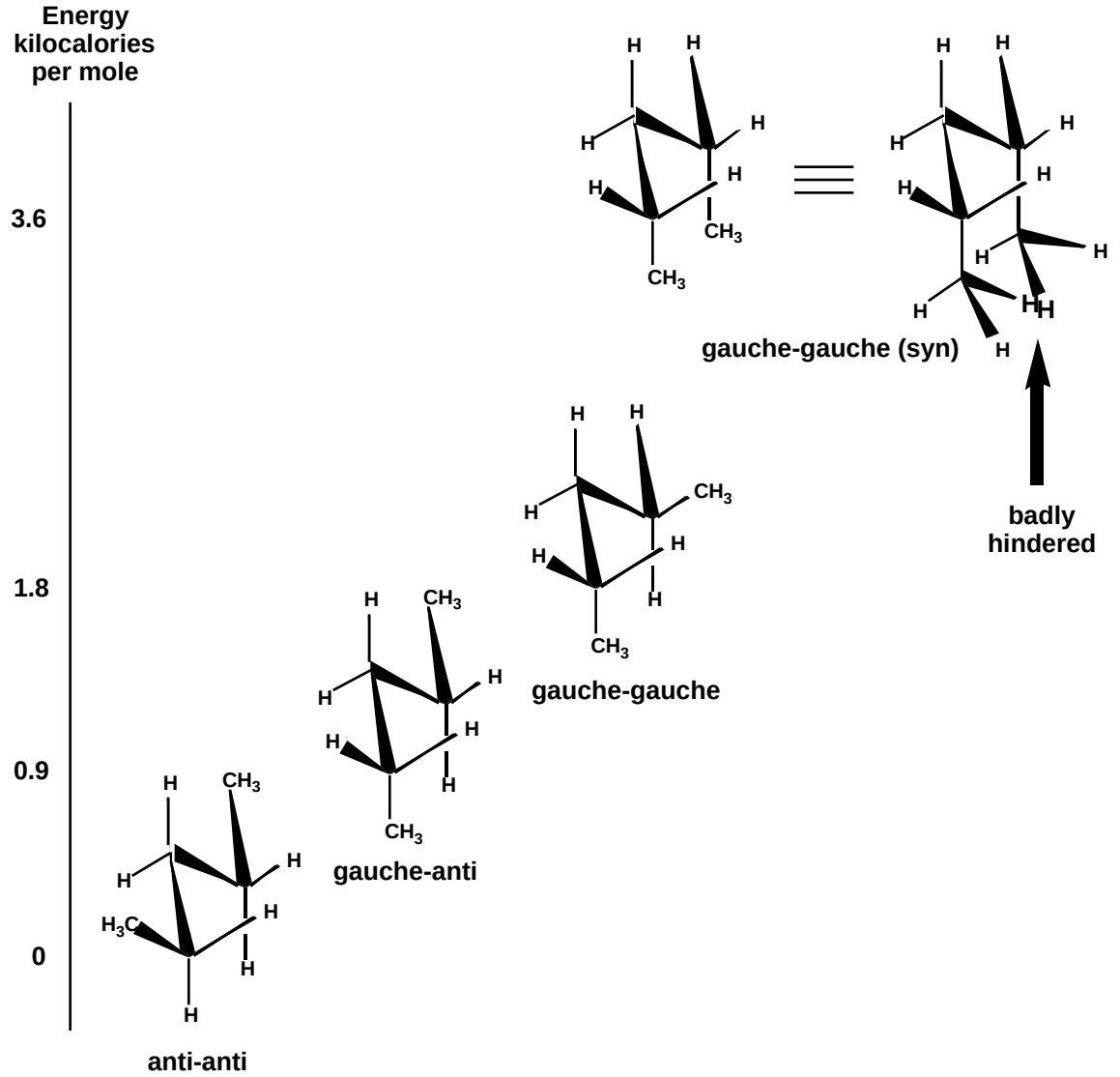
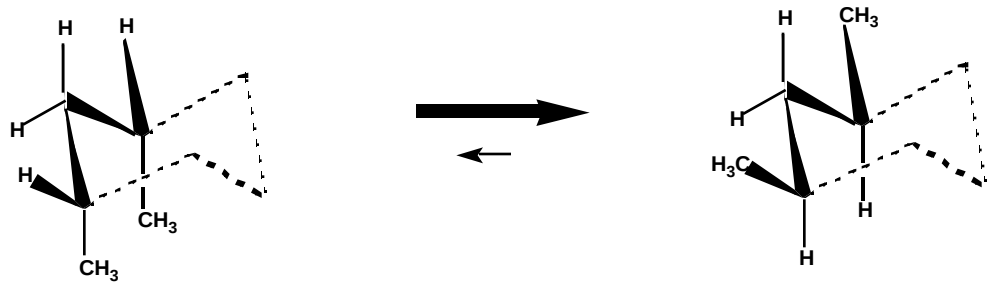
Text Related to Segment 2.04 ©2002 Claude E. Wintner

An examination of the conformational possibilities for normal pentane, $CH_3CH_2CH_2CH_2CH_3$, reveals aspects of similarity to the case of normal butane, but in addition discovers the problem of a new and unfavorable type of interaction. For our purpose n-pentane may be treated as 1,3-dimethylpropane. As in propane, rotation can take place independently about each of the two interior bonds; and in each case the situation is analogous to that for rotation about the central bond in n-butane, that is, the relationship of the carbon atoms flanking the bond in question can be anti or gauche. Among the nine variations obtained as a result of having three staggered rotamers for each of two bonds, and then excluding all equienergetic conformers (ones that are either congruent with or the non-congruent mirror images of cases that already have been counted), the analysis finds four conformations, differing in energy. In order of increasing energy, and hence decreasing population, these are termed anti-anti, anti-gauche, and gauche-gauche. However, there are two distinct gauche-gauche variations, with the one labeled "gauche-gauche (syn)" being extraordinarily hindered; for, as a result of having its two terminal methyl groups adjacent and parallel, it is saddled with obligatory hydrogen-hydrogen interactions which are greatly destabilizing. Hence, the gauche-gauche (syn) conformation is strongly disfavored. As a direct consequence, we shall see important extensions of this phenomenon in the cyclohexane series, for example, in *cis*-1,3-dimethylcyclohexane, for which the conformational equilibrium lies very strongly to the right as shown, so that the gauche-gauche (syn) interaction is avoided.

conformations of n-pentane







application of above to case of *cis*-1,3-dimethylcyclohexane