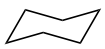
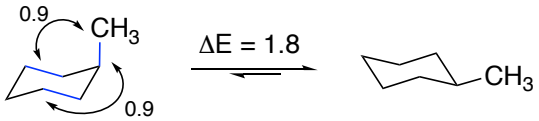
Conformational Analysis of Substituted Cyclohexanes



cyclohexane
$E_{rel} = 0$

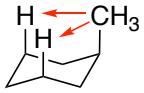
Interactions:
gauche = 0.9 kcal/mol
syn-pentane = 3.7 kcal/mol



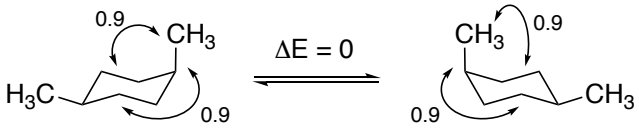
$E_{rel} = 0.9 \times 2$
$= 1.8$ kcal/mol

$E_{rel} = 0$

Rather than looking for "gauche" groups, it is often easier to count the number of 1,3-diaxial interactions between the substituent and hydrogens.



2 x 0.9 = 1.8 kcal/mol



$E_{rel} = 0.9 \times 2$
$= 1.8$ kcal/mol

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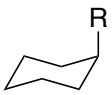
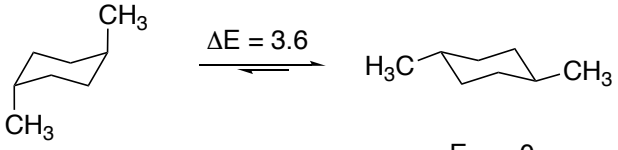
$= 1.8$ kcal/mol

Typical A-Values

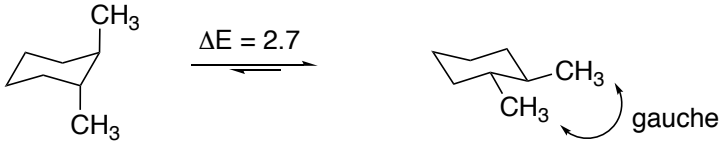
R	A-Value
F	0.25
Cl	0.53
Br	0.5
I	0.46
OH	0.7
OCH_3	0.75
NH_2	1.23
SH	1.21
CH_3	1.74
CH_2CH_3	1.79
$CH(CH_3)_2$	2.21
$C(CH_3)_3$	4.8
$CH{=}CH_2$	1.6
CHO	0.6
COOH	1.4
Ph	2.8





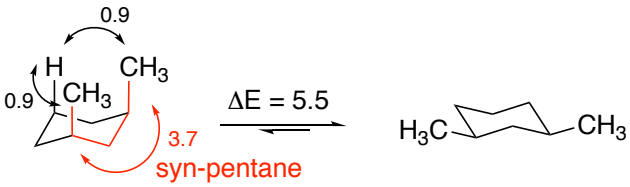
$E_{rel} = 0.9 \times 4$
$= 3.6$ kcal/mol

$E_{rel} = 0$



$E_{rel} = 0.9 \times 4$
$= 3.6$ kcal/mol

$E_{rel} = 1 \times 0.9$
$= 0.9$ kcal/mol



$E_{rel} = 0.9 \times 2 + 3.7$
$= 5.5$ kcal/mol

$E_{rel} = 0$