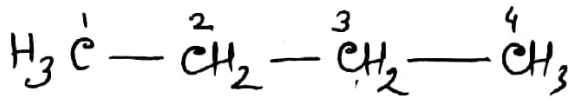


# Conformation

①

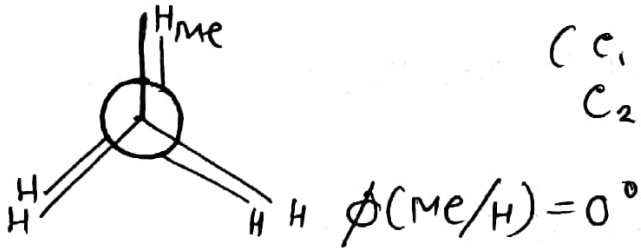
## class-3

Potential energy diagram of n-butane

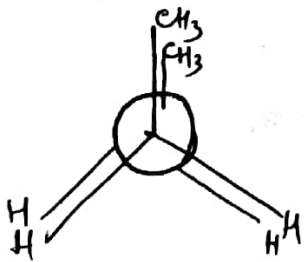


In n-butane unlike n-propane conformational isomerism arises both due to  $\text{C}_1-\text{C}_2$  and  $\text{C}_2-\text{C}_3$  single bond rotation.

If we assume free rotation around  $\text{C}_1-\text{C}_2$  single bond we can start from ( $\text{C}_1 = \text{Front carbon}$  or  $\text{C}_2 = \text{Back carbon}$ ).

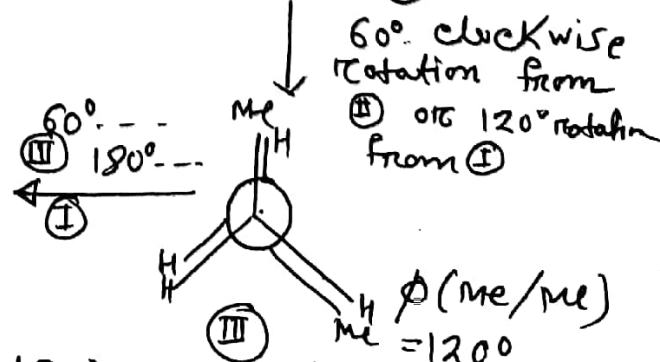
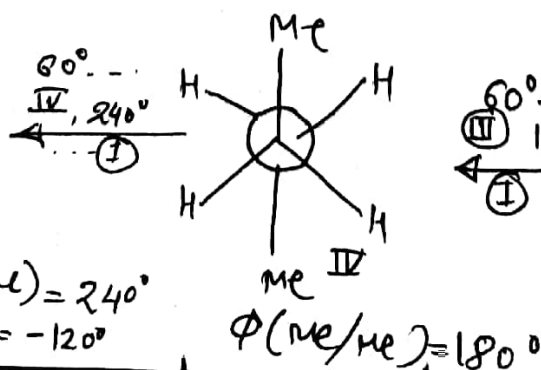
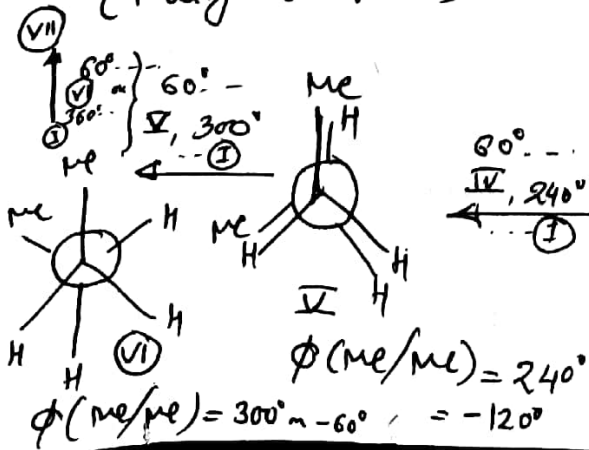
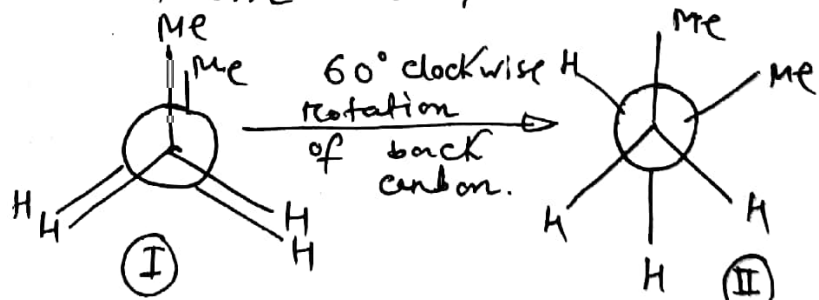


But if we assume free rotation around  $\text{C}_2-\text{C}_3$  single bond we can start from



(Fully eclipsed)

Let's see more isomers from this structure.



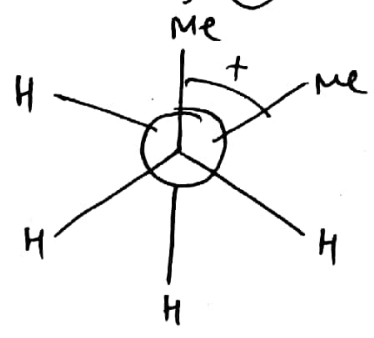
Stability order (increasing order)

I, VII < III, V < II, VI < IV

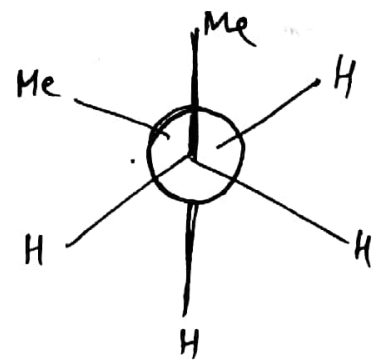
Mind it

in n-butane at room temperature Anti staggered ≈ 66% and Gauche (both P+M) ≈ 34%.

II, VI → Gauche structure

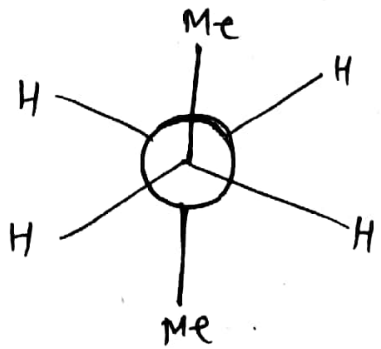


$\phi(\text{Me/Me}) = +60^\circ$   
P-gauche



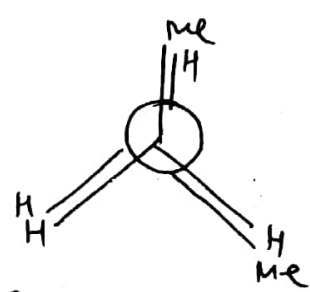
$\phi(\text{Me/Me}) = -60^\circ$   
M-gauche

IV → Anti staggered.



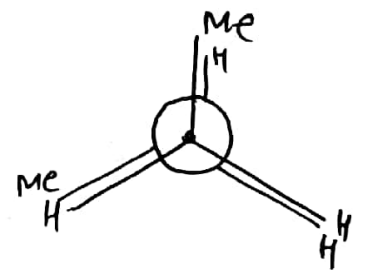
$\phi(\text{Me/Me}) = 180^\circ$   
(most stable)

III, V → Eclipsed.



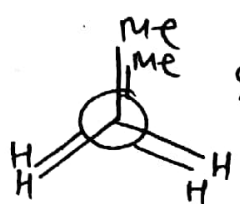
$\phi(\text{Me/Me}) = +120^\circ$   
 $\phi(\text{Me/H}) = 0^\circ$

(Repulsion betw<sup>n</sup> Me/H makes it less stable)



$\phi(\text{Me/Me}) = -120^\circ$  OR  $+240^\circ$   
 $\phi(\text{Me/H}) = 0^\circ$

I, VII → identical.



$\phi(\text{Me/Me}) = 0^\circ$   
Fully eclipsed

Energy profile diagram OR Torsional curve

