***online* Chemistry 331 Learning Module 3.3**
Conformational analysis of monosubstituted cyclohexanes

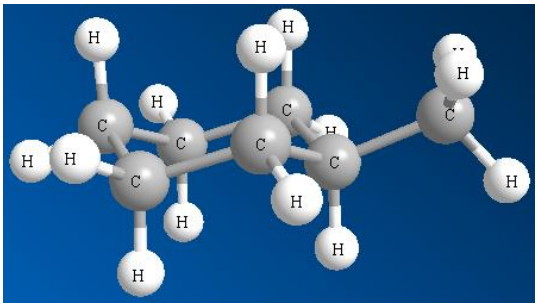
## An overview

In this learning module we will consider the chair conformations of various monosubstituted cyclohexanes. In particular we will identify and quantify any destabilizing interactions.

## Methylcyclohexane

equatorial methyl group

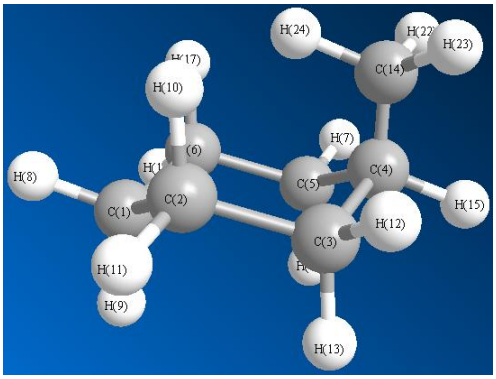
**View from the side**



***Please see Video Learning Module 3.3A***

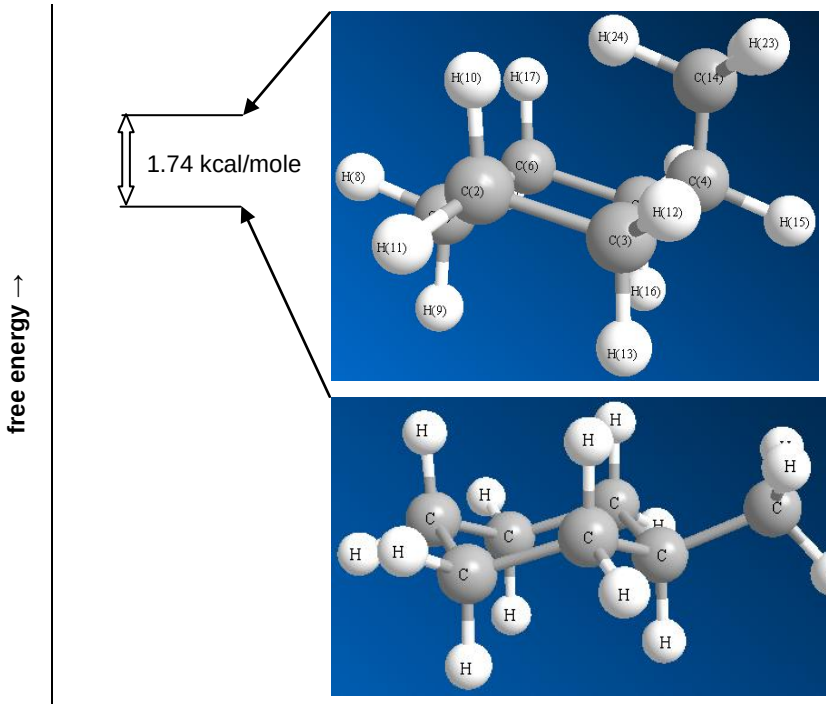
axial methyl group

**View from the side**




***Please see Video Learning Module 3.3B***

Relative stabilities (least stable conformation at the top of the graph)



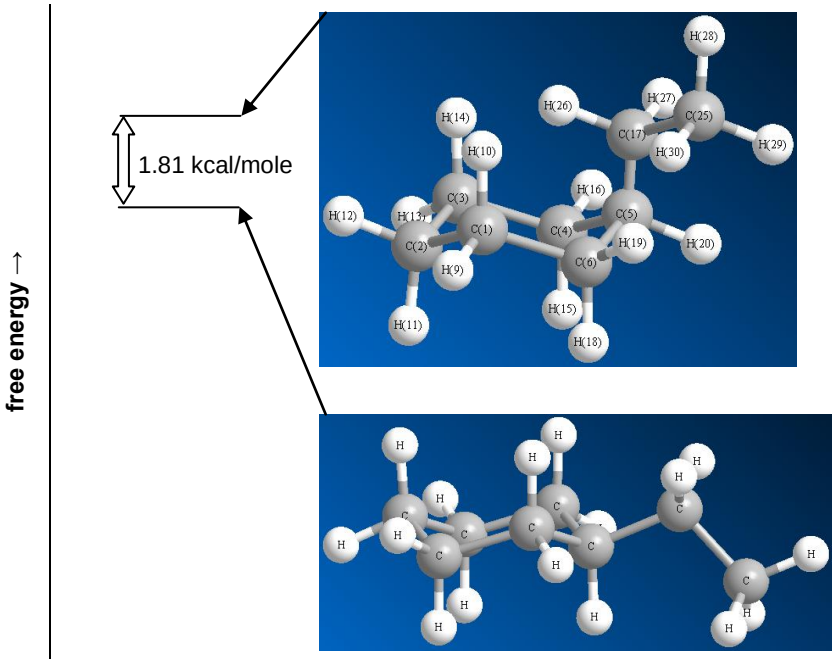

This conformation of methylcyclohexane is destabilized by two H:$CH_3$ 1,3-diaxial interactions:
-between H(10) and the C(14) $CH_3$ group
-between H(17) and the C(14) $CH_3$ group

If the total strain energy of this chair conformation is 1.74 kcal/mole then the **strain energy associate with one H:$CH_3$ 1,3-diaxial interaction must be 0.87 kcal/mole**

**In the accompanying *Video Learning Module* H(10) is color-coded red and H (17) is color-coded green**

***Please see Video Learning Module 3.3C***

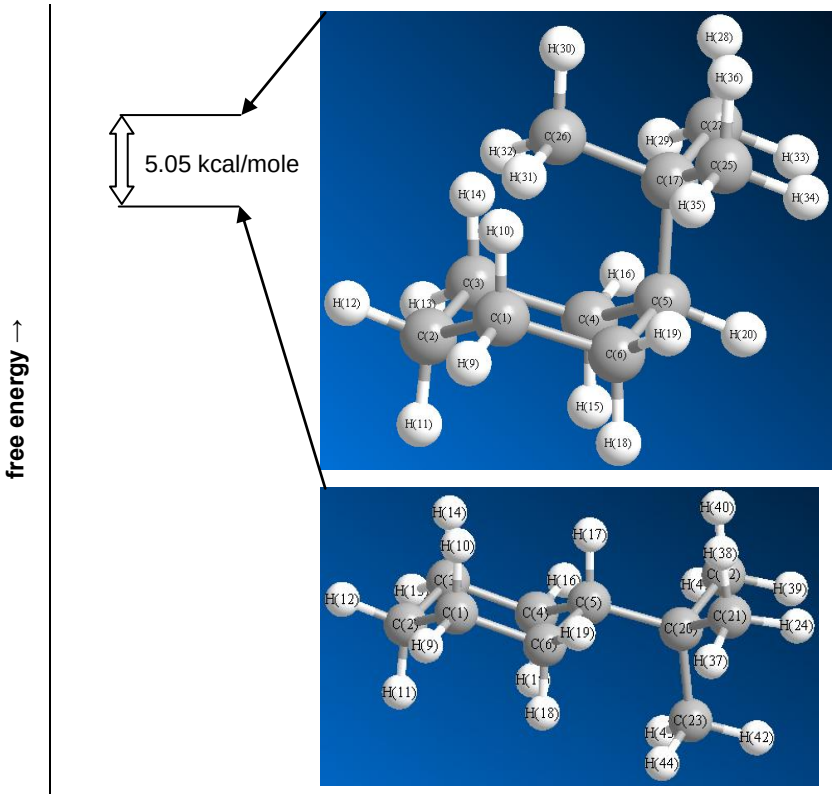
## Ethylcyclohexane




This conformation of ethylcyclohexane is destabilized by two H:$CH_2CH_3$ 1,3-diaxial interactions:
-between H(14) and the C(17) $CH_2CH_3$ group
-between H(10) and the C(17) $CH_2CH_3$ group

If the total strain energy of this chair conformation is 1.81 kcal/mole then the **strain energy associate with one H:$CH_2CH_3$ 1,3-diaxial interaction must be 0.91 kcal/mole**

## *Tert*-butylcyclohexane

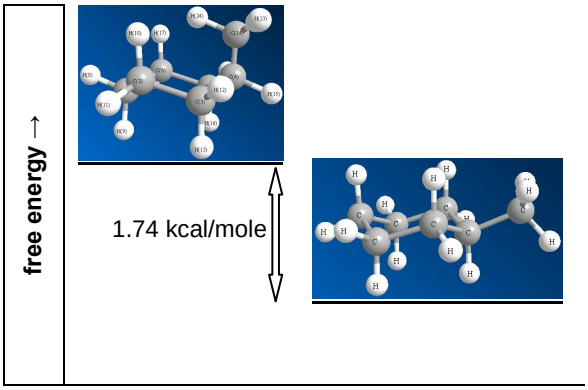



This conformation of *tert*-butylcyclohexane is destabilized by two H:$C(CH_3)_3$ 1,3-diaxial interactions:
-between H(14) and the C(17) $C(CH_3)_3$ group
-between H(10) and the C(17) $C(CH_3)_3$ group

If the total strain energy of this chair conformation is 5.05 kcal/mole then the **strain energy associate with one H:$C(CH_3)_3$ 1,3-diaxial interaction must be 2.53 kcal/mole**

## Calculating the equilibrium constant and composition at equilibrium

Methylcyclohexane




$\Delta G°$?
$\Delta G°$ = -1.74 kcal/mole

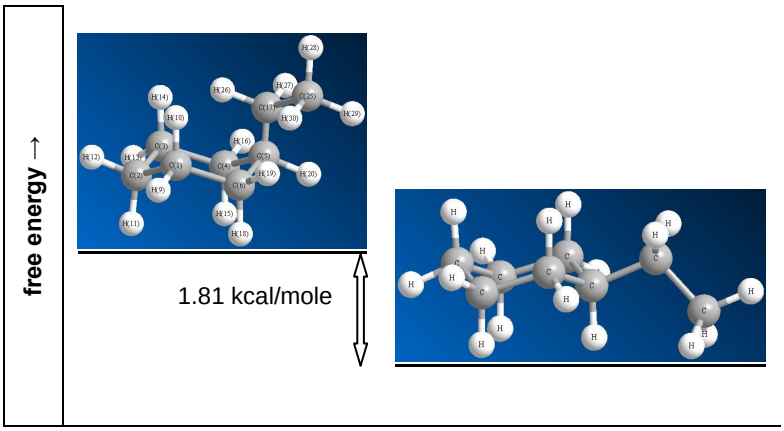
$K_{eq}$?
$K_{eq} = 10^{-\Delta G°/2.3RT}$
$K_{eq} = 10^{-(-1.74)/(1.364)} = 18.9$

$$K_{eq} = \left[\frac{\text{cyclohexane, equatorial R group}}{\text{cyclohexane, axial R group}}\right] = \frac{18.9}{1}$$

$$\%\ \text{equatorial R group} = \left[\frac{18.9}{1+18.9}\right] x100 = 95\%$$

$$\%\ \text{axial R group} = \left[\frac{1}{1+18.9}\right] x100 = 5\%$$

Ethylcyclohexane




$\Delta G°$?
$\Delta G°$ = -1.81 kcal/mole

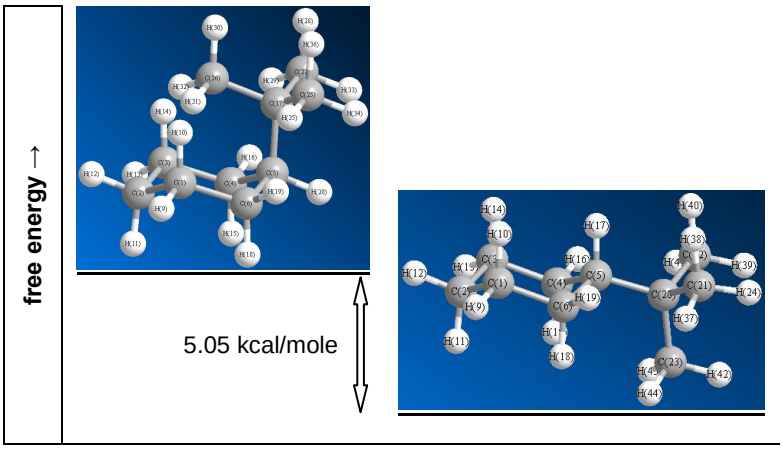
$K_{eq}$?
$K_{eq} = 10^{-\Delta G°/2.3RT}$
$K_{eq} = 10^{-(-1.81)/(1.364)} = 21.2$

$$K_{eq} = \left[\frac{\text{ethylcyclohexane, equatorial R group}}{\text{ethylcyclohexane, axial R group}}\right] = \frac{21.2}{1}$$

$$\%\ \text{equatorial R group} = \left[\frac{21.2}{1+21.2}\right] x100 = 95.5\%$$

$$\%\ \text{axial R group} = \left[\frac{1}{1+21.2}\right] x100 = 4.5\%$$

*Tert*-butylcyclohexane




$\Delta G°$?
$\Delta G°$ = -5.05 kcal/mole

$K_{eq}$?
$K_{eq} = 10^{-\Delta G°/2.3RT}$
$K_{eq} = 10^{-(-5.05)/(1.364)} = 5039$

$$K_{eq} = \left[\frac{\text{tert-butylcyclohexane, equatorial R group}}{\text{tert-butylcyclohexane, axial R group}}\right] = \frac{5039}{1}$$

$$\%\ \text{equatorial R group} = \left[\frac{5039}{1+5039}\right] x100 = 99.98\%$$

$$\%\ \text{axial R group} = \left[\frac{1}{1+5039}\right] x100 = 0.02\%$$