

Alkane and Cycloalkane Conformations

A. Alkane Conformations

1. Bond rotation

a) Ethane

-two basic conformations relative to _____

eclipsed	staggered
Newman projections	

-staggered is _____ by ~12 kJ/mol (~3 kcal/mol)

-higher E associated with _____ conformation is called _____.

[E available at room temp. is ~80 kJ/mol or 20 kcal/mol]

Conformational analysis energy diagram for ethane

b) Basis of preference for staggered

-What do you think drives this preference?

Two reasons advanced:

(1) Preference is due to avoidance of _____.

(2) _____ between C-H sigma bond and C-H sigma* on adjacent C:

Key concept: Delocalizing or sharing electrons is _____!!!

c) Larger alkanes

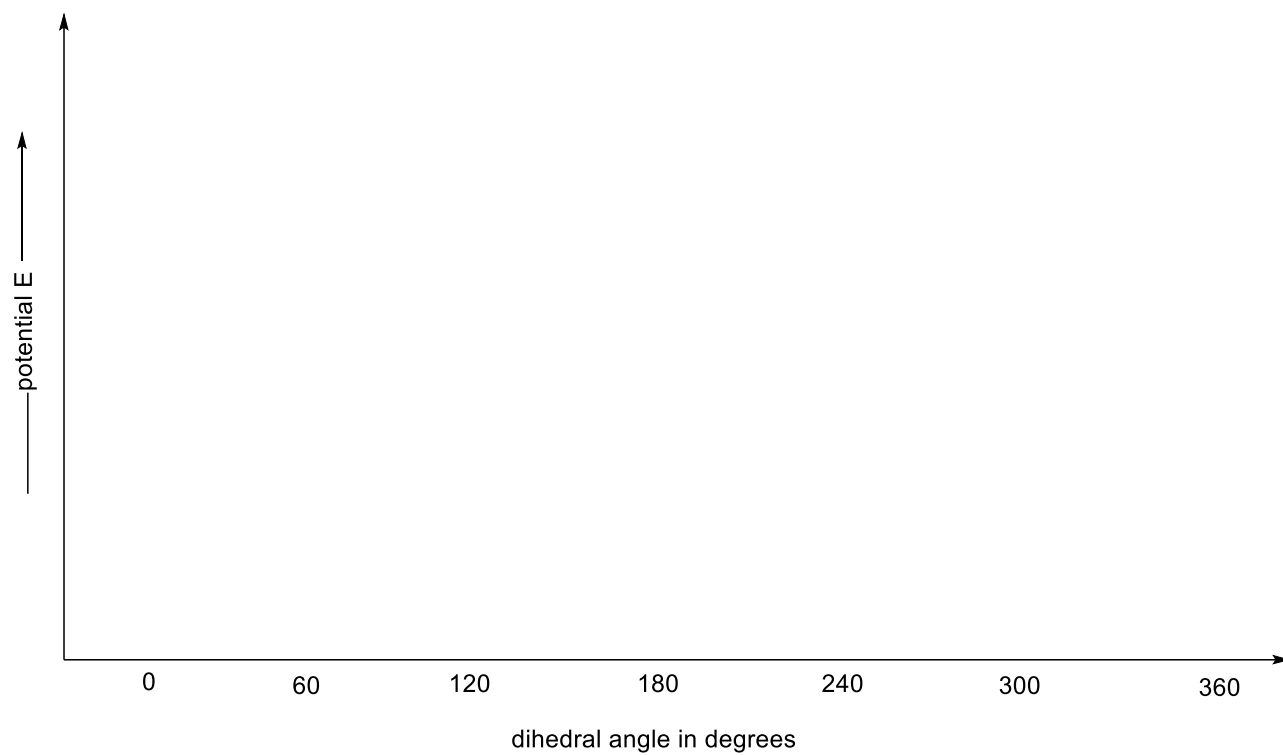
-basically the same principle applies and alkanes prefer a _____ conformation. This leads to _____ backbone pattern.

e.g. butane:

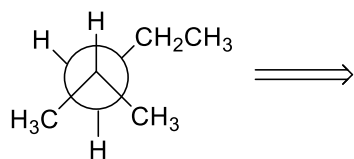
eclipsed	staggered
Newman projections	

-one little additional orientation: _____

-Conformational energy diagram for 1,2-dichloroethane conformers:



Newman projections → Sawhorse depiction

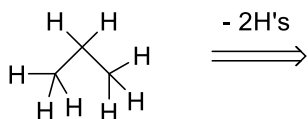


B. Cycloalkanes and Their Conformations

Ring	Ring size	ΔH_f per $-\text{CH}_2-$ (kJ/mol)	Ring strain energy per CH_2 (kJ/mol)
cyclopropane			
cyclobutane			
cyclopentane			
cyclohexane			
cycloheptane			
cyclooctane			

1. Cyclopropane, the simplest cycloalkane

a) Introduction



Draw pseudo-3 D model:

b) Ring Strain

(1) _____ strain:

-What will the C-C-C internal angles of cyclopropane? _____

-What is the hybridization of the C atom? _____

-What angle does that hybridization of C prefer? _____

*This difference....

(2) _____ strain

-What do you notice about the H atoms? _____

2. Cyclobutane and Ring Strain

a) Ring strain....

(1) angle strain?

(2) torsional strain?

**Adjacent atoms are also known as _____.*

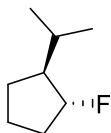
3. Cyclopentane

a) Ring Strain

-angles? _____ preferred? _____

-torsional strain?

a)



b) Conformations

4. Cyclohexane

a) Ring Strain

b) Drawing Cyclohexane (Find your inner artist!)

-note equatorial and axial groups!

Reason for names:

c) Conformations of Cyclohexane

-show: chair form, twist boat, boat

-interconversion and energy relationship → Called the _____

Important notes:

1)

2)

*boat structure also has _____ interactions on sides!

Youtube video with cyclohexane chair flip:

<http://www.youtube.com/watch?v=38YKPG1r30Q>

or <http://www.youtube.com/watch?v=Dux32urvZvQ>

Expectations: Know how to draw chair and boat structures.

5. Monosubstituted Cyclohexane

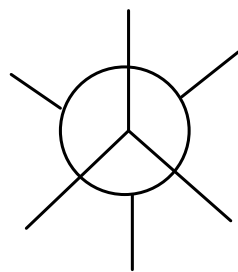
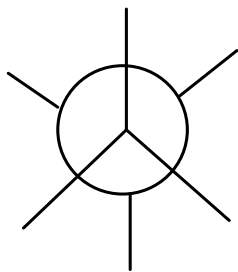
-preference for equatorial position to reduce _____

a) 2 reasons for equatorial preference

(1)

(2)

-show example:

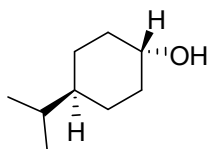


6. Disubstituted Cyclohexane

-preference for two groups to be equatorial or largest group to be equatorial

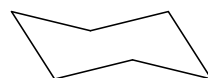
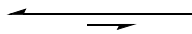
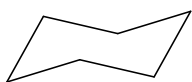
-cis vs. trans configurations:

a)



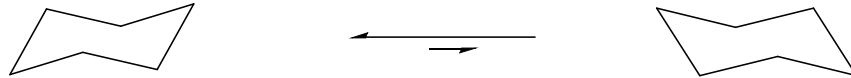
*called _____

Analyze chair structures....



Alternative depiction: Haworth projections....

b) cis isomer



7. Polysubstituted Cyclohexane

- same principles apply
- example: D-glucose

Special case: tert-butyl group →