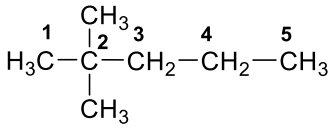
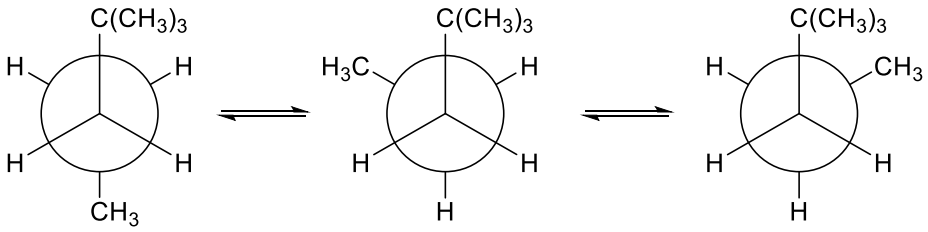
Tutorial 4

Q1. Write Newman projections for all three staggered conformations of 2,2-dimethylpentane, looking down the C3-C4 bond. Select the most stable conformation.



2,2-dimethylpentane

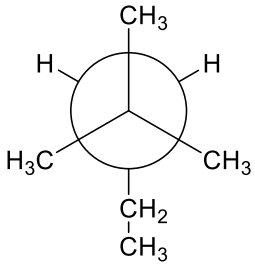
Answer 1.



most stable

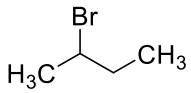
Q2. For 2,2-dimethylpentane, write one Newman projection looking down the C2-C3 bond. Explain why the view down the C3-C4 bond (in the question above) is more informative in identifying the best conformation.

Answer 2.



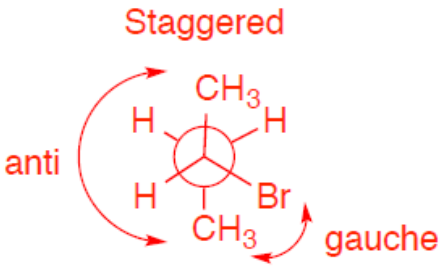
Since all substituents on C2 are the same, there are no distinctive conformations to choose from. Looking down the C2-C3 bond, there is only one eclipsed and staggered conformation, and hence it does not provide a complete idea about other conformations that may exist.

Q3. Consider 2-bromobutane (shown). Sighting along the C2-C3 bond and using Newman projections, answer the following questions using the data provided in the table below.



Interaction	kcal·mol^{-1}
H,H eclipsed	1.0
H,CH_3 eclipsed	1.4
CH_3,CH_3 eclipsed	2.6
H,Br eclipsed	1.7
CH_3,Br gauche	0.9
CH_3,CH_3 gauche	0.9
CH_3,Br eclipsed	3.8

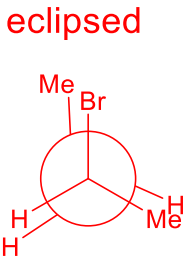
a. Draw the most stable conformer and calculate the total interaction energy.



Most stable

total PE is 0.9 kcal/mol for CH_3/Br gauche

b. Draw the least stable conformer and calculate the total interaction energy.

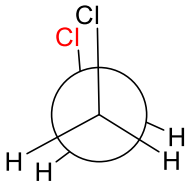


Total PE = 1.4 (H, Me eclipsed) + 1.0 (H, H eclipsed) + 3.8 (CH_3, Br eclipsed) = 6.2 kcal/mol

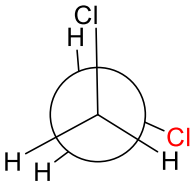
Q4. Consider the molecule 1,2-dichloroethane and answer the following questions.

(a) Draw Newman projections for all eclipsed conformations formed by rotation from 0^o to 360^o about the C-C bond.

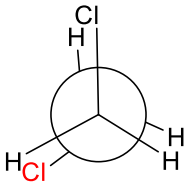
Answer:



(I)



(II)



(III)

(b) Which eclipsed conformation(s) has the lowest energy? Which will have the highest energy?

Answer: Conformation **(I)** will have highest energy (i.e. lowest stability) due higher torsional strain between C-Cl bonds due to stronger steric repulsion between two chlorides along with dipole-dipole repulsion between them. Conformations **(II)** and **(III)** will be lower in energy (they have same energy) as these conformations can avoid higher energy Cl-Cl torsional strain as well as repulsive electronic interaction (dipole-dipole interaction) between chlorides.