

LEC (7)

CHEM 30A

Oct 18th

(1)

① CONFORMATIONAL ANALYSIS

② PROPERTIES

Quiz 1: AVERAGE 26/30

Readings: Rest of Chapter 2

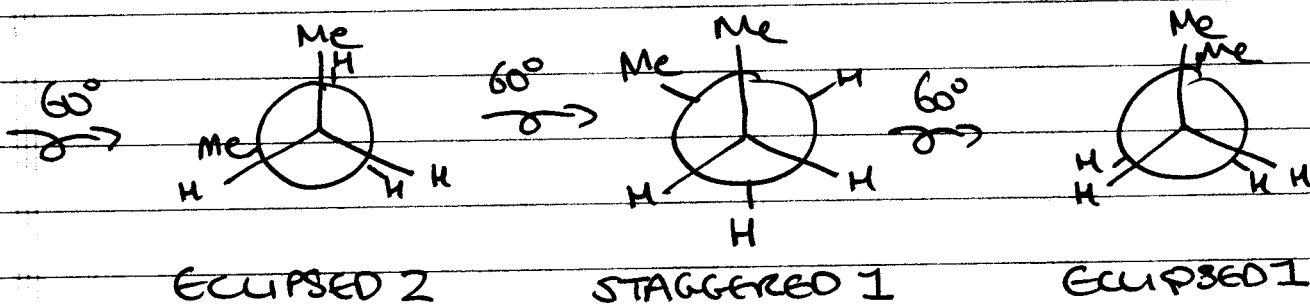
Problems: NO NEW ONES

① CONFORMATIONAL ANALYSIS

- start at Pg 4 from lecture 6

(1 kcal = 4.18 kJ)

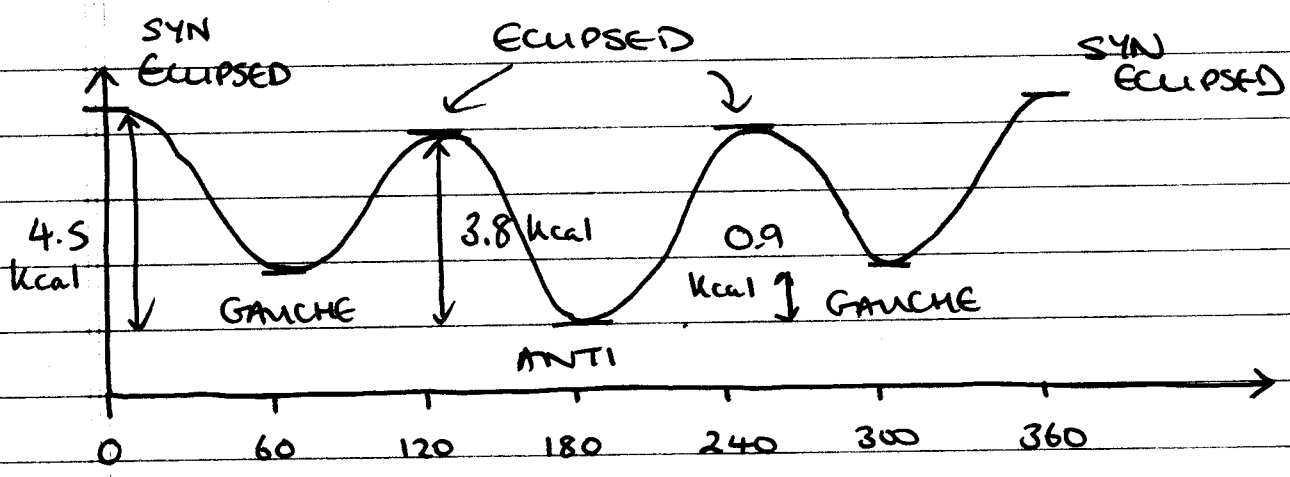
continue from end of Pg 8 Lec 6



(Mirror image)
to other
ECLIPSED 2

(Mirror image)
to other
STAGGERED 1

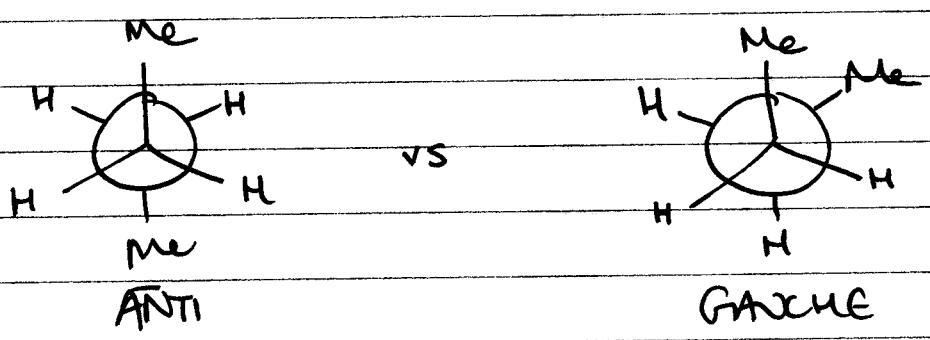
2



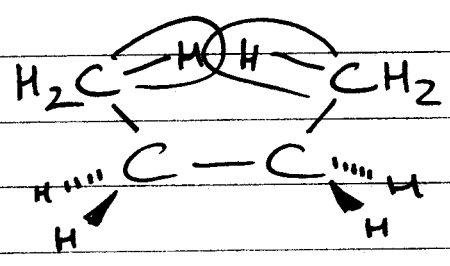
Each eclipsed conformer is a MAXIMA
Each staggered conformer is a MINIMA

BUT different MINIMA / MAXIMA ENERGIES

Consider



Neither is ECLIPSED, BUT ANTI IS MORE STABLE THAN GAUCHE - difference in energy is due to STERIC STRAIN



↓
forcing atoms closer together than atomic radii allow

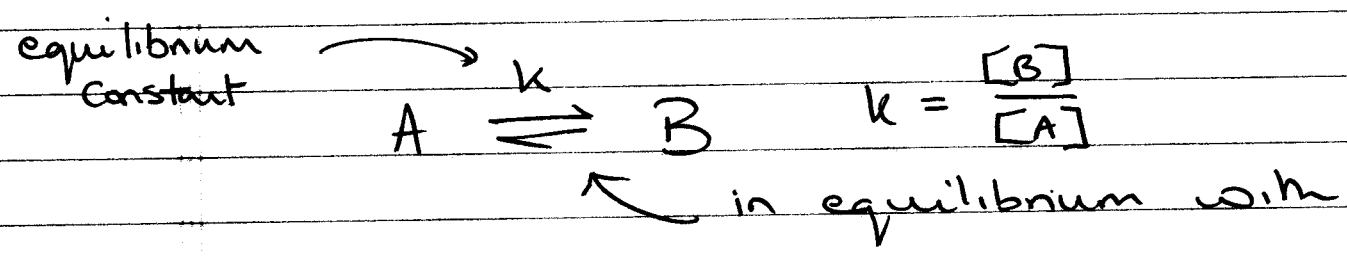
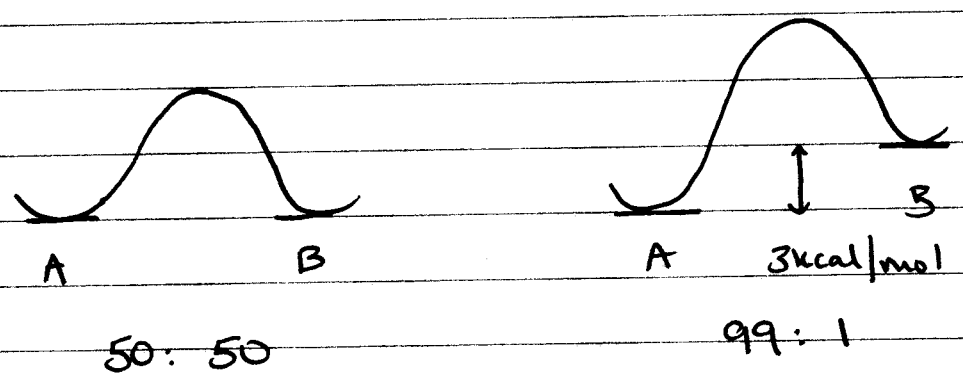
3

At room temperature, BUTANE is rapidly equilibrating between conformers

~80 : 20 anti : gauche

NOTE: v. small differences in energy barriers result in very different ratios of conformational isomers

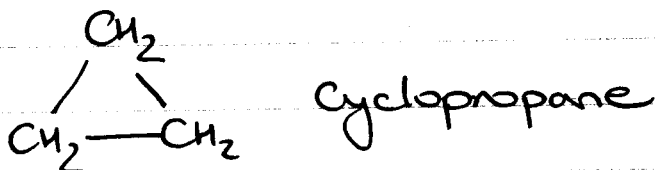
At room temp:



$$\Delta G^\circ = -RT \ln k$$

energy difference
(free energy)

- CYCLOALKANES

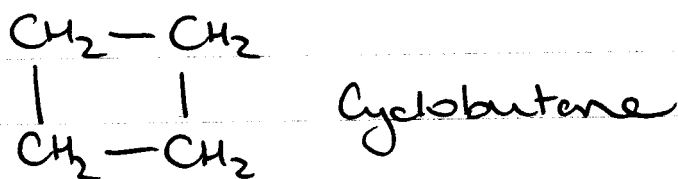


Ring strain of $\sim 28 \text{ kcal/mol}$



ANGLE STRAIN - most

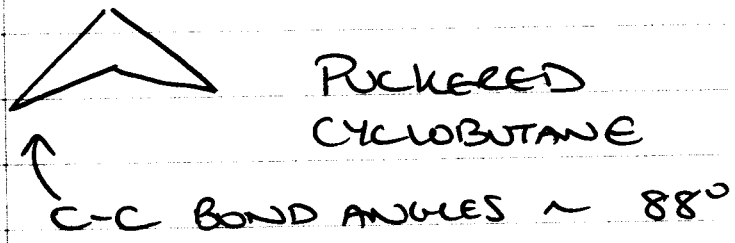
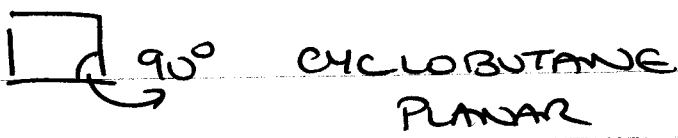
eclipsed C-H bonds, and cannot be any other way \Rightarrow TORSIONAL STRAIN



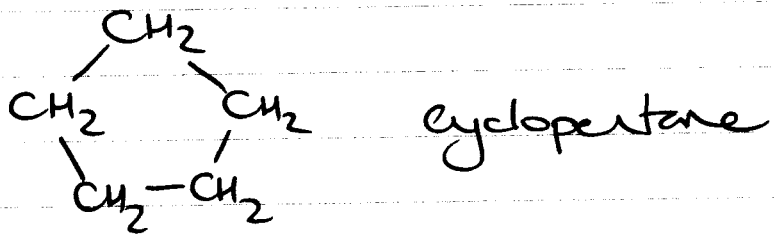
If planar, all C-Hs are eclipsed, so ring is puckered \rightarrow reduces TORSIONAL STRAIN

BUT increases ANGLE STRAIN

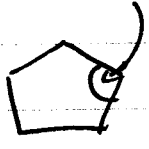
Ring strain is $\sim 26 \text{ kcal/mol}$



ALL CYCLOALKANES
LARGER THAN
CYCLOPROPANE
ADOPT NONPLANAR
CONFORMATIONS



If it was planar, internal angles would be 108°

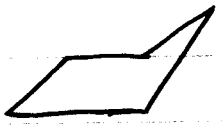


cf 109.5° for tetrahedral



VERY LITTLE ANGLE STRAIN

But again, all C-H bonds would be eclipsed



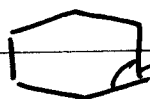
4 in PLANE,
1 OUT

ENVELOPE CONFORMATION
(FIVE EQUIVALENT ONES)
EQUILIBRIUM

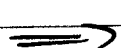
Ring strain is ~ 7 kcal/mol

6

cyclohexane



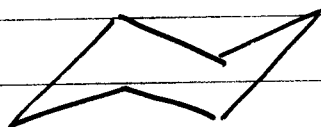
120°



would lead to
angle strain &
torsional strain,

BUT CYCLOHEXANE is almost strain free

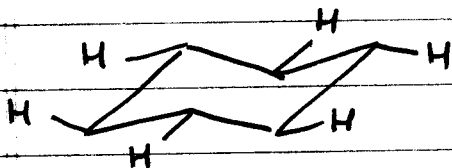
CHAIR CONFORMATION



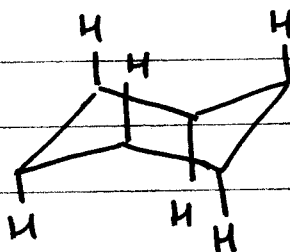
C-C-C angles $\sim 109.5^\circ$
NO ANGLE STRAIN

HYDROGENS ON ADJACENT CARBONS ARE
STAGGERED — NO TORSIONAL STRAIN

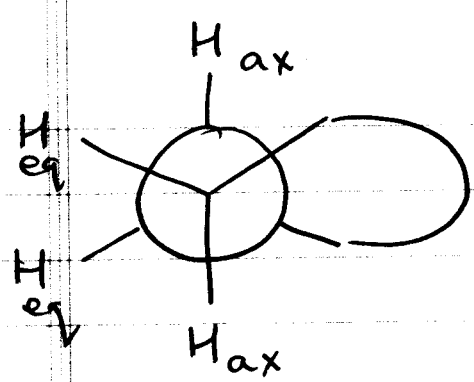
NO STERIC STRAIN



EQUATORIAL



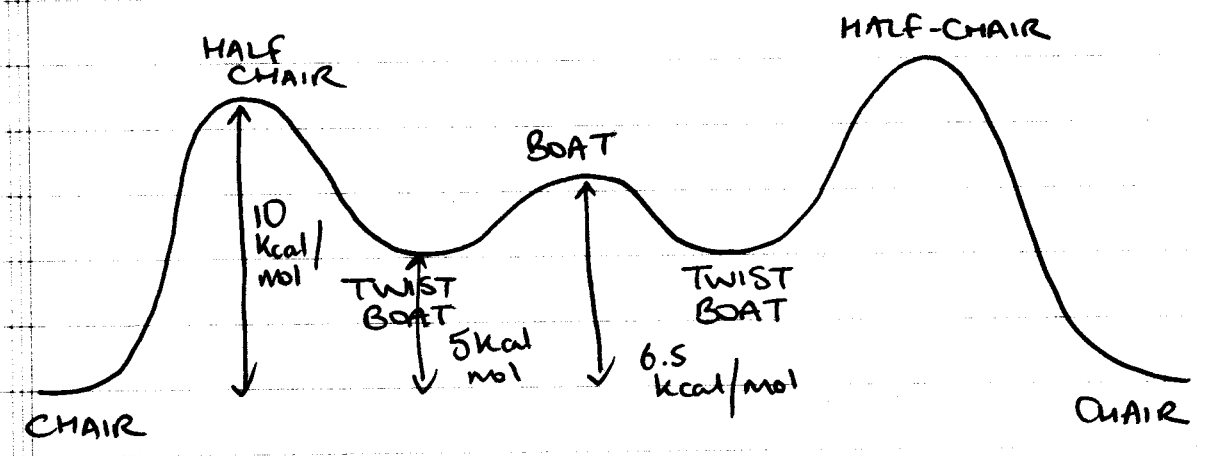
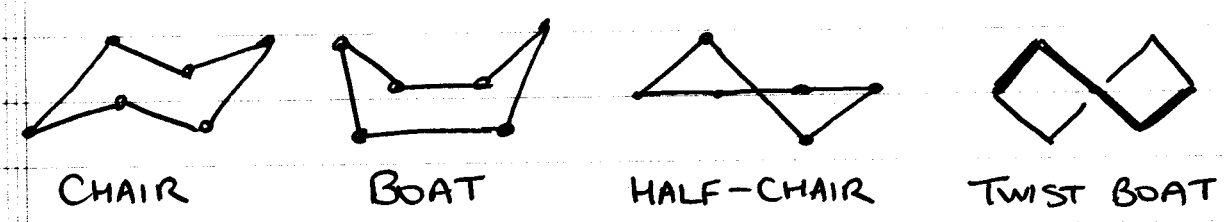
AXIAL



LOOKING DOWN ANY
C-C AXIS

NEWMAN PROJ

- OTHER CYCLOHEXANE CONFORMATIONS



ROOM TEMP - CHAIR > 99.99% of
equilibrium mixture

DYNAMICS OF THE CYCLOHEXANE RING