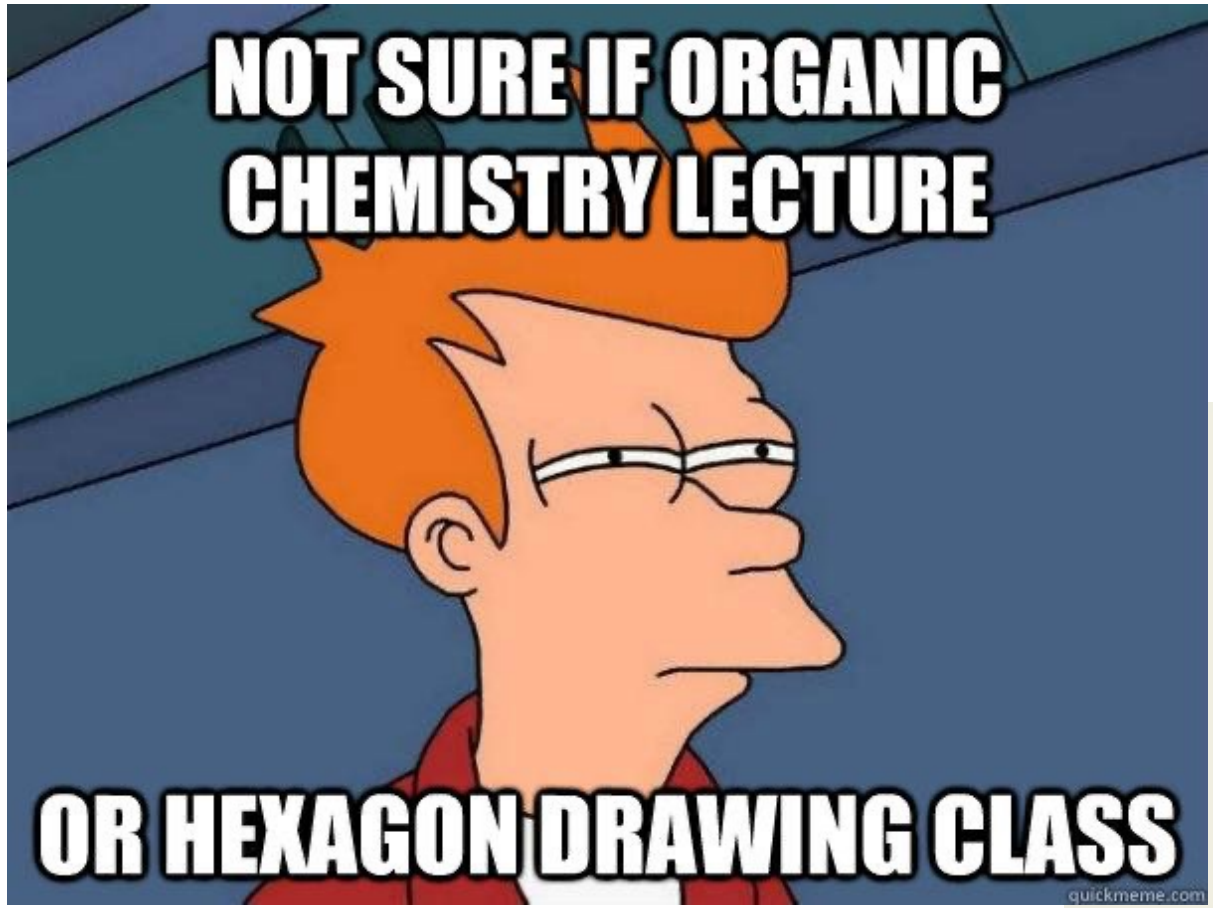
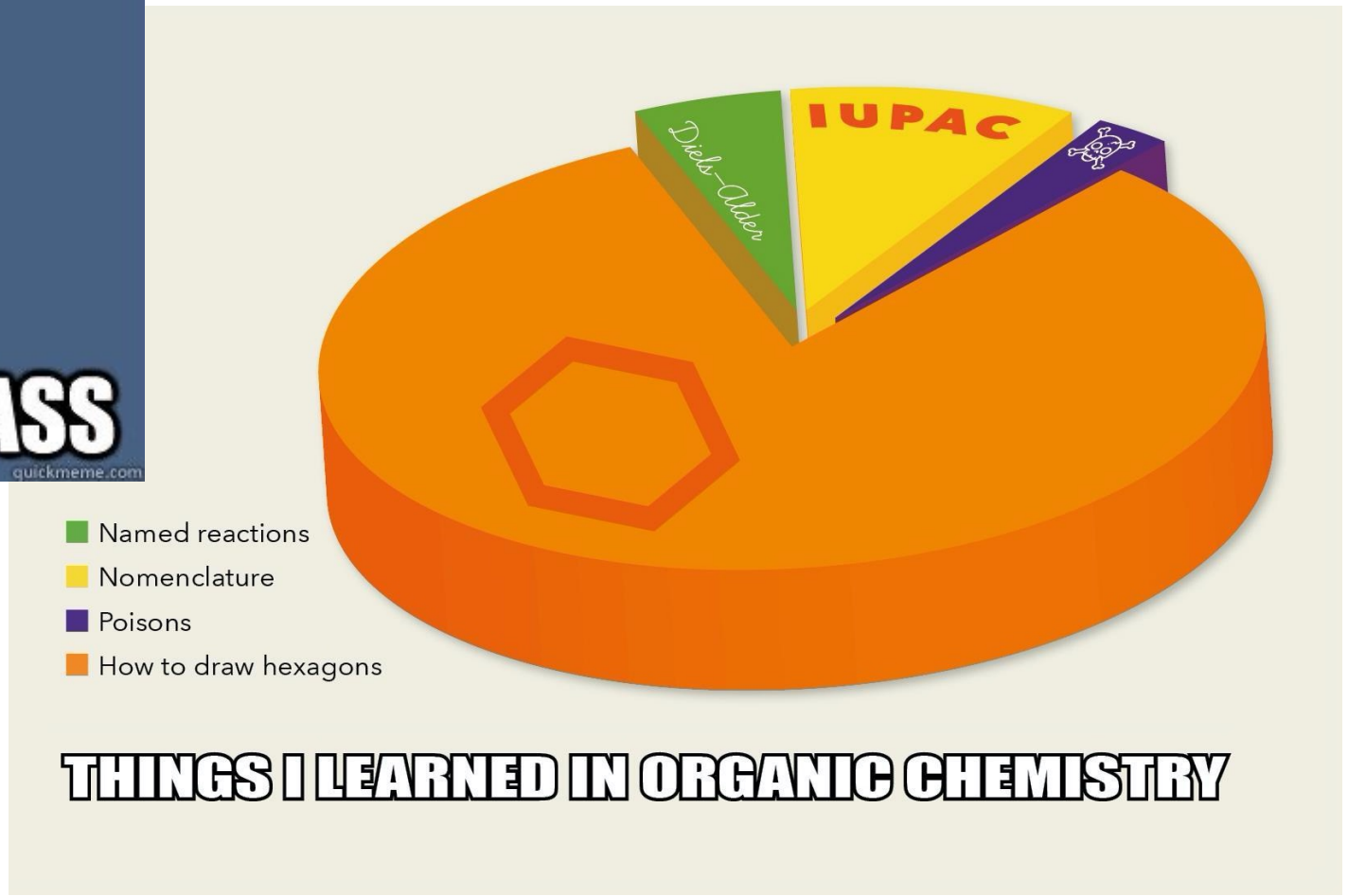


ALKANES & CONFORMERS

CH. 4



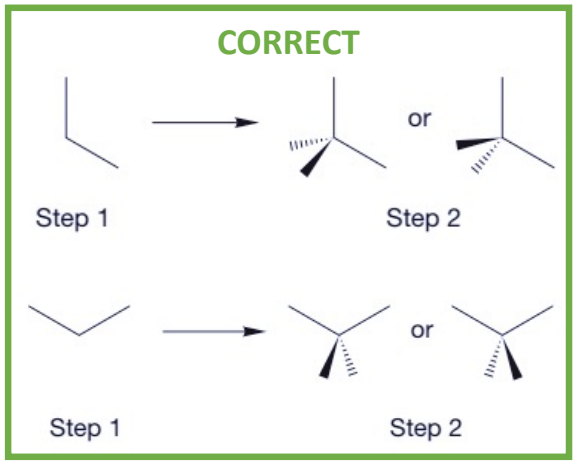
PROPERTIES & HOW TO DRAW

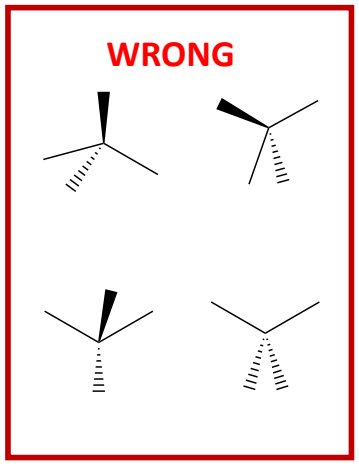
Alkanes all have similar molecular formula C_nH_{2n+2}, which expresses that these carbons are fully "saturated" with hydrogen atoms (i.e. there *no double/triple bonds* and *no rings* in the molecule).

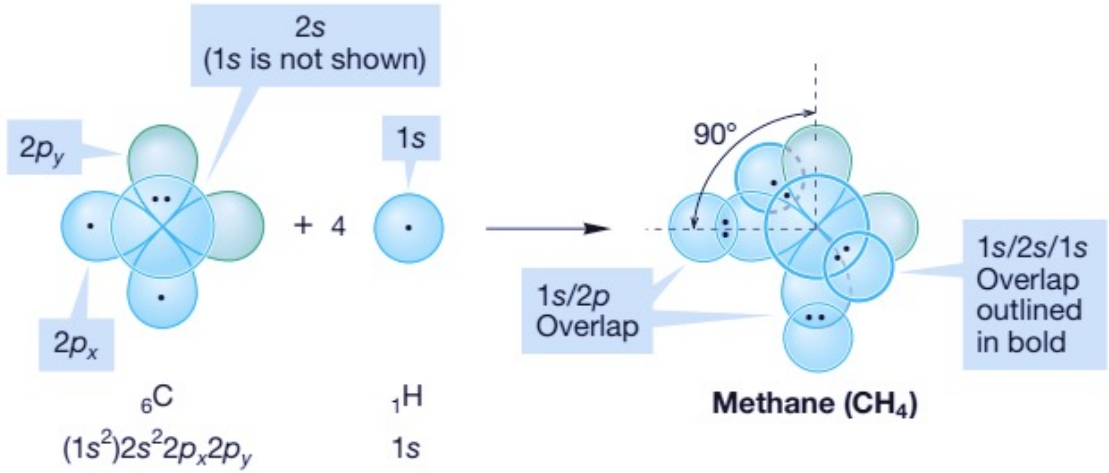
The simplest alkane is **methane** (sp^3, tetrahedral). You should know how to draw the orbitals and the correct tetrahedral structure.

Alkanes are **typically unreactive** with most reagents, due to their nearly non-polar C–H bonds.

Alkanes can be found as open-chain structures, with or without branching, and as cyclic rings.



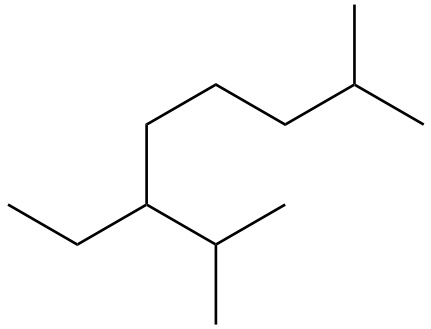


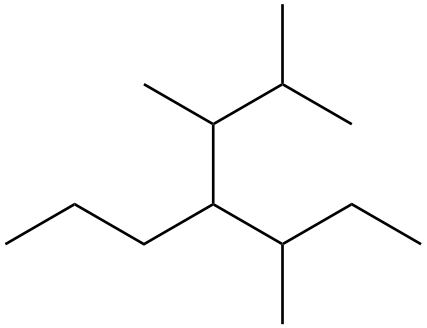


1

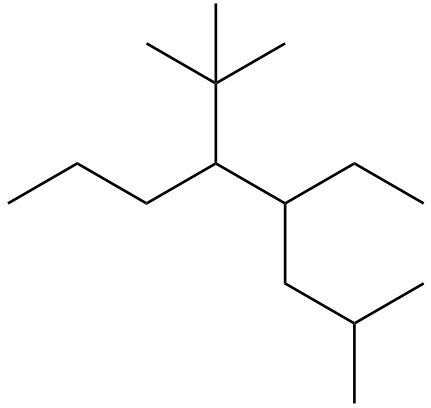
Provide a systematic IUPAC name for these compounds.

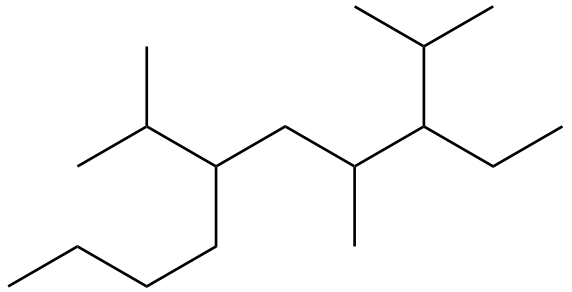
(1) Select Parent
  – longest chain
  – w. most substituents
(2) Name Substituents
(3) Assign # to Substituents to have the lowest #-ing possible
(4) Alphabetize Substituents
  – ignore “di-, tri-” when alphabetizing





1	*methyl*
2	*ethyl*
3	*propyl*
4	*butyl*
5	*pentyl*
6	*hexyl*
7	*heptyl*
8	*octyl*
9	*nonyl*
10	*decyl*

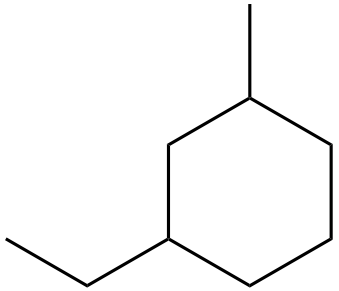


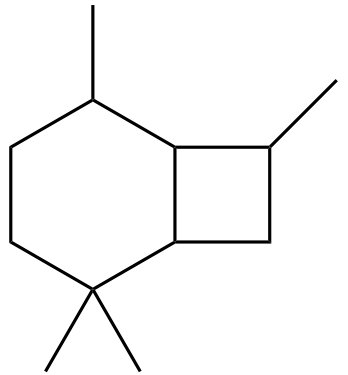


Naming Ringed Structures

Monocyclics

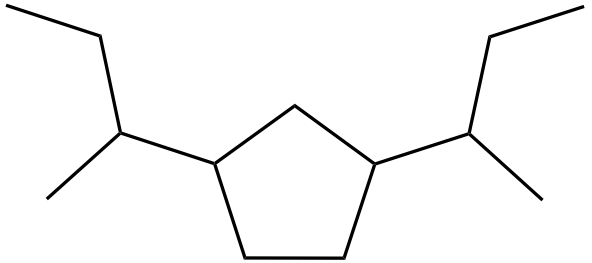
1. Which has more Carbons?
   - Ring – This is the parent
   - Chain – This is the parent
2. Name according to alkane rules

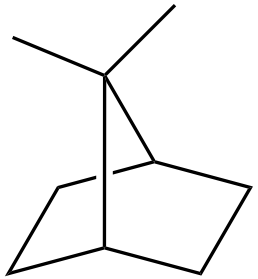


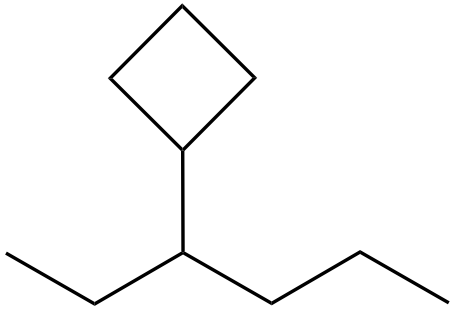


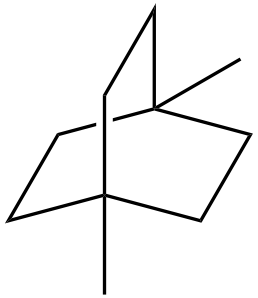
Bicyclics

1. Identify bridgeheads
   – point at which rings are fused
2. Count # of carbons for each “path”
   – do not include bridgehead carbons in #
   – list in order of largest to smallest
   – place within brackets
3. Name the parent
   – add the #s in the brackets
   – name as if all C’s were in single ring
4. Identify substituents
   – Number parent starting with the longest path.
   – Include bridgehead C in this count.









3 Draw the following compounds from the IUPAC names.

a) 3-isopropyl-2,4-dimethylpentane

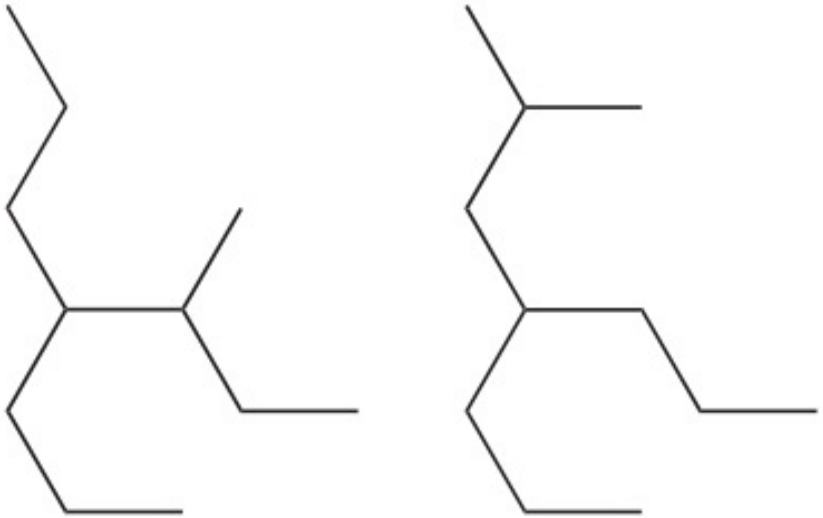
b) 1,1,2,2-tetramethylcyclopropane

c) 8,8-diethylbicyclo[3.2.1]octane

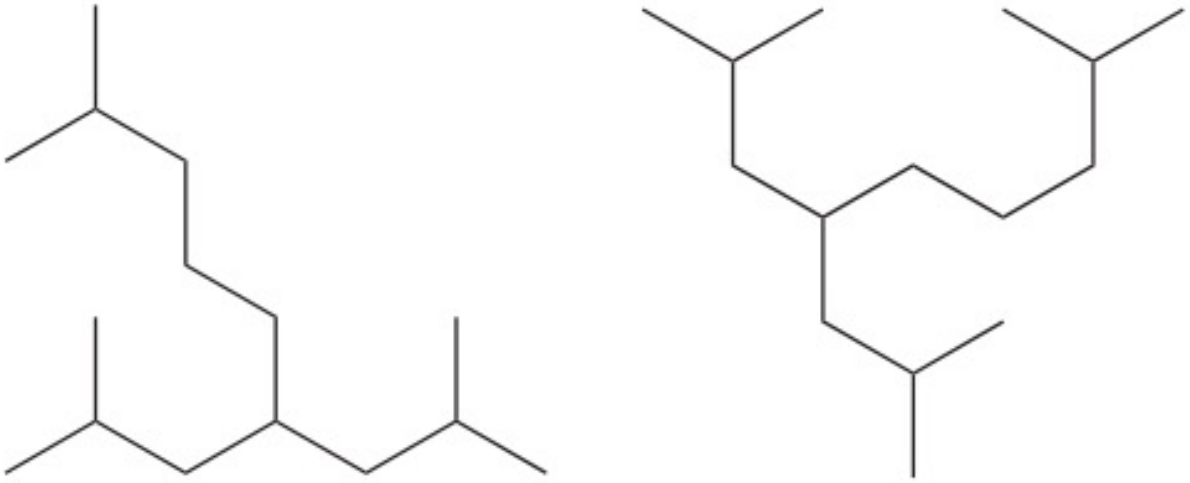
d) 3-isopropylbicyclo[3.2.0]heptane

4 Identify is these compounds are constitutional isomers, identical, or non-isomeric.

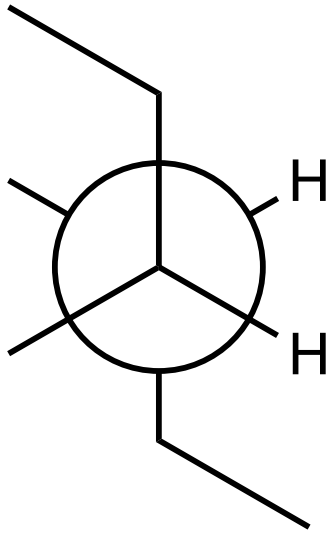
a)

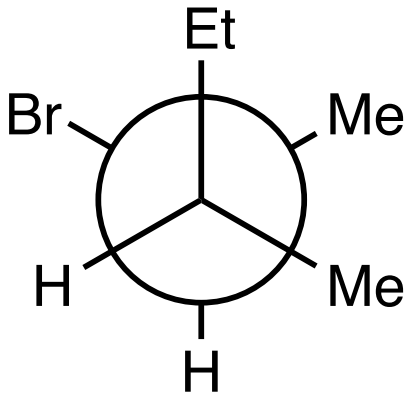


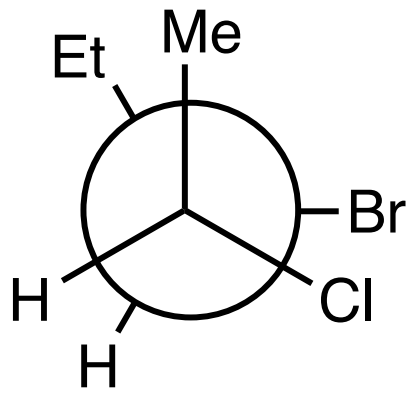
b)



5 Draw and name the following Newman projections. Include stereochemistry.



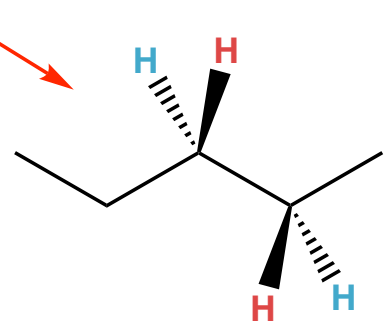


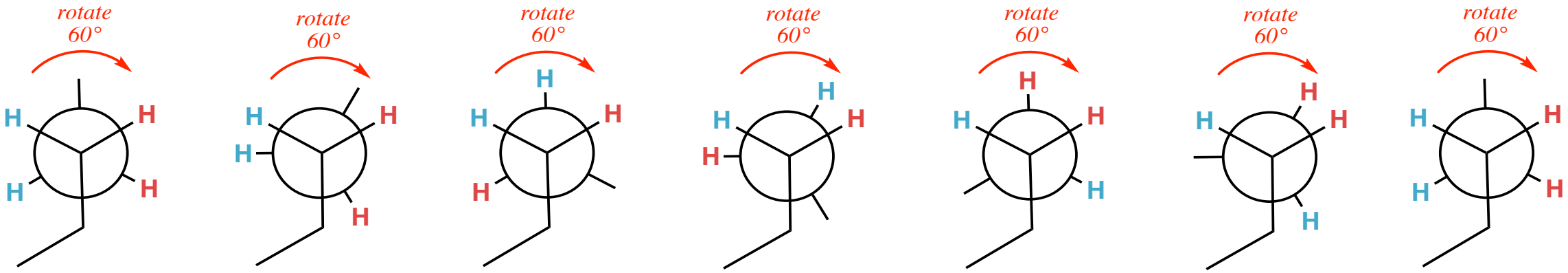


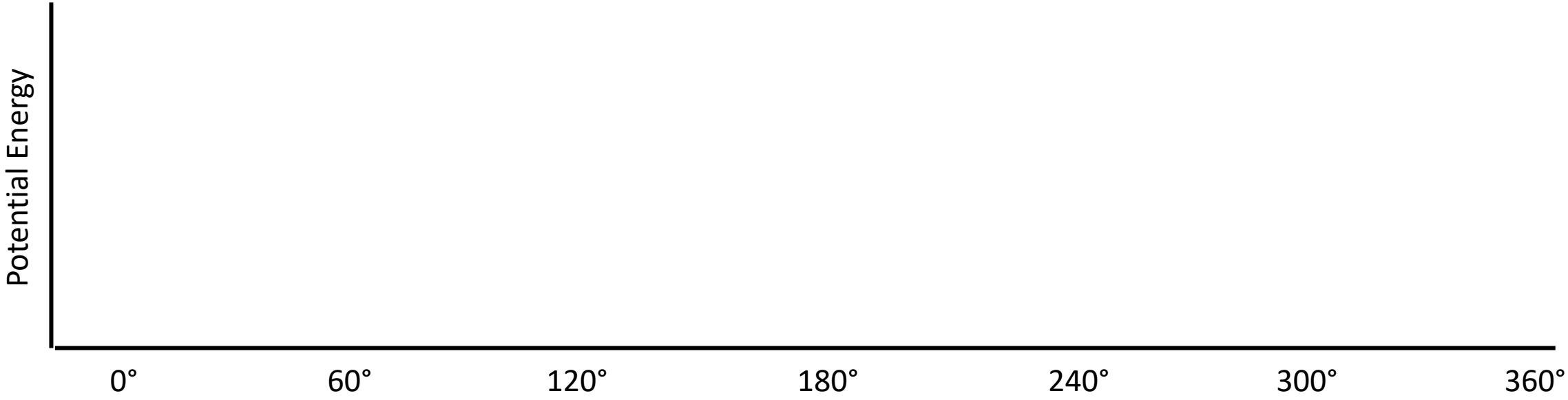
5 Draw and name the following Newman projections. Include stereochemistry.

6

Draw the Energy Diagram for Hexane.

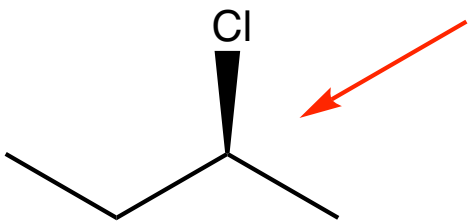


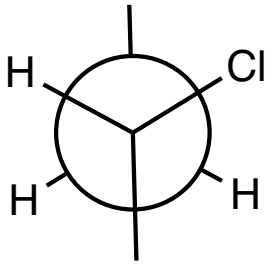




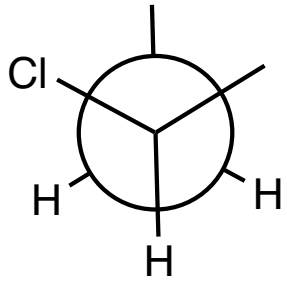
7

Select the Newman projection of the conformer of the following compound where the two methyl groups are *anti*.

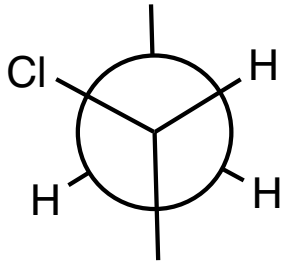




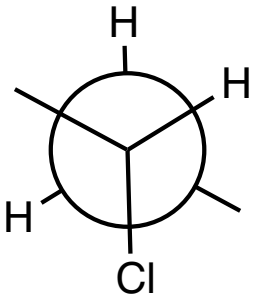
I.



II.

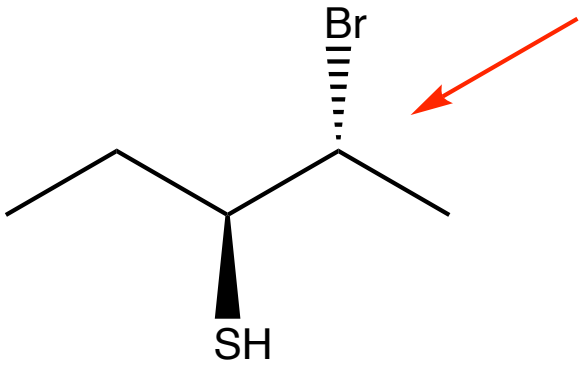


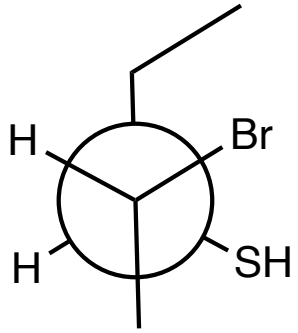
III.



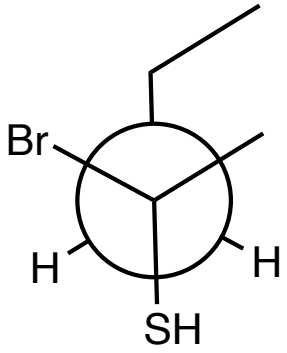
IV.

Select the Newman projection of the conformer of the following compound.

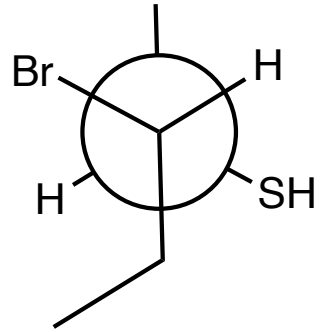




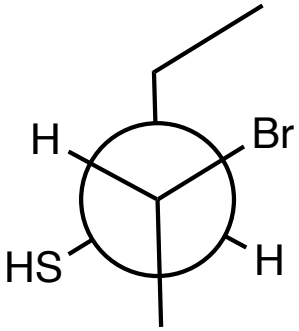
I.



II.



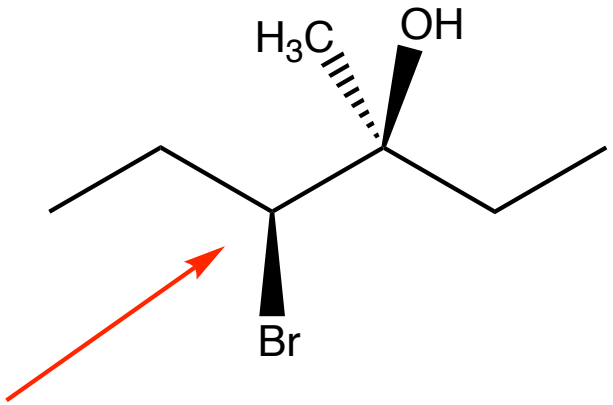
III.

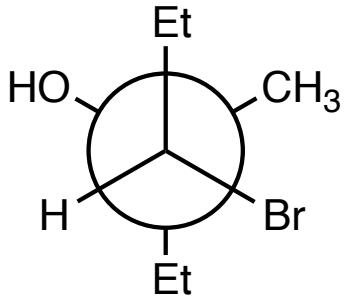


IV.

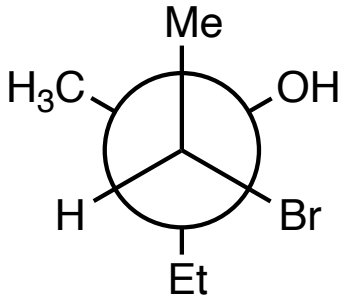
8

Select the Newman projection of the conformer of the following compound.

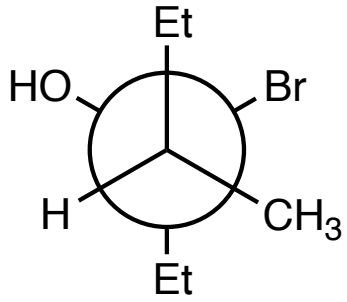




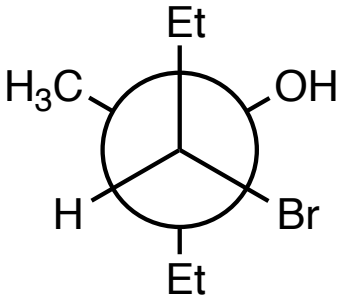
I.



II.

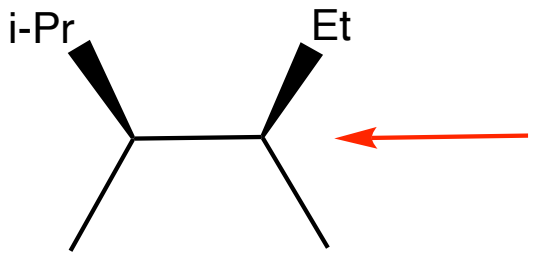


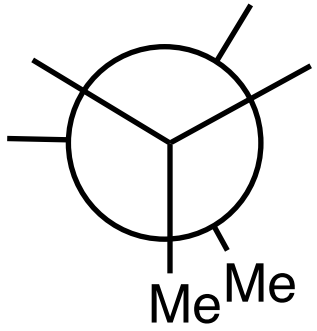
III.

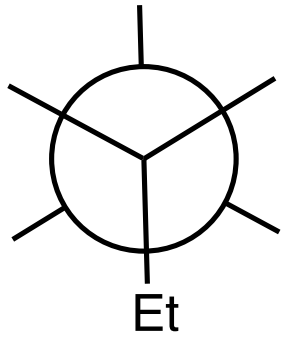


IV.

Draw the Newman projection for the following conformer, then draw the most stable conformer.





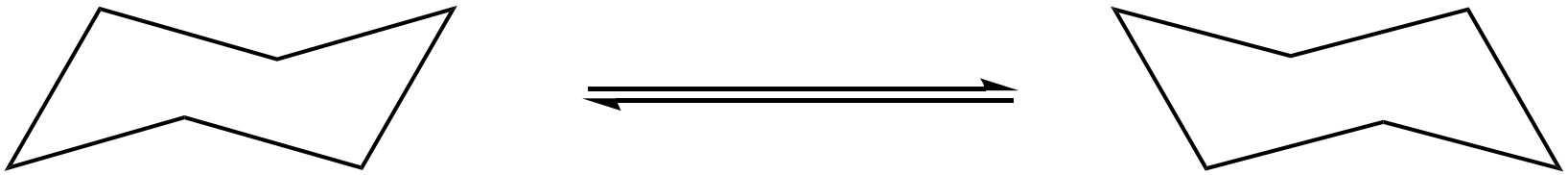


Approximate Gauche Energy Values (kcal/mole)

	H	Me	Et	i-Pr	t-Bu	Ph
H	0	0	0.1	0.2	0.5	0.2
Me	0	0.8	0.9	1.1	2.7	1.4
Et	0.1	0.9	1.1	1.6	3.0	1.5
i-Pr	0.2	1.1	1.6	2.0	4.1	2.1
t-Bu	0.5	2.7	3.0	4.1	8.2	3.9
Ph	0.2	1.4	1.5	2.1	3.9	2.3

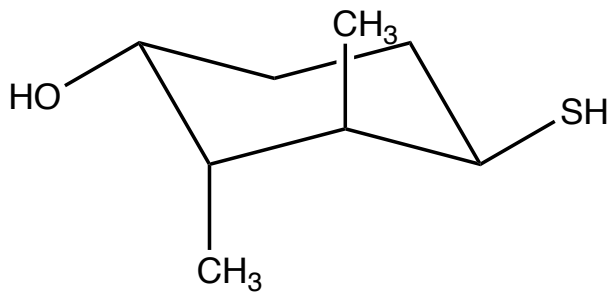
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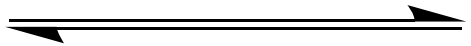
Label axial (H) and equatorial (H) hydrogens on conformer A. Draw where they shift to in conformer B.



A B

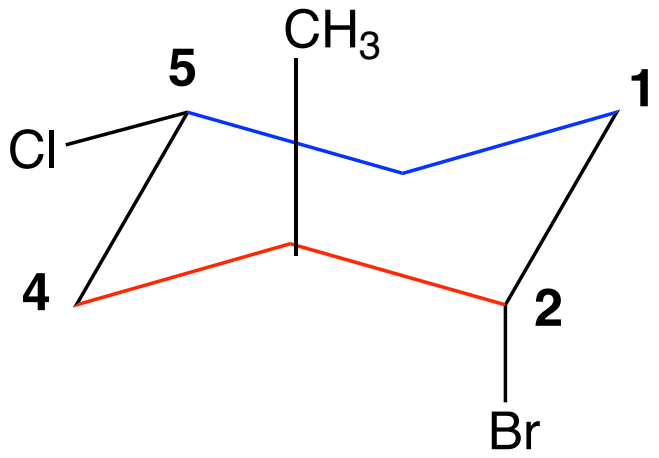
Draw the chair conformer for the following compound. Select which is more stable.





10

Convert the chair to its Newman projection looking down the C4-C5 and C2-C1 bonds.



CYCLOALKANES

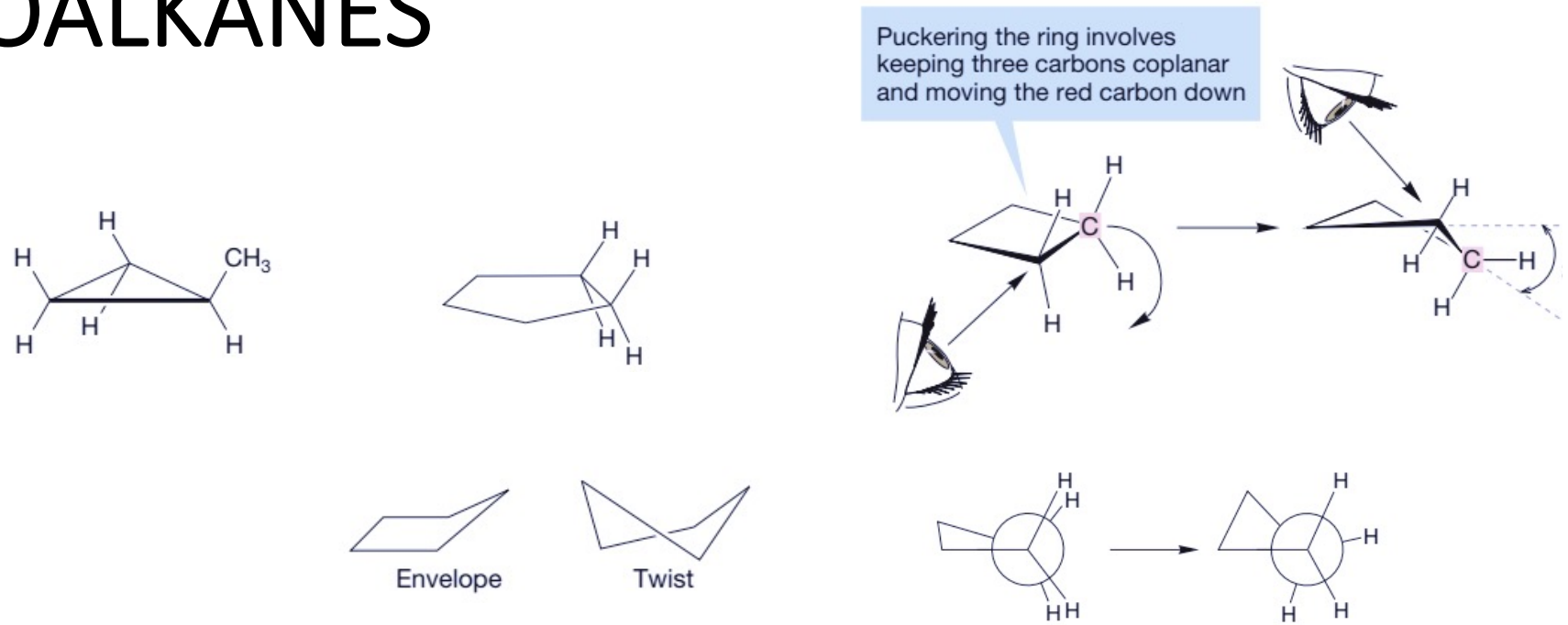
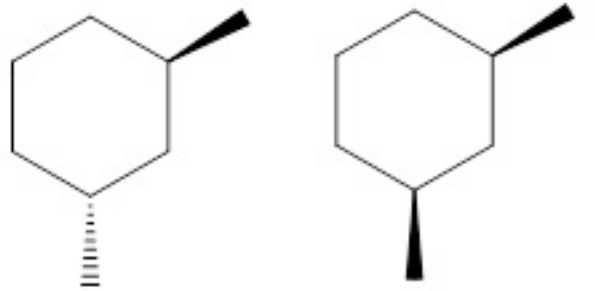


***Table* 1:** *Heats of combustion of select hydrocarbons*

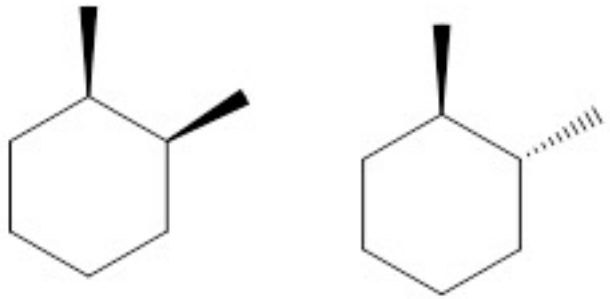
Cycloalkane $(CH_2)_n$	**CH_2 Units** n	**$\Delta H^{25°}$** kcal/mole	**$\Delta H^{25°}$** per CH_2 Unit	**Ring Strain** kcal/mole
Cyclopropane	n = 3	468.7	156.2	27.6
Cyclobutane	n = 4	614.3	153.6	26.4
Cyclopentane	n = 5	741.5	148.3	6.5
Cyclohexane	n = 6	882.1	147.0	0.0
Cycloheptane	n = 7	1035.4	147.9	6.3
Cyclooctane	n = 8	1186.0	148.2	9.6
Cyclononane	n = 9	1335.0	148.3	11.7
Cyclodecane	n = 10	1481	148.1	11.0
$CH_3(CH_2)_mCH_3$	m = large	—	147.0	0.0

11 Circle the more stable isomer.

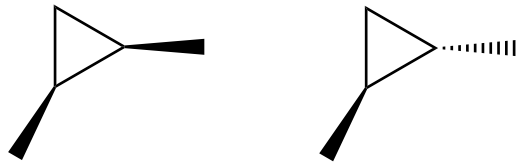
a)



b)

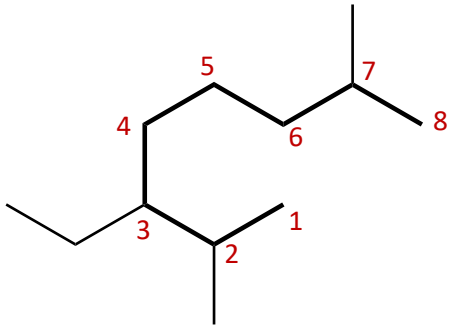


c)

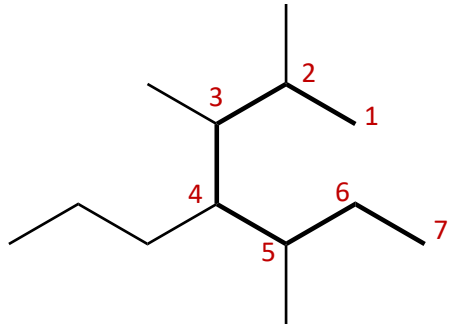


ANSWER KEY

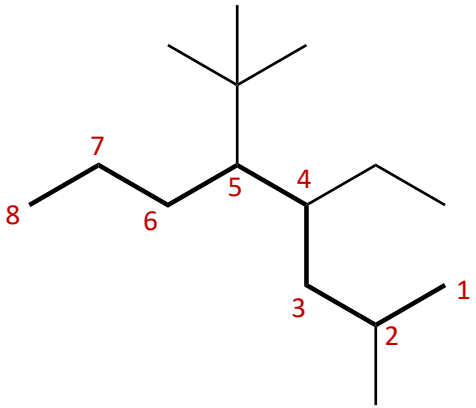
1 Provide a systematic IUPAC name for these compounds.



3-ethyl-2,7-dimethyloctane



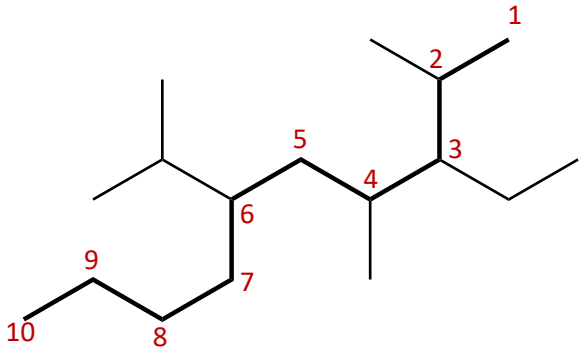
2,3,5-trimethyl-4-propylheptane



4-ethyl-5-(1,1-dimethylethyl)-2-methyloctane

or

5-(*tert*-butyl)-4-ethyl-2-methyloctane

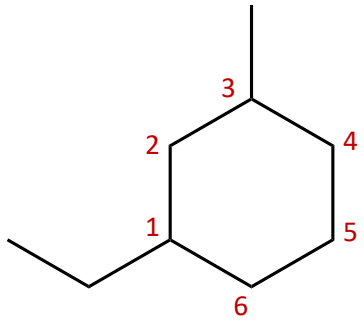


3-ethyl-6-(1-methylethyl)-2,4-dimethyldecane

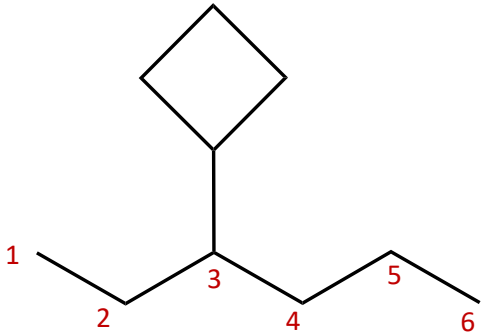
or

3-ethyl-6-isopropyl-2,4-dimethyldecane

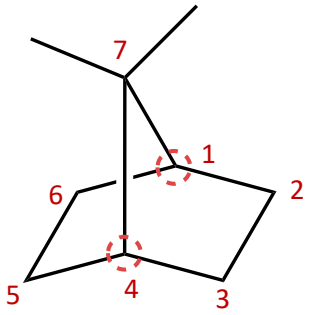
2 Naming Ringed Structures



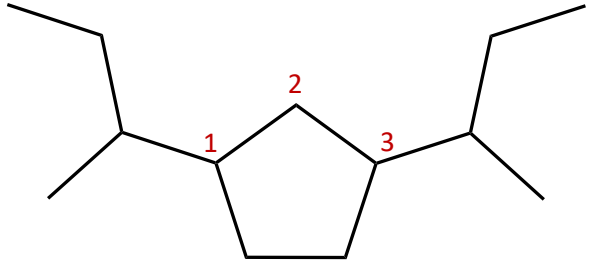
1-ethyl-3-methylcyclohexane



3-cyclobutylhexane



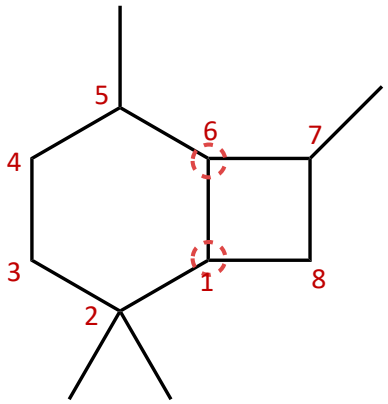
7,7-dimethylbicyclo[2.2.1]heptane



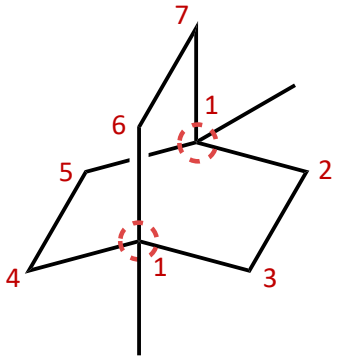
1,3-di-*sec*-butyl-cyclopentane

or

1,3-di(1-methylpropyl)cyclopentane



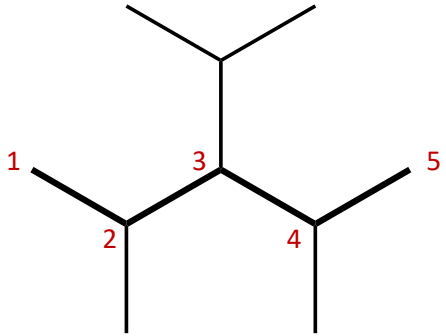
2,2,5,7-tetramethylbicyclo[4.2.0]octane



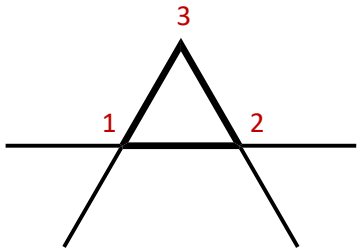
1,4-dimethylbicyclo[2.2.2]octane

3 Draw the following compounds from the IUPAC names.

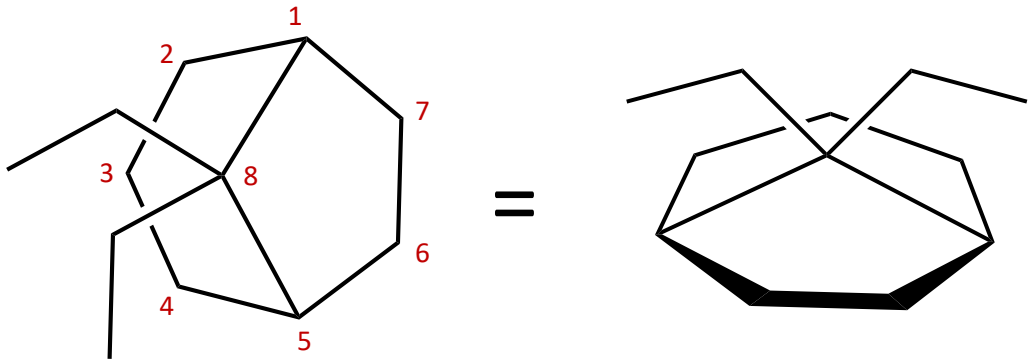
a) 3-isopropyl-2,4-dimethylpentane



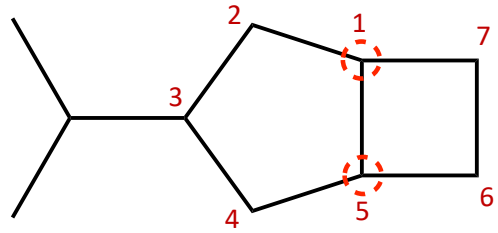
b) 1,1,2,2-tetramethylcyclopropane



c) 8,8-diethylbicyclo[3.2.1]octane

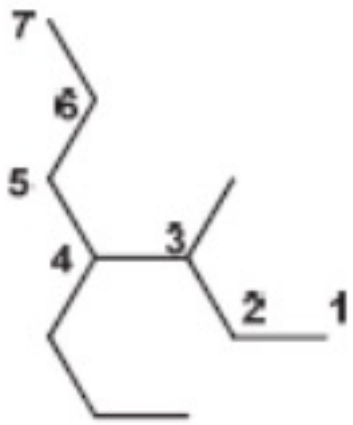


d) 3-isopropylbicyclo[3.2.0]heptane

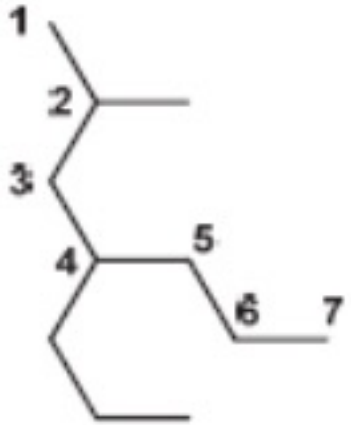


4 Identify is these compounds are constitutional isomers, identical, or non-isomeric.

a)

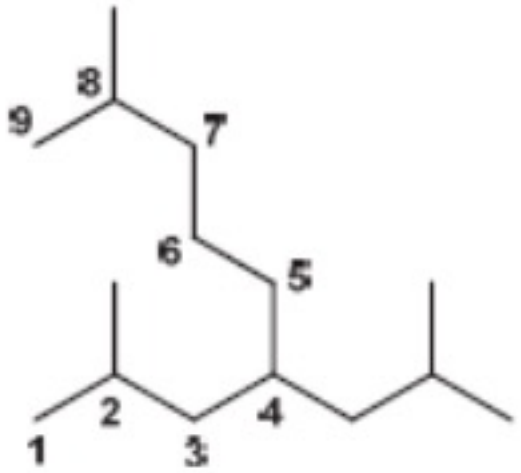


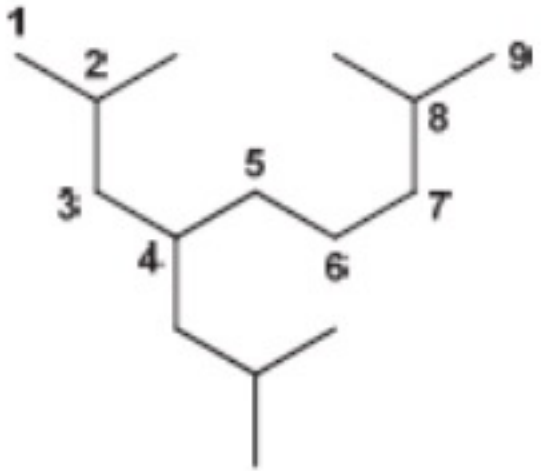
3-methyl-4-propylheptane



2-methyl-4-propylheptane

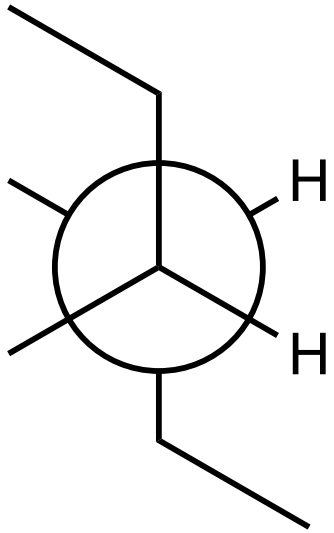
b)

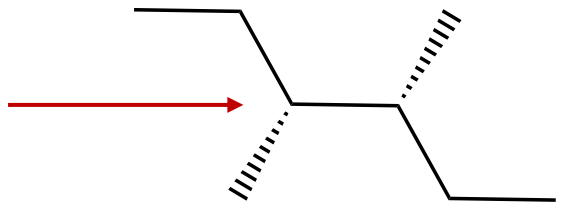




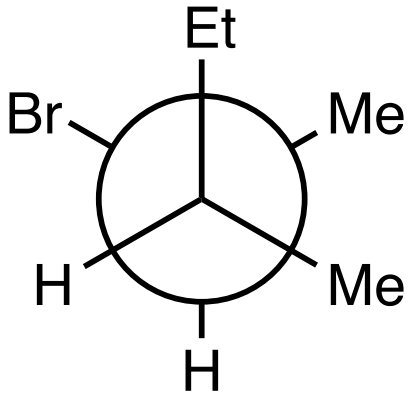
Both are 4-isobutyl-2,8-dimethylnonane

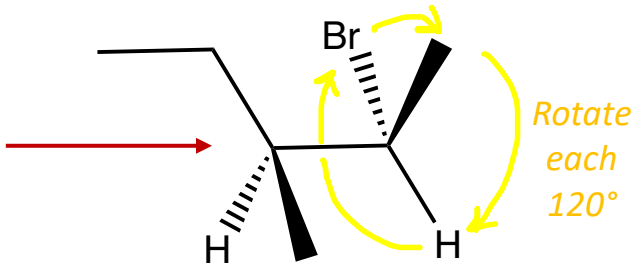
5 Draw and name the following Newman projections. Include stereochemistry.

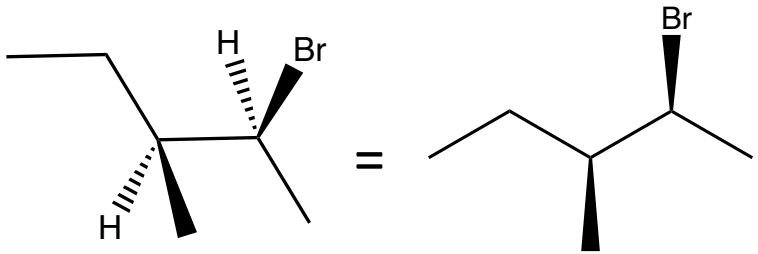




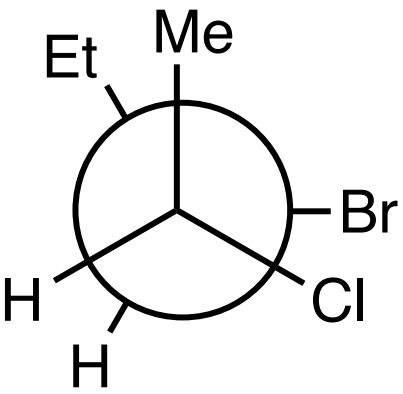
3,4-dimethylhexane

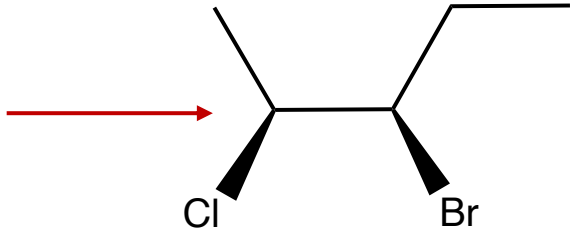






2-bromo-3-methylpentane

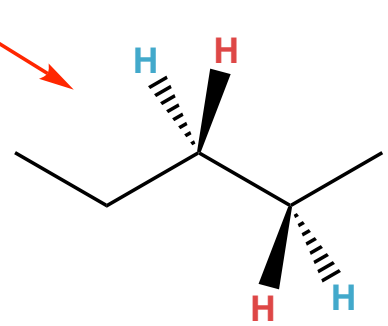


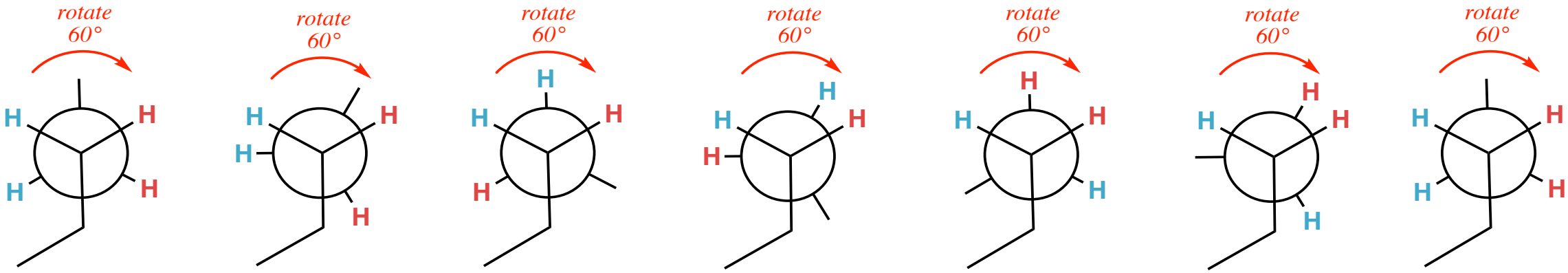


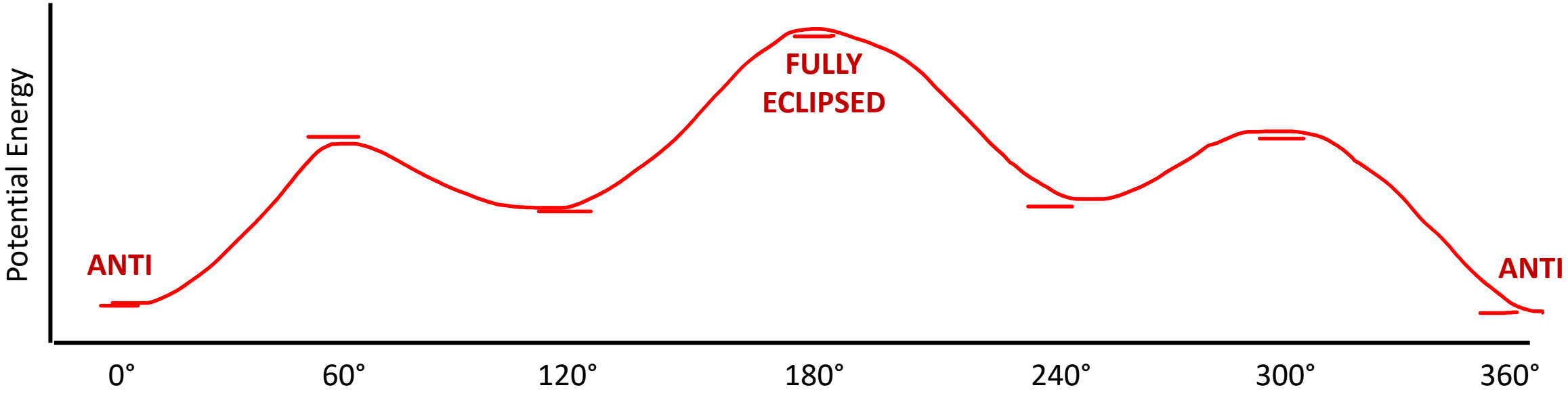
3-bromo-2-chloropentane

6

Draw the Energy Diagram for Hexane.

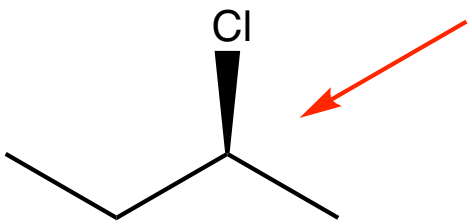


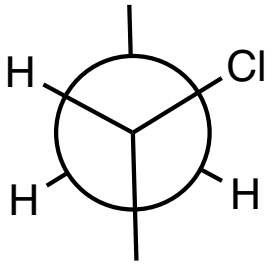




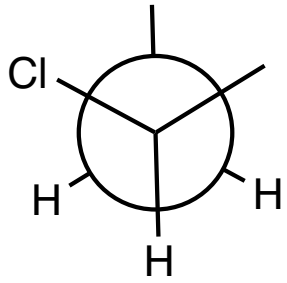
7

Select the Newman projection of the conformer of the following compound where the two methyl groups are *anti*.

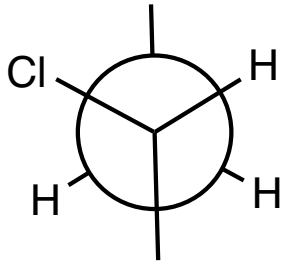




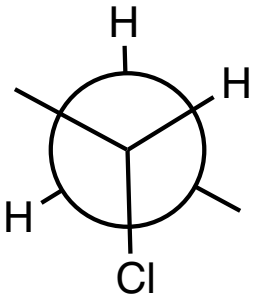
I.



II.

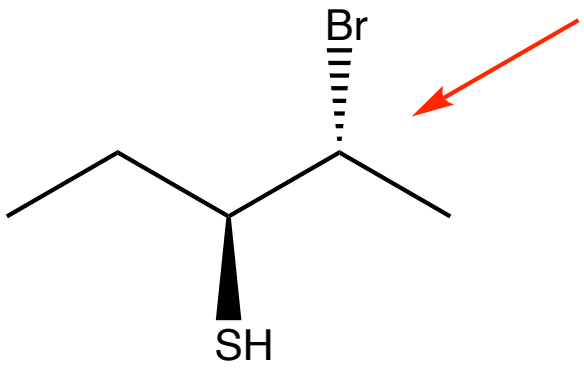


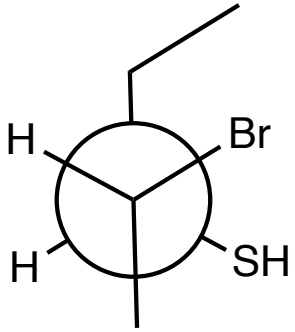
III.



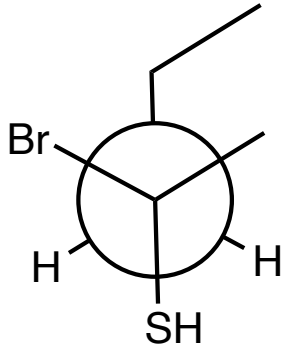
IV.

Select the Newman projection of the conformer of the following compound.

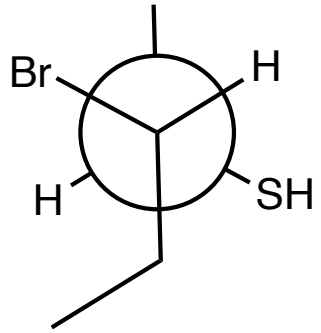




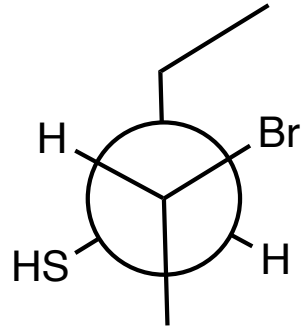
I.



II.

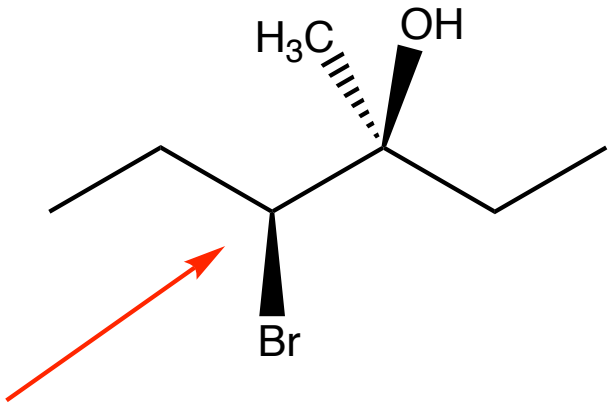


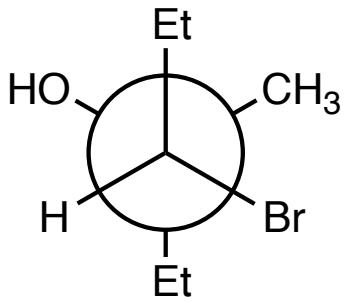
III.



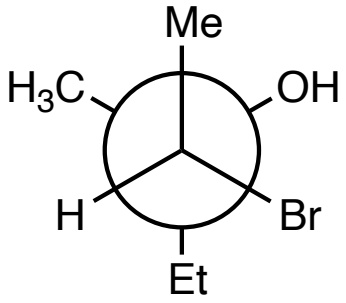
IV.

8 Select the Newman projection of the conformer of the following compound.

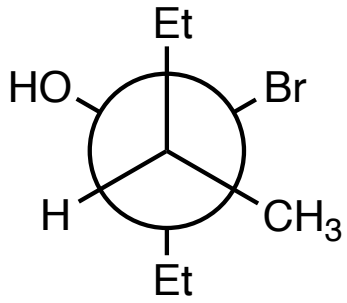




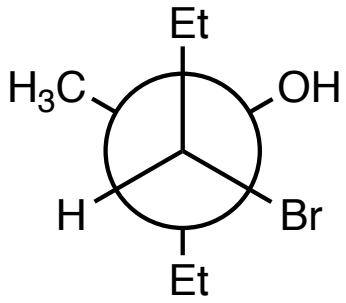
I.



II.

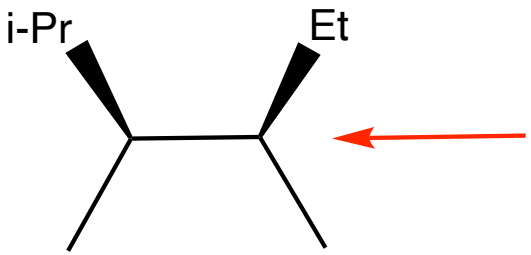


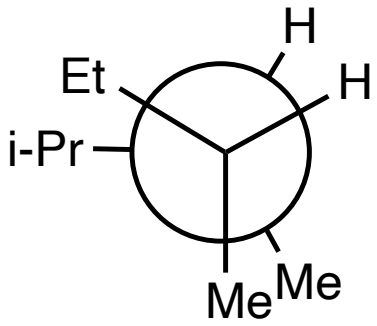
III.

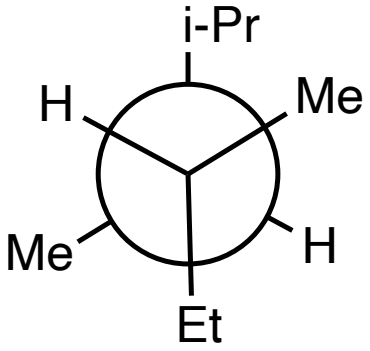


IV.

Draw the Newman projection for the following conformer, then draw the most stable conformer.







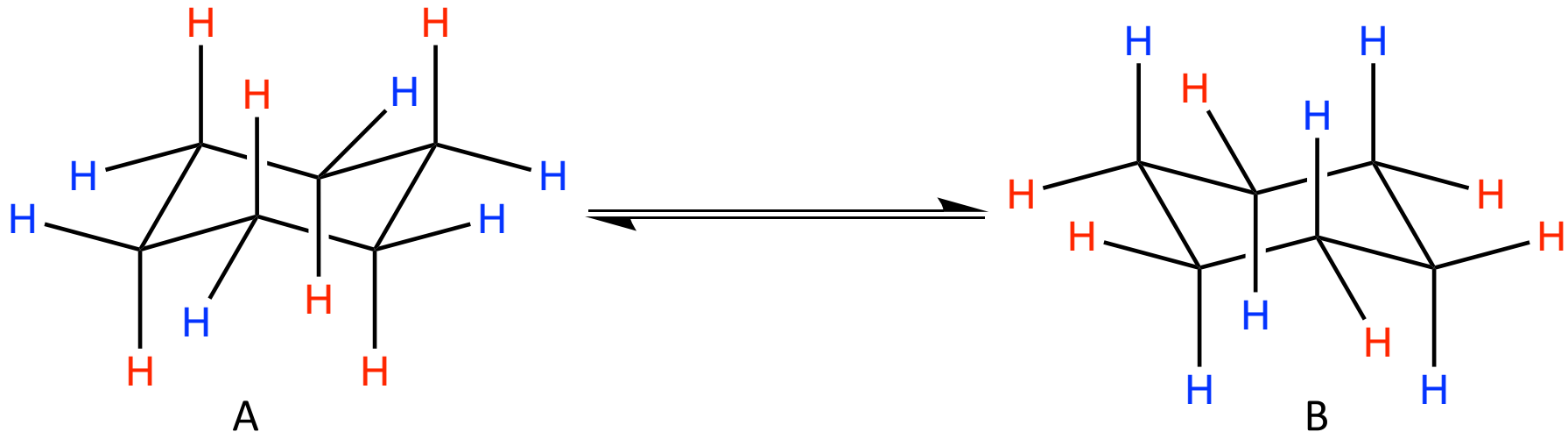
Gauche	
i-Pr-Me	1.1
Me-Et	0.9
H-*i*-Pr	0.2
H-Et	0.1
2 H-Me	0.0
	2.3

Approximate Gauche Energy Values (kcal/mole)

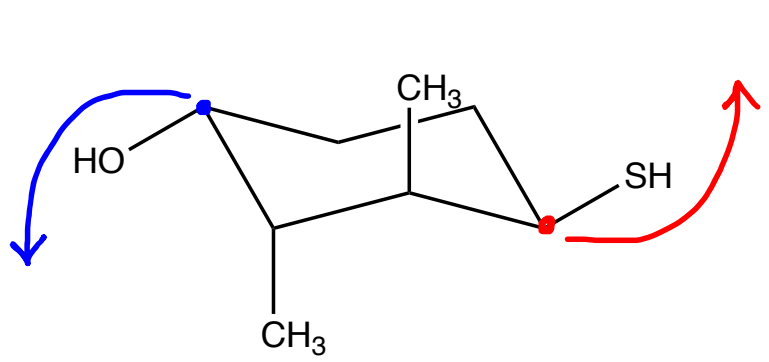
	H	Me	Et	i-Pr	t-Bu	Ph
H	0	0	0.1	0.2	0.5	0.2
Me	0	0.8	0.9	1.1	2.7	1.4
Et	0.1	0.9	1.1	1.6	3.0	1.5
i-Pr	0.2	1.1	1.6	2.0	4.1	2.1
t-Bu	0.5	2.7	3.0	4.1	8.2	3.9
Ph	0.2	1.4	1.5	2.1	3.9	2.3

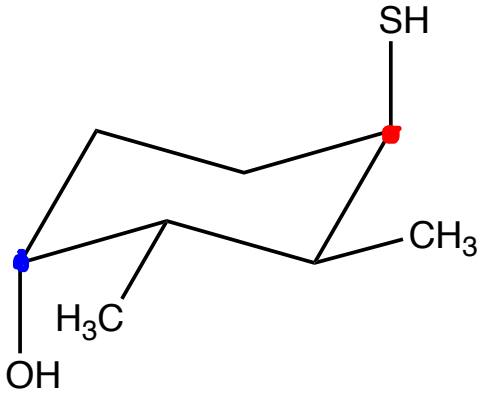
9

Label axial (H) and equatorial (H) hydrogens on conformer A. Draw where they shift to in conformer B.



Draw the chair conformer for the following compound. Select which is more stable.

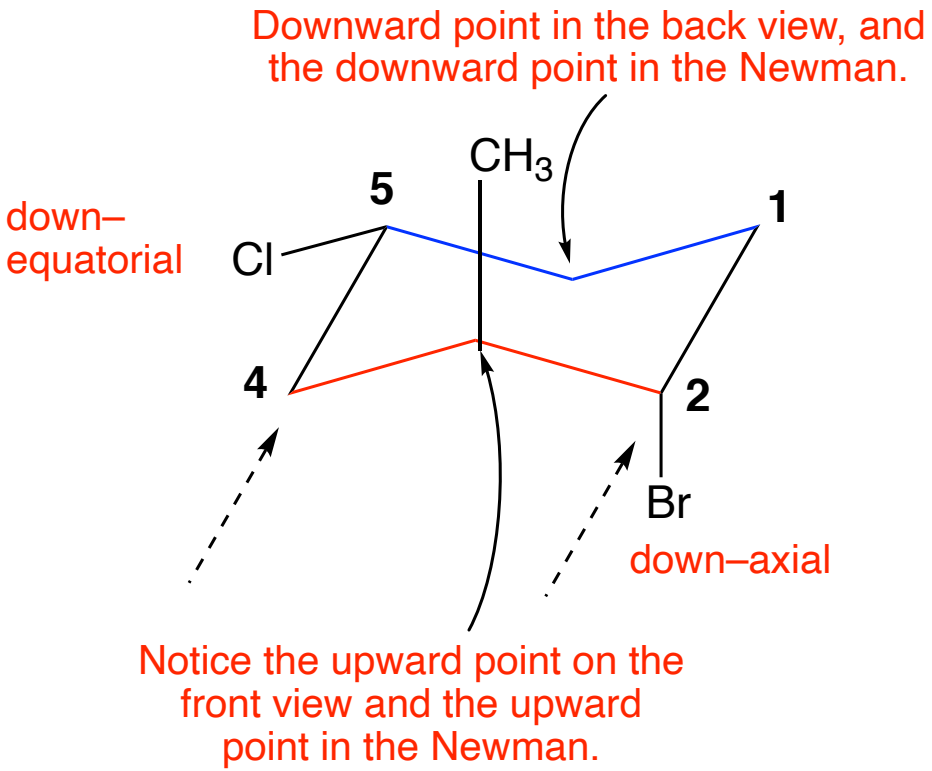


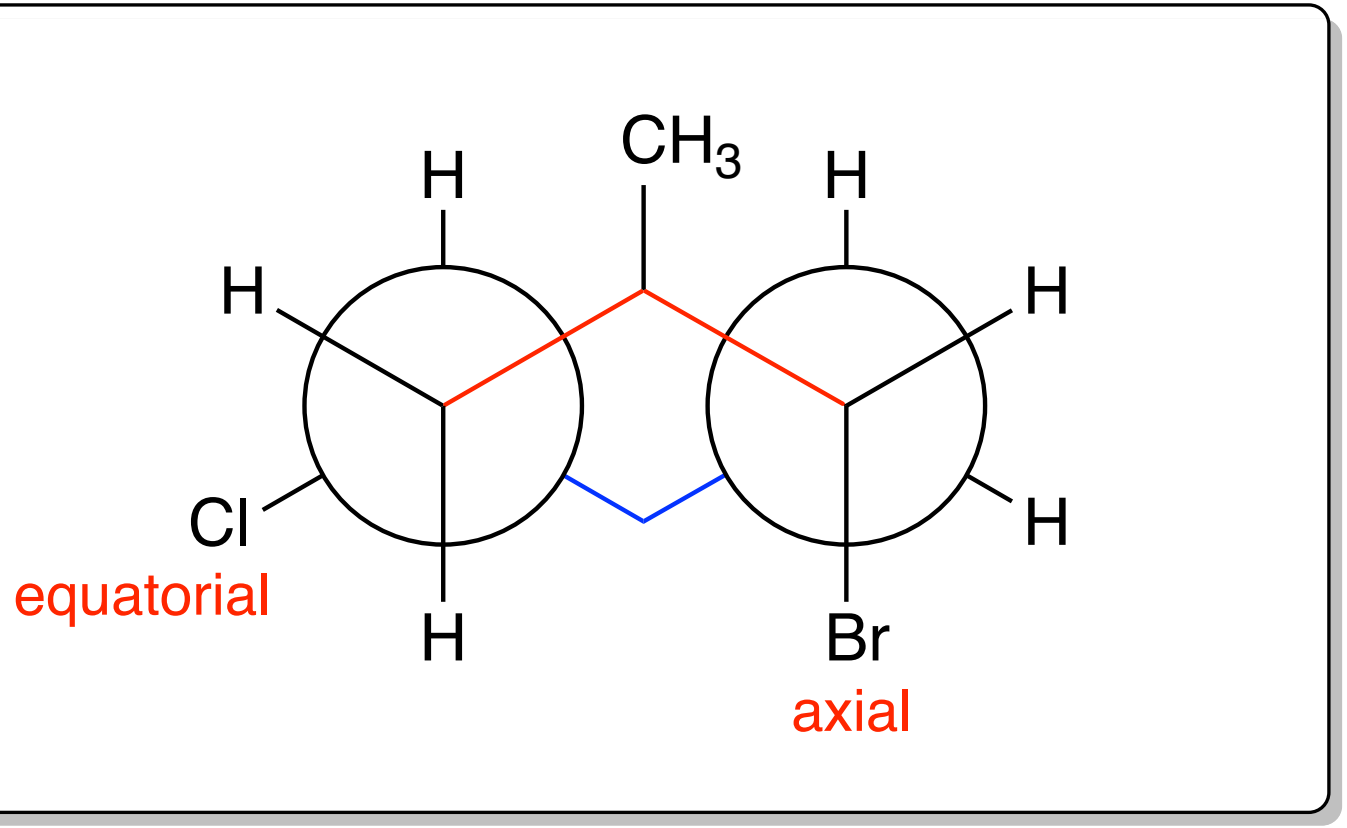


MORE STABLE

The methyl groups are bulkier than OH and SH groups, so the chair conformer with methyl equatorial is most stable.

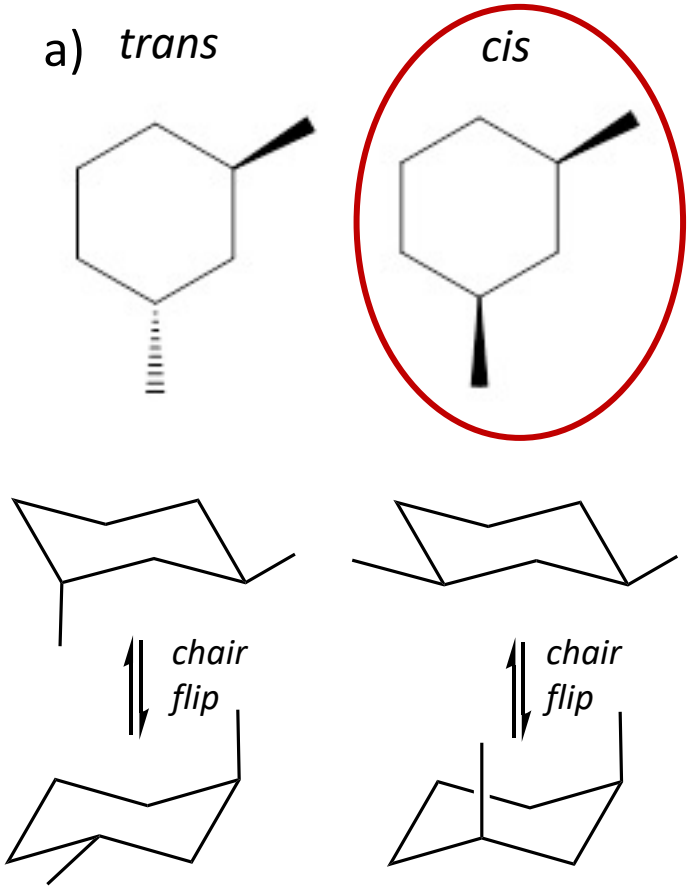
10 Convert the chair to its Newman projection looking down the C4-C5 and C2-C1 bonds.





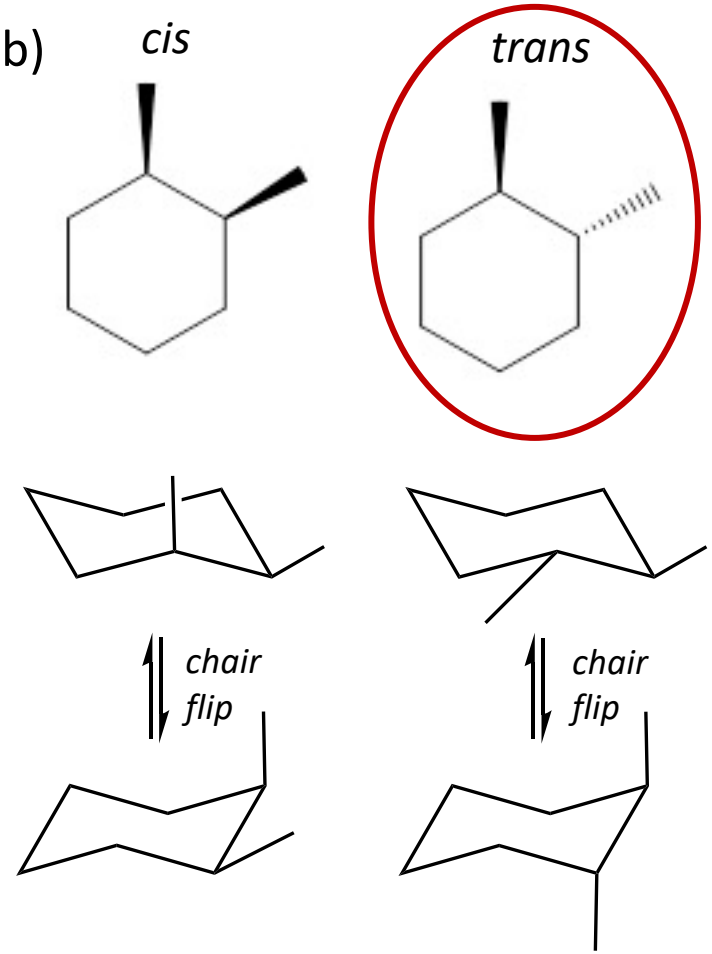
11 Circle the more stable isomer.

a) *trans* *cis*



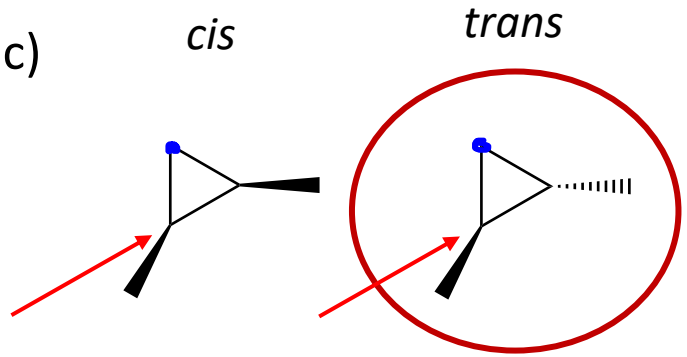
Both methyl groups can be either equatorial or axial. Equatorial conformer is most stable.

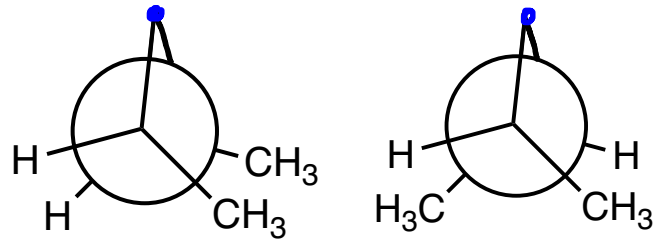
b) *cis* *trans*



Both methyl groups can be either equatorial or axial. Equatorial conformer is most stable.

c) *cis* *trans*





Avoids CH_3-CH_3 eclipsing strain.

** The ring is locked in an eclipsed conformer.