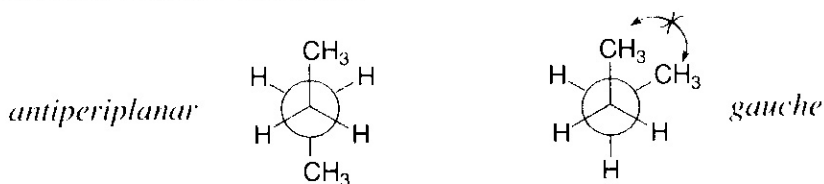


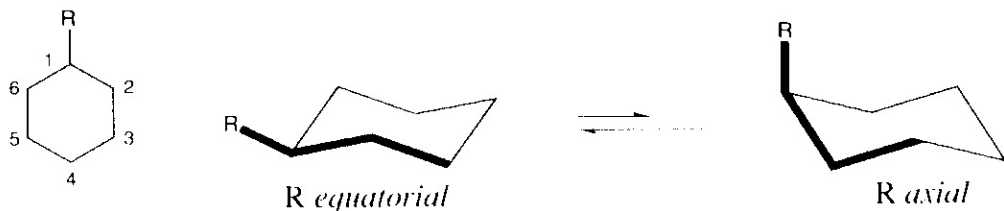
# Conformations of Alkylcyclohexanes

We use AM1 semi-empirical calculations to assign conformational preferences in alkylcyclohexanes, and to interpret these preferences in terms of steric effects.

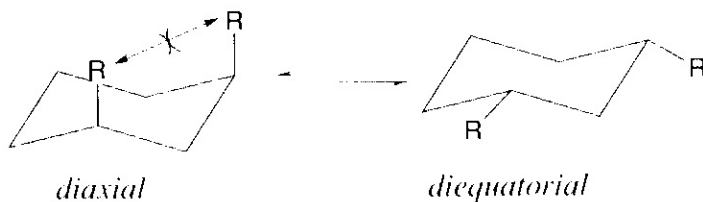
Alkyl groups prefer *equatorial* positions on cyclohexane.<sup>1</sup> The *equatorial* conformer of methylcyclohexane is 1.7 kcal/mol lower in energy than the *axial* conformer. The difference increases to 5.4 kcal/mol in *tert*-butylcyclohexane. The usual preference for *equatorial* substitution in cyclohexane is consistent with the fact that the terminal methyl groups in the ground-state conformer of *n*-butane are *antiperiplanar* rather than *gauche*; this minimizes unfavorable steric interactions between them, i.e.,



Inspection of substituted cyclohexanes reveals that equatorial substituents are *antiperiplanar* to  $C_2C_3$  and  $C_5C_6$ , but that axial substituents are *gauche*, i.e.,



Conformational preferences in disubstituted rings can be predicted by adding together substituent effects, and significant deviations from additivity are indicative of interactions between substituents. Direct steric interaction between alkyl groups in a 1,3-*diaxial* (a/a) conformer will give an especially large preference for the diequatorial (e/e) conformer.



1. Carey and Sundberg A, p. 130; Lowry and Richardson, p. 138; March, p. 143.