LEC (6) CHEM 30A Oct 12th

(1) NOMENCLATURE (Common names)
(2) CONFORMATIONAL ANALYSIS

READ 2.6-2.8 PROBLEMS 2.8, 2.32-2.35

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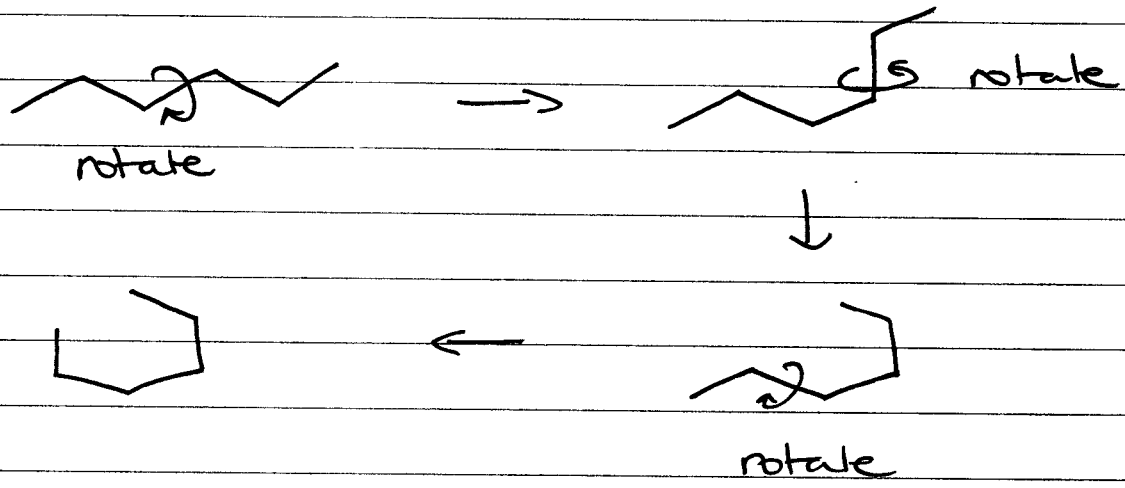
(1) Common NAMES
Pages (5)+(6) from Lec 5

(2) CONFORMATIONAL ANALYSIS

- Consider HEXANE

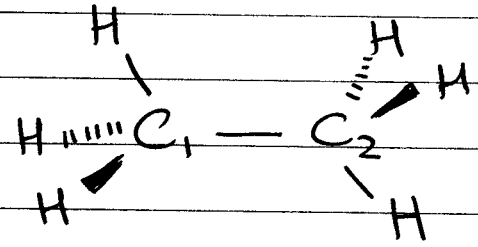


THESE ARE ALL THE SAME MOLECULE...

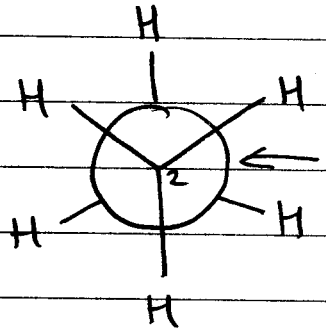
Different arrangements of atoms that result ONLY from single bond rotations are called CONFORMATIONS.

At room temperature, all single bonds are constantly rotating

- consider C_2H_6



← look from here

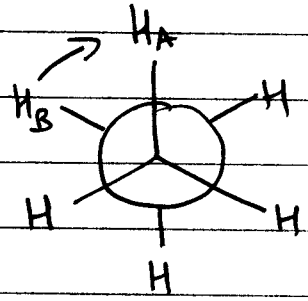


← C_1 is at back

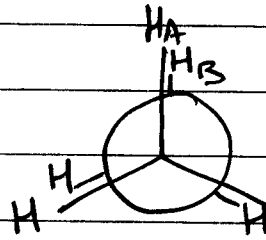
Look down C–C bond => NEWMAN PROJECTION

- TWO METHYL GROUPS CAN ROTATE WRT ONE ANOTHER (0 - 360°)
=> infinite number of conformations

At rt, rate of rotation is ~ 10 BILLION s^{-1}
but ROTATION is not completely UNHINDERED



rotate → 60°

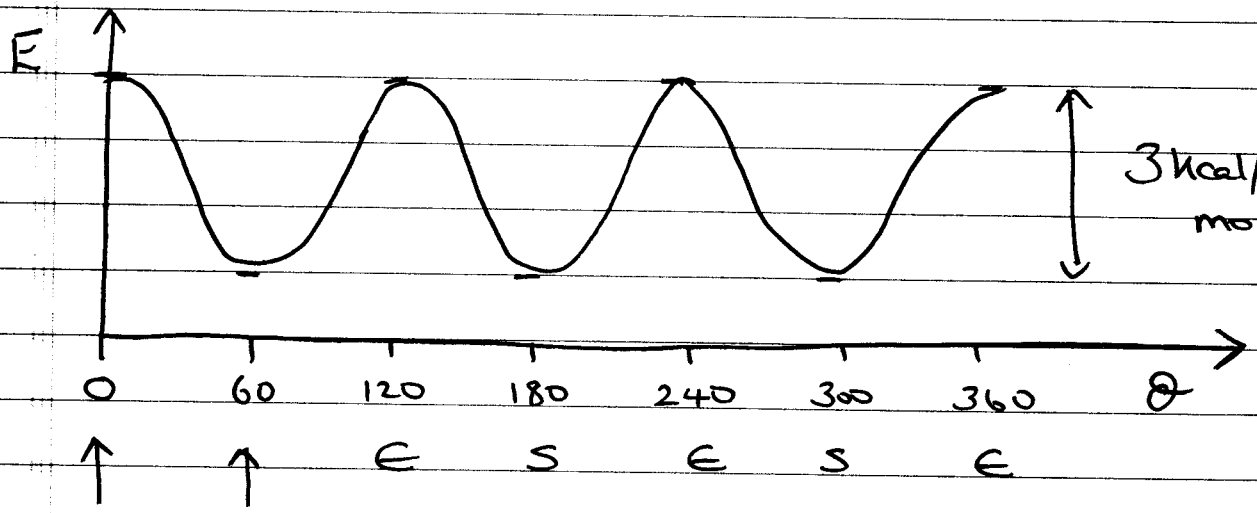


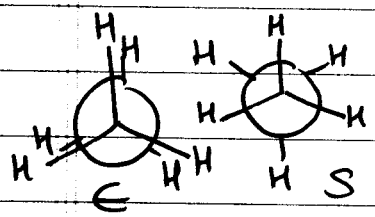
Higher in energy by 3 kcal/mol

STAGGERED ($\theta = 60°$)

ECLIPSED ($\theta = 0°$)

θ (DIHEDRAL ANGLE) – angle between 2 intersecting planes $H_A C_2 C_1$ & $H_B C_1 C_2$

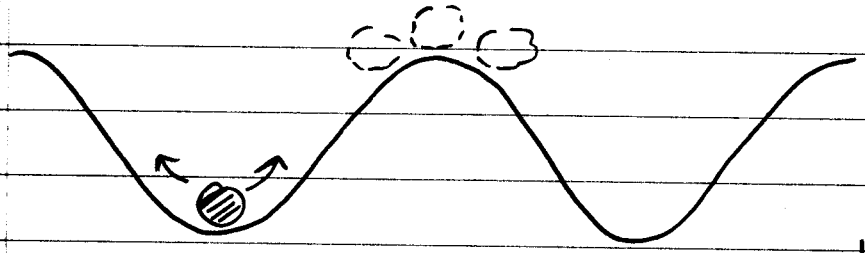




ENERGY BARRIER also REFERRED TO AS TORSIONAL STRAIN

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.

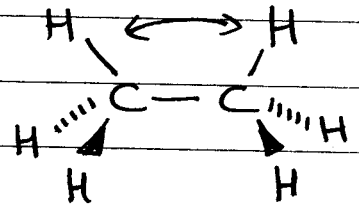
EQUILIBRIUM



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

WHY IS THERE A BARRIER?

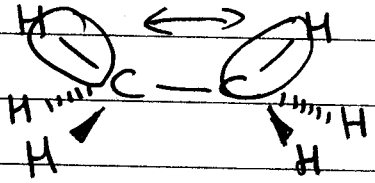
(i) STERIC INTERACTION?



BUT H ATOMS are VERY SMALL

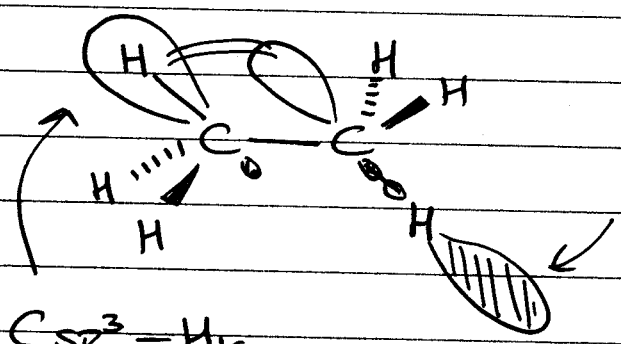
sterics account for ~10% of BARRIER

(ii) ELECTRON PAIR REPULSION



BIGGEST FACTOR

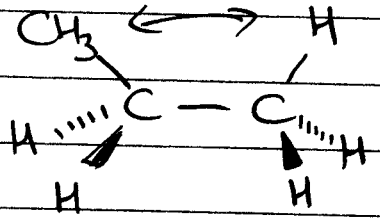
(iii) ATTRACTIVE INTERACTIONS



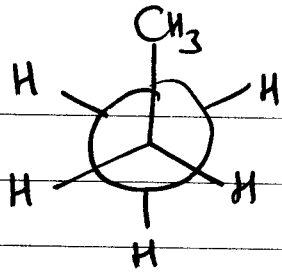
$Csp^3 - H_{1s}$ σ^* empty antibonding orbital

$Csp^3 - H_{1s}$ σ filled bonding orbital

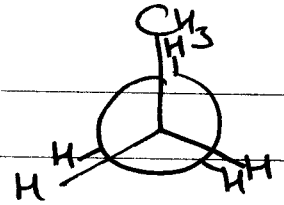
CONFORMATIONS OF PROPANE?



Bigger repulsive interaction than C–H/C–H



rotate ↻

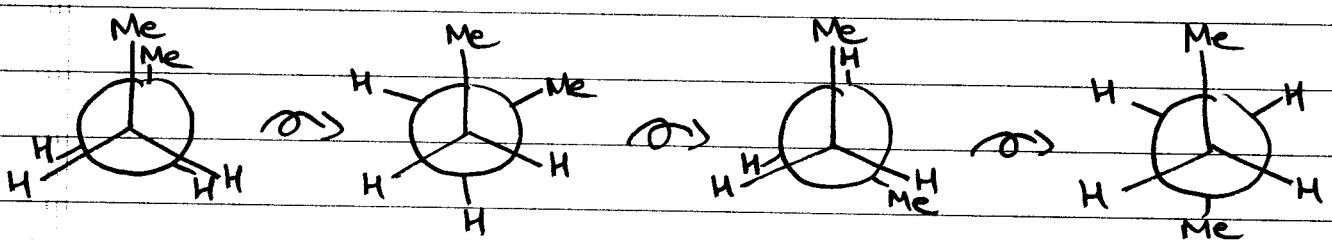


Same profile as ETHANE, but higher barrier (3.4 kcal/mol)

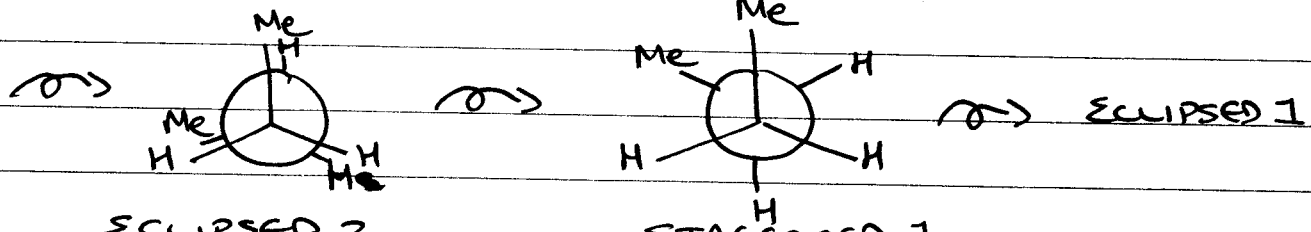
Staggered

Eclipsed

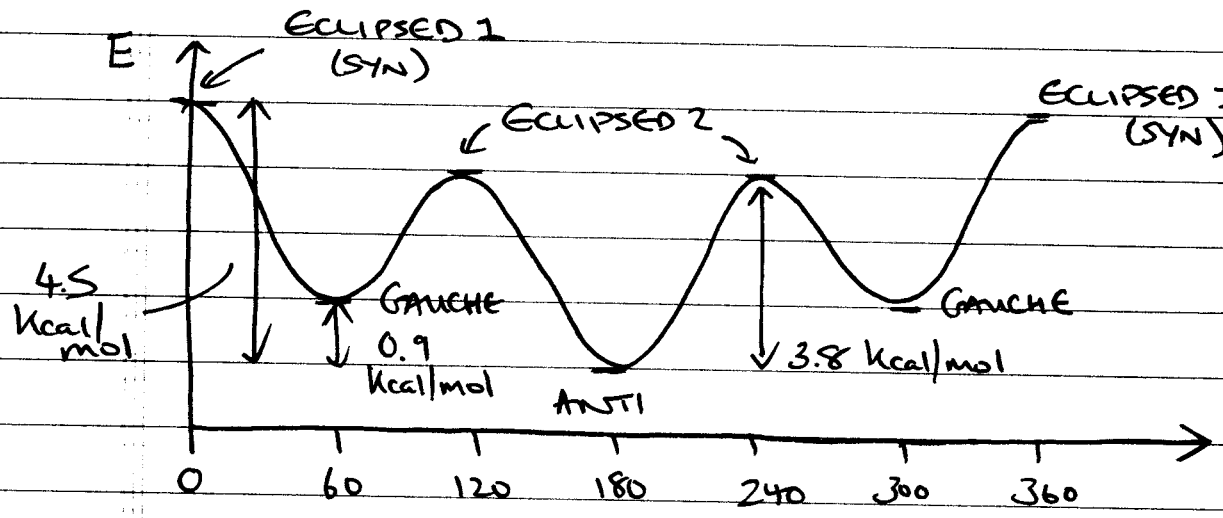
– CONFORMATIONS OF BUTANE



ECLIPSED 1 → STAGGERED 1 (GAUCHE) → ECLIPSED 2 → STAGGERED 2 (ANTI)

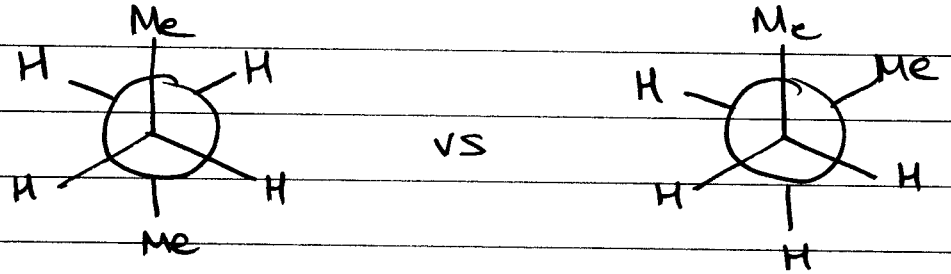


→ ECLIPSED 2 (mirror image of E1) → STAGGERED 1 (GAUCHE) (mirror image of other one) → ECLIPSED 1



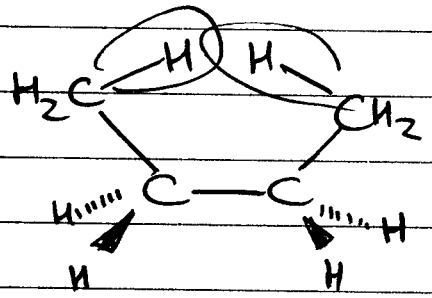
Each ECLIPSED conformer is a MINIMA
Each STAGGERED conformer is a MAXIMA

BUT different MINIMA/MAXIMA energies



ANTI (180°) GAUCHE (60°)

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



forcing atoms closer together than atomic radii will allow

At room temp, BUTANE is rapidly equilibrating between CONFORMERS

~80:20 anti/gauche