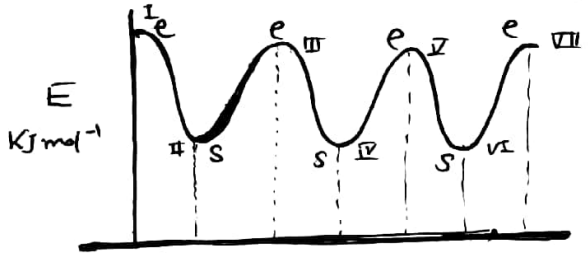
Conformational Isomerism

Class-2

$H_3C - CH_3$

Energy Profile diagram or Potential energy diagram or Torsional curve.



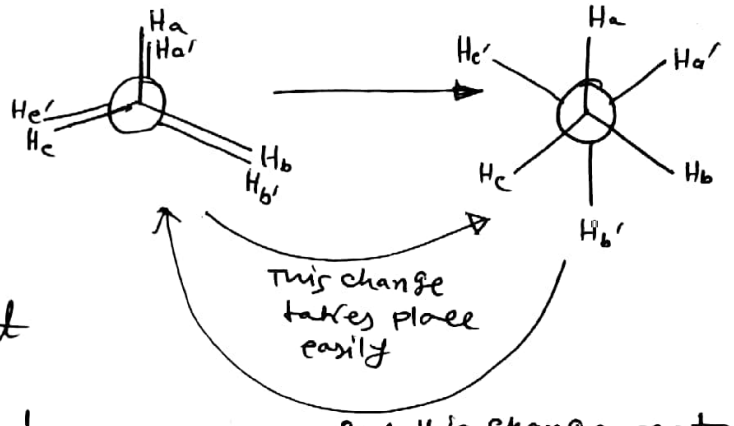
ϕ (H/H)
[more specifically ϕ (Ha/Ha')]

e → eclipsed. (I, III, V, VII)
s → staggered (II, IV, VI).

(Two extreme energy set, all other isomers falls within this energy set).

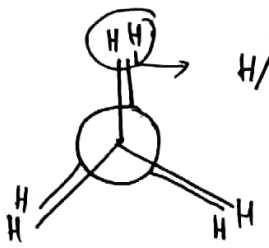
i.e there are three equivalent energy minima corresponds to staggered, these are called Conformer or rotamer. with ϕ - 60°, 180°, -60°. ϕ = dihedral angle or torsion angle.
(Stn-II) (Stn-IV) (Stn-VI)

Torsion angle ?



But this change not occur easily because it will lead to more energy structure, so energy is to be supplied to rotate through this angle (60°) i.e. a torsion is being Produced because of C-H/e-H eclipsing state (called Pitzer strain) so this angle also, called torsional angle and from this concept energy Profile diagram is a torsional curve

* On the other hand three equivalent energy state that corresponds to eclipsed structures having torsional angle ϕ = 0°; 120°, -120°
(Stn-I) (Stn-III) (Stn-V).



H/H → distance (below 0.23 nm. Vandeawaal radius)

H/H → eclipsing energy = 4 KJ mol⁻¹

Total energy = 12 KJ mol⁻¹ (for 3 eclipsing H/H pair)

The energy barrier of ethane thus 12 KJ mol⁻¹

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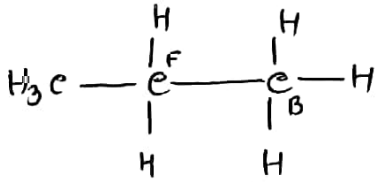
In case of ethane two extreme sets of energy → Eclipsed, staggered

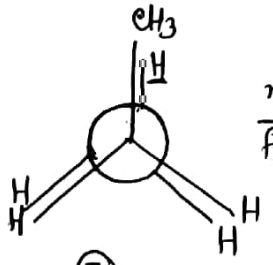
If there was another str. within this energy then gauche or skew str. will come.

For n-Propane :

$H_3C - CH_2 - CH_3$

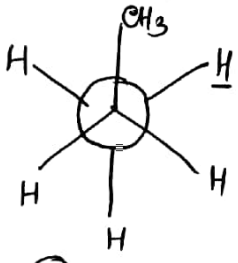


F = Front
B = Back



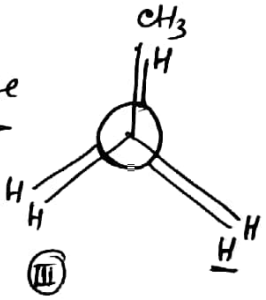
(I) $\phi(CH_3/\underline{H}) = 0°$

60° clockwise rotation of front carbon through $C_F - C_B$ bond



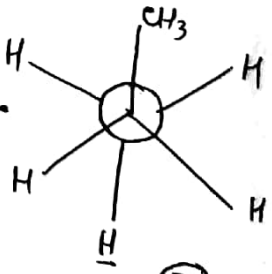
(II) $\phi(CH_3/\underline{H}) = 60°$

60° clockwise rotation of front carbon (120° rotation from I)



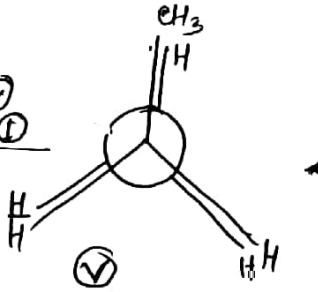
(III) $\phi(CH_3/\underline{H}) = 120°$

60° rotation from (III) / 180° rotation



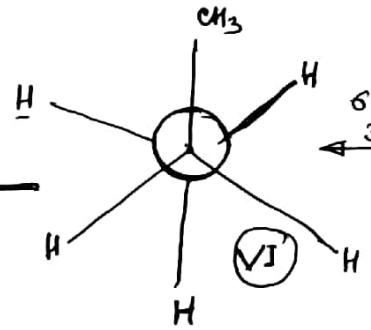
(IV) $\phi(CH_3/H) = 180°$

60° — (IV) / 240° — (I)

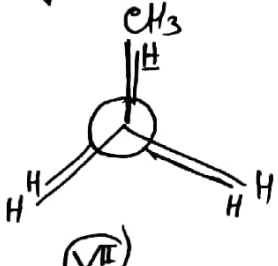


(V) $\phi(CH_3/H) = 240°$

60° — (V) / 300° — (I)



(VI) $\phi(CH_3/H) = 300°$

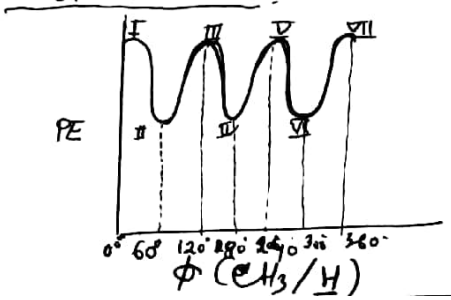


(VII)

I, III, V, VII → Eclipsed

II, IV, VI → staggered

Torsional Curve.



Difference in energy between the conformations P_E and P_S is 14 KJ mol^{-1} (2 KJ mol^{-1} is higher than that of ethane).

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