


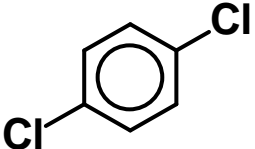
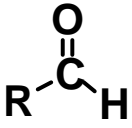
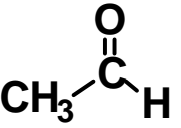
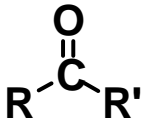
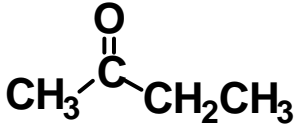
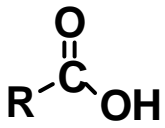
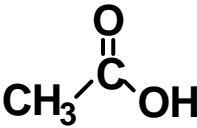
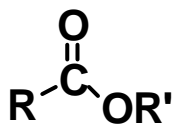
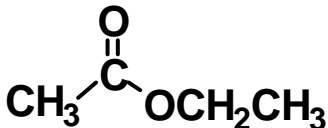


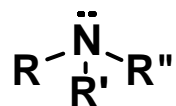
# Chapter 2

## Organic Compounds

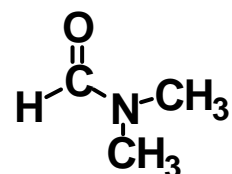
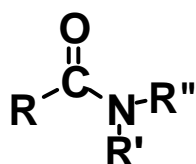
### Classification by Functional Group

Class	Functional Group	Example
Alkane	R-H	CH <sub>3</sub> CH <sub>3</sub>
Alkene		CH <sub>3</sub> -CH=CH <sub>2</sub>
Alkyne		CH <sub>3</sub> -C≡C-H
Aromatic		
Alkyl halide	R-X, X = F, Cl, Br, I	CH <sub>3</sub> CH <sub>2</sub> Cl
Alcohol	R-OH	CH <sub>3</sub> CH <sub>2</sub> OH
Ether	R-O-R	CH <sub>3</sub> CH <sub>2</sub> -O-CH <sub>2</sub> CH <sub>3</sub>
Aldehyde		
Ketone		
Carboxylic acid		
Ester		

Amine



Amide



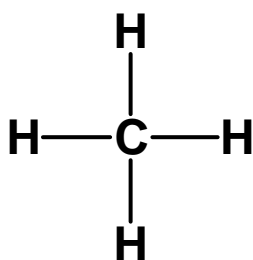
## Alkanes

### *Saturated hydrocarbons (Aliphatic)*

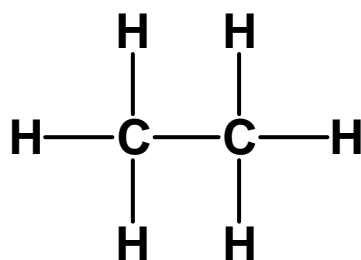
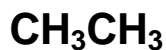
- Hydrocarbons – Contain only C and H atoms.
- Saturated – Only single bonds.
- Aliphatic – “Fat” like.

Can be acyclic (no rings) or cyclic (cycloalkanes)

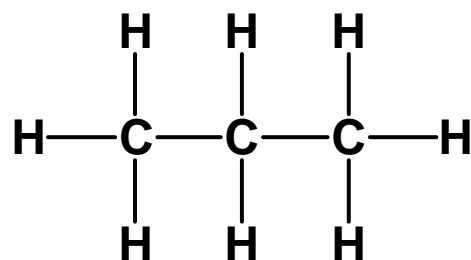
Methane

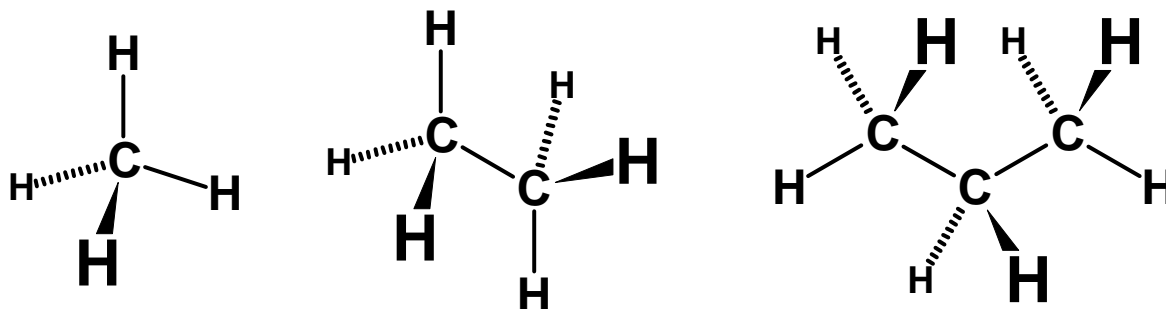


Ethane



Propane





Name	Formula
Methane	CH <sub>4</sub>
Ethane	CH <sub>3</sub> CH <sub>3</sub>
Propane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>
Butane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>
Pentane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>
Hexane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>
Heptane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>
Octane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>
Nonane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>
Decane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>

### Isomerism

Starting with C<sub>4</sub>H<sub>10</sub> Isomers are possible.  
Compare the hydrogens in propane, we have two different ones.



Normal Butane

Isobutane

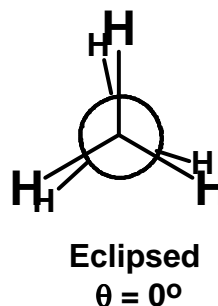
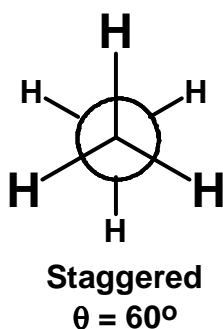
***Constitutional Isomers***

**Isomerism:** The phenomenon whereby certain chemical compounds have structures that are different although the compounds possess the same elemental composition.

**Isomers:** Two or more chemical substances having the same elementary composition and molecular weight but differing in structure.

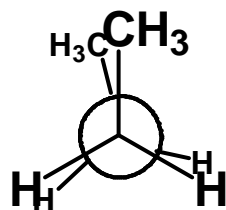
### Conformational Isomers

#### Ethane



$$\Delta G^\ddagger \sim 3 \text{ kcal/mol}$$

#### Butane



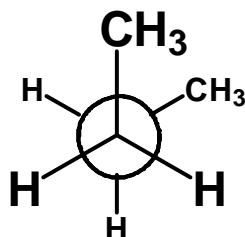
$\theta$

$0^\circ$

*syn-periplanar*

$\Delta G^\circ$

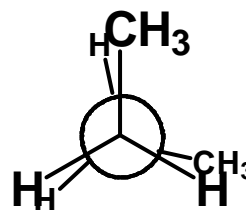
6.1 kcal/mol



$60^\circ$

*syn-clinal (gauche)*

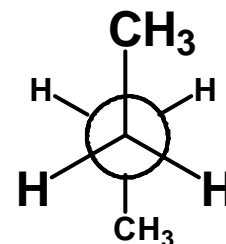
0.9 kcal/mol



$120^\circ$

*anti-clinal*

3.4 kcal/mol



$180^\circ$

*anti-periplanar (trans)*

0 kcal/mol

## Nomenclature of Alkanes

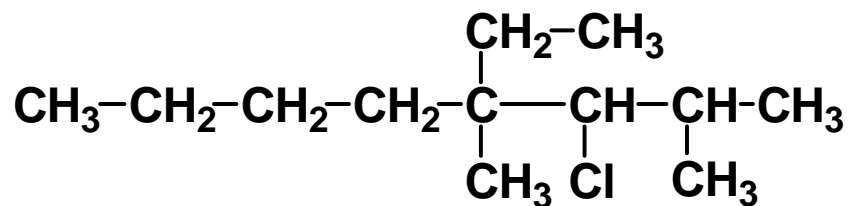
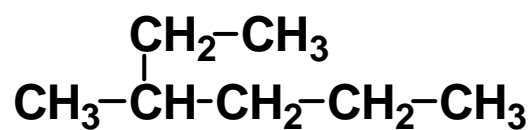
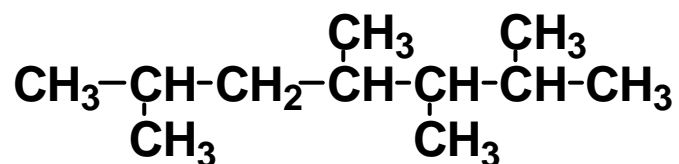
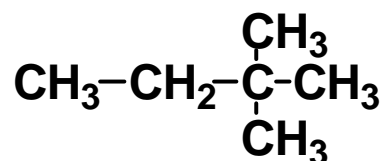
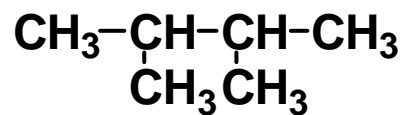
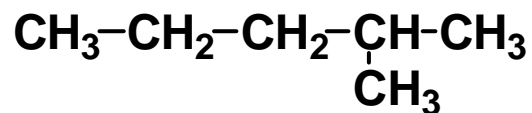
### Names and Formulas of Selected Alkyl Groups

Formula	Name	Formula	Name
CH <sub>3</sub> -	methyl	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> -	<i>n</i> -butyl
CH <sub>3</sub> CH <sub>2</sub> -	ethyl	(CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> -	isobutyl
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> -	<i>n</i> -propyl	CH <sub>3</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )-	sec-butyl
(CH <sub>3</sub> ) <sub>2</sub> CH-	isopropyl	(CH <sub>3</sub> ) <sub>3</sub> C-	tert-butyl

## IUPAC Rules for Naming Alkanes

1. Select the longest continuous chain of carbon atoms as the parent compound.
2. Number the carbon atoms in the parent carbon chain starting from the end closest to the first carbon atom that has an alkyl or other group.
3. Name the alkyl group and designate the position on the parent carbon chain by a number.
4. When the same alkyl group branch chain occurs more than once, indicate this repetition by a prefix (*di-*, *tri-*, *tetra-*, and so forth).
5. When several different alkyl groups are attached to the parent compound, list them in alphabetical order.

Examples: Name the following compounds:



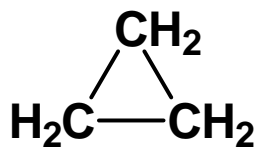
**Examples: Write structural formulas for the following:**

**3-ethylpentane**

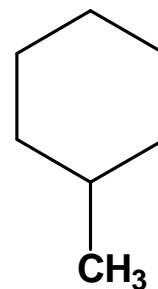
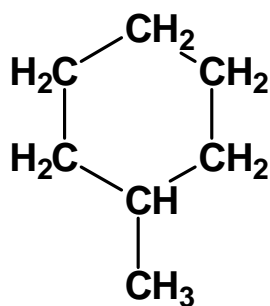
**2,2,4-trimethylpentane**

- **Primary C**
- **Secondary C**
- **Tertiary C**
- **Quaternary C**

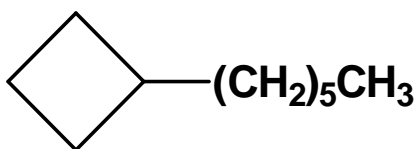
# Cycloalkanes



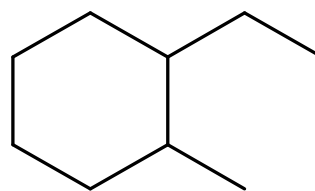
**Cyclopropane**



**Methylcyclohexane**

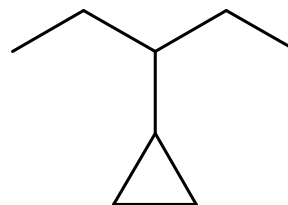
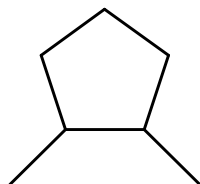
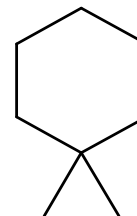


**1-Cyclobutylhexane**

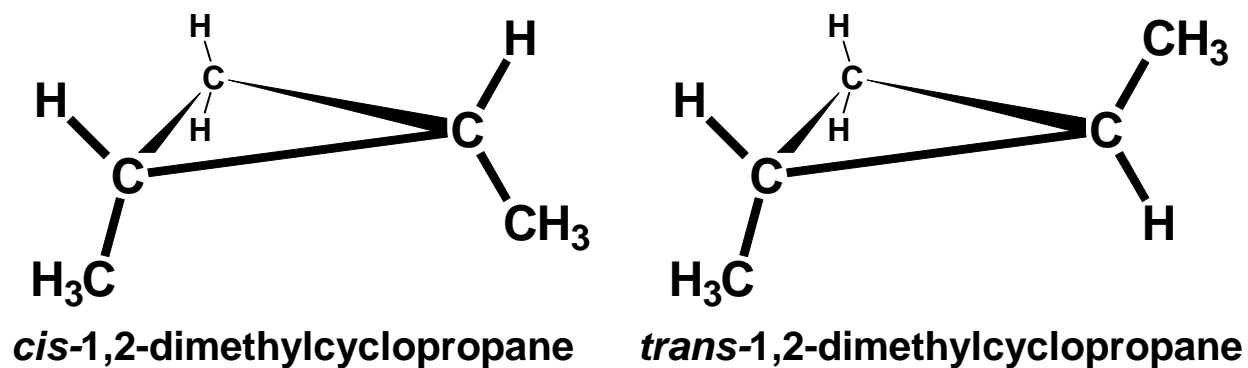


**1-Ethyl-2-methylcyclohexane**

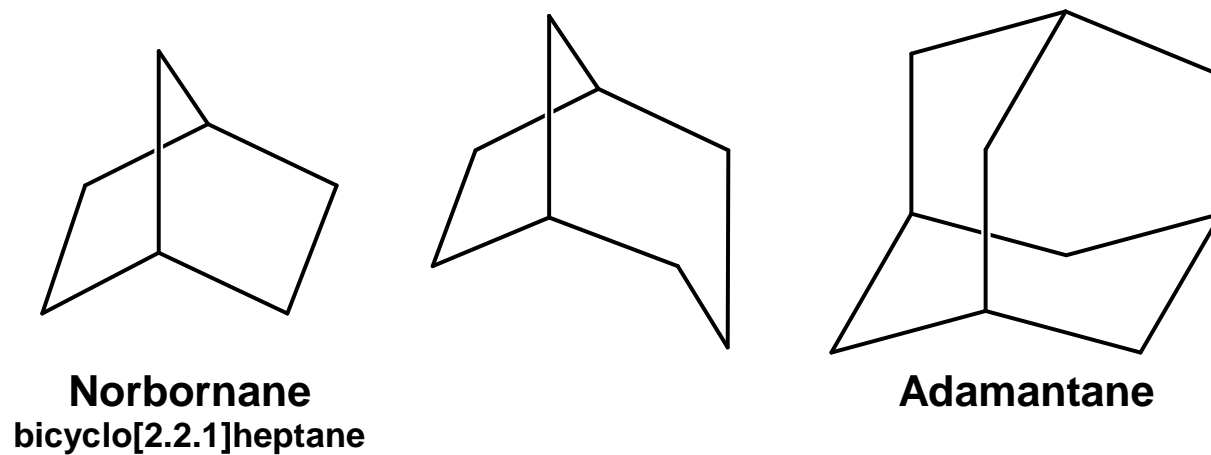
**Name the following compounds:**



## *cis-trans* Isomerism in Cycloalkanes

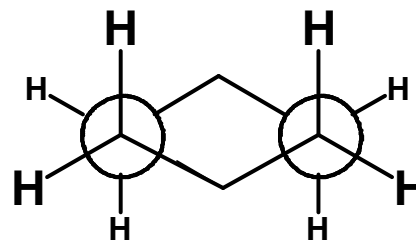
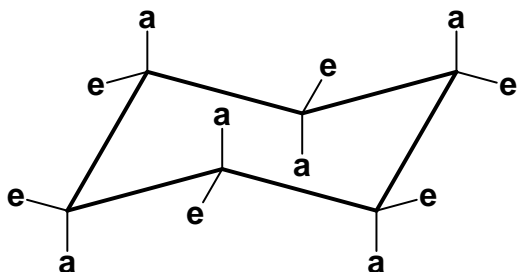


## Polycyclic Alkanes



## Conformations of Cyclohexane

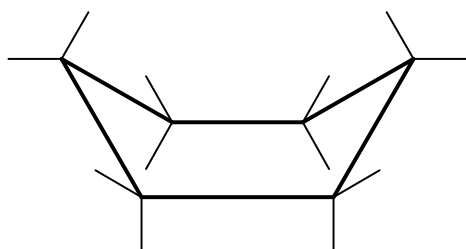
### “chair” (rigid) form



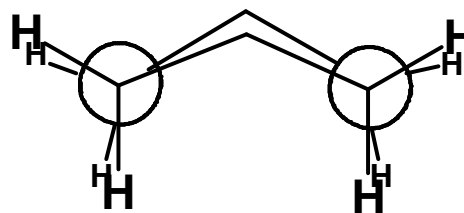
Free of torsional strain (Pitzer strain). All bonds are staggered.

Free of ring strain (Baeyer strain). All bond angles are  $\sim 109.5^\circ$ .

### “boat” form

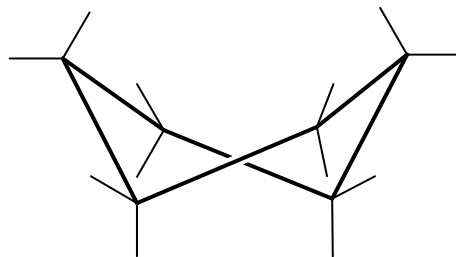


Transannular 1,4 steric interactions



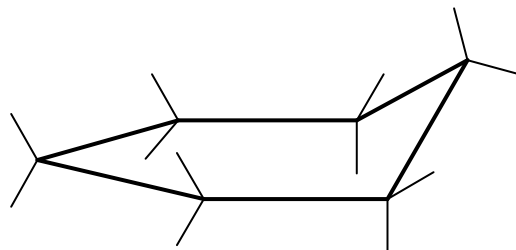
Eclipsing

### “twist”, “twist-boat”, “skew” (flexible) form

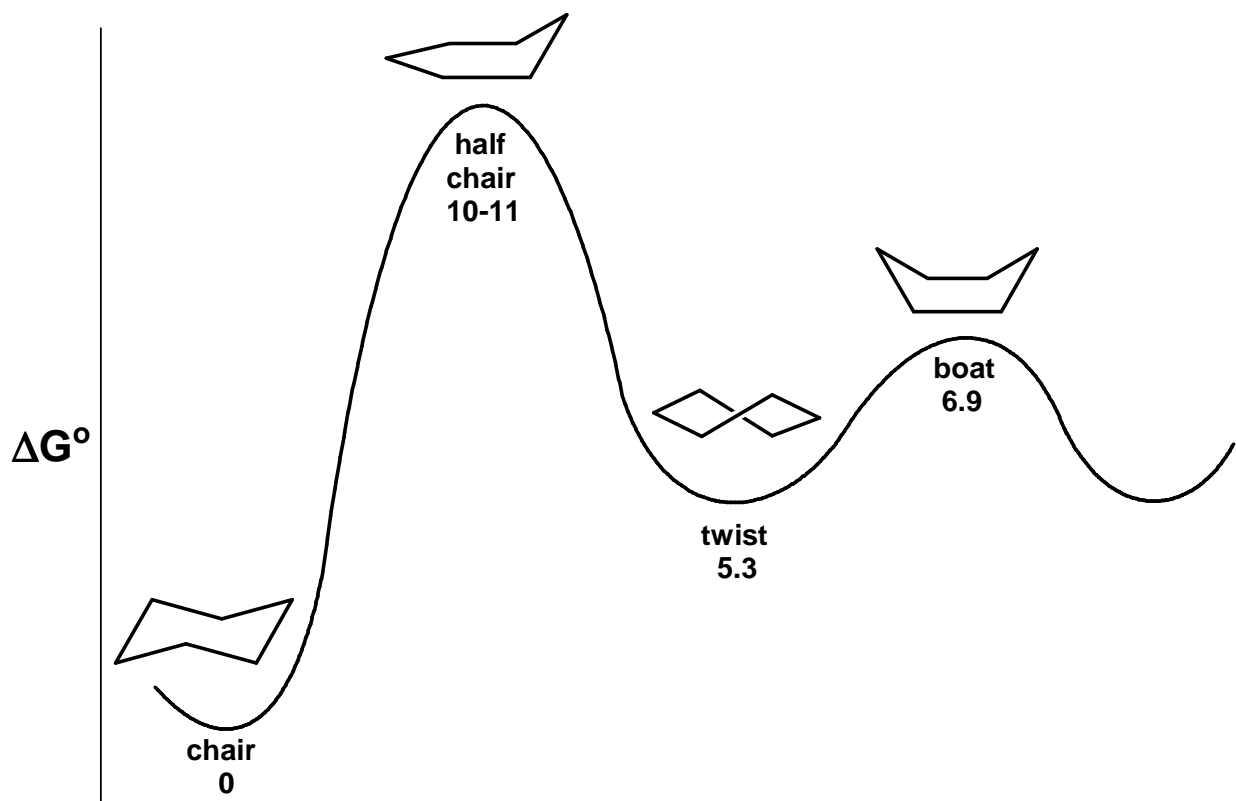


Avoids eclipsing, avoids 1,4 interactions.

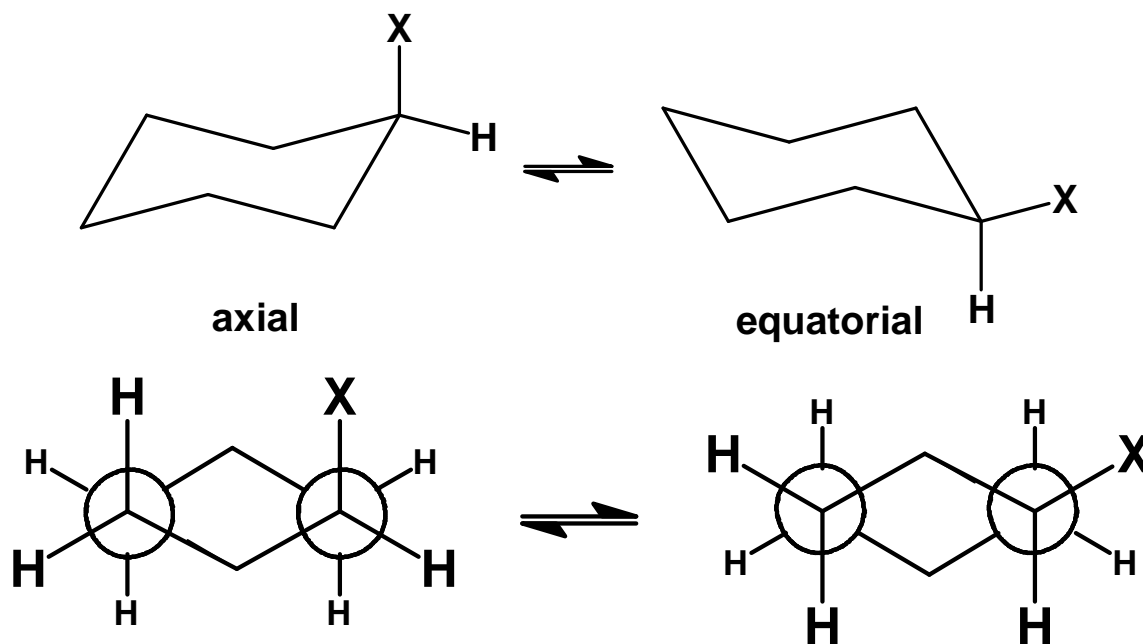
## “half-chair” or “chaise longue” form



Severe torsional strain (eclipsing).  
Severe angle deformation strain  
( $\sim 120^\circ$ , *NOT*  $109.5^\circ$ ).



## Monosubstituted Cyclohexanes



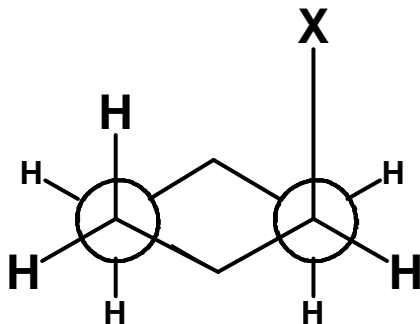
The **CONFORMATIONAL ENERGY** of a substituent, X, is the excess energy of the axial conformation over the equatorial conformation.

Table of Conformational Energies

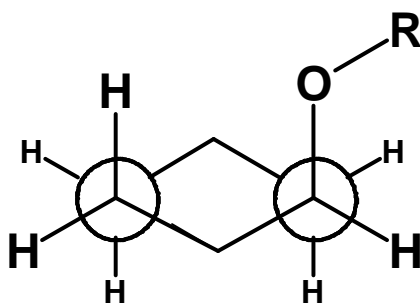
Atom or Group	$-\Delta G^\circ$ (kcal/mol)	Atom or Group	$-\Delta G^\circ$ (kcal/mol)
F	0.15	OH (protic)	0.87
Cl	0.43	OCH <sub>3</sub>	0.60
CN	0.17	OCH <sub>2</sub> CH <sub>3</sub>	0.94
CH <sub>3</sub>	1.70	NH <sub>2</sub> (protic)	1.60
CH <sub>2</sub> CH <sub>3</sub>	1.75	NHMe	1.0
CH(CH <sub>3</sub> ) <sub>2</sub>	2.15	NMe <sub>2</sub>	2.1
C(CH <sub>3</sub> ) <sub>3</sub>	>5.0 (ca. 12.0)	NO <sub>2</sub>	1.10
C <sub>6</sub> H <sub>5</sub>	3.0	SH	0.9
COOH	1.35	SCH <sub>3</sub>	0.7
CO <sub>2</sub> Et	1.20	HgBr	0.0

**Some interesting points:**

- ◆ Little change going from  $F \rightarrow Cl \rightarrow Br \rightarrow I$
- ◆ Little change going from  $OH \rightarrow SH \rightarrow HgBr$



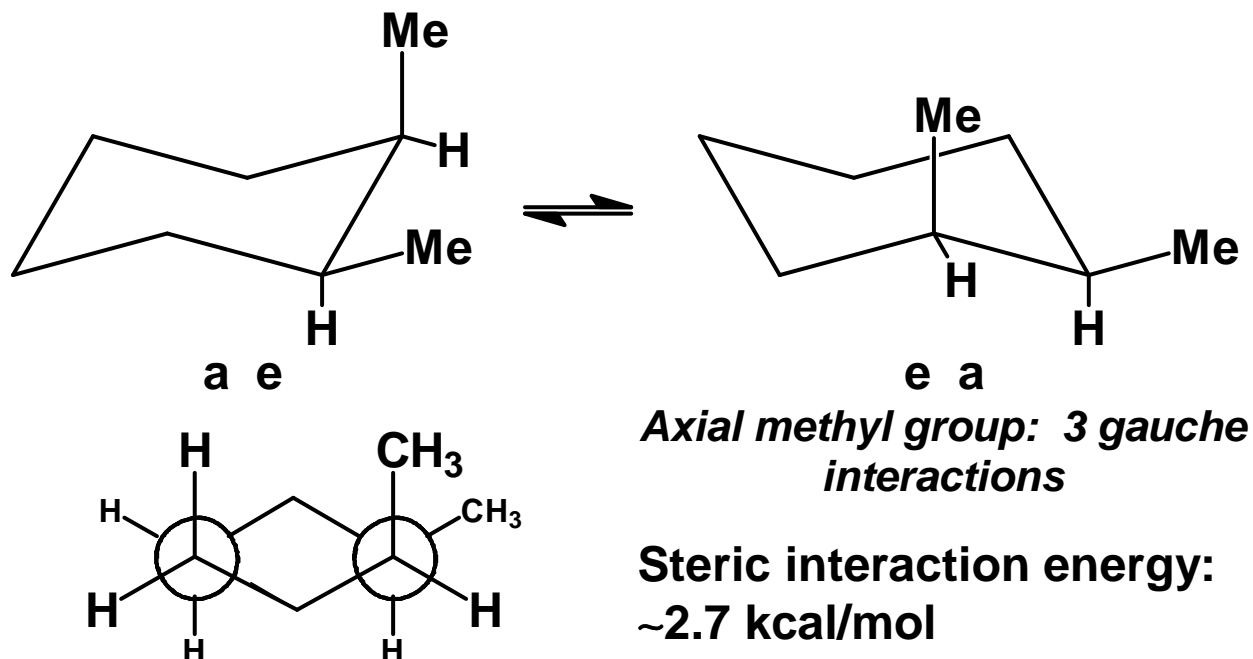
- ◆ Little change going from  $OH \rightarrow OMe \rightarrow OEt$



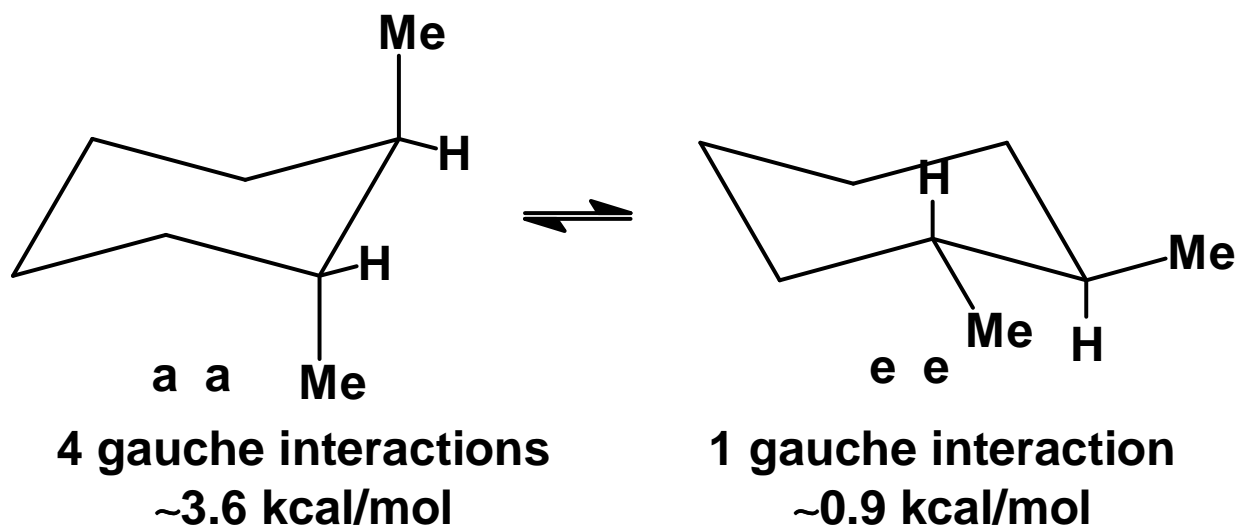
- ◆ But,  $CH_3 \rightarrow CH_2CH_3 \rightarrow CH(CH_3)_2 \rightarrow C(CH_3)_3$

## Disubstituted Cyclohexanes

### *cis*-1,2-Dimethylcyclohexane

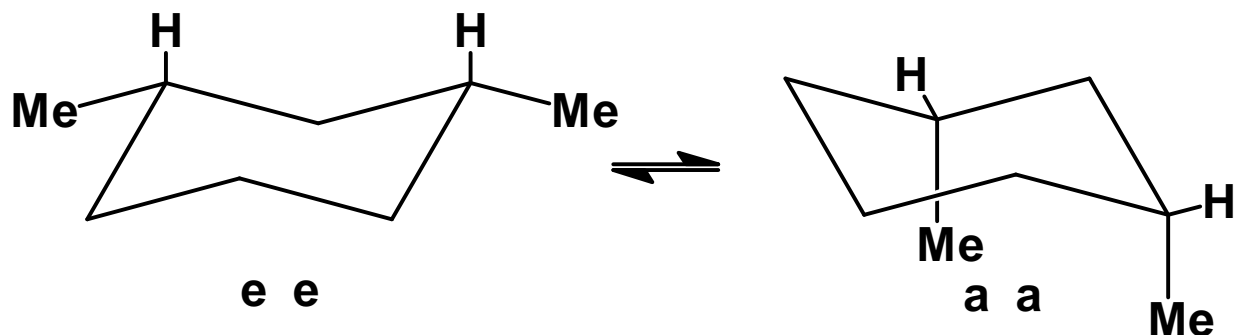


### *trans*-1,2-Dimethylcyclohexane



$$\Delta E \sim 2.7 \text{ kcal/mol}$$

So, equilibrium strongly favors **e e** over **a a**.

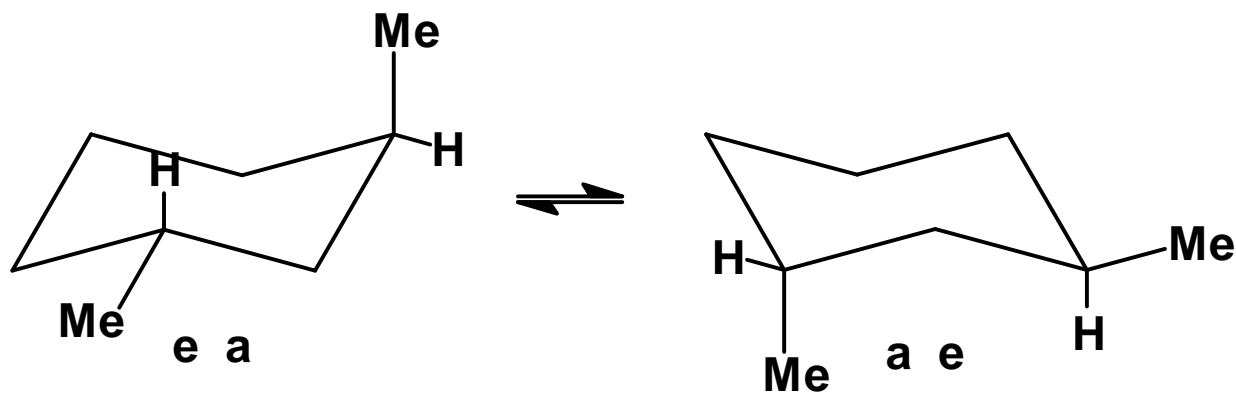
***cis*-1,3-Dimethylcyclohexane**

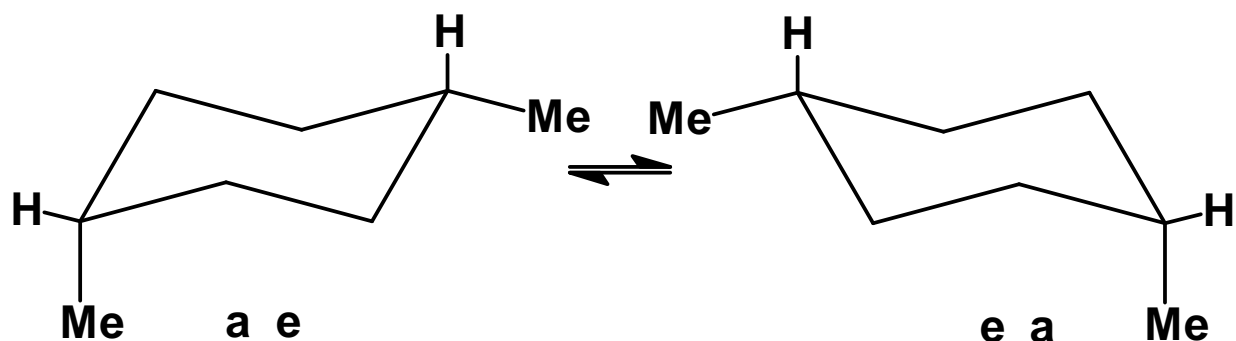
0 gauche interactions

4 gauche interactions  
(3.6 kcal/mol)+ 1,3-diaxial interaction  
(~1.9 kcal/mol)

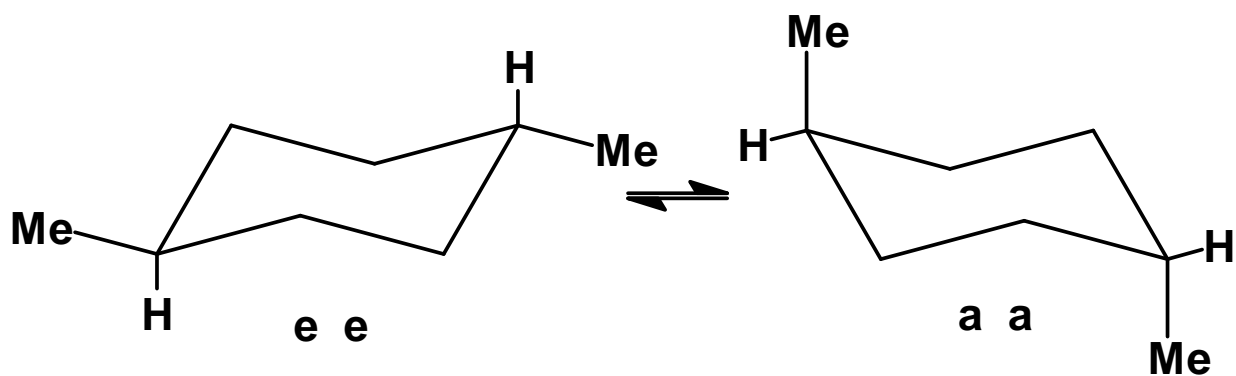
= ~5.5 kcal/mol

0

***trans*-1,3-Dimethylcyclohexane**2 gauche interactions  
~1.8 kcal/mol

***cis*-1,4-Dimethylcyclohexane**

2 gauche interactions  
~1.8 kcal/mol

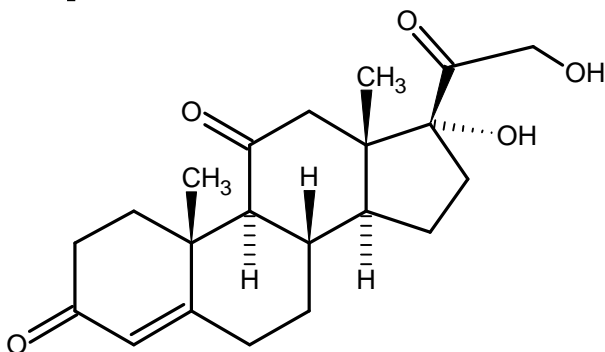
***trans*-1,4-Dimethylcyclohexane**

0 gauche interactions

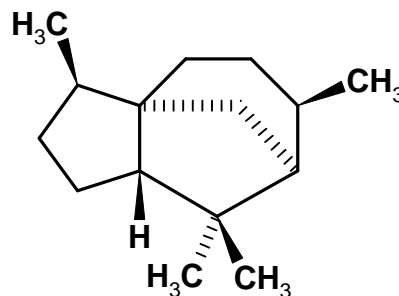
4 gauche interactions  
~3.6 kcal/mol

## Polycyclic Ring systems:

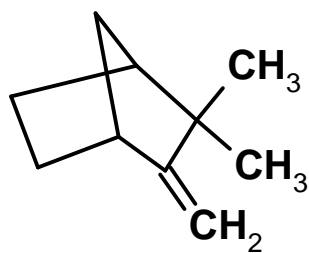
These compounds are very common in terpenes and steroids.



**cortisone**



**cedrane**



**camphene**