

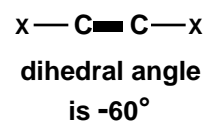
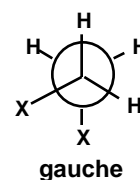
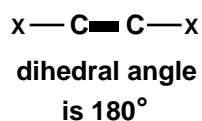
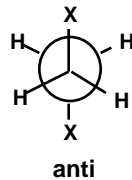
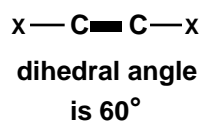
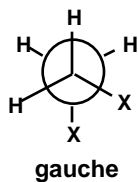
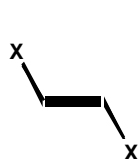
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The next variation of molecular formula takes us to C_4H_{10} , and again it is interesting to consider the conformational situation. Of the three carbon-carbon connections in normal butane, $CH_3CH_2CH_2CH_3$, the two exterior bonds present a situation comparable to that just discussed for propane. On the other hand, the case of rotation about the central carbon-carbon bond in normal butane merits further attention. From the point of view of energy there is less degeneracy than was the case for ethane, because of the relative positioning of the two terminal methyl groups. To describe this situation clearly it is helpful first to introduce some new terminology. We already have determined that, in considering rotation about the central bond of a 3-bond-4-atom system (the bond between atoms 2 and 3), we should concentrate our attention on staggered forms:

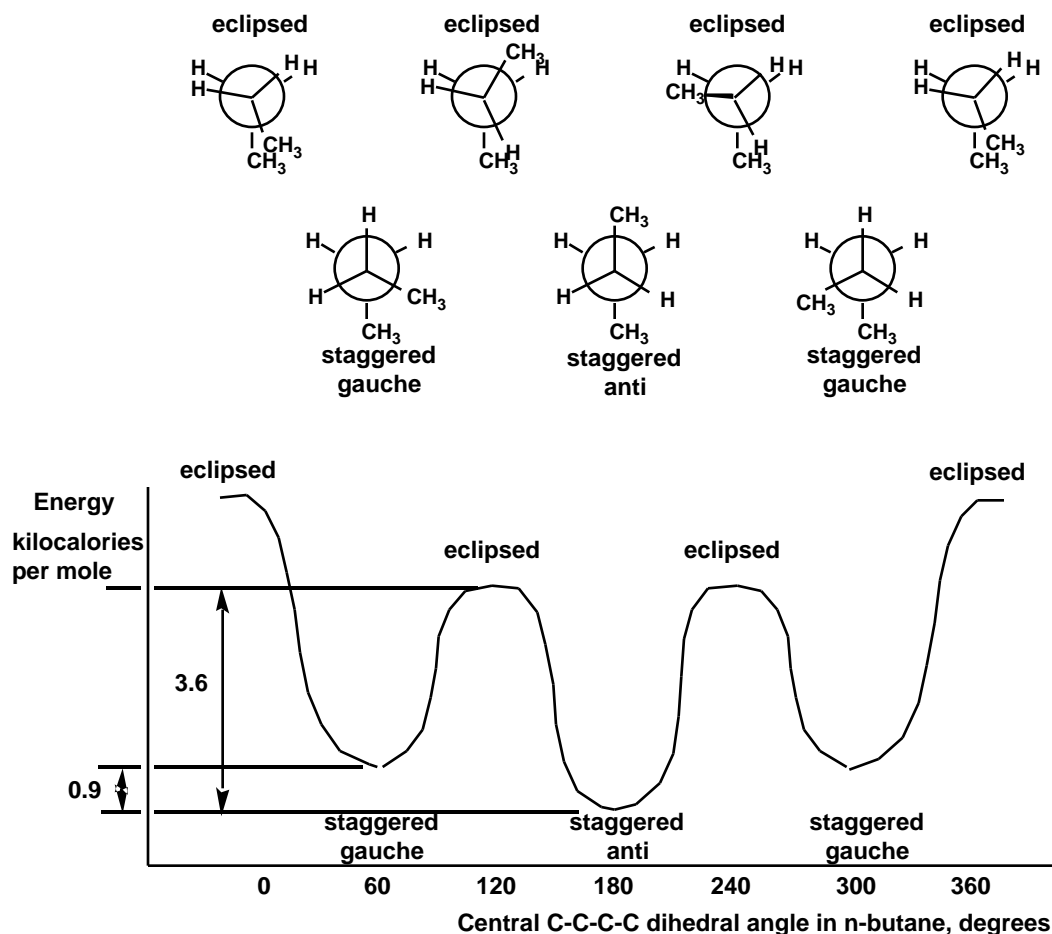


Now, when there is a group X other than hydrogen at each of the termini positions, then there exist three staggered possibilities, differing in the dihedral angle defined between the two groups X relative to each other about the central bond. Two of these possibilities — the ones with a dihedral angle of (absolute value) 60° — will be degenerate as regards energy (although, as will be emphasized later, they are non-congruent mirror images of one other: conformational, though NOT configurational, enantiomers). The third case, with dihedral angle 180° , clearly is in a different energetic situation. The 60° cases are termed gauche conformers, the 180° case is termed the anti conformer. In simple hydrocarbon cases such

as n-butane, where there are no electrostatic effects, the anti conformer is more stable for steric reasons. (However, in some other cases — for example, involving halogen atoms — strong electrostatic forces can lead to the so-called gauche effect, which may dictate more stable gauche conformers.)

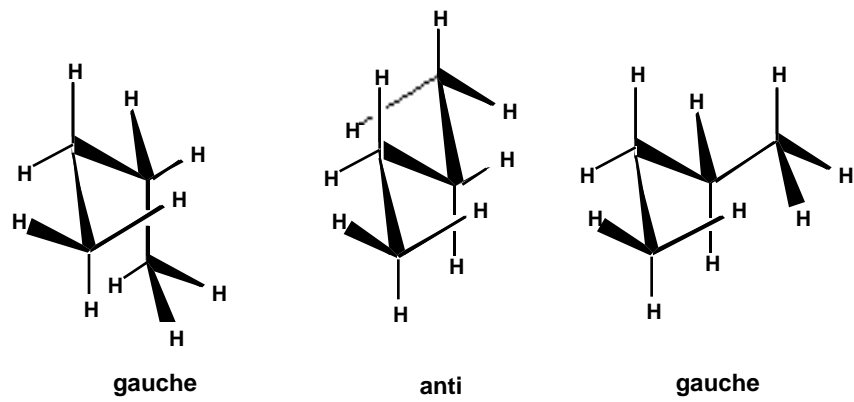


Applying these ideas to n-butane we find the following:



The anti form, offering the opportunity for minimum steric interaction between the terminal methyl groups, is lower in energy, by about 0.9 kilocalorie per mole, than the two gauche forms.

Wedge projection formulae also are used to depict these ideas, as is shown below for n-butane. The visualization of such formulae is not, for most of us, so easy on the first try, and models should be used to help in understanding the perspective that is meant. Then, after some practice, the formula — without the model — often will suffice.



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