LEC (6) CHEM 30A Oct 18th

(1) NOMENCLATURE
(2) CONFORMATION } ALKANES
(3) PROPERTIES

A PENCIL
B ELECTRONIC
C STOP WRITING

HMK: READ: 2 – 2.6
PROBLEMS: 2.9, 2.27, 2.28

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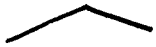
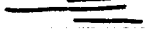
(1) NOMENCLATURE

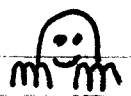
PREFIX – INFIX – SUFFIX

PROP — 3 Cs
AN — single bonds
E — hydrocarbon


INFIX
- AN –  PROPANE
- EN –  PROPENE
- YN –  PROPYNE

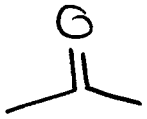
SUFFIX
- –E  PROPANE
- –OL  PROPANOL
- –AL  PROPANAL
- (–AMINE)  PROPYL AMINE
- –ONE PROPANONE
- –OIC ACID  PROPANOIC ACID

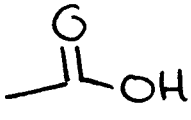
N – HERE YOU GO – S

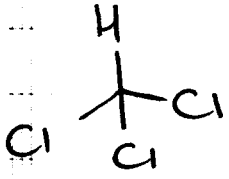


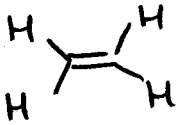
- COMMON NAMES / STRUCTURES / ACRONYMS

- KEEP A NOTEBOOK

 ~~PROPANONE~~ ACETONE

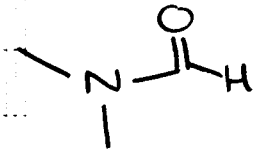
 ~~ETHANOIC~~ ACETIC ACID

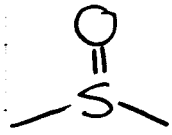
 ~~TRICHLOROMETHANE~~ CHLOROFORM

 ~~ETHENE~~ ETHYLENE

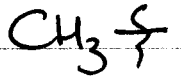
ALL ABOUT COMMON NAMES

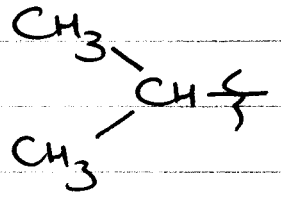
 TETRAHYDROFURAN THF

 DIMETHYLFORMAMIDE DMF

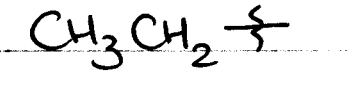
 DIMETHYLSULFOXIDE DMSO

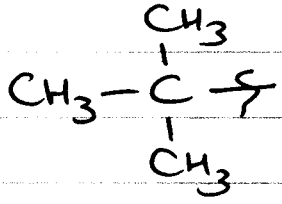
- other common abbreviations

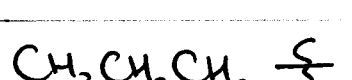
 Me

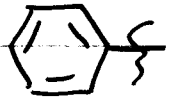
 ^{i}Pr

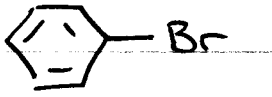
 Et

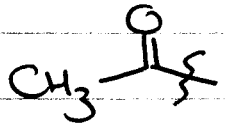
 Pr

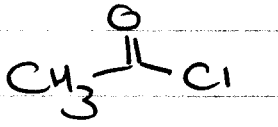
 ^{t}Bu

 Bu

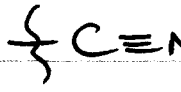
 Ph
PHENYL

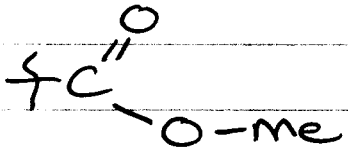
i.e.  = PhBr

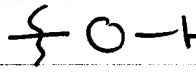
 Ac
ACETYL

i.e.  = AcCl

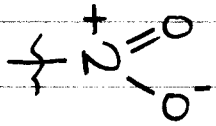
- functional groups

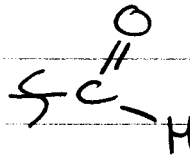
 - CN

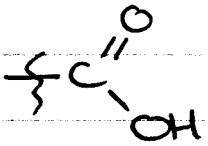


 - OH

- CO_2Me

 - NO_2

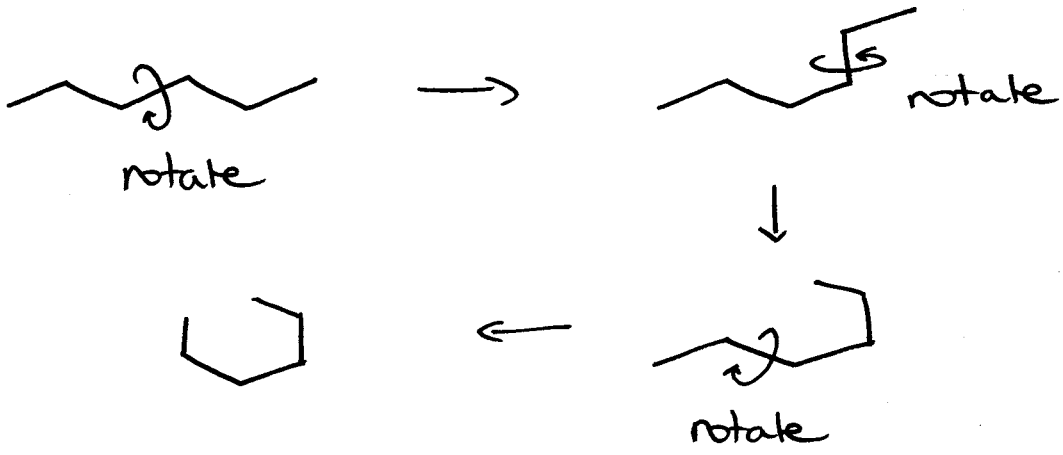


 - CO_2H

- CHO

(2) CONFORMATIONAL ANALYSIS

- consider HEXANE

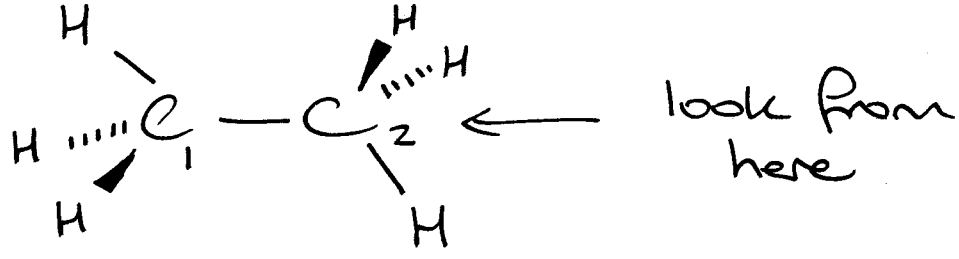


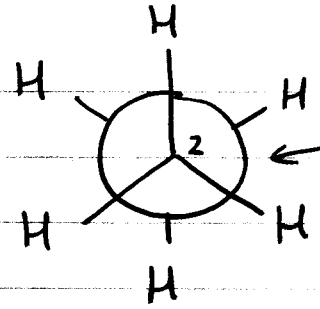
THESE ARE ALL THE SAME MOLECULE

Different arrangements of atoms that result from ONLY single bond rotations are called CONFORMATIONS

At room temp, all single bonds are constantly rotating

Consider C_2H_6





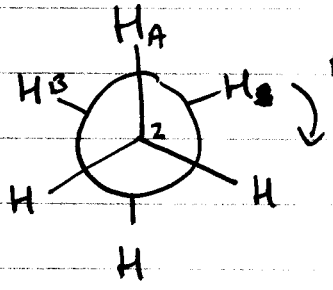
← C_1 is at back

LOOKING DOWN C–C bond

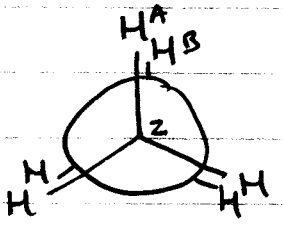
NEWMAN PROJECTION

- TWO METHYL GROUPS CAN ROTATE WRT ONE ANOTHER i.e. 0 – 360° (INFINITE NUMBER OF CONFORMATIONS)
- AT RT, rate of rotation ~ 7000000 s^{-1} ! or 10000000000 s^{-1} !

HOWEVER, rotation is not completely unhindered



rotate 60°



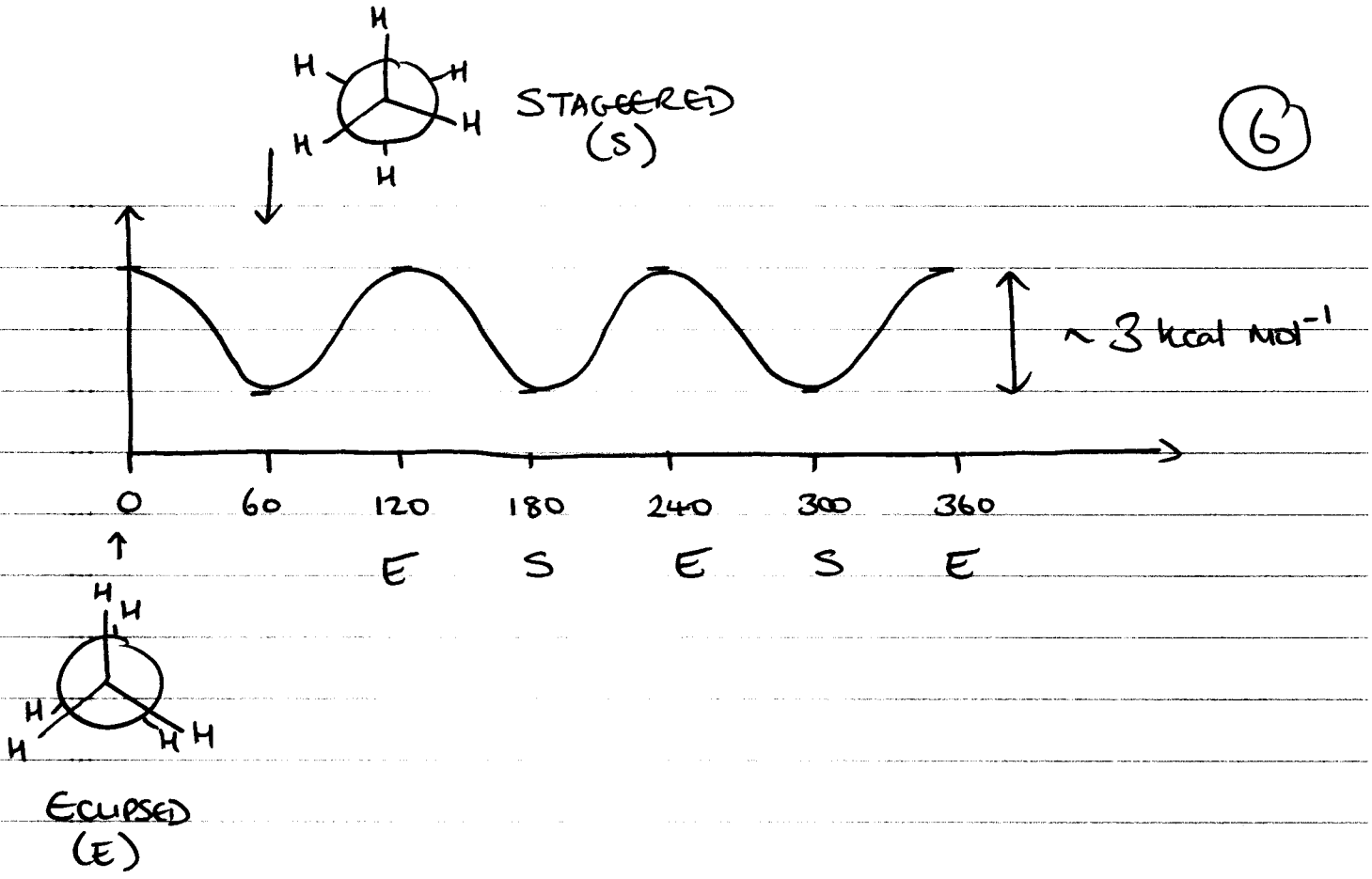
HIGHER ENERGY by ~ 3kcal mol^{-1}

STAGGERED ECLIPSED

DIHEDRAL ANGLE – angle between two intersecting planes (Θ)

$H_A C_2 C_1$
$H_B C_1 C_2$ 60°

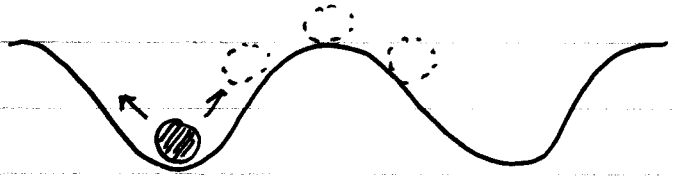
0°



Energy barrier is also called TORSIONAL STRAIN

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

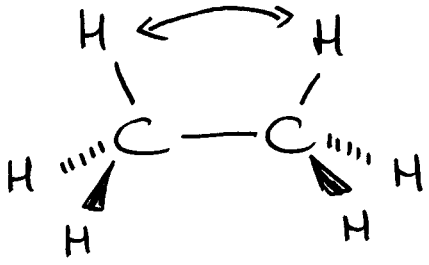
EQUILIBRIUM



Enough energy → will go over barrier, but won't spend a lot of time there

WHY IS THERE A BARRIER?

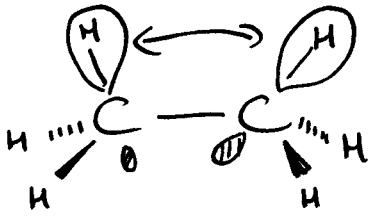
(i) STERIC INTERACTION?



BUT H ATOMS are VERY SMALL

STERICS ACCOUNT FOR ~ 10% of BARRIER

(ii) ELECTRON PAIR REPULSION

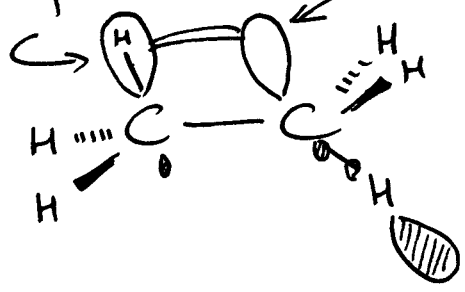


(iii) ATTRACTIVE INTERACTIONS

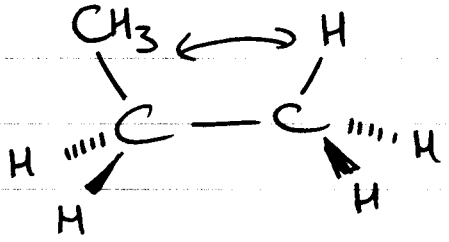
$C_{sp^3}-H_{1s}$ σ

$C_{sp^3}-H_{1s}$ σ^*

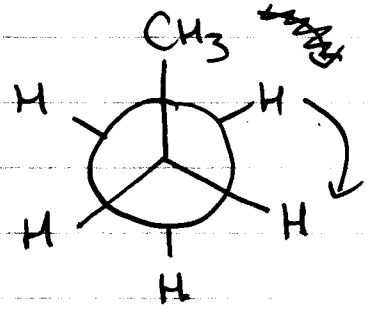
EMPTY ANTIBONDING ORBITAL



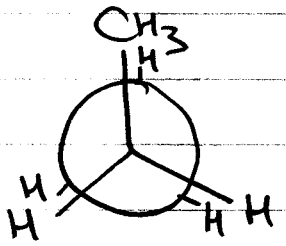
– CONFORMATIONS OF PROPANE



Bigger repulsive interaction than C–H C–H



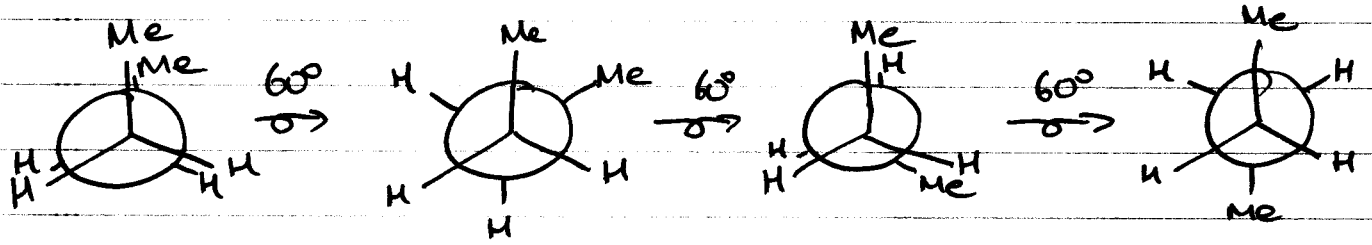
STAGGERED



ECLIPSED

So, same energy profile as ETHANE, but barrier is now 3.4 kcal mol^{-1} (cf 3.0 kcal mol^{-1})

– CONFORMATIONS OF BUTANE



ECLIPSED 1 STAGGERED 1 ECLIPSED 2 STAGGERED 2

GAUCHE ANTI