

LEC ⑥

CHEM 30 A

①  
Apr 15<sup>th</sup>

- ① NOMENCLATURE
- ② CONFORMATIONAL ANALYSIS
- ③ CYCLOALKANES

Quiz  
Max 18/30  
Low 0  
High 35

READ 2.6-2.8

HMK 2.8, 2.9, 2.24-2.30 (3<sup>rd</sup>)

2.7, 2.8, 2.28-2.37 (4<sup>th</sup>)

## ① NOMENCLATURE

General rules: PREFIX-INFIX-SUFFIX



PROP

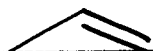
AN

E

3CS

single  
bonds

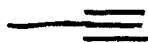
hydrocarbon



PROPENE

-EN-

double bonds



PROPYNE

-YN-

triple bonds

SUFFIXES → functional groups

- E



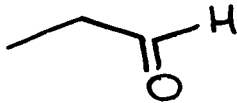
PROPANE

- OL



PROPANOL

- AL



PROPANAL

- ONE



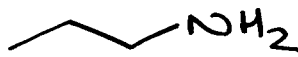
PROPANONE

- OIC ACID



PROPANOIC ACID

(- AMINE)



PROPYL AMINE  
(not PROPANAMINE)

- CYCLOALKANES - easy

- BICYCLOALKANES - don't worry about it.

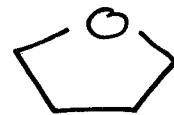
Common Names / Structures / Acronyms  
(Keep a notebook)



acetone



pyridine

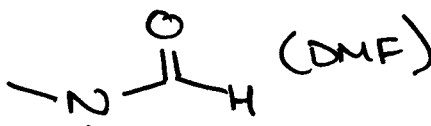


(THF)

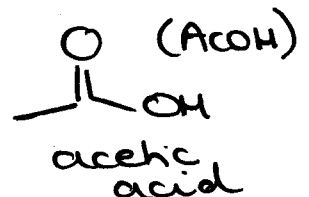
tetrahydrofuran



dimethyl sulfoxide

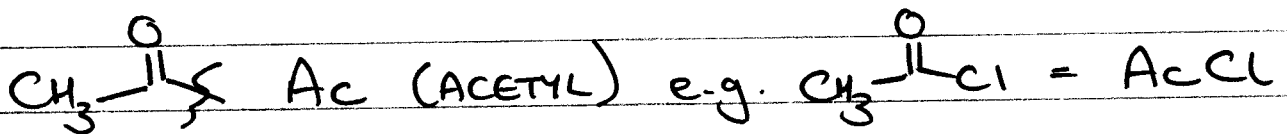
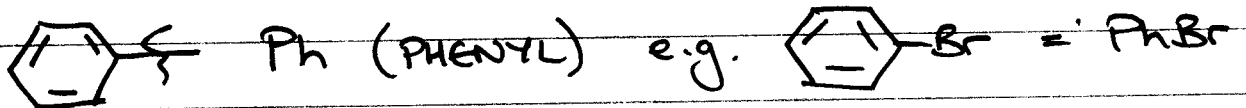
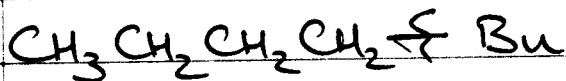
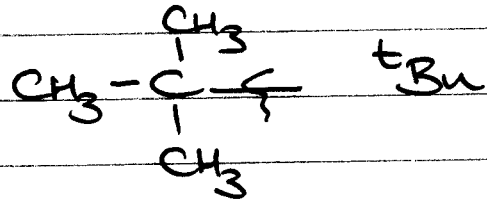
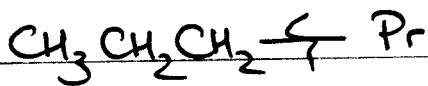
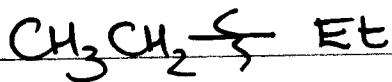
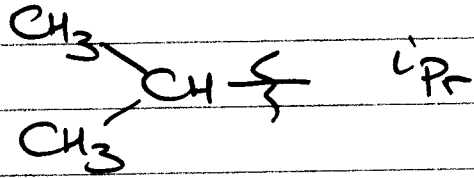
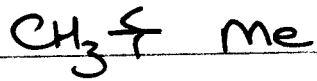


dimethylformamide



acetic acid

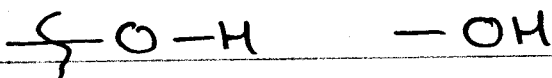
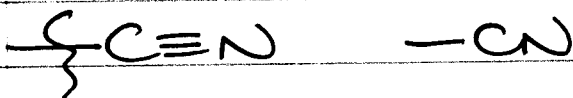
- other common abbreviations

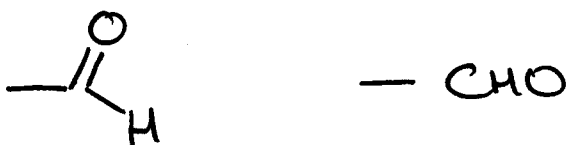
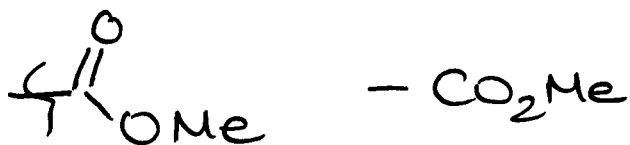
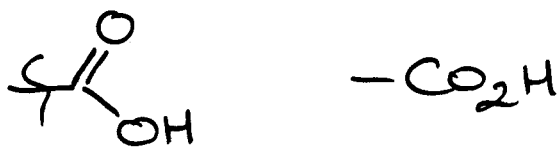


R GROUPS - stuff dangling off the area of interest in a molecule

e.g. R-Cl, R-OH, R-CO<sub>2</sub>H  
chloride      alcohol      carboxylic acid

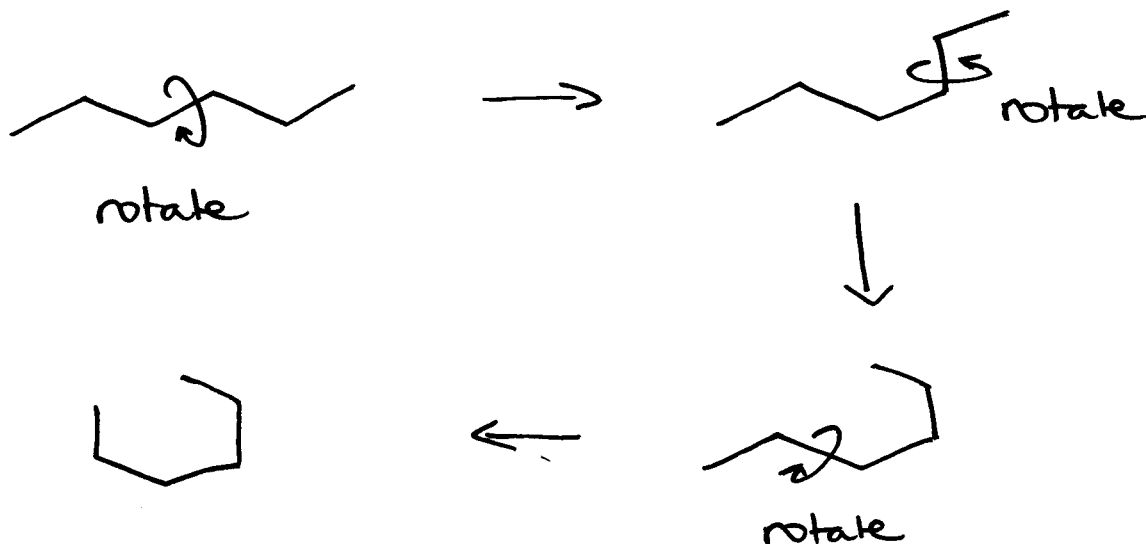
FUNCTIONAL GROUPS





② CONFORMATIONAL ANALYSIS

- consider HEXANE

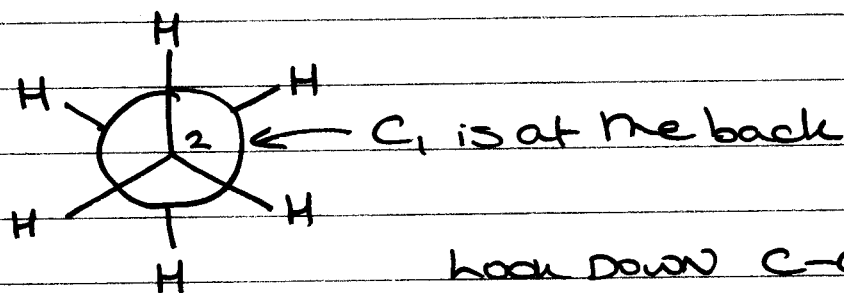
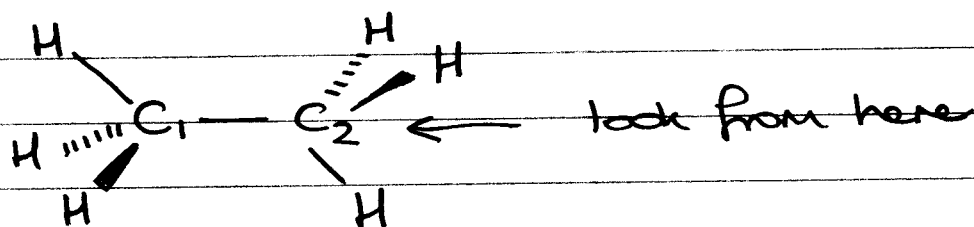


THESE ARE ALL THE SAME MOLECULE...  
 Different arrangements of atoms that result from ONLY single bond rotations are called CONFORMATIONS

5

At room temperature all single bonds are constantly rotating

- consider  $C_2H_6$

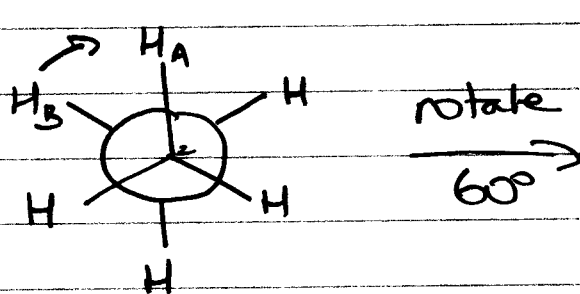


LOOK DOWN C-C BOND  
NEWMAN PROJECTION

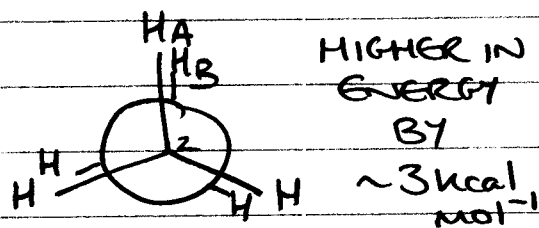
- Two METHYL GROUPS CAN ROTATE wrt ONE ANOTHER ( $0-360^\circ$ )

$\Rightarrow$  INFINITE NUMBER OF CONFORMATIONS

At RT, rate of rotation is  $\sim 10$  BILLION  $s^{-1}$   
but rotation is not completely UNHINDERED



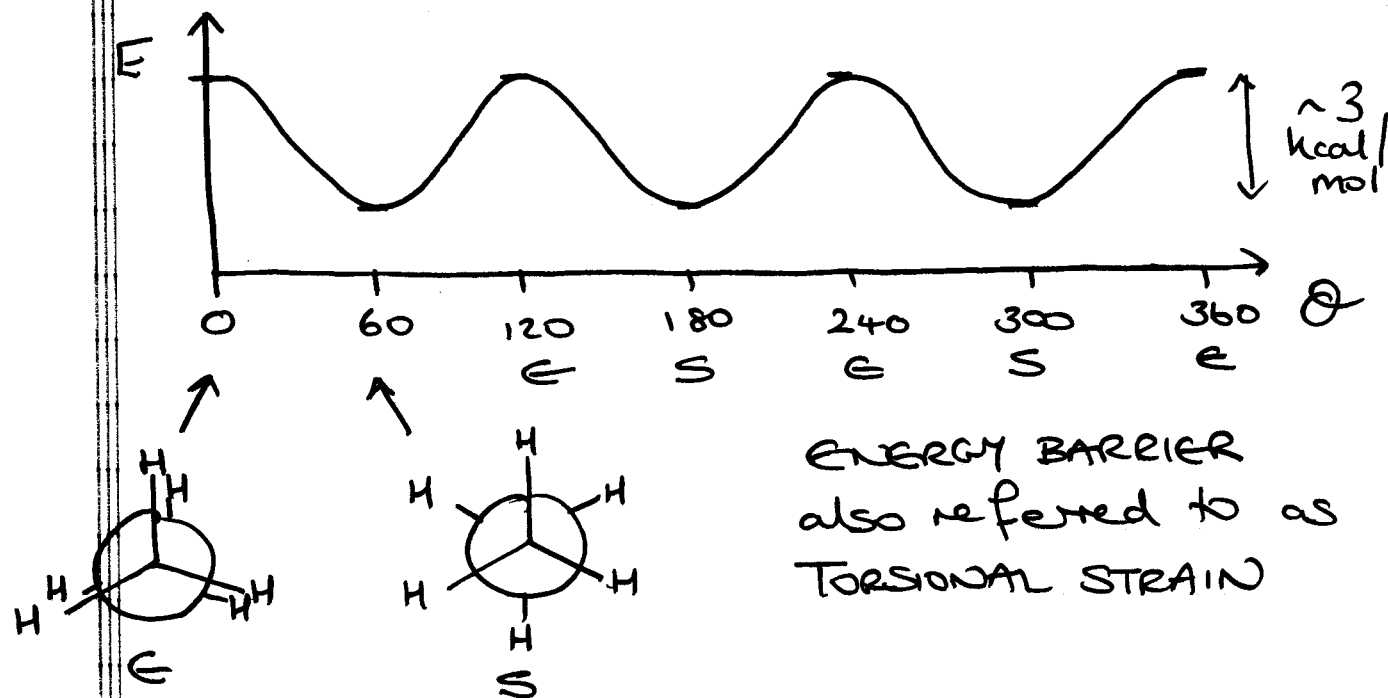
STAGGERED ( $\theta = 60^\circ$ )



ECLIPSED ( $\theta = 0^\circ$ )

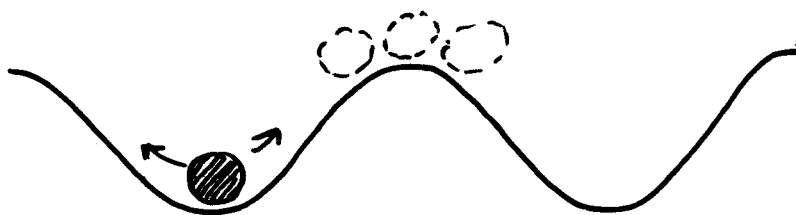
6

Q (DIHEDRAL ANGLE) - angle between 2 intersecting planes  $H_A C_2 C_1$  &  $H_B C_1 C_2$



Any given molecule will spend most of its time in a staggered or nearly staggered conformation (LOWEST ENERGY) and will only briefly pass through the eclipsed conformation on its way to the next staggered conformation

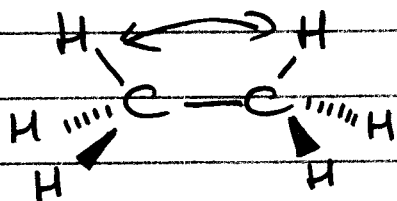
EQUILIBRIUM



enough energy and it will pass over the barrier, but won't spend a lot of time there.

# WHY IS THERE A BARRIER?

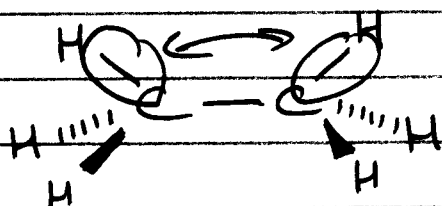
## (i) STERIC INTERACTION?



BUT H ATOMS are VERY SMALL

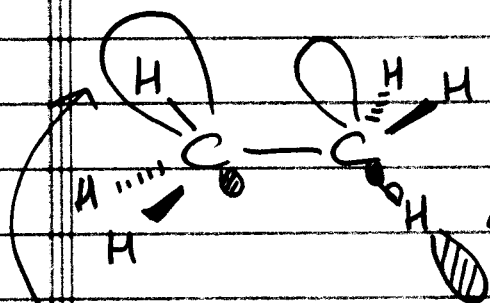
Sterics account for ~10% of BARRIER

## (ii) ELECTRON PAIR REPULSION



BIGGEST FACTOR

## (iii) ATTRACTIVE INTERACTIONS

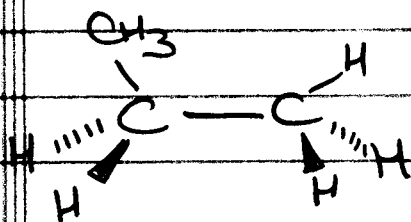


$C_{sp^3}-H_{1s} \sigma^*$

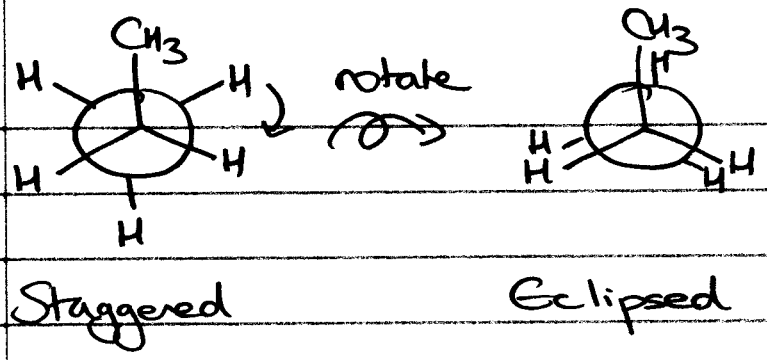
empty anti bonding orbital

$C_{sp^3}-H_{1s} \sigma$  filled bonding orbital

## — CONFORMATIONS OF PROPANE ?

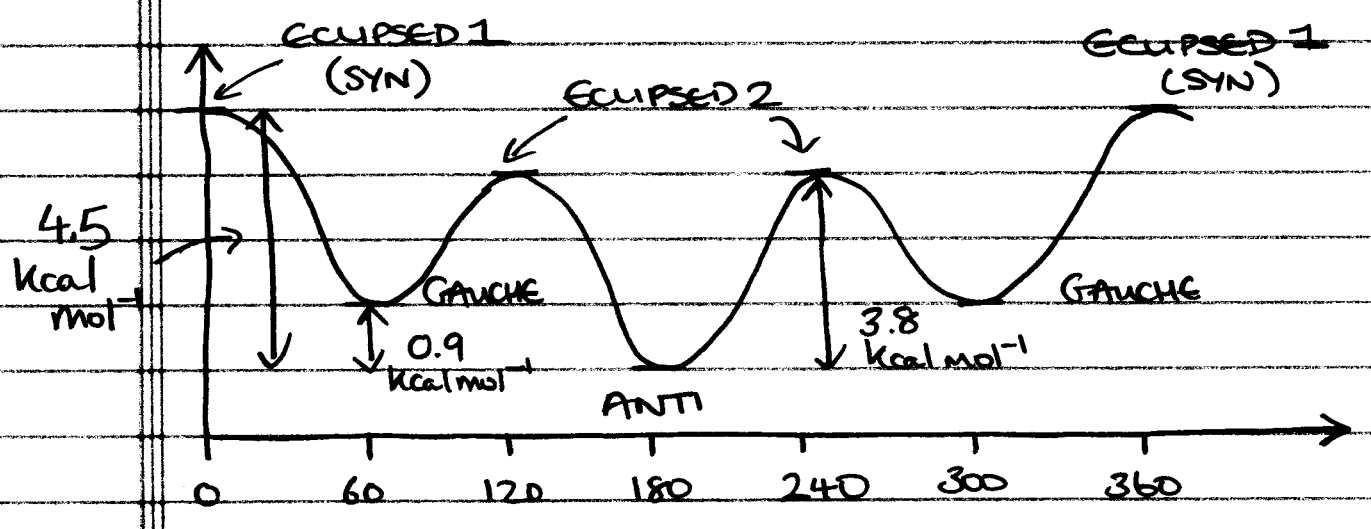
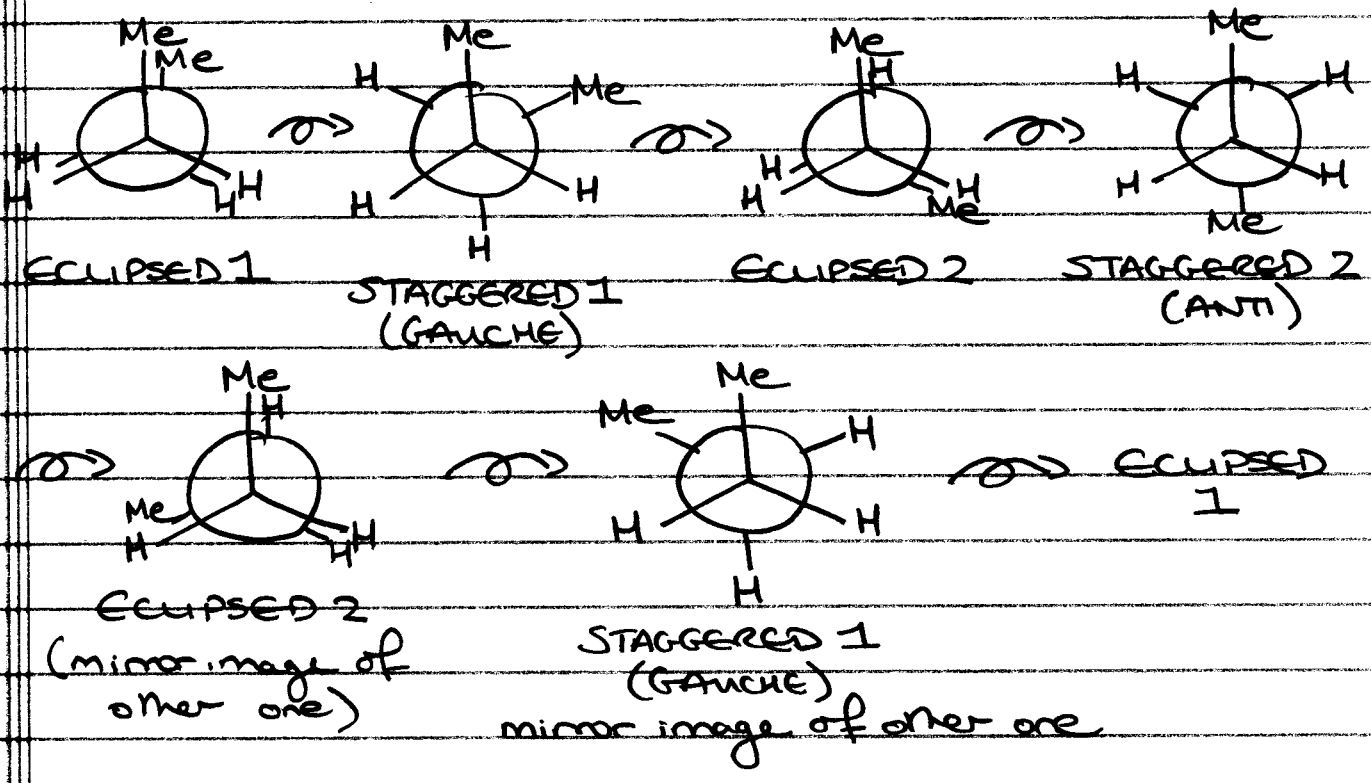


Bigger repulsive interaction than C-H / C-H



Same profile as ETHANE, but higher barrier (3.4 kcal/mol)

CONFORMATIONS OF BUTANE

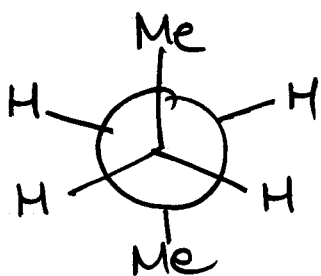




9

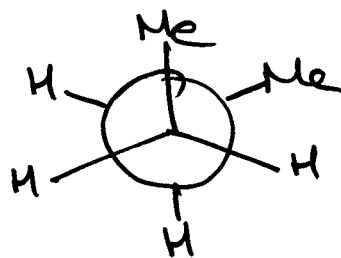
Each ECLIPSED conformer is a MINIMA  
Each STAGGERED conformer is a MAXIMA

But different MINIMA / MAXIMA energies



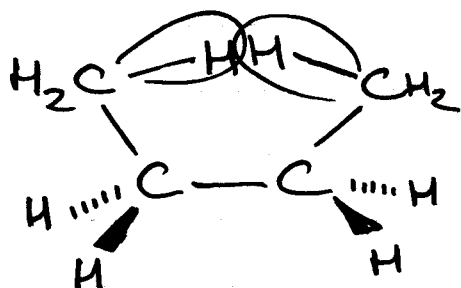
ANTI (180°)

VS



GAUCHE (60°)

Neither is ECLIPSED, but ANTI is more stable than GAUCHE - difference in energy due to STERIC STRAIN



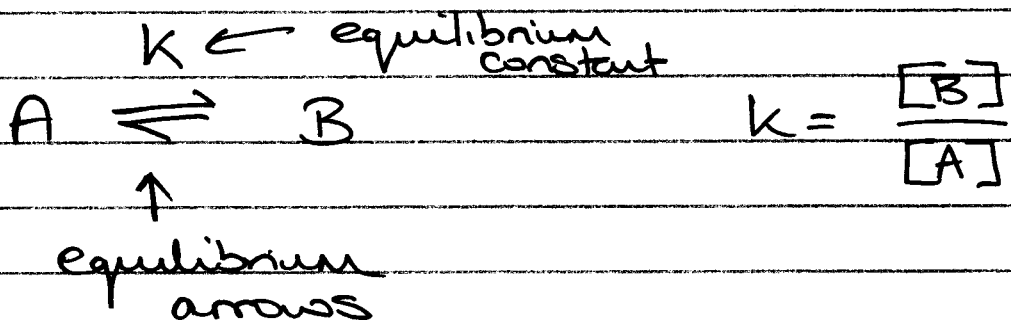
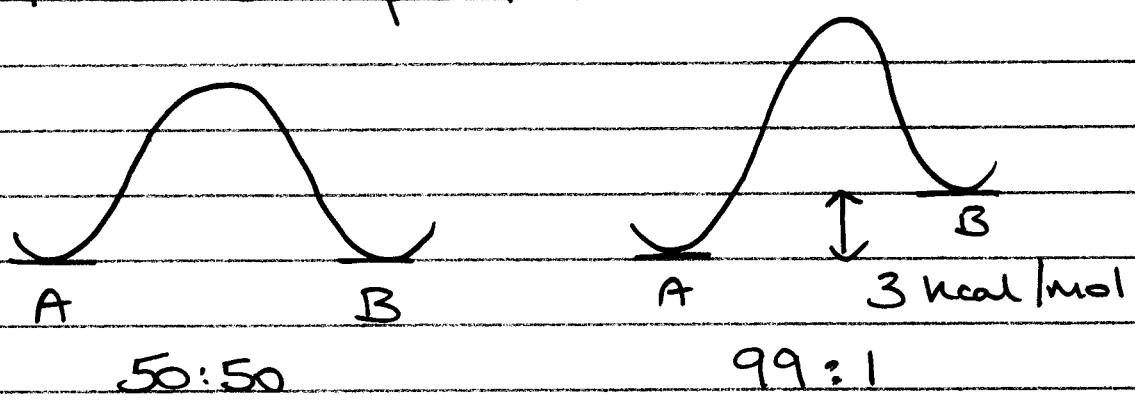
↓  
bring atoms closer together than atomic radii allow

At room temperature, BUTANE is rapidly equilibrating between conformers

~80:20 anti / gauche

Note: very small differences in energy result in very different ratios of conformational isomers

At room temperature:



$\Delta G^\circ = -RT \ln K$   
 $\uparrow$   
 difference in free energy

next up: CYCLOALKANES