

## 3.12

### Disubstituted Cycloalkanes: Stereoisomers

Stereoisomers are isomers that have same constitution but different arrangement of atoms in space

*Isomers*

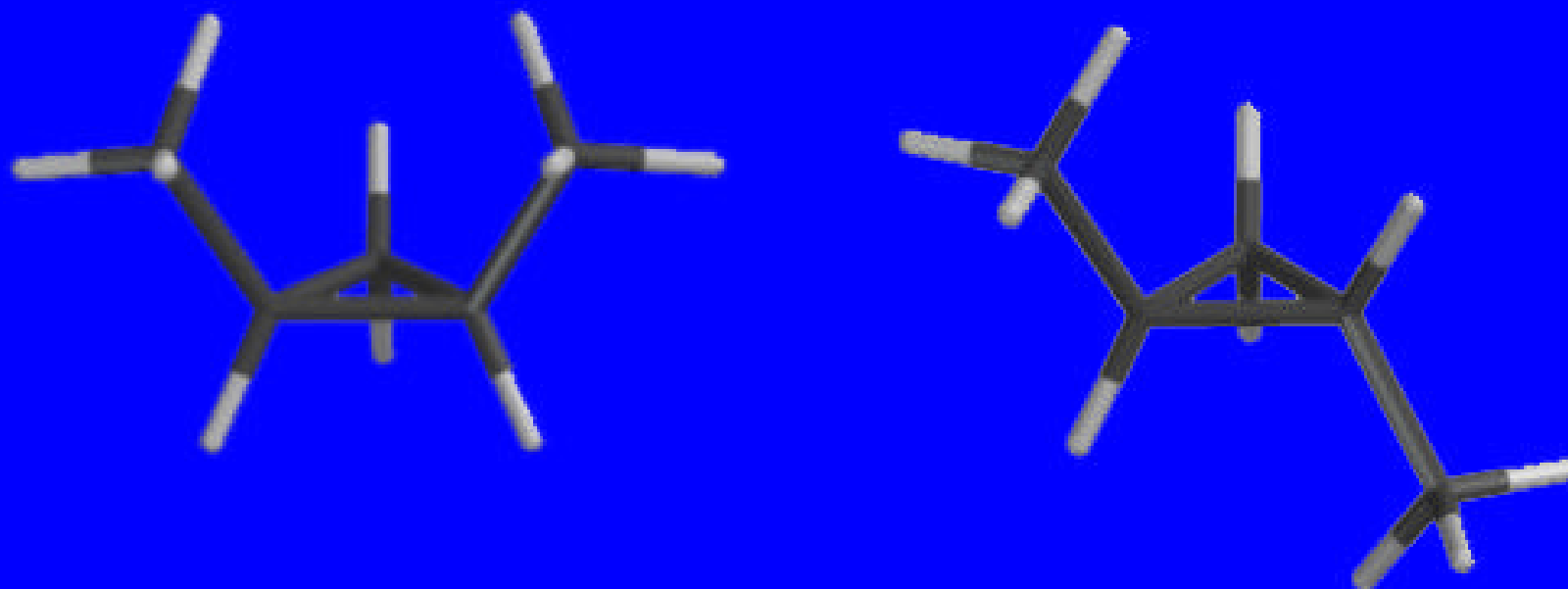
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graph TD; A[Isomers] --> B[Constitutional isomers]; A --> C[Stereoisomers];
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The diagram is a simple tree structure. At the top is a cyan box labeled 'Isomers'. A vertical yellow line descends from the bottom center of this box. This line meets a horizontal yellow line that branches out to the left and right. From the left end of this horizontal line, a vertical yellow line descends to a green box labeled 'Constitutional isomers'. From the right end of the horizontal line, a vertical yellow line descends to an orange box labeled 'Stereoisomers'. All boxes have a black drop shadow.

*Constitutional isomers*

*Stereoisomers*

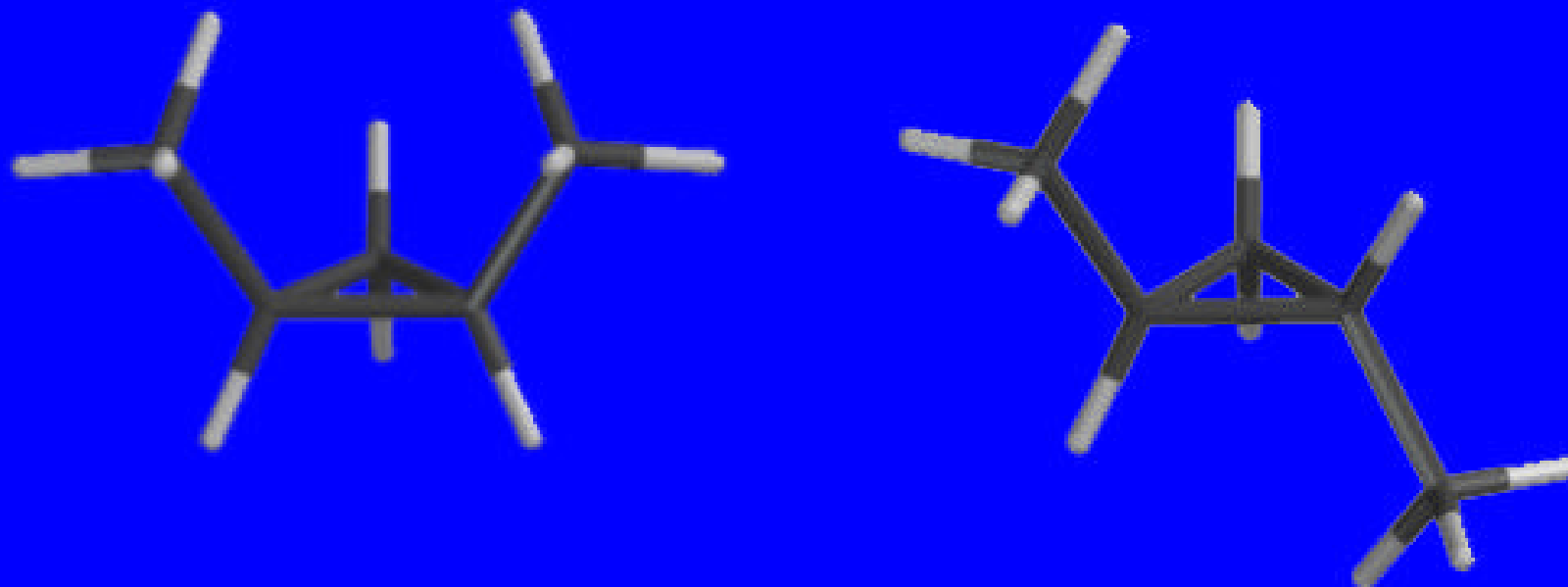
## *1,2-Dimethylcyclopropane*



There are two stereoisomers of  
1,2-dimethylcyclopropane.

They differ in spatial arrangement of atoms.

## 1,2-Dimethylcyclopropane



*cis*-1,2-Dimethylcyclopropane has methyl groups on same side of ring.

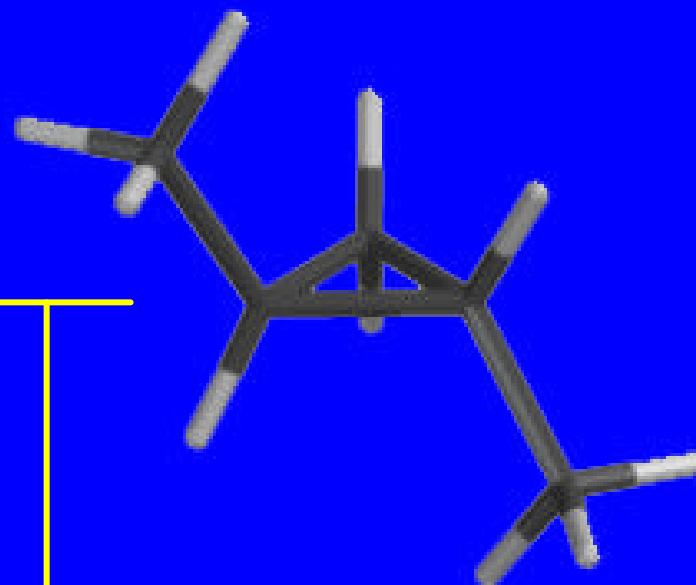
*trans*-1,2-Dimethylcyclopropane has methyl groups on opposite sides.

Relative stabilities of stereoisomers may be determined from heats of combustion.

van der Waals strain makes cis stereoisomer less stable than trans



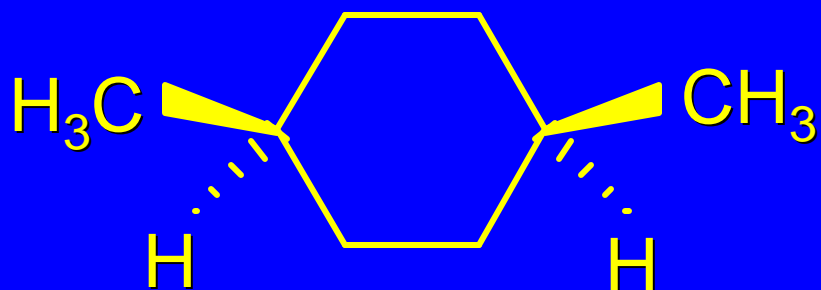
3371 kJ/mol



3366 kJ/mol

3.13  
Conformational Analysis  
of Disubstituted Cyclohexanes

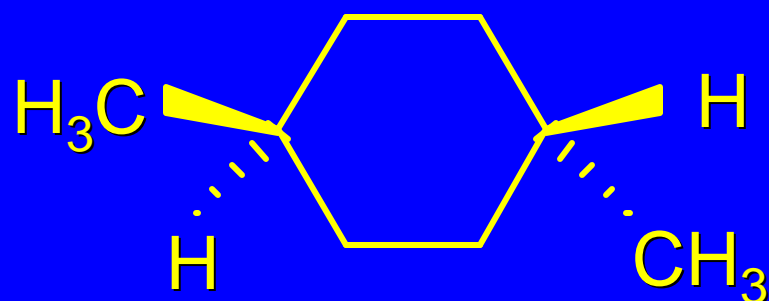
## 1,4-Dimethylcyclohexane Stereoisomers



cis

5219 kJ/mol

less stable



trans

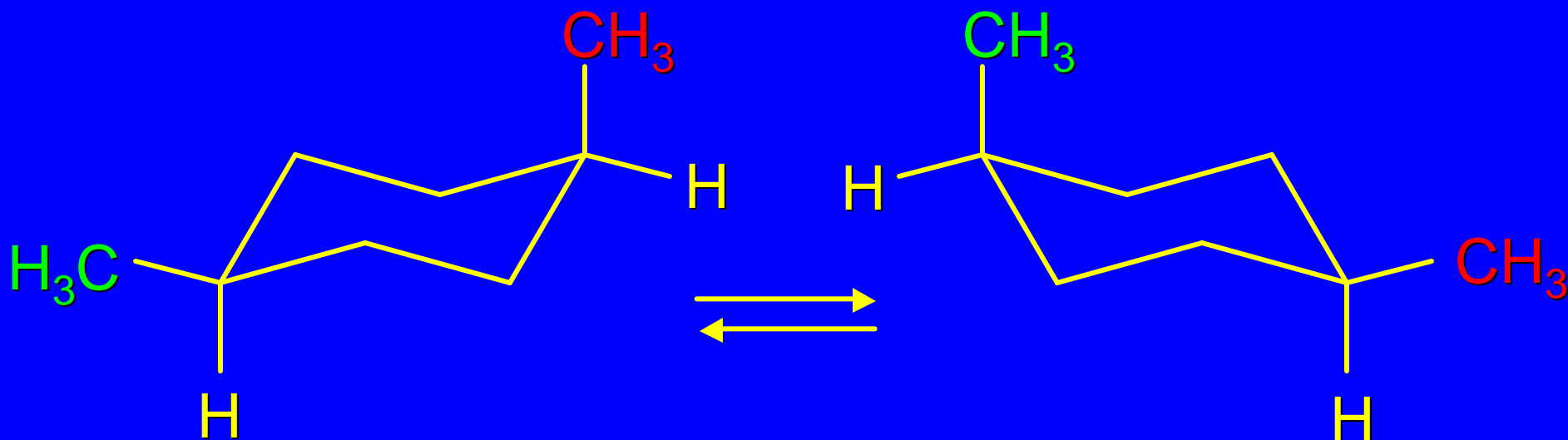
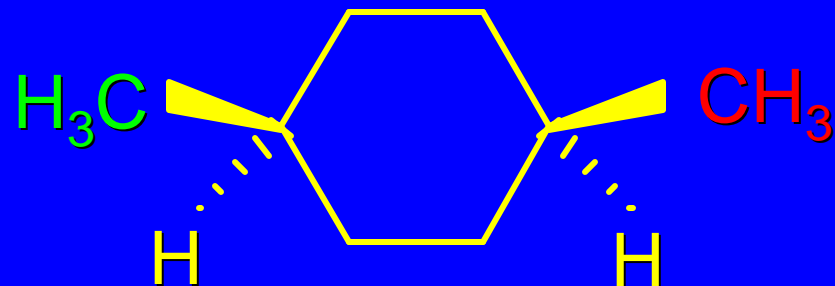
5212 kJ/mol

more stable

Trans stereoisomer is more stable than cis, but methyl groups are too far apart to crowd each other.

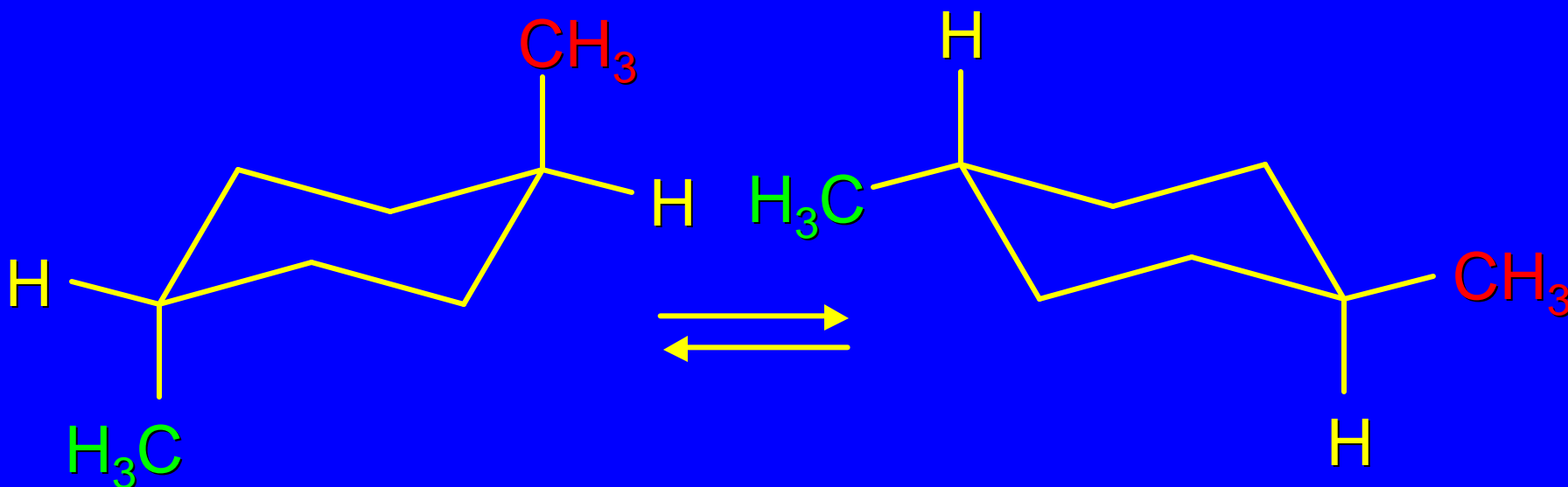
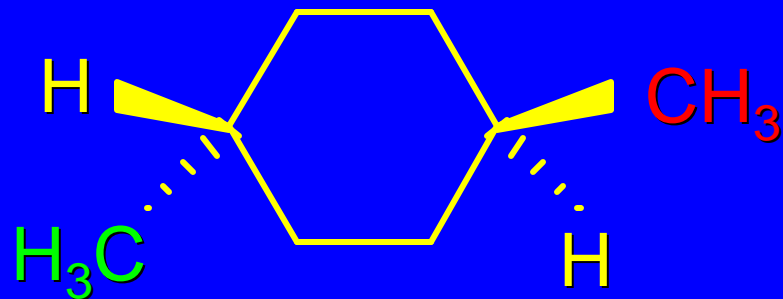


Conformational analysis of  
*cis*-1,4-dimethylcyclohexane



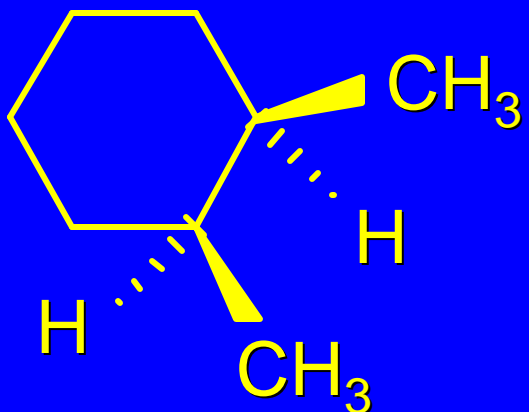
Two equivalent conformations; each has one axial methyl group and one equatorial methyl group

Conformational analysis of  
*trans*-1,4-dimethylcyclohexane



Two conformations are not equivalent; most stable conformation has both methyl groups equatorial.

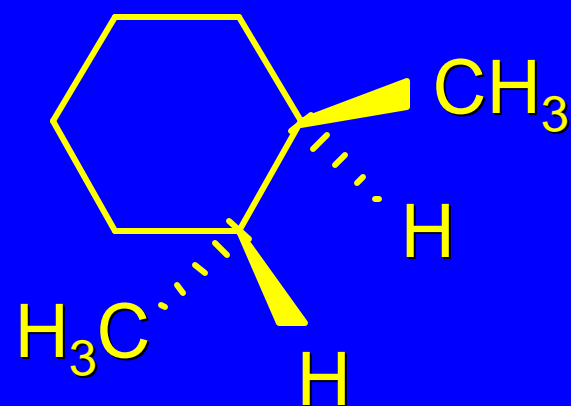
## 1,2-Dimethylcyclohexane Stereoisomers



cis

5223 kJ/mol

less stable



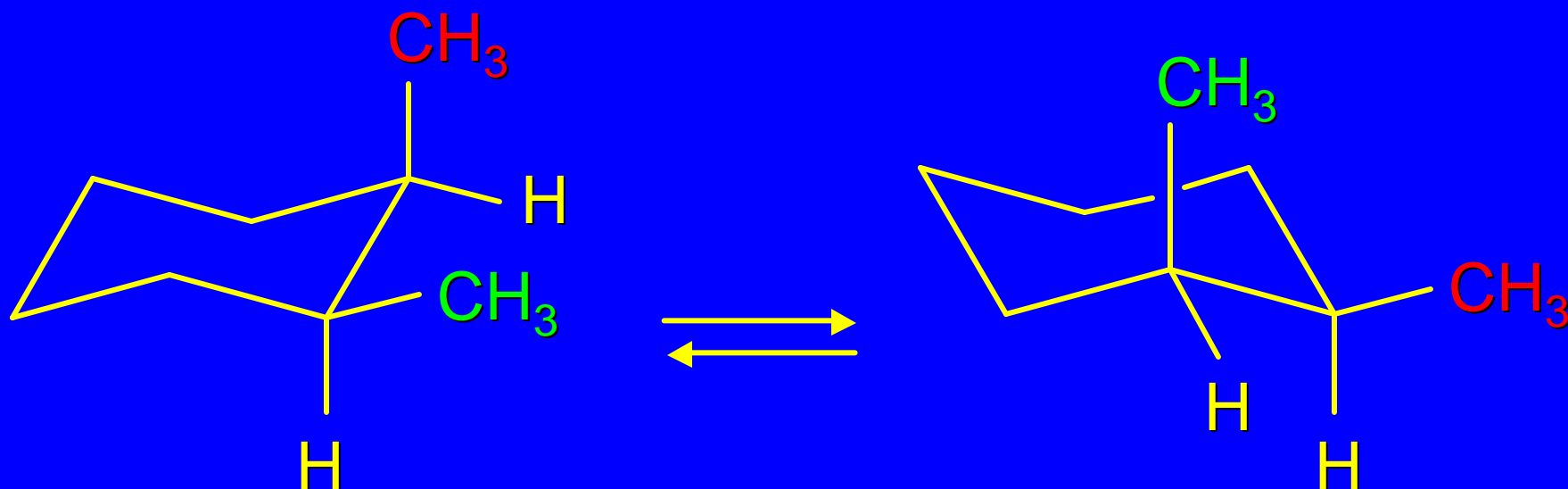
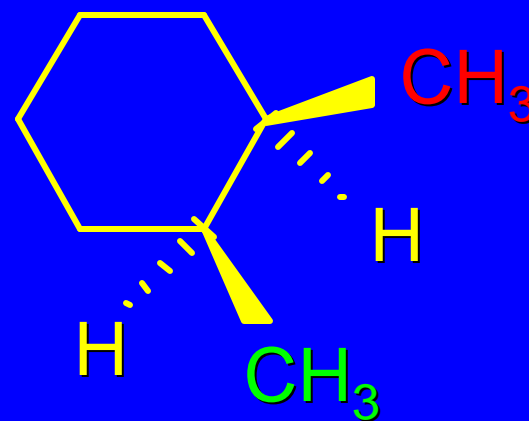
trans

5217 kJ/mol

more stable

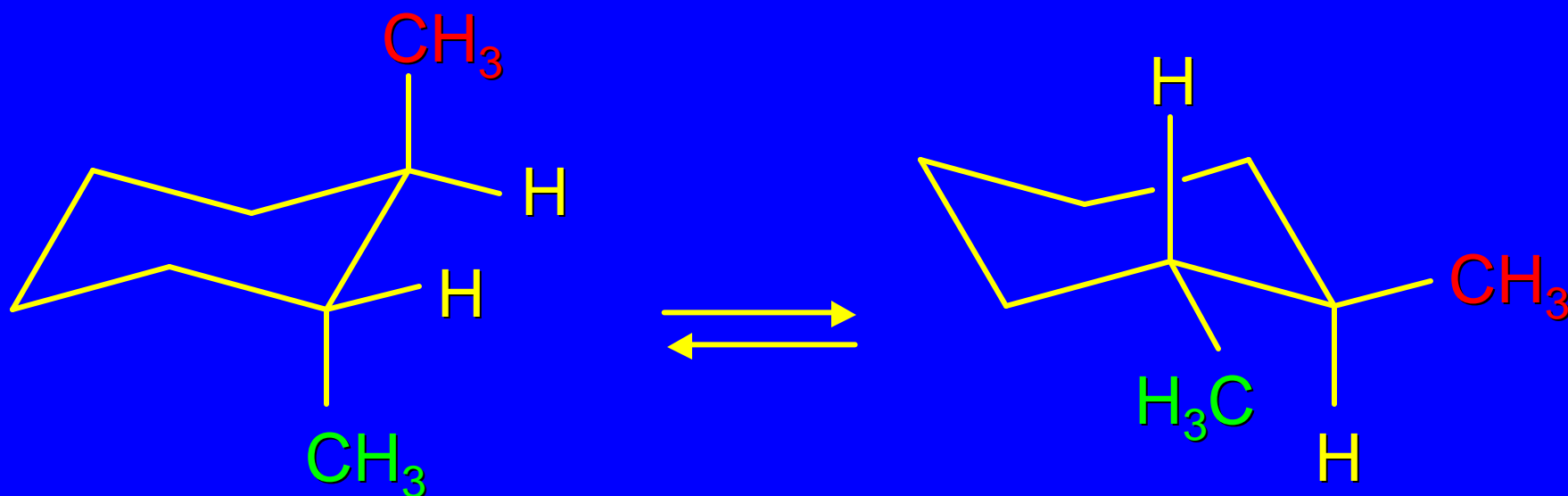
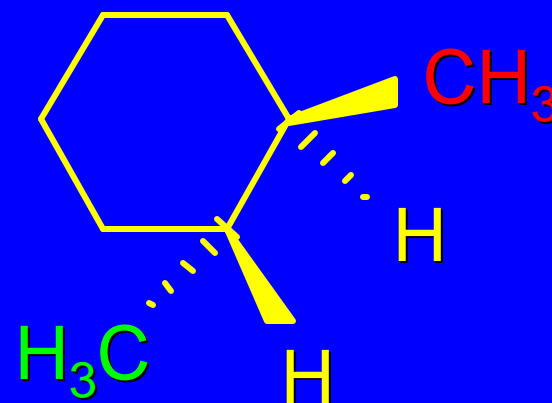
Analogous to 1,4 in that trans is more stable than cis.

Conformational analysis of *cis*-1,2-dimethylcyclohexane



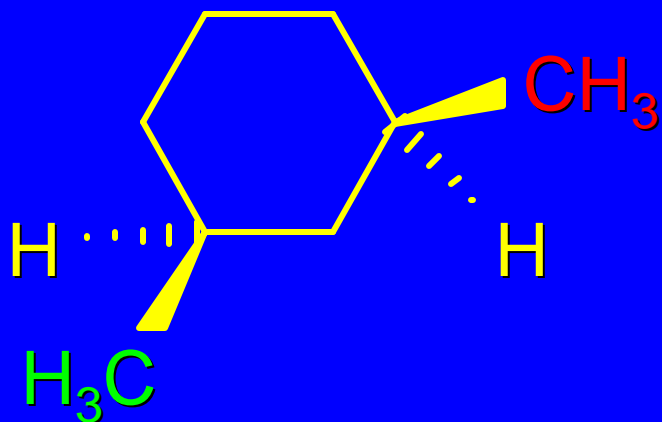
Two equivalent conformations; each has one axial methyl group and one equatorial methyl group

Conformational analysis of  
*trans*-1,2-dimethylcyclohexane



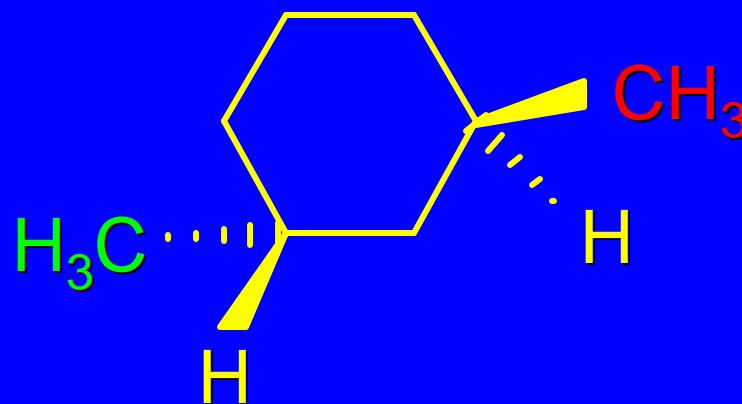
Two conformations are not equivalent; most stable conformation has both methyl groups equatorial.

## 1,3-Dimethylcyclohexane Stereoisomers



cis

5212 kJ/mol  
more stable

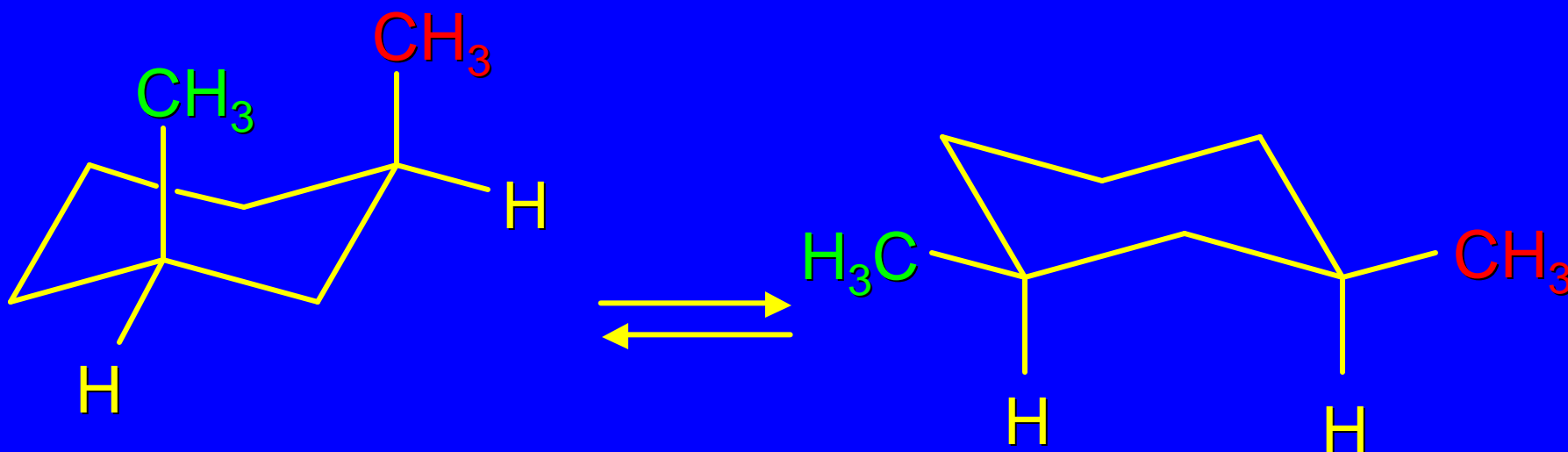
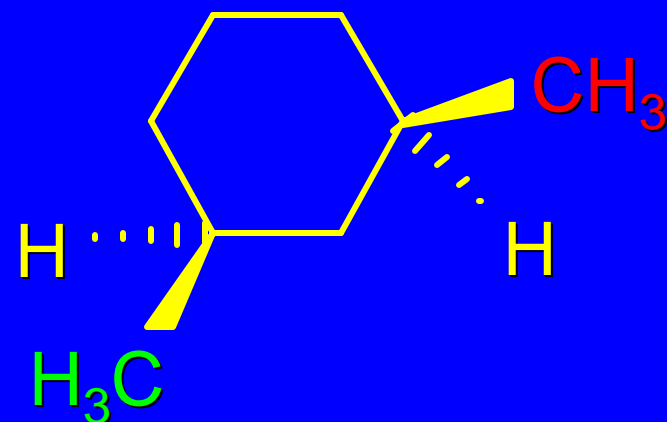


trans

5219 kJ/mol  
less stable

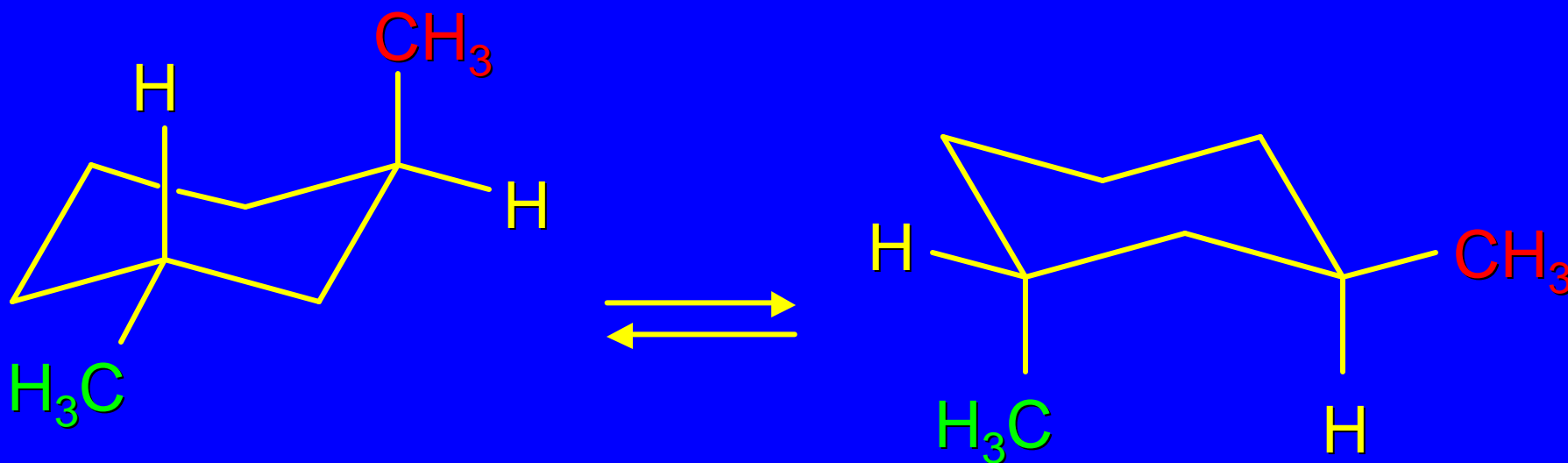
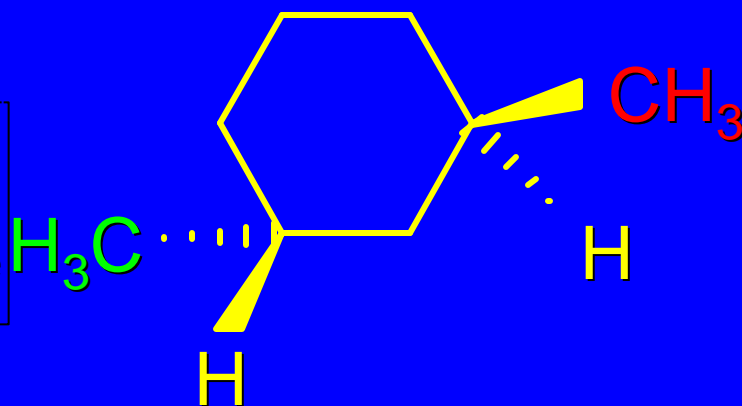
Unlike 1,2 and 1,4; cis-1,3 is more stable than trans.

Conformational analysis of *cis*-1,3-dimethylcyclohexane



Two conformations are not equivalent; most stable conformation has both methyl groups equatorial.

Conformational analysis of  
*trans*-1,3-dimethylcyclohexane



Two equivalent conformations; each has one axial and one equatorial methyl group.



Table 3.2 Heats of Combustion of Isomeric Dimethylcyclohexanes

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Compound	Orientation	$-\Delta H^\circ$
<i>cis</i> -1,2-dimethyl	ax-eq	5223
<i>trans</i> -1,2-dimethyl	eq-eq	5217*
<i>cis</i> -1,3-dimethyl	eq-eq	5212*
<i>trans</i> -1,3-dimethyl	ax-eq	5219
<i>cis</i> -1,4-dimethyl	ax-eq	5219
<i>trans</i> -1,4-dimethyl	eq-eq	5212*

\*more stable stereoisomer of pair