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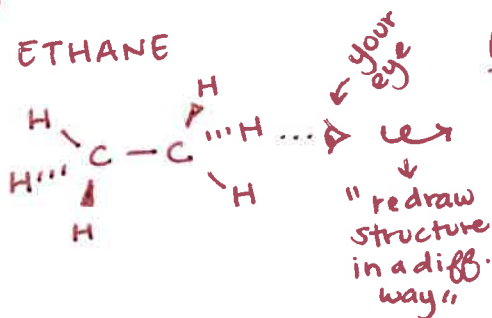
Recall Alkanes

- molecules containing only C+H and only single bonds
 CH_4 - methane ; CH_3CH_3 - ethane ; $\text{CH}_3\text{CH}_2\text{CH}_3$ - propane ; etc.

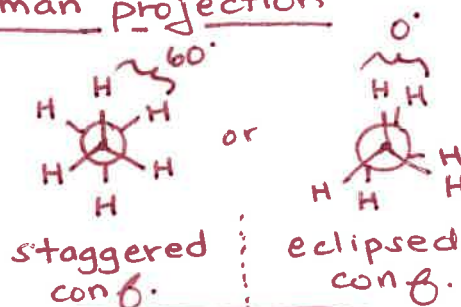
SHAPES of alkane molecules...

- alkane conformations
- for most alkanes, shape can vary because of rotation about C-C bond(s)

- consider ETHANE

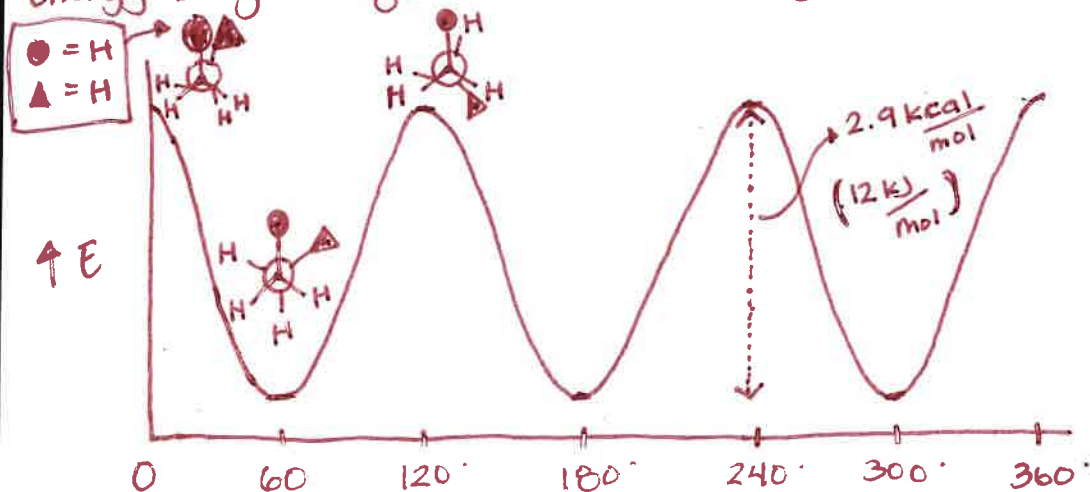


Newman projection



Note: two circles indicate looking down a C-C bond

Energy Diagram for C-C rotation of ethane



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1) Energy minimum (plural minima)
 → energy is lowest, at least locally

2) Energy maximum (plural maxima)
 → energy is highest

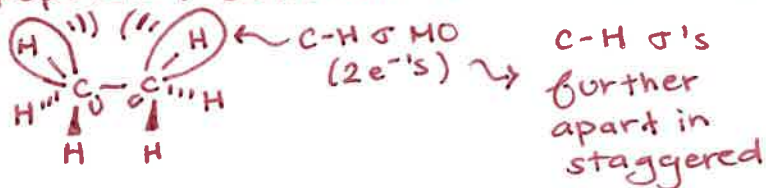
3) Minima are stable forms; maxima are unstable
 ↳ ("transition state")

↙ can not be isolated

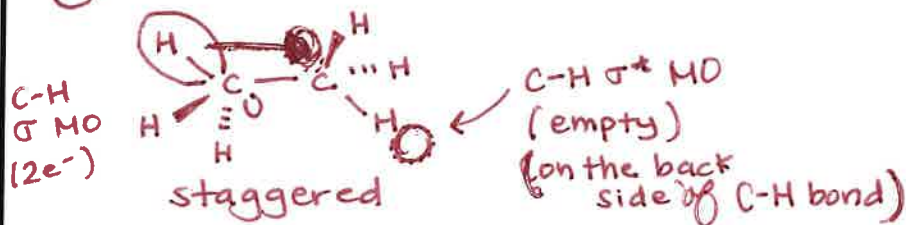
→ Eclipsed = max. (unstable) vs. Staggered = min. (stable)

Why is staggered a minimum, or why is eclipsed a maximum?

① Repulsion between C-H σ e^- 's destabilizes eclipsed.



② $\sigma \rightarrow \sigma^* e^-$ delocalization stabilizes the staggered conf.

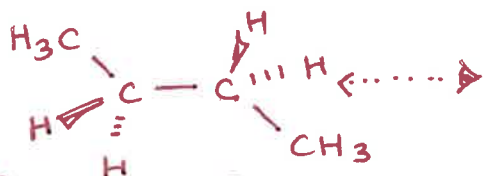


- reduce $e^- - e^-$ repulsion in C-H σ by the e^- 's going into the C-H σ^*
 ↳ overall, net stabilization of staggered

butane
 →

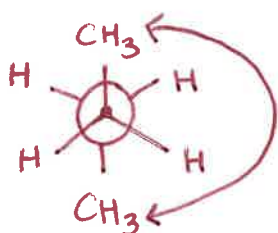
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Butane = $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$



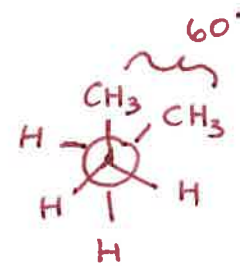
lower symmetry!

• Now, there are 2 different staggered forms.



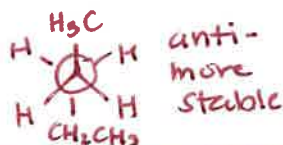
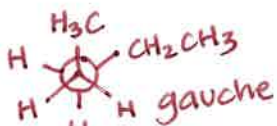
"anti"

180° VS.

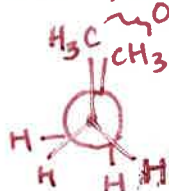


"gauche"

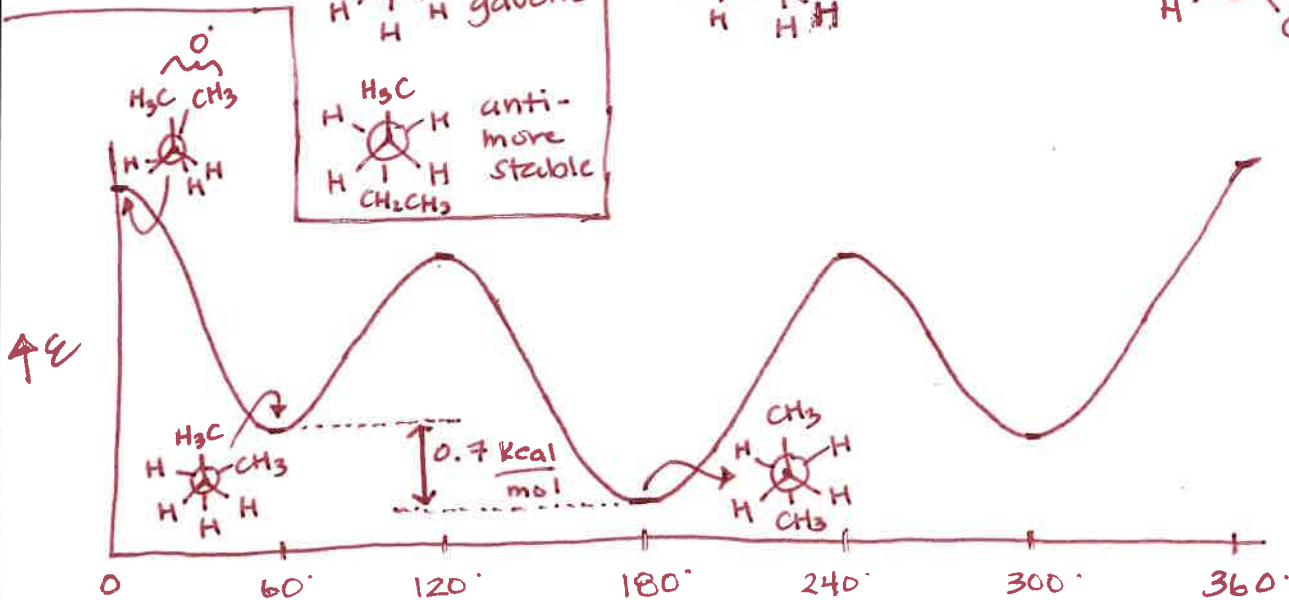
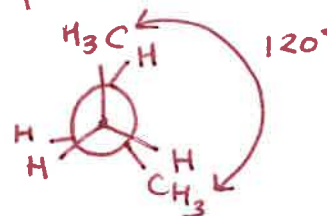
• These principles extend to other alkanes



• also, 2 different eclipsed



VS.



→ ANTI = Global energy minimum (most stable; more so than gauche)
 Why? ⇒ "STERICS"



methyl-methyl steric repulsion destabilizes gauche relative to anti

Disclaimer: BETTER IMAGES in BOOK!