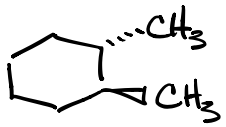
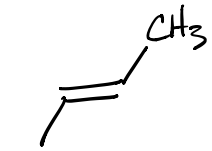
Organic Chemistry Lecture

Monday March 30, 2020

- Determining the lowest energy conformation of Cyclohexane derivatives.
- Moving from 2D- line drawings to Haworth to 3D-Chair Conformations and assessing 1,3-diaxial interactions and goache interactions in Newman projections.

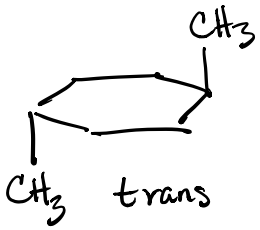


trans-1,2-dimethylcyclohexane

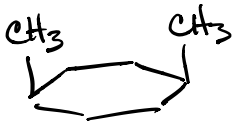


trans

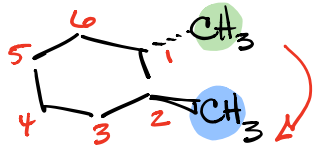
Cis



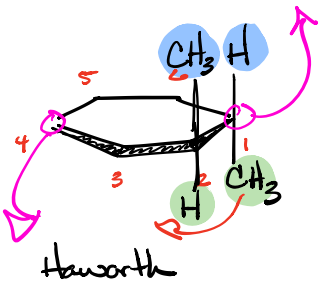
trans



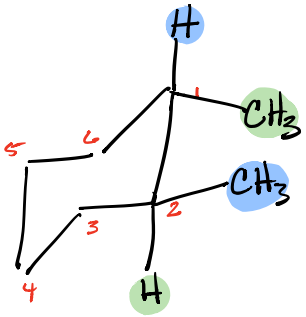
Cis



2D line drawing

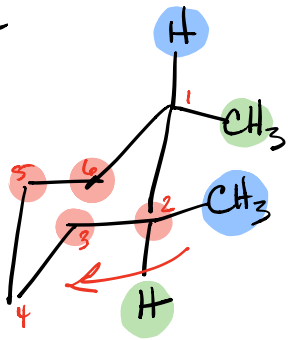


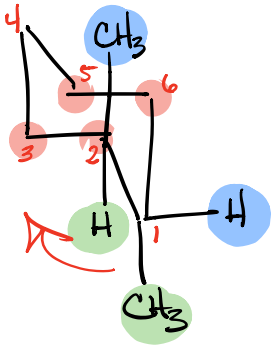
Haworth



Hash Back in Space

Wedge forward in Space

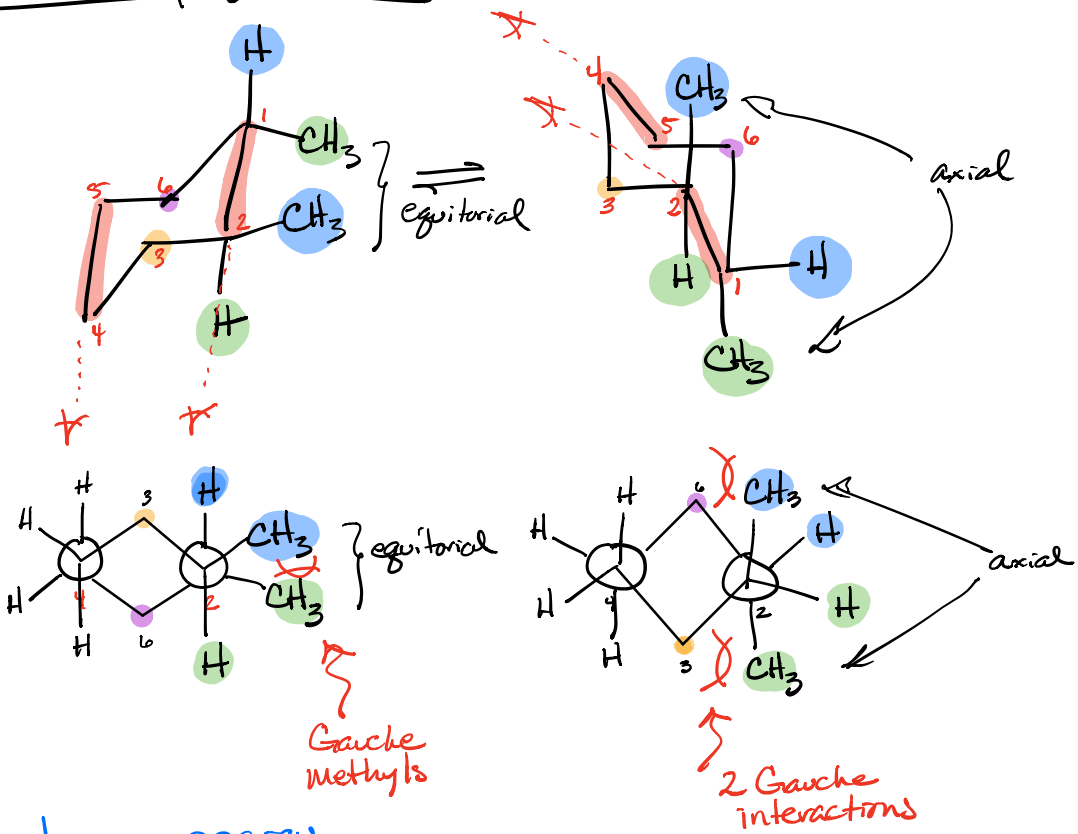




Two important factors to Consider

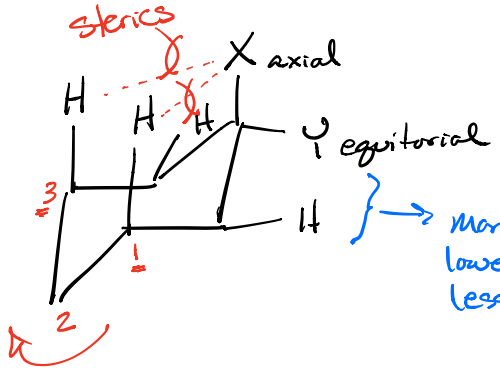
- # of Gauche interactions vs. anti in Newman projection
- 1,3-diaxial interaction in Chair Conformations

Newman projections



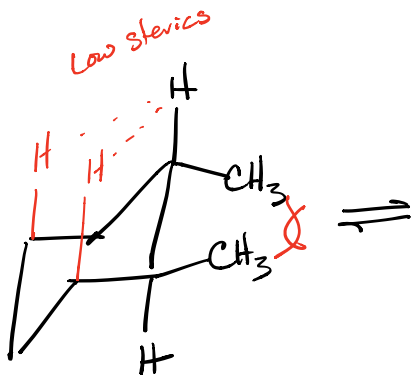
Lower energy due to decreased # of Gauch interactions

1,3-Diaxial Interactions



Sterics is a repulsive force that increase molecular energy.

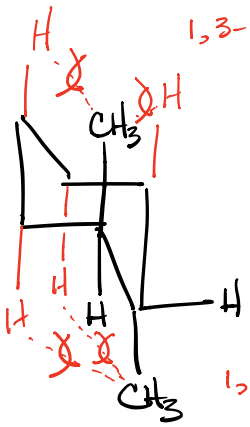
→ more space
lower energy
less sterics



no 1,3-diaxial

1 - Gauch between methyls

Lower Energy Conformation



→ Sterics

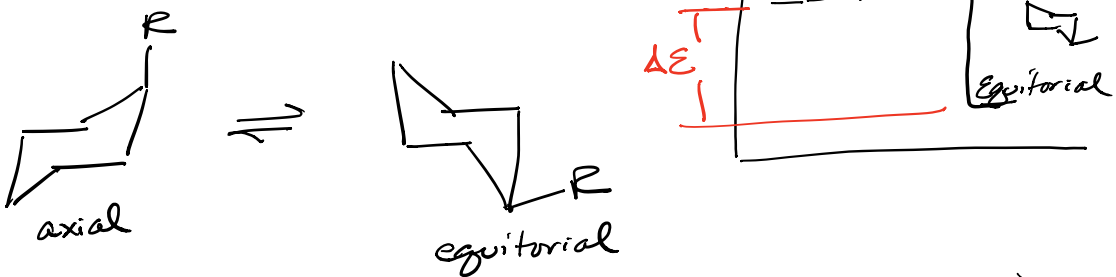
1,3-diaxial

2 1,3-diaxial w/ methyls

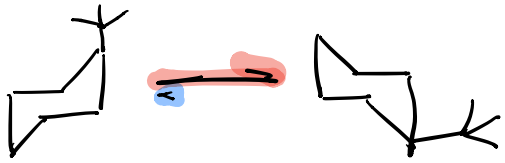
2 Gauche interactions w/ methyls & Ring (Newman)

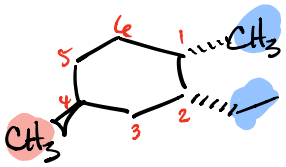
A-Values

% of Molecules w/ Substituent in the equitorial Orientation



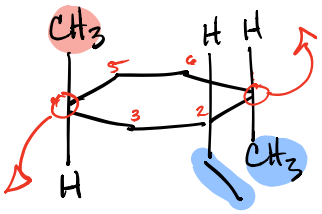
R Group	% molecules in equitorial (A-value)
– F	60%
– Cl	70%
– OH	83%
– CH_3	95%
Ethyl	96%
– ipr	97%
– ^tBu	99.9% Locking Group

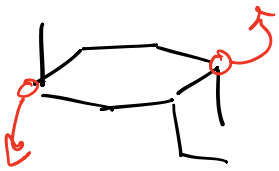


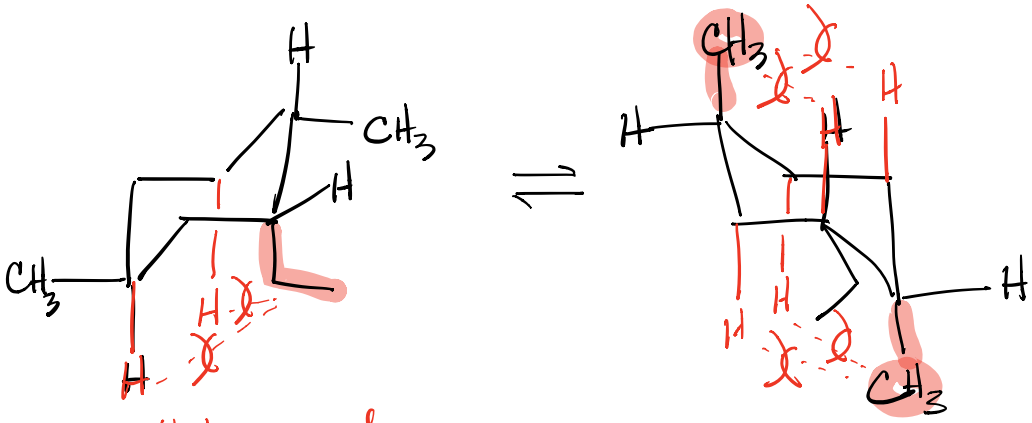


Draw the lowest energy chair conformation for the molecule shown to the left.

① 2D → ② Haworth → ③ Chair → ④ Newman
1,3-diaxial Gauche



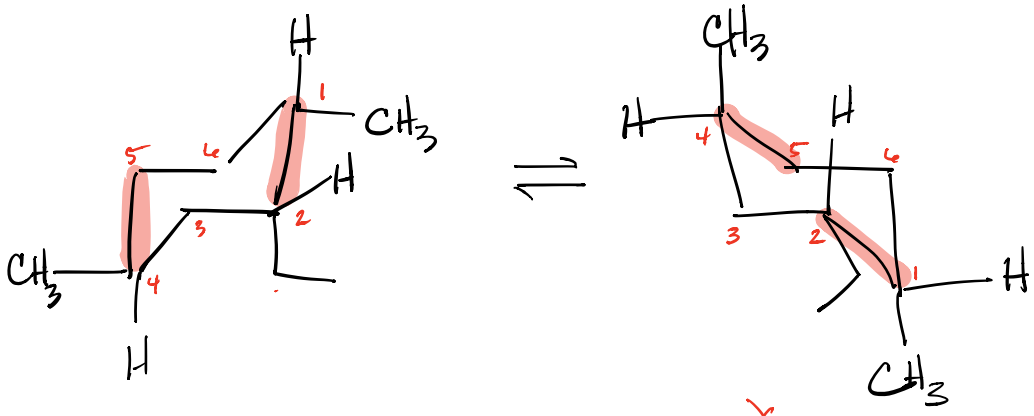


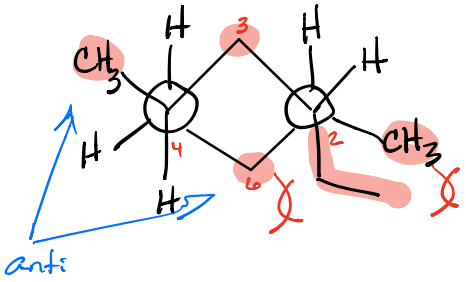


Ethyl in axial
w/ 1,3-diaxial interactions
w/ hydrogens

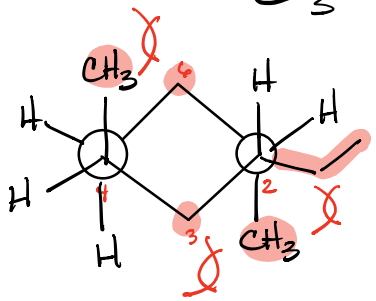
Lower energy
1-diaxial

Both methyls are axial
and have diaxial interactions
w/ hydrogens



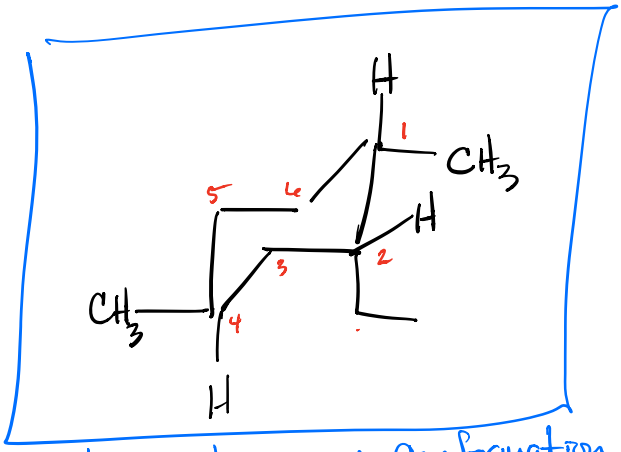


2 Gauche



3 Gauche interactions

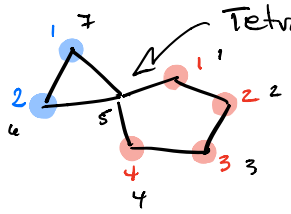
Lower Energy due to
lower # of Gauche interactions

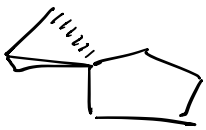


Lowest energy Conformation
Lower 1,3-diaxials
& less Gauche interactions

Bicyclic Ring Systems

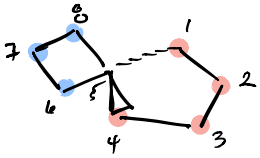
Spiro type - Rings joined at 1 Carbon





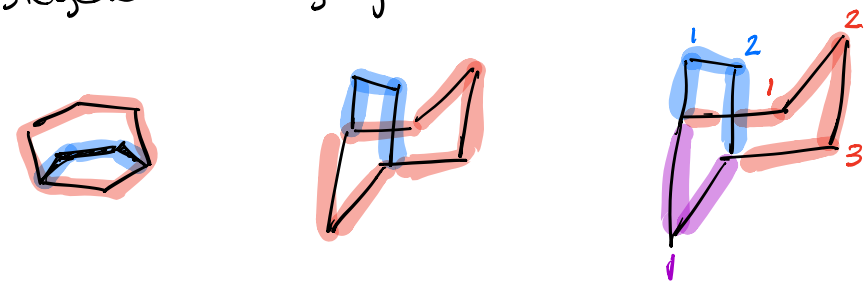
Spiro [2.4] Septane

Increasing #



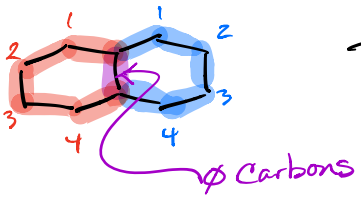
Spiro [3.4] Octane

Bicyclo - Rings joined at 2 different Carbons



Bicyclo [3.2.1] Octane

decreasing



Bicyclo [4.4.0] decane