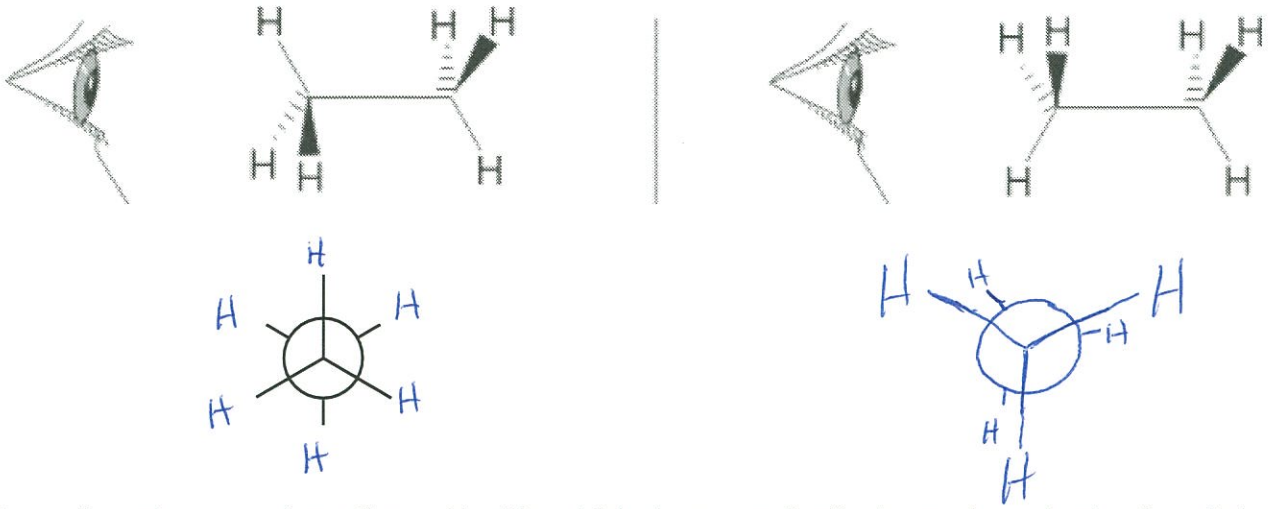
CHAPTER 3: ORGANIC COMPOUNDS AND ALKANES

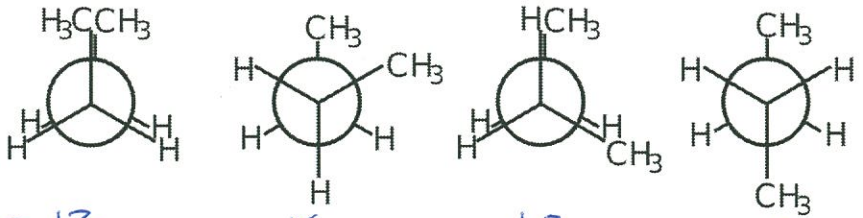
Conformations of Alkanes. Draw Newman projections for the staggered and eclipsed conformations of ethane, using the perspectives indicated below. I've started you off by drawing the skeleton of the Newman projection for the left conformation - you can draw the one on the right.



From the above conformations, identify which is energetically favored, and why the disfavored conformation is higher in energy (e.g. identify and calculate the rotational strain energy).

Useful Conformational Strain Data
σ-σ torsional strain = 4 kJ/mol
CH_3-H eclipsing steric strain = 2 kJ/mol
CH_3-CH_3 gauche steric strain = 3.8 kJ/mol
CH_3-CH_3 eclipsing steric strain = 7 kJ/mol

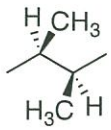
For the Newman projections of butane, below, calculate the strain energy for each and identify which is the energetically most favored conformation.



Torsional = 12		X	12	X
CH_3-CH_3 eclipsing = 7		X	X	X
CH_3-CH_3 Gauche = X		3.8	X	X
CH_3-H eclipsing = X			2+2	X
	19	3.8	16	0

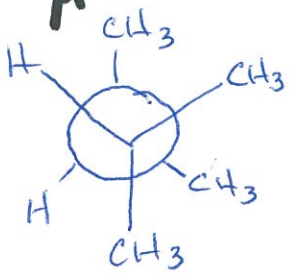
Seven

Draw Newman projections that represent 60° rotations around the C2-C3 bond of 2,3-dimethylbutane, beginning with the conformation that is shown here to the right. This should result in ~~six~~ Newman projections, where the first and last represent the initial conformation. For each, calculate the total strain energy. Finally, generate a graph that plots energy (kJ/mol) versus rotational conformation.



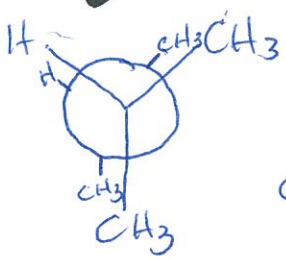
2,3-dimethylbutane

A



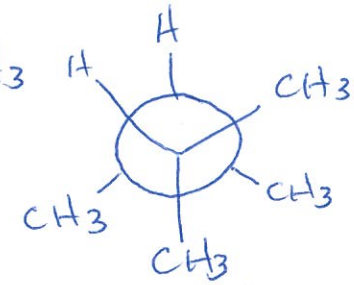
3 x GAUCHE

B



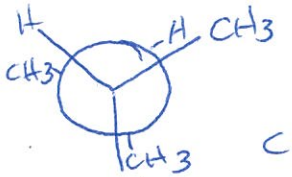
torsional +
2 x CH_3-CH_3 eclipsing

C



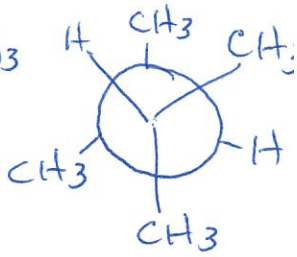
3 x GAUCHE

D



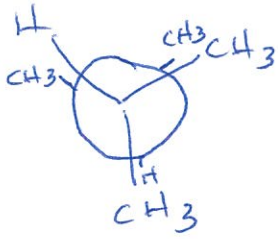
torsional +
CH_3-CH_3 eclipsing +
2 x CH_3-H eclipsing

E



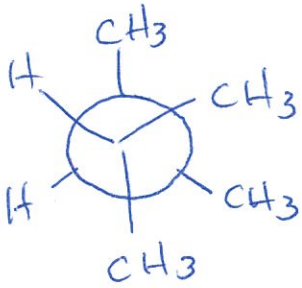
2 x GAUCHE

F

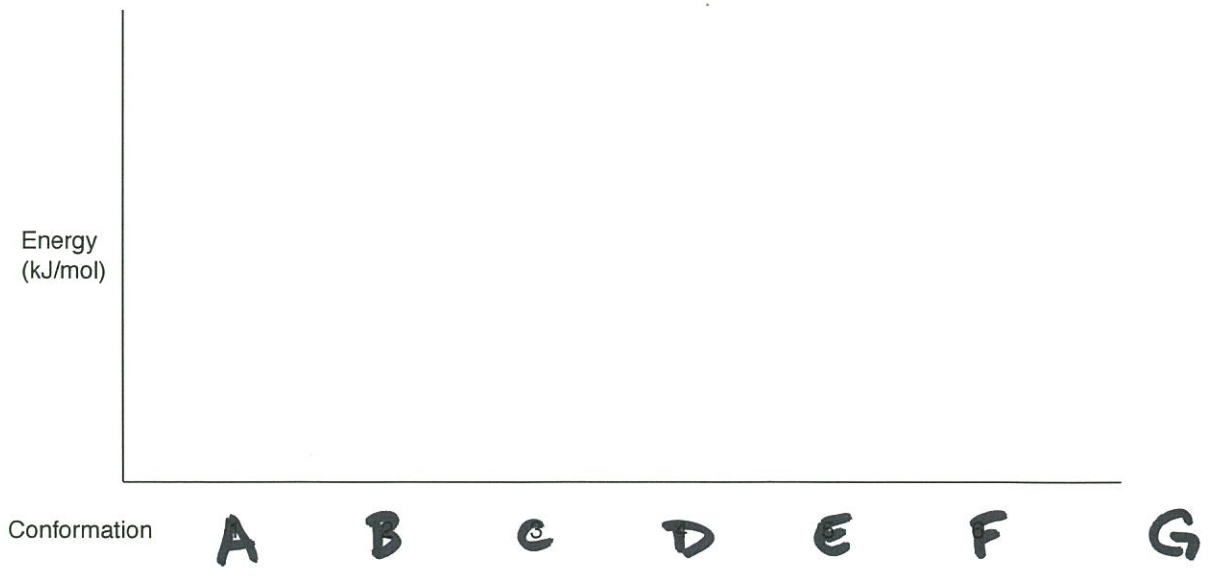


torsional +
CH_3-CH_3 eclipsing +
2 x CH_3-H eclipsing

G



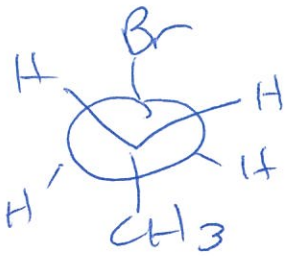
3 x GAUCHE



Consider 1-bromopropane, $CH_3CH_2CH_2Br$.

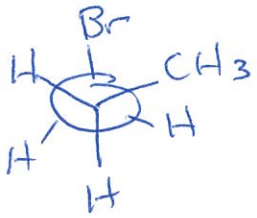
(a) Draw the Newman projection for the conformation in which -CH_3 and -Br are anti (dihedral angle 180°.
(b) Draw the Newman projection for the conformation in which -CH_3 and -Br are gauche (dihedral angle 60°.
(c) Which of these is the lowest energy conformation?

a)

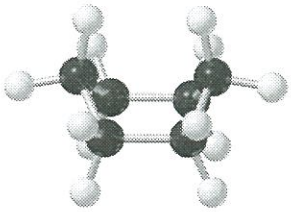


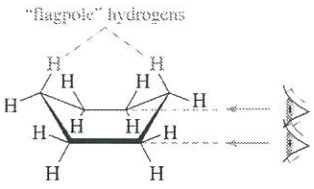
← lowest energy

b)

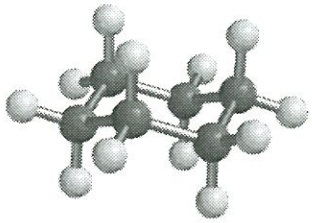


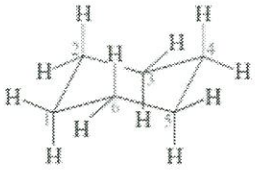
In chapter 4, we'll be discussing cyclohexane rings and their preference for a 'chair' conformation. A relatively high-energy (unstable) conformation is called a 'boat' conformation. Examine the two figures below and provide a reason for the relatively high-stability of the 'chair' conformation. There's a hint given to you in the first image - the two eyes.





boat conformation





chair conformation