Naming Alkanes and Alkyl Groups

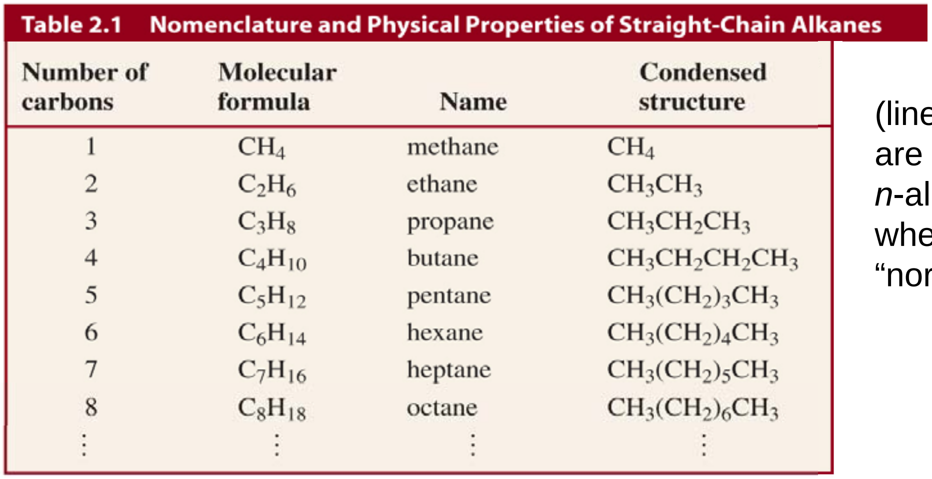
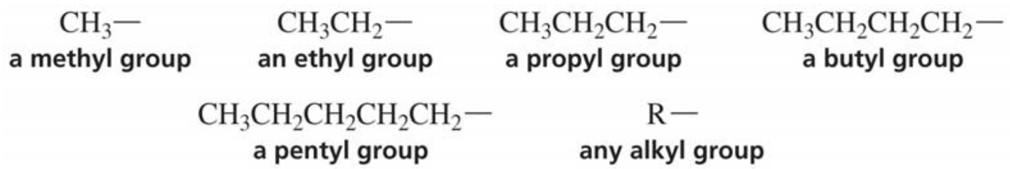


Table 2.1 Nomenclature and Physical Properties of Straight-Chain Alkanes

Number of carbons	Molecular formula	Name	Condensed structure
1	CH_4	methane	CH_4
2	C_2H_6	ethane	CH_3CH_3
3	C_3H_8	propane	$CH_3CH_2CH_3$
4	C_4H_{10}	butane	$CH_3CH_2CH_2CH_3$
5	C_5H_{12}	pentane	$CH_3(CH_2)_3CH_3$
6	C_6H_{14}	hexane	$CH_3(CH_2)_4CH_3$
7	C_7H_{16}	heptane	$CH_3(CH_2)_5CH_3$
8	C_8H_{18}	octane	$CH_3(CH_2)_6CH_3$
⋮	⋮	⋮	⋮

(linear alkanes are also called *n*-alkanes, where *n* is "normal")

Names of alkyl fragments derive from alkanes:



$CH_3—$ **a methyl group**

$CH_3CH_2—$ **an ethyl group**

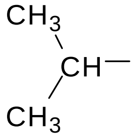
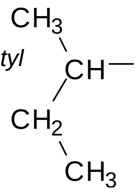
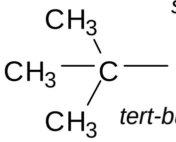
$CH_3CH_2CH_2—$ **a propyl group**

$CH_3CH_2CH_2CH_2—$ **a butyl group**

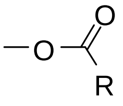
$CH_3CH_2CH_2CH_2CH_2—$ **a pentyl group**

$R—$ **any alkyl group**

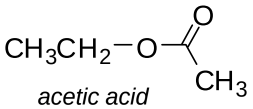
Naming Functionalized Alkanes

CH_4 *methane*	$CH_3—$ *(or* $H_3C—$*)* *methyl*
CH_3CH_3 *ethane*	$CH_3CH_2—$ *ethyl*
$CH_3CH_2CH_3$ *propane*	$CH_3CH_2CH_2—$ *n-propyl*  *iso-propyl*
$CH_3CH_2CH_2CH_3$ *butane*	$CH_3CH_2CH_2CH_2—$ *n-butyl*  *sec-butyl*  *tert-butyl*

—OH *alcohol* → $CH_3—OH$ *methyl alcohol (methanol)*

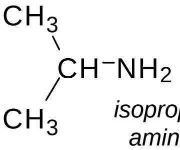


ester →

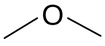


acetic acid ethyl ester (ethyl acetate)

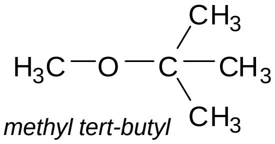
$—NH_2$ *amine* →



isopropyl amine

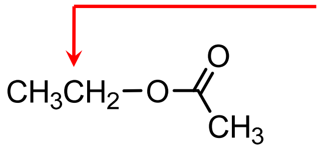


ether →



methyl tert-butyl ether (MTBE)

Naming Functionalized Alkanes



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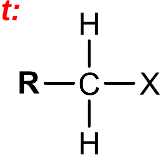
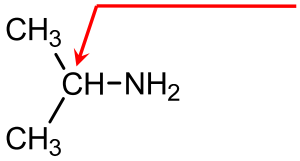


$\mathbf{R}-\overset{H}{\underset{H}{C}}-X$

Primary carbon, forms primary ester.



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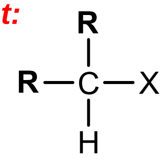
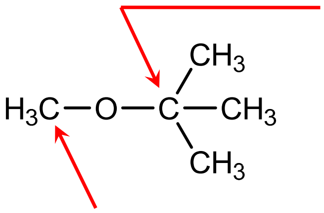


$\mathbf{R}-\overset{\mathbf{R}}{\underset{H}{C}}-X$

Secondary carbon, forms secondary amine.



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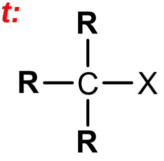
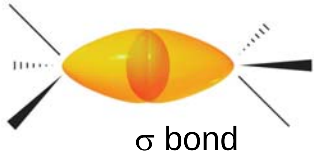


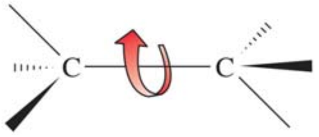
$\mathbf{R}-\overset{\mathbf{R}}{\underset{\mathbf{R}}{C}}-X$

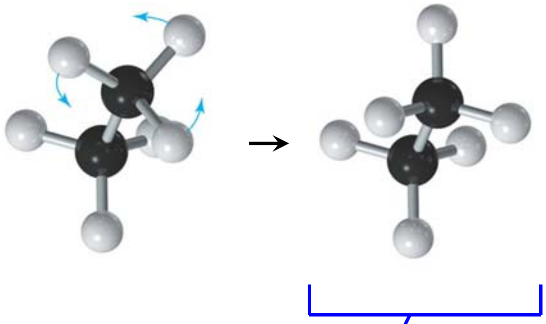
Tertiary carbon, forms tertiary ether.

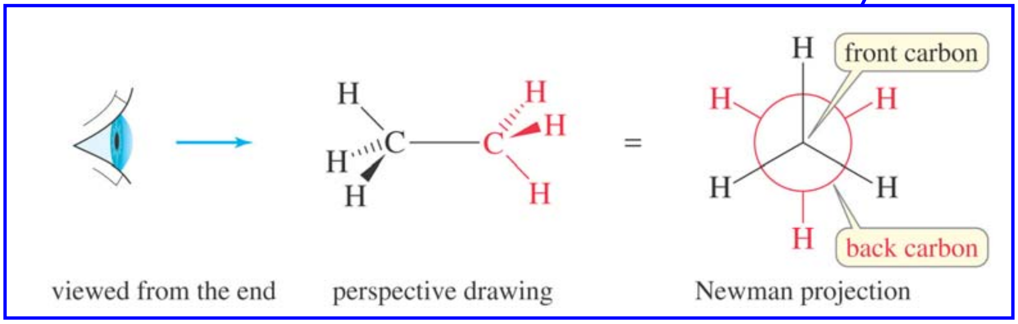
Just **methyl**, not primary.

Bond Rotation and Newman Projections

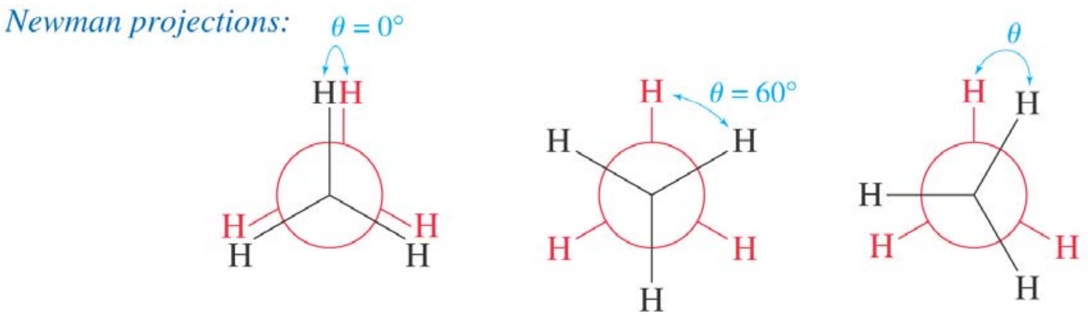








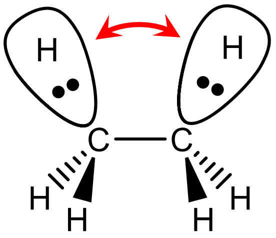
Rotation About Single Bond in Ethane



“eclipsed”

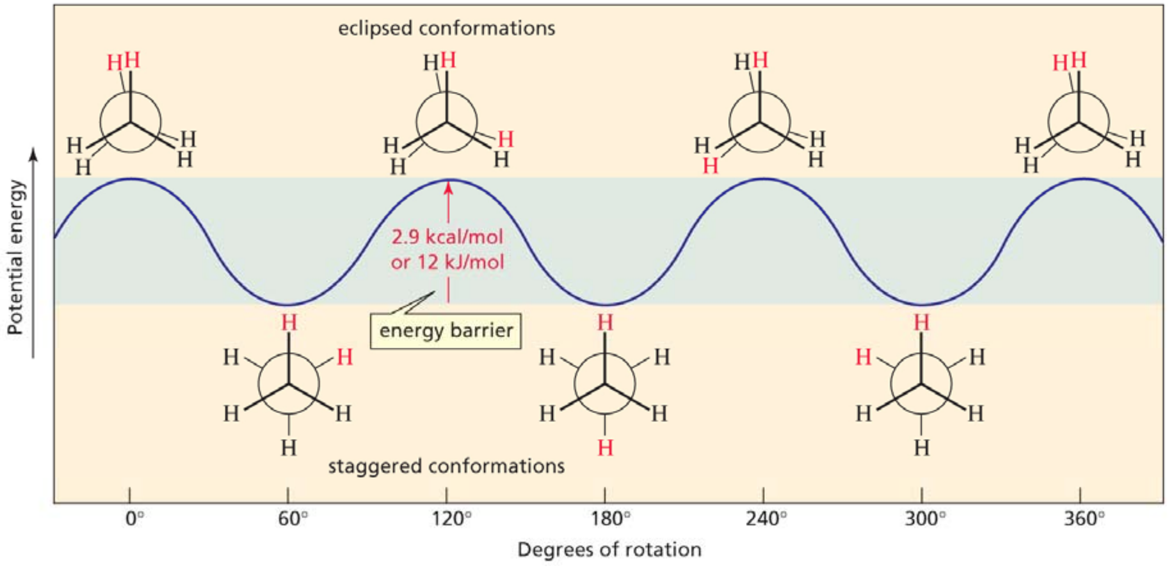
“staggered”

“skew”



In “eclipsed” conformation, electron-pair repulsion between σ bonds is maximized.

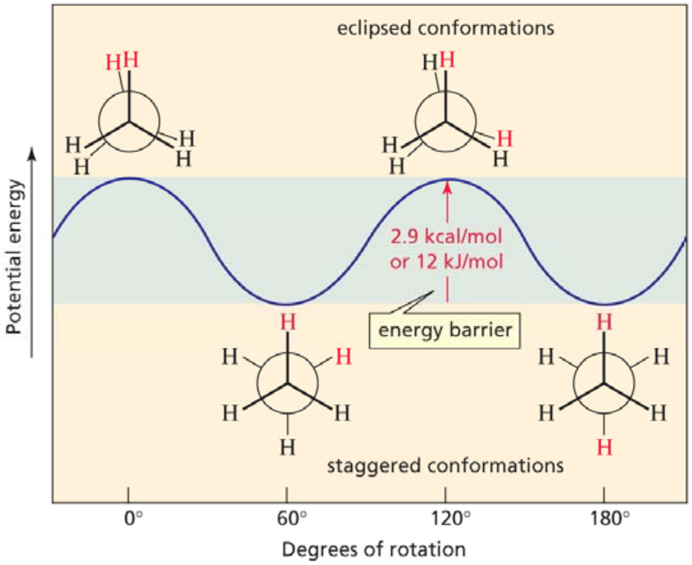
Rotation About Single Bond in Ethane

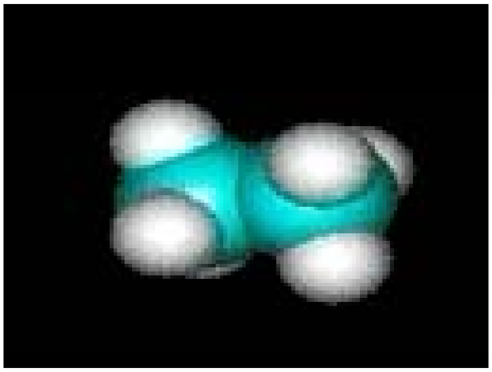


Torsional energy of 2.9 kcal/mol must be overcome to rotate 120°.

Timescale of that happening: once every 100 femtoseconds (at room temp).

Rotation About Single Bond in Ethane

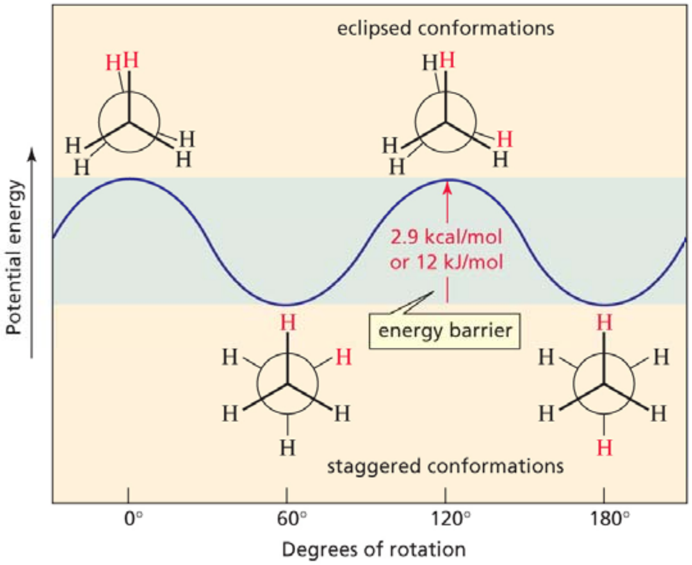


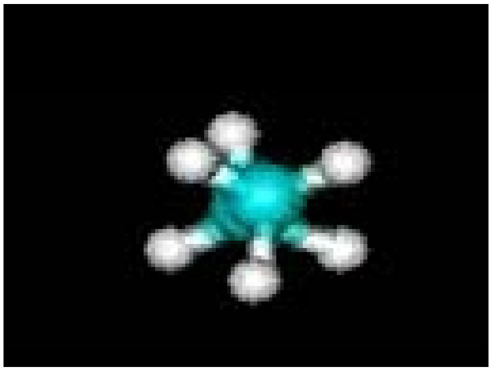


Video: Ethane, 273 K, 500 fs

(Simulation performed by molecular dynamics, using standard rotational and vibrational potentials.)

Rotation About Single Bond in Ethane





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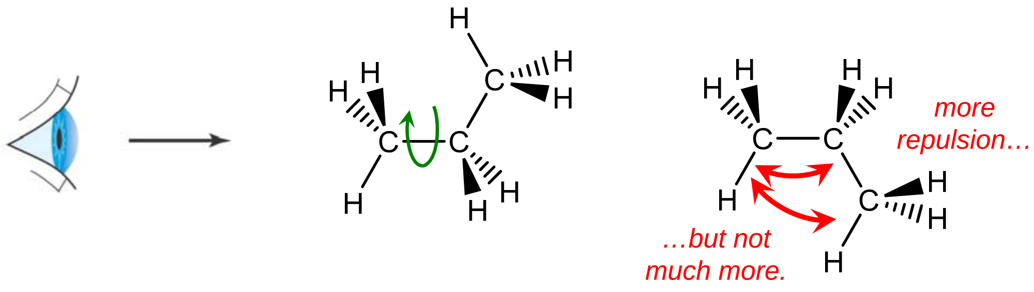
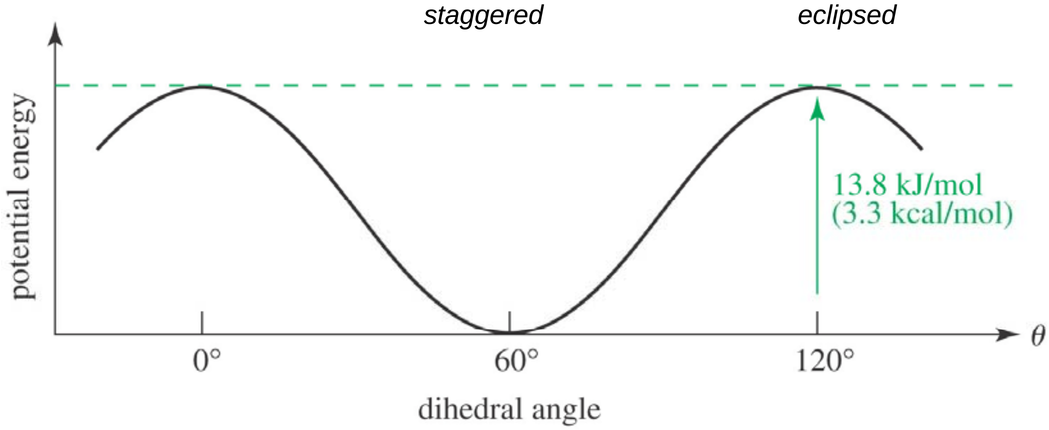
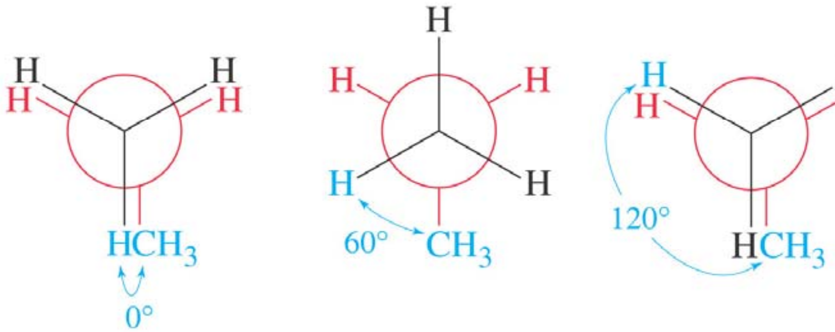
Rotation About Single Bond in Propane

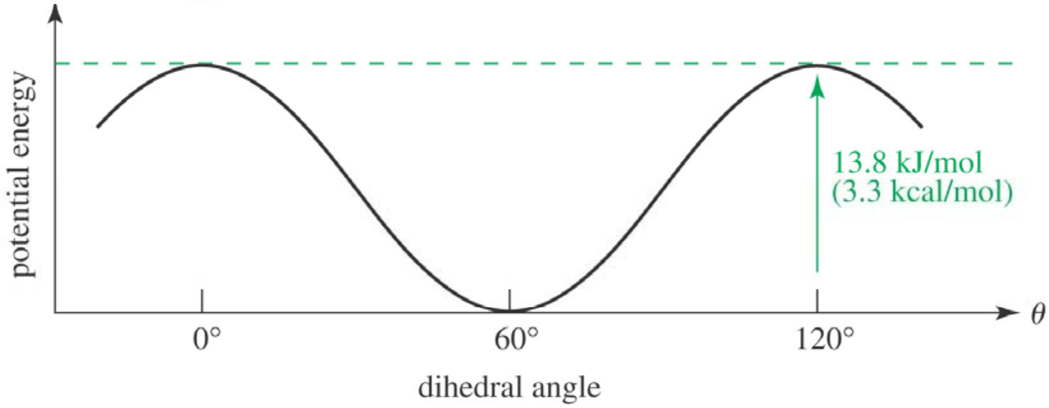


staggered *eclipsed*

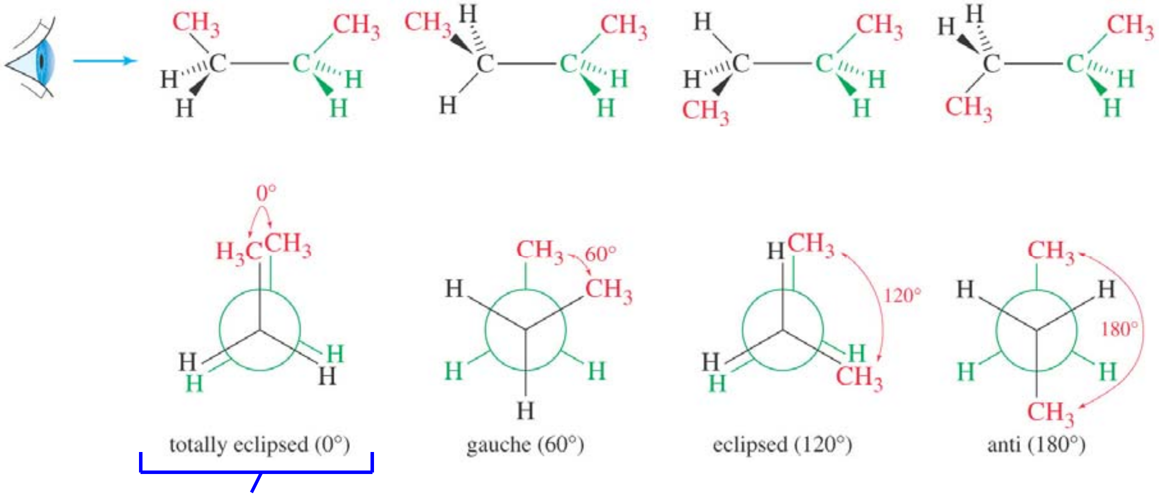


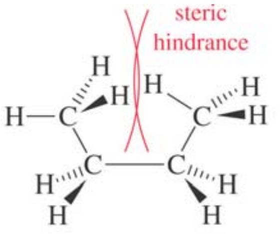
Rotation About Single Bond in Propane

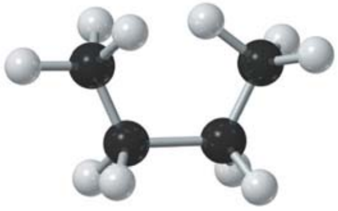




Rotation About Single Bond in Butane



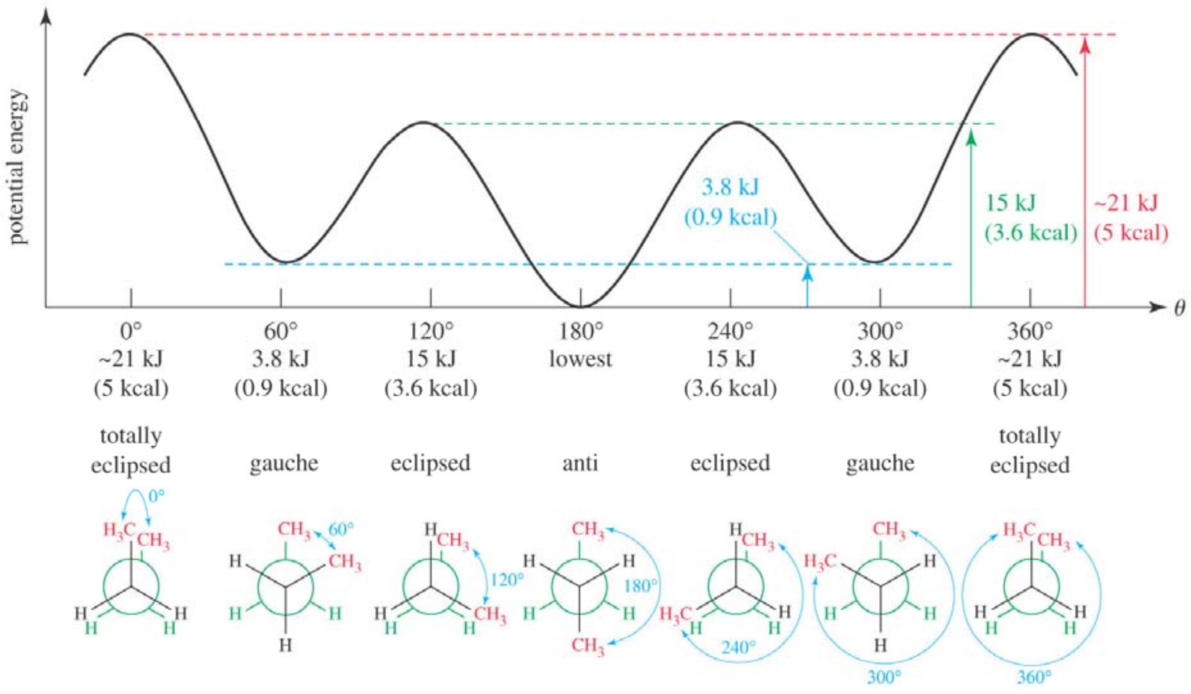




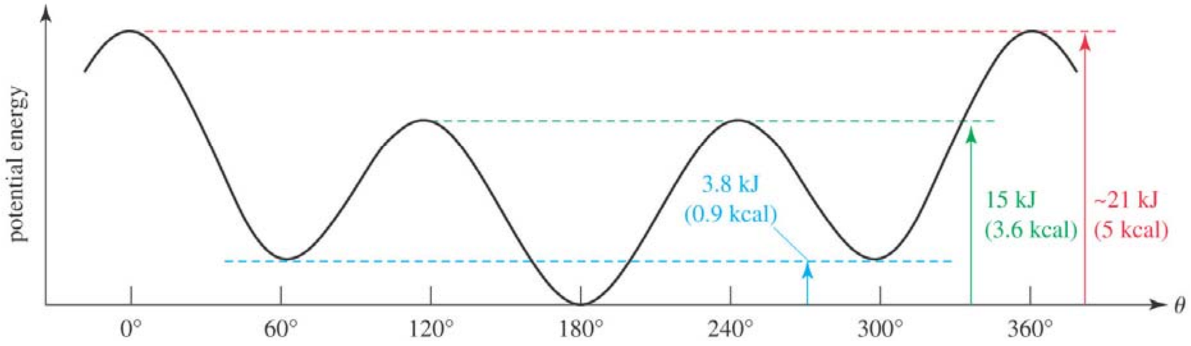
H-H steric interaction is unavoidable.

So, “totally eclipsed” is higher in energy than “eclipsed”.

Rotation About Single Bond in Butane



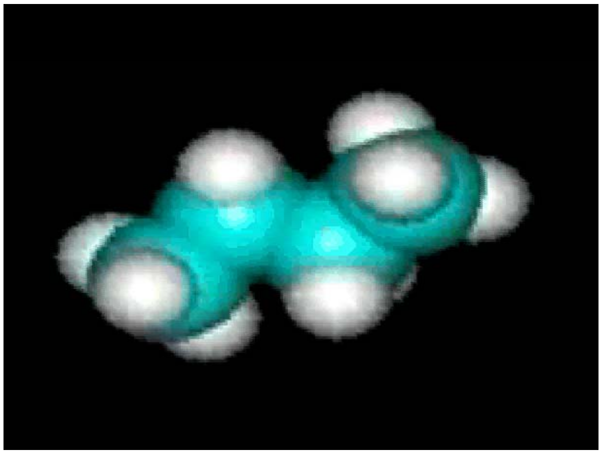
Rotation About Single Bond in Butane



Points to note:

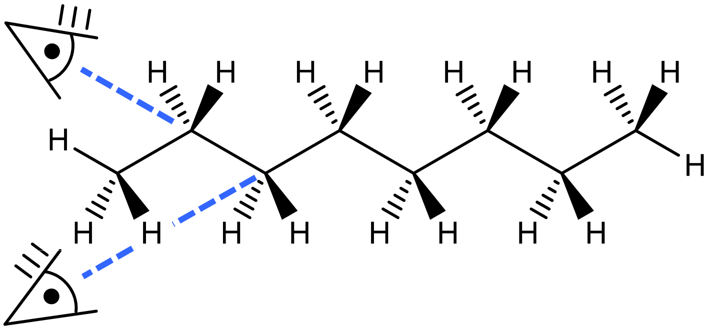
Gauche is not that much less stable than anti; so, butane spends plenty of time in gauche conformation.

Barrier to rotation of end methyl groups (3.3 kcal/mol) is less than that of internal C-C bond (5 kcal/mol).



Conformational Preferences Extend to Higher Alkanes

For linear alkanes, the all-anti conformation is preferred…



What Newman projections would you draw for these two perspectives?

Conformational Preferences Extend to Higher Alkanes

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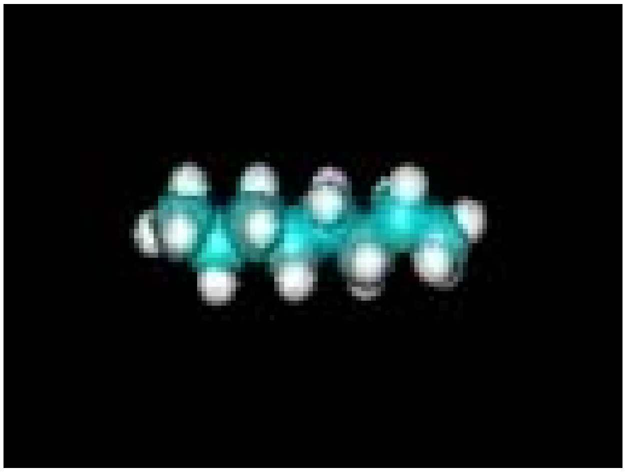

…but not by much. Gauche conformers frequently observed.