1. Draw the Newman projection representing the most stable conformation of *n*-butane (*n* meaning acyclic, or straight chain). Use $C_2$-$C_3$ bond as the projection axis.

2. Sketch an approximate potential energy diagram (E vs Rotation Angles) for the $360^0$ rotation of 2-methylbutane about the $C_2$-$C_3$ bond. For each unique energy maximum and minimum, illustrate the conformation using a Newman projection.

3. Perform the conformational analysis along the $C_2$-$C_3$ bond of 2,2,3,3-tetramethylbutane by drawing the Newman projections and creating a sketch of potential energy diagram (Y-axis: Potential Energy, X-axis: rotational angle by $60^o$) *Make sure to clearly distinguish or indicate the energy of each conformation in the diagram*. Indicate the conformations that are energy maxima and minima.

4. Draw Newman projections for (a) the chair conformation of cyclohexane, and (b) two chair conformations of isopropylcyclohexane.

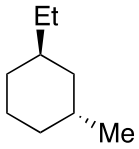
5. Draw both chair conformations of bromocyclohexane. Indicate which of the two chair conformation is more stable, and explain why.

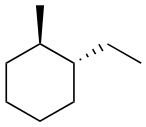
6. Draw 3-dimensional structural formulas for the two chair conformations of (a) *cis*-1-isopropyl-3-methylcyclohexane and (b) *trans*-1-isopropyl-3-methylcyclohexane. Indicate which of the two conformations in (a) and (b) is more stable.

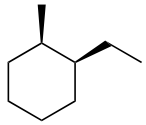
7. Draw Newman projections for all possible chair conformations of *cis*- and *trans*-1,2-dimethylcyclohexane. Indicate which chair conformation is most stable.

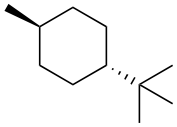
8. It was found experimentally that the predominant chair conformation of *trans*-1,4-dichlorocyclohexane is diequatorial, whereas that of *trans*-1,2-dichlorocyclohexane is diaxial. Provide a reasonable explanation for these results.

9. Determine whether the substituents on the following disubstituted cyclohexanes have *cis*- or *trans*-stereochemical relationships. Name each compound including *cis*- or *trans*- designation and draw both chair conformations of each compound. Determine which of the two chair conformations is more stable.

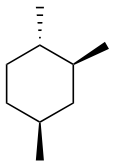
a) 

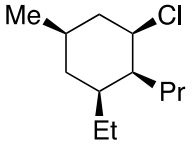

b) 

c) 

d) 

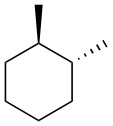
10. Draw both chair conformations for each of the following tri-substituted cyclohexanes. Determine which of the two chair conformations from each compound is more stable.

a) 

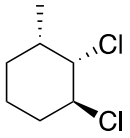
b) 

11. Draw the **lowest** energy chair conformation for each of the following compounds:

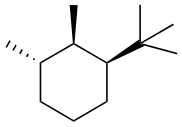
a)



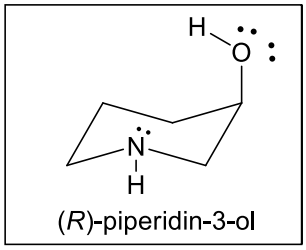
b)




c)



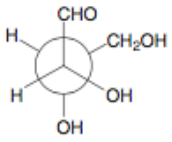
12. The most stable conformation of (R)-piperidin-3-ol has the OH group in an axial position, rather than an equatorial position. Draw the Newman projection of this compound from the given 3-D structure, and provide an explanation for this observation. (Hint: intermolecular force)



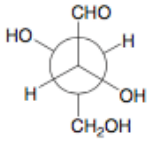
(*R*)-piperidin-3-ol

*hydrogens are not drawn in

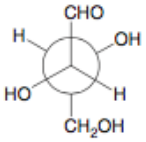
13. Consider Newman projections (**A** – **D**) for four-carbon molecules. Convert each Newman projection into 3D bond-line representation and determine the stereochemical relationships (identical, enantiomers or diastereomers) of (a) **A** and **B**; (b) **A** and **C**; (c) **A** and **D** and (d) **C** and **D**.



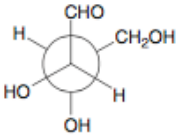
**A**



**B**



**C**

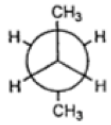


**D**

## Solutions

1.

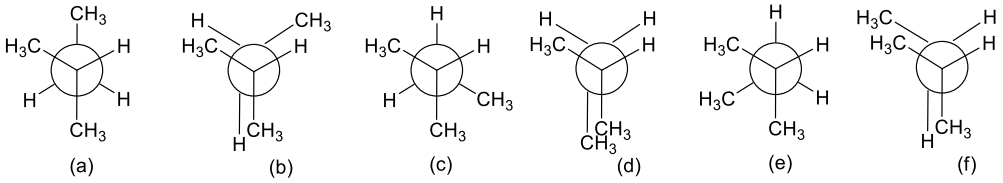
$C_2$-$C_3$ projection



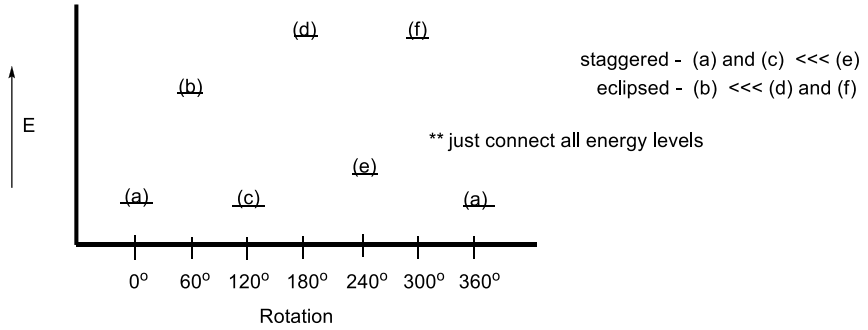
2.

2-methylbutane

Rotating the distal carbon clockwise



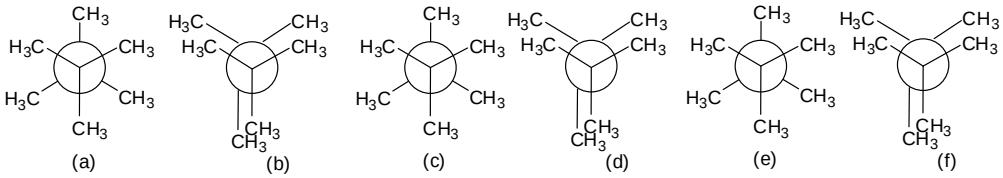
(a) (b) (c) (d) (e) (f)



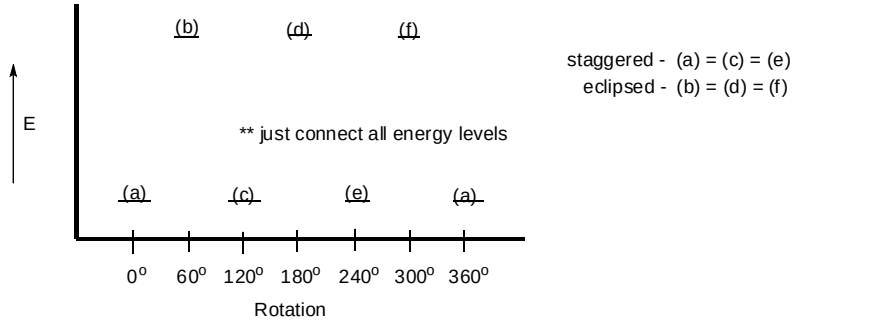

3.

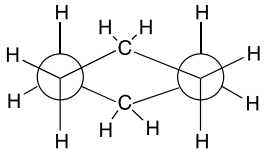
2,2,3,3-tetramethylbutane

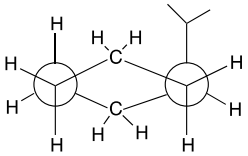
Rotating the distal carbon clockwise



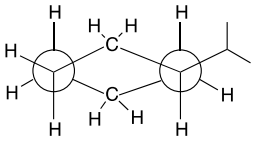
(a) (b) (c) (d) (e) (f)



4. (a) 

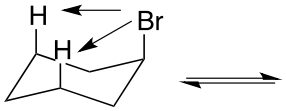
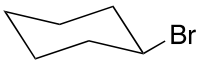
(b) 

When isoproyl group is axial



When isoproyl group is equatorial

5. *hydrogens are omitted for simpler drawing

(1)    Br (2)

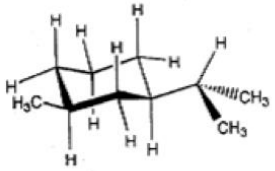
With axial bromine

1,3-diaxial interaction

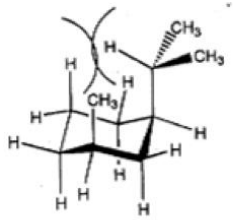
With equatorial bromine

**MORE STABLE**

Bromine (or substituent) is not creating 1,3-diaxial interaction

6. (a) 

ring-flip



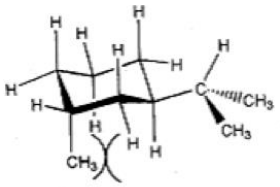
cis e,e

more stable

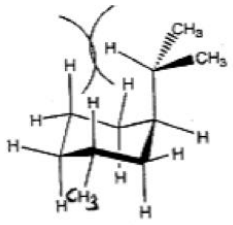
cis a,a

1,3-diaxial interactions are very severe

less stable

(b) 

ring-flip



trans a,e

1,3-diaxial interactions are less severe due to the smaller size of $CH_3$

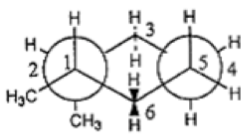
more stable

trans e,a

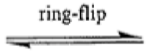
1,3-diaxial interactions are more severe

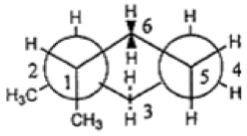
less stable

7.



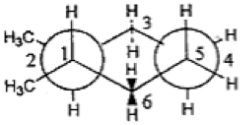
cis e,a



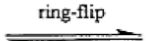



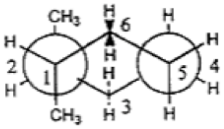
cis a,e

For cis-1,2-dimethylcyclohexane, Both chair conformations have equal stability.



trans e,e



trans a,a

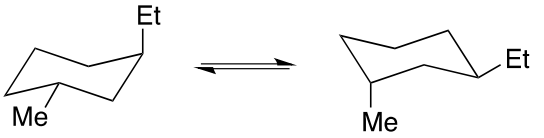
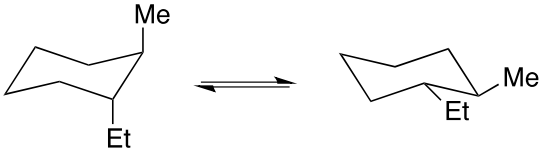
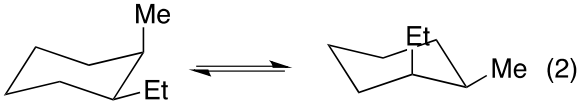
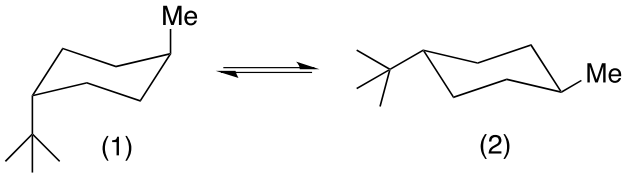
For trans-1,2-dimethylcyclohexane, chair conformation on the left has considerably more stability due to the absence of 1,3-diaxial interactions.

8.

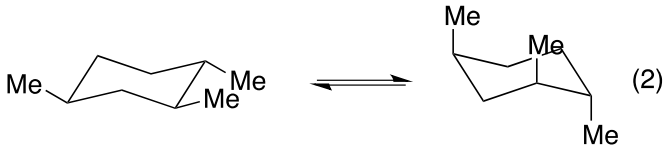
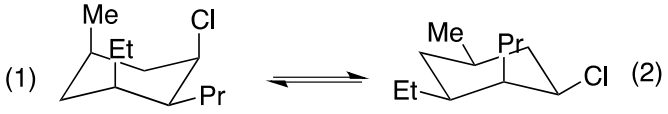
- Please draw the chair conformation of each compound.

For *trans*-1,4-dichlorocyclohexane, placing both chlorines in equatorial positions is preferred so that steric strain between chlorine and axial hydrogens are minimized. For *trans*-1,2-dichlorocyclohexane, both chlorines in equatorial positions place them in very close proximity (*N.B.* Chlorine is much BIGGER and more electron rich than methyl or H; if you draw the Newman Projection of this compound, you will see the two chlorines are GAUCHE to each other), and steric strain by two large chlorines would be caused. Therefore, it would rather place both chlorines in axial position at the expense of 1,3-diaxial interaction. So for *trans*-1,2-dichlorocyclohexane, the notion of "placing the large substituent in equatorial positions would lead to a more stable conformation" does not apply.

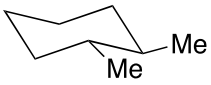
9.

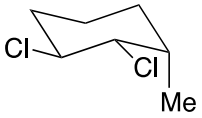
| | Name | Chair conformations | More stable? |
|---|---|---|---|
| a) | *trans*-1-ethyl-3-methylcyclohexane | (1)  (2) | (2) |
| b) | *trans*-1-ethyl-2-methylcyclohexane | (1)  (2) | (2) |
| c) | *cis*-1-ethyl-2-methylcyclohexane | (1)  (2) | (1) |
| d) | *trans*-1-(*tert*-butyl)-4-methylcyclohexane |  | (2) |

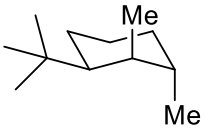
10.

| | | Chair conformations | More stable? |
|---|---|---|---|
| a) | (1)   | | (1) |
| b) | (1)   | | (2) |

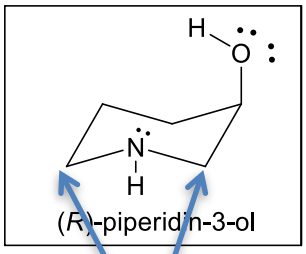
11. The lowest energy (most stable) chair conformations

a)  

b)  

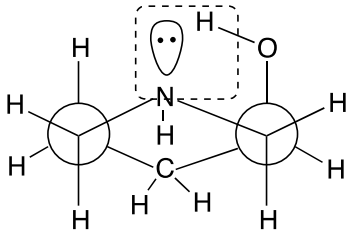
c)  

12.

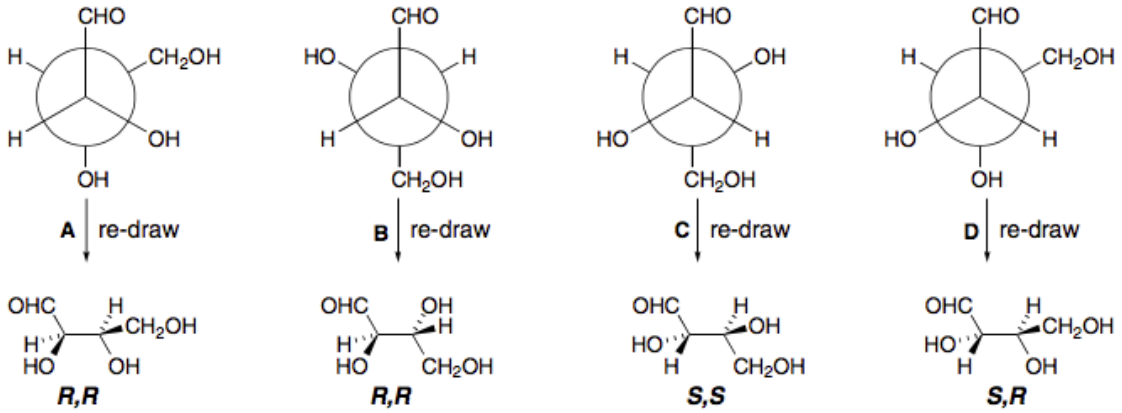



*hydrogens are not drawn in

Look along these C-C bonds when drawing the Newman Projection

| Newman Projection | Explanation |
|---|---|
| Hydrogen Bonding   | Hydrogen bonding, a form of stabilizing intermolecular force, is achieved, when OH is placed axially, rather than in equatorial. |

13.




a. **A** and **B** are identical.
b. **A** and **C** are enantiomers.
c. **A** and **D** are diastereomers.
d. **C** and **D** are diastereomers.