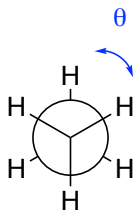
Saturated Acyclic Hydrocarbons

from chapter(s) _____ in the recommended text

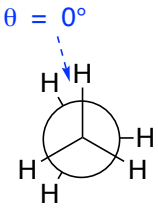
A Introduction

B Conformations Of Acyclic Hydrocarbons

Ethane

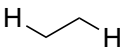


staggered

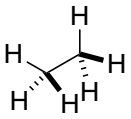


shown slightly offset but direct allignment is assumed

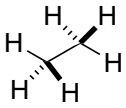
eclipsed



staggered



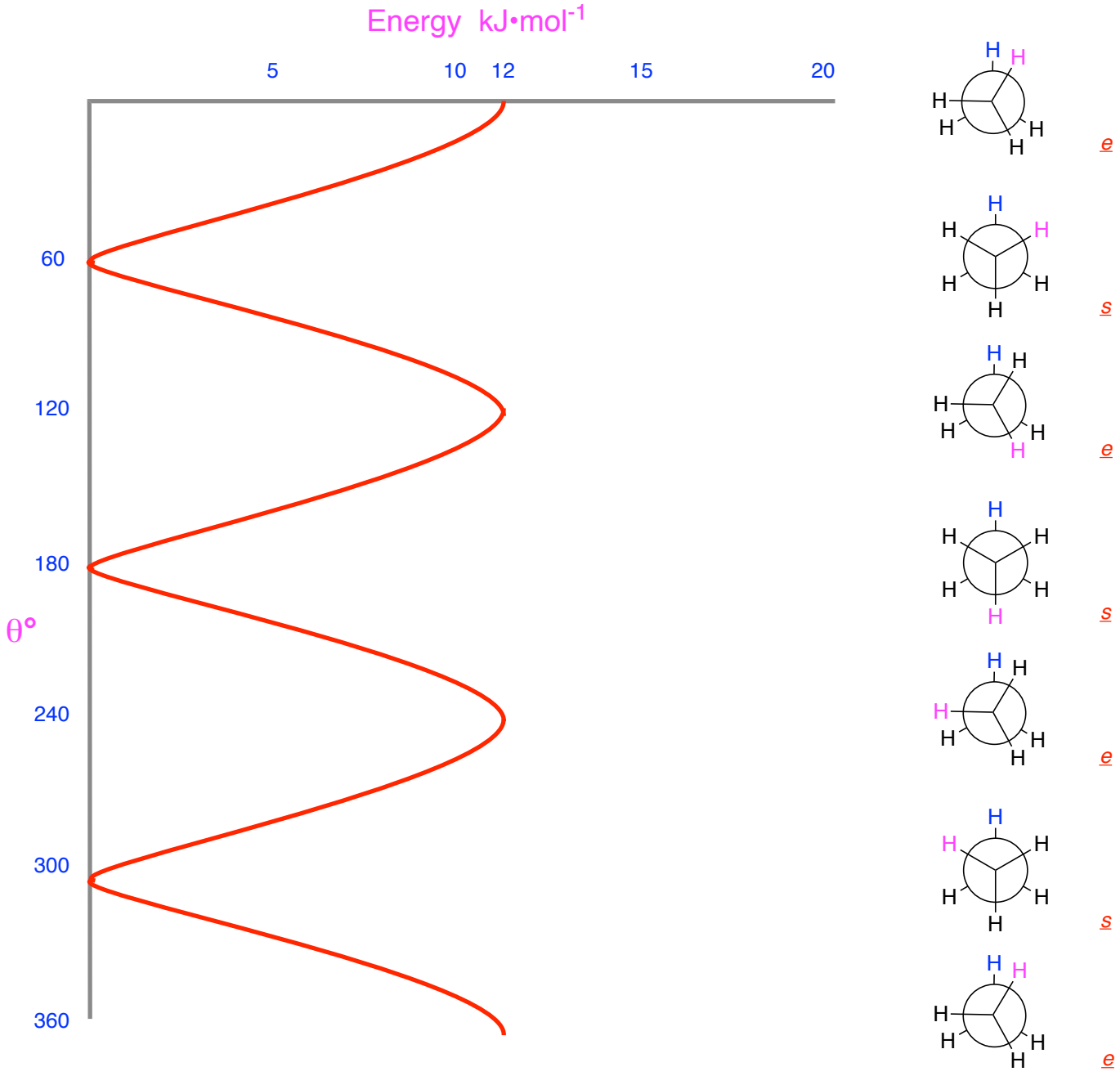
eclipsed



staggered

eclipsed

The *staggered* ethane conformer is more stable

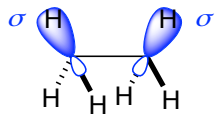


that repulsion is called *torsional* strain.

molecular orbital diagrams to indicate *destabilizing* interactions
and *stabilizing* interactions

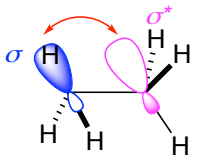
σ-orbital contributes *2* e
an empty one donates *0 e*

repulsive

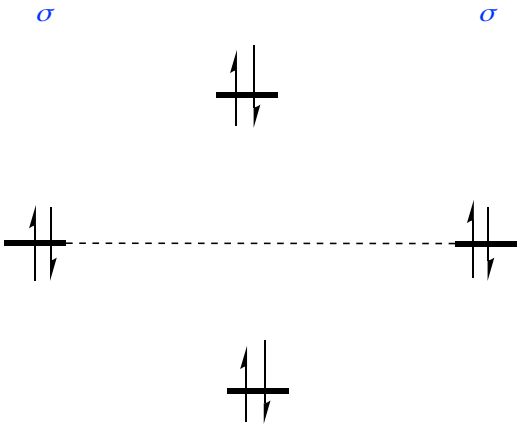


torsional strain

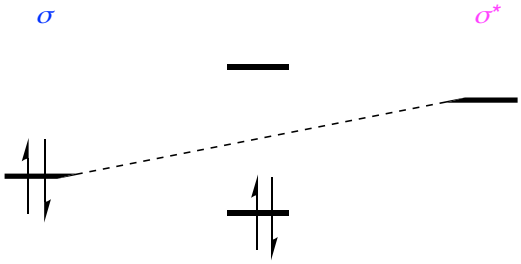
attractive



add electrons to the diagrams below and indicate bond orders:



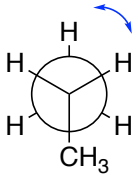
non-bonding



bonding

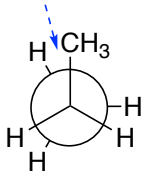
Propane

θ = 60°



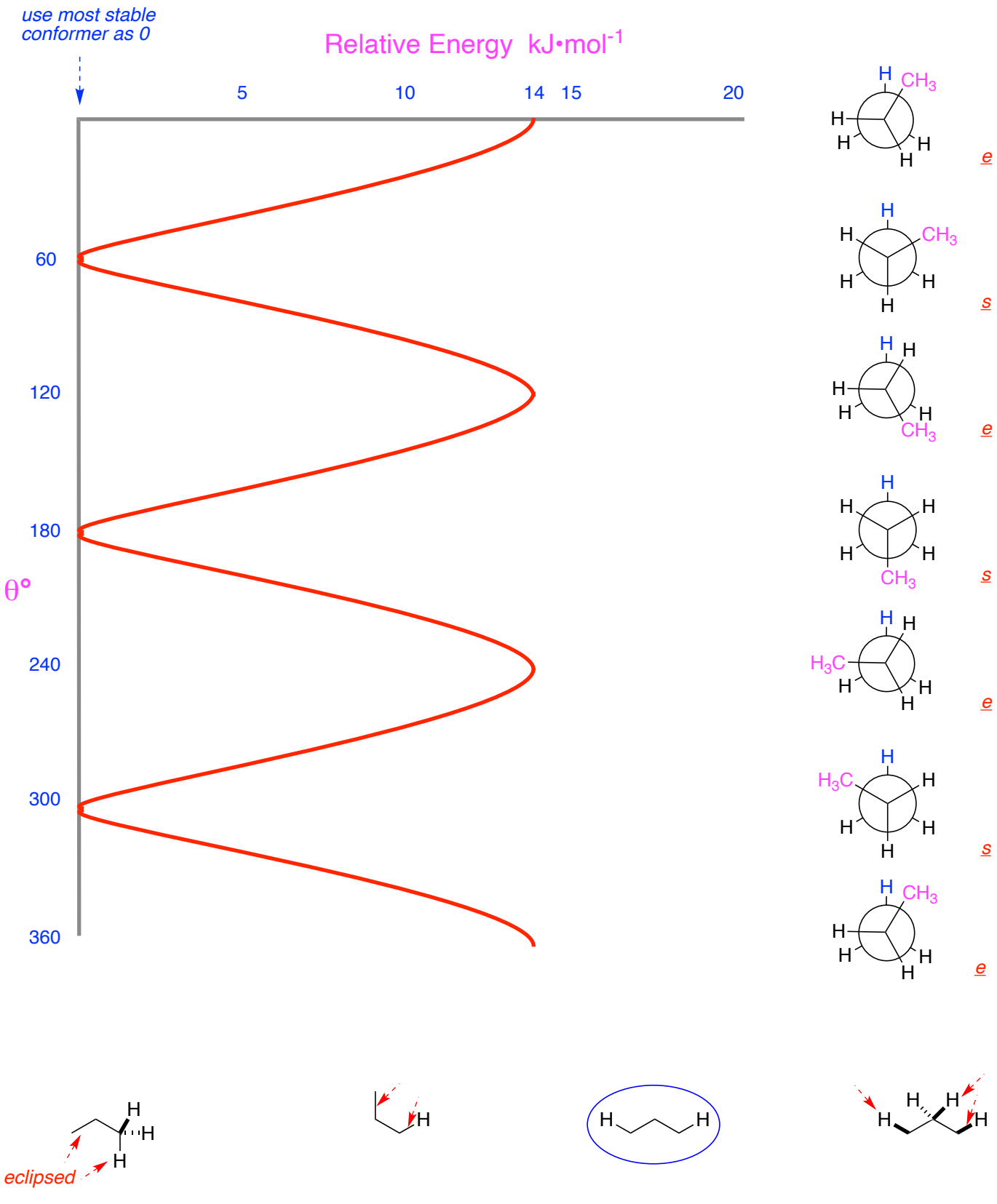
staggered

θ = 0°

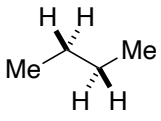


eclipsed

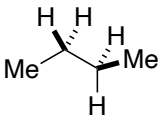
shown slightly offset but direct allignment is assumed


use most stable conformer as 0
Relative Energy kJ•mol-1
5
10
14
15
20
60
120
180
240
300
360
θ°
e
s
e
s
e
s
e
eclipsed

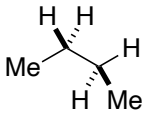
Butane



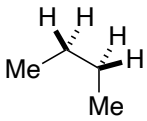
very low



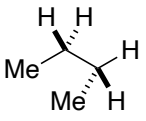
high



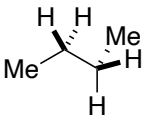
low



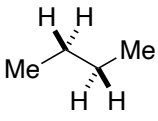
very high



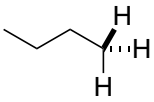
low

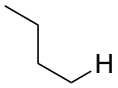


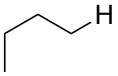
high

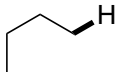


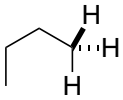
very low

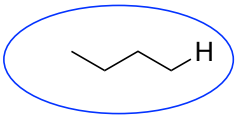


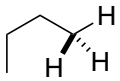


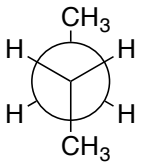




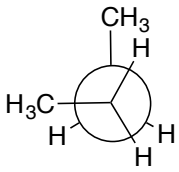








a



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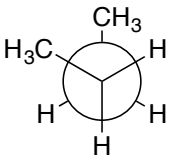

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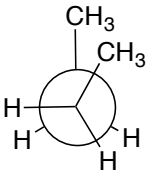

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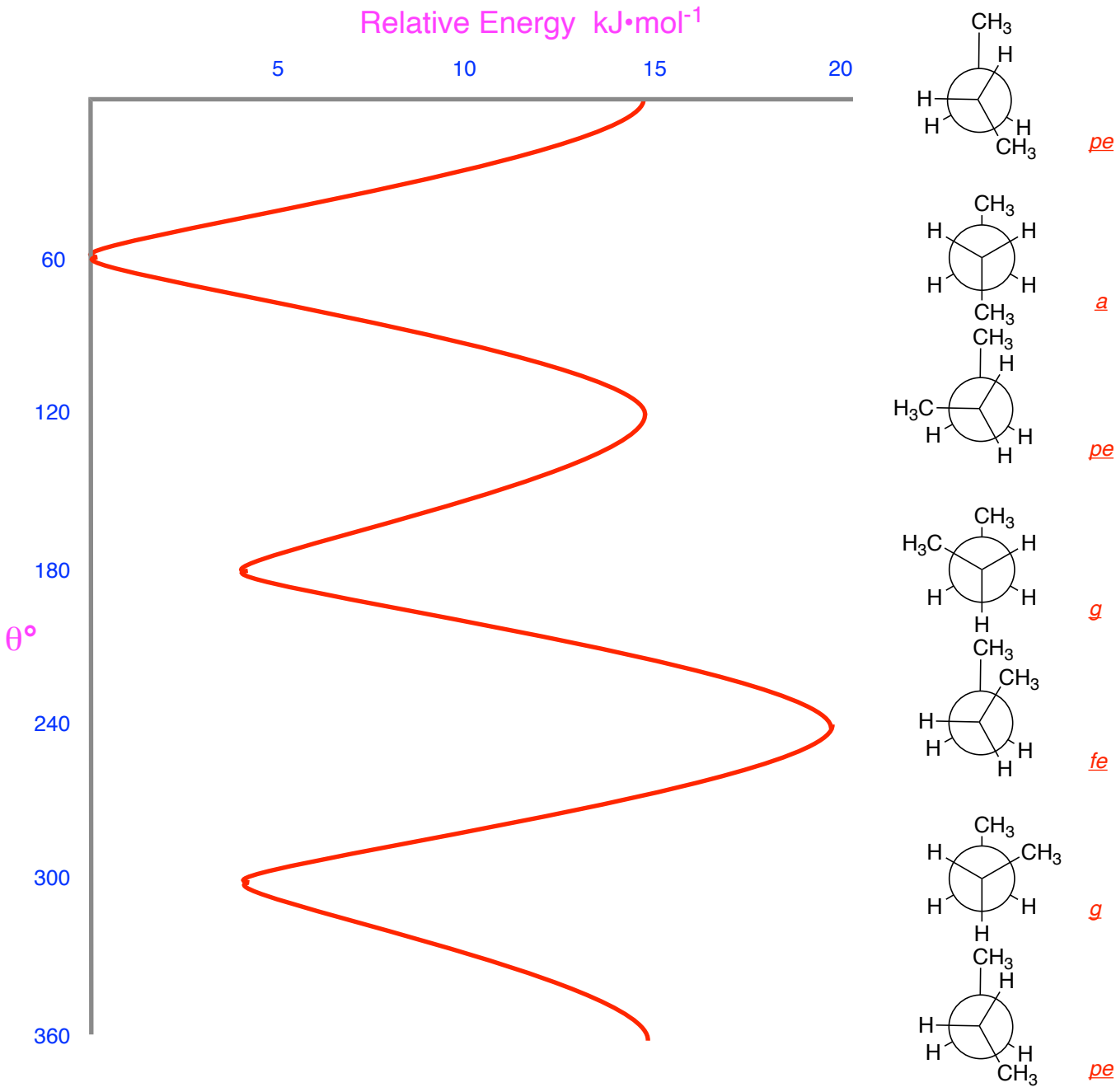


Destabilization of butane in the totally eclipsed conformation is a result of combinations of *torsional / steric* strain.

Steric strain between the methyl groups in butane is that which results when atoms compete for the same region of space.

C Art In Organic Chemistry

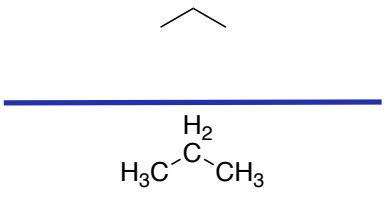
Two Dimensional Diagrams Of Organic Molecules

is one bond to an apex that {terminal point} represents *CH_3*
two bonds to an apex means it is a *CH_2*
three bonds to a branch point represent *CH*.
this means there are *0* hydrogen atoms on that carbon.

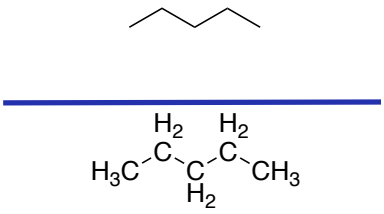
Zigzag conformations represent *staggered* conformers

it *does not* matter if the chains zigzag

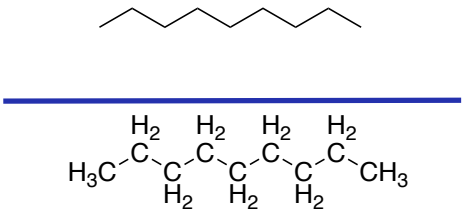
propane



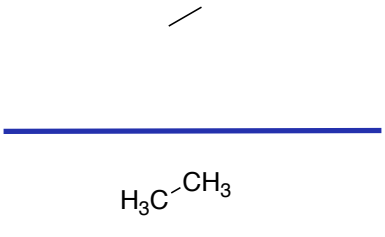
pentane



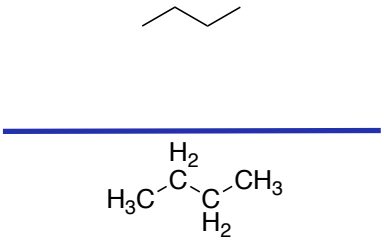
nonane



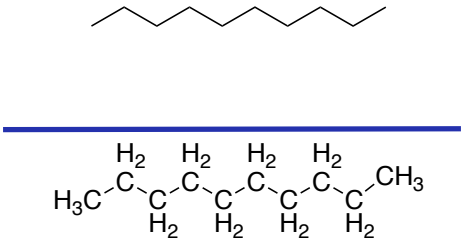
ethane



butane

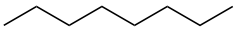


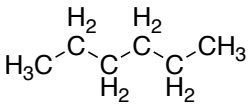
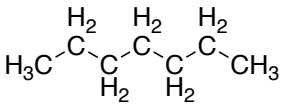
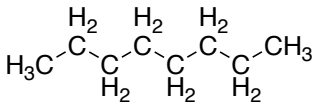
decane



hexane *heptane* *octane*





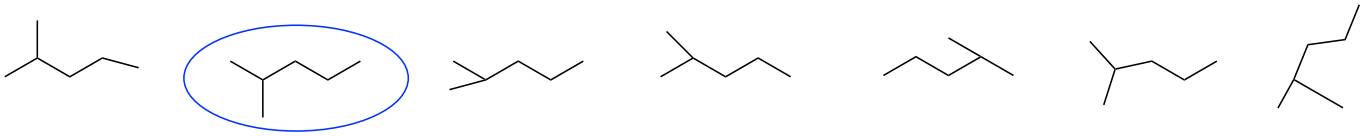
ideal bond (*H*-*C*-*H*) angles for sp^3-hybridized carbons ~*109°*

has *4* bonds to other atoms.

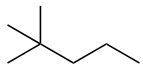
carbon atoms in organic structures *always* have
C-atoms in common organic molecules *never*

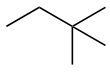
hybridization state of the carbons in the above molecules is *sp^3 because* they have *4* atoms attached.

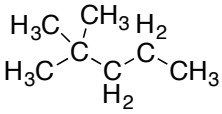
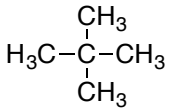
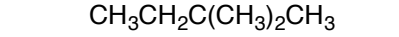
corners of a *tetrahedral* shape
ideally about *109°*

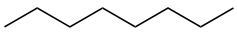


2,2-dimethylpentane *2,2-dimethylpropane* *2,2-dimethylbutane*



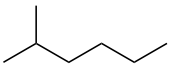




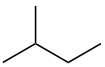
octane

heptane

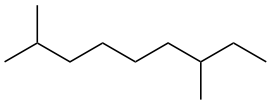


2-methylhexane

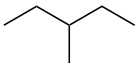
methylpropane



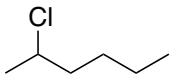
2-methylbutane



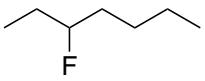
2,7-dimethylnonane



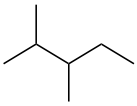
3-methylpentane



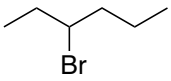
2-chlorohexane



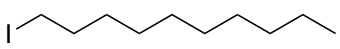
3-fluoroheptane



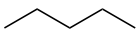
2,3-dimethylpentane



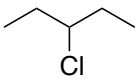
3-bromohexane



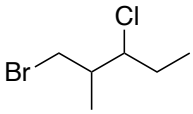
1-iododecanane



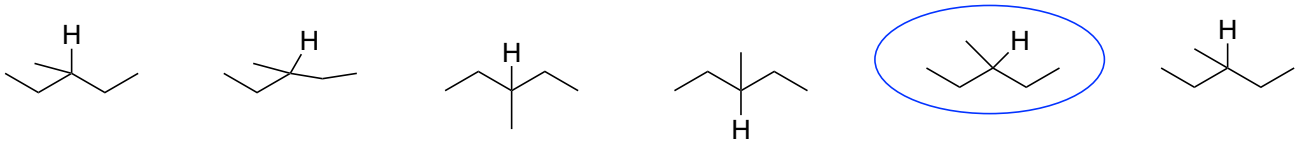
$CH_3CH_2CH_2CH_2CH_3$



$CH_3CH_2CHClCH_2CH_3$



$BrCH_2CH(CH_3)CHClCH_2CH_3$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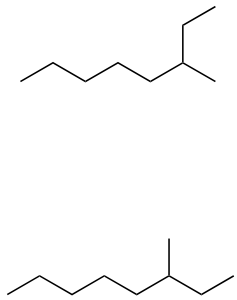

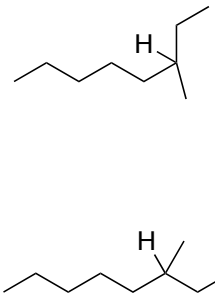
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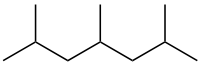

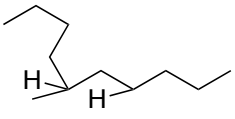
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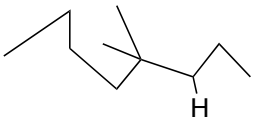
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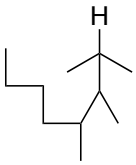
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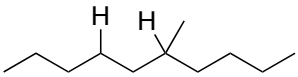
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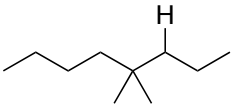
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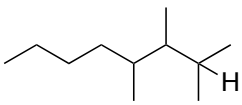
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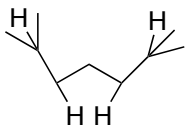
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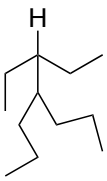
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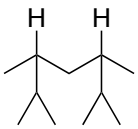
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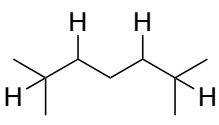
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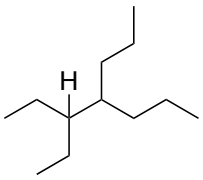
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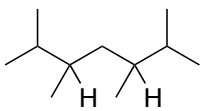
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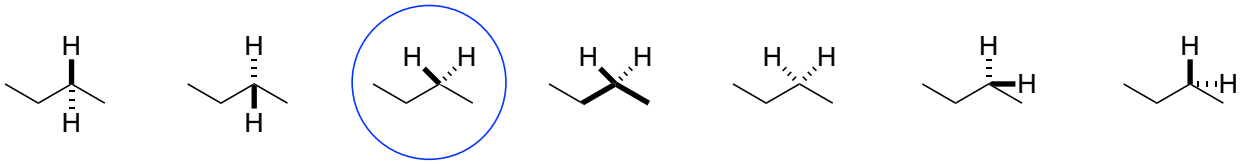
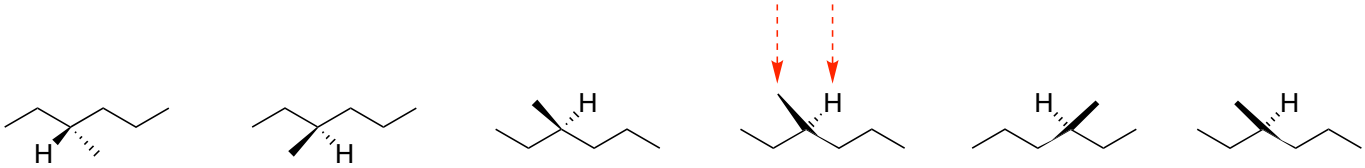
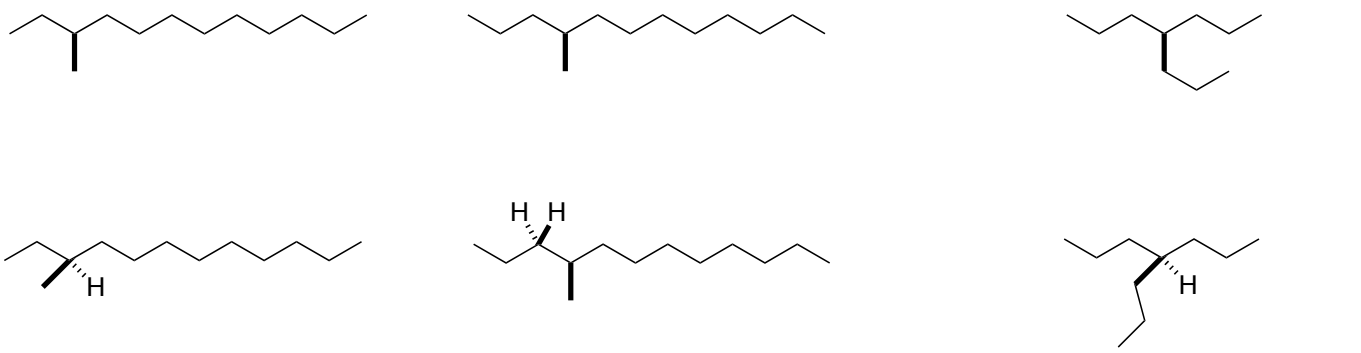
Three Dimensional Diagrams Of Organic Molecules



wedges wrong way around





.... the C^3 hydrogen

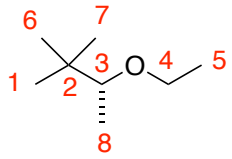
.... both hydrogens on C^3

.... the H on unique C

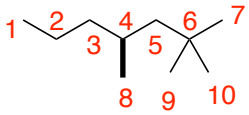
Alkyl Fragments

In Acyclic Hydrocarbons

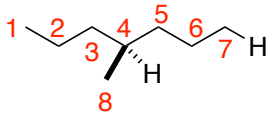
carbon connected to three hydrogens is called a *methyl*
Methylene fragments (of molecules) are those that have CH_2 connected
Methine is the name given to *CH* fragments
CH_3 connected to anything is called a *methyl*
A quaternary *C* has *0* hydrogen



C1, C5, C6, C7, C8 methyl
C2 quarternary
C3 methine
C4 methylene



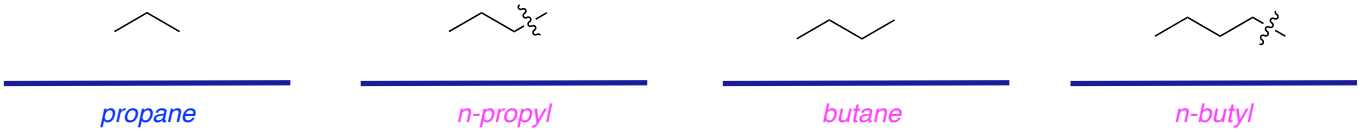
C1, C7, C8, C9, C10 methyl
C2, C3, C5 methylene
C4 = methine
C6 = quarternary



C1, C7, C8 methyl
C2, C3, C6 methylene
C4 = methine

removed and replaced with something else *ie substituted*
represented as *CH_3, Me*
represented as *CH_3CH_2, Et*
ethyl group *cannot* be isolated and put in a bottle; it *is not* a discrete compound, but it *is* a molecular fragment
the fragment *is* attached to something else

Propane contains *2* types of
gives *different* outcomes
chain gives *a normal* propyl
represented as *$MeCH_2CH_2$, $EtCH_2$, ^nPr*
a(n) *iso-* propyl group
can be represented as *^iPr, $(CH_3)_2CH$*



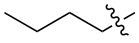
propane *n-propyl* *butane* *n-butyl*

3 types of hydrogen
butyl chain gives a *normal* butyl group
represented as *$MeCH_2CH_2CH_2$, $^nPrCH_2$, $CH_3CH_2CH_2CH_2$*

a(n) *sec* butyl group
represented as *$CH_3CH_2CHCH_3$*

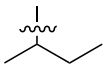
2-Methylpropane is an *isomer* of butane: it has __2__ chemically inequivalent hydrogen
ie a *^iBu* group.

ie *^tBu*.

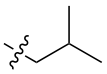


n-butyl

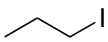
tert-butyl



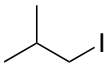
sec-butyl



iso-butyl

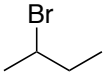


^{n}PrI



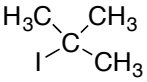
^{i}BuI

^{i}PrCl

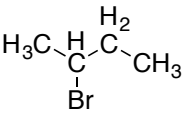


^{s}BuBr

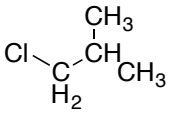
MeBr



^{t}BuI

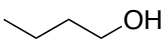


^{s}BuBr

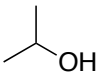


^{i}BuCl

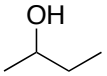
^{t}BuOH



^{n}BuOH



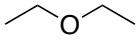
^{i}PrOH



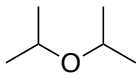
^{s}BuOH

EtOH

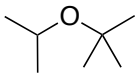
^{t}BuOMe



EtOEt
an anesthetic



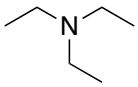
^{i}PrO^{i}Pr



^{t}BuO^{i}Pr

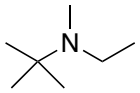
MeOMe

^{t}BuNHMe



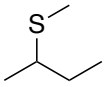
Et_3N

^{i}PrNH$_2$

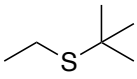


^{t}BuNMeEt

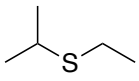
MeNH$_2$



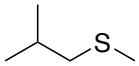
^{s}BuSMe



EtS^{t}Bu

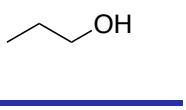


^{i}PrSEt



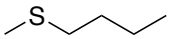
^{i}BuSMe

Me_2S



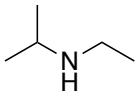
$HO^{n}Pr$

alcohol



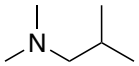
$MeS^{n}Bu$

thioether



$^{i}PrNHEt$

amine



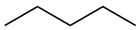
$^{i}BuNMe_{2}$

amine

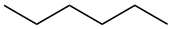
name functional groups as alcohol, amine, ether, or thioether on the dashed lines

D Conclusion

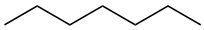
These *are* zigzag conformations.



pentane



hexane



heptane

decane

linear hydrocarbons *can* be represented