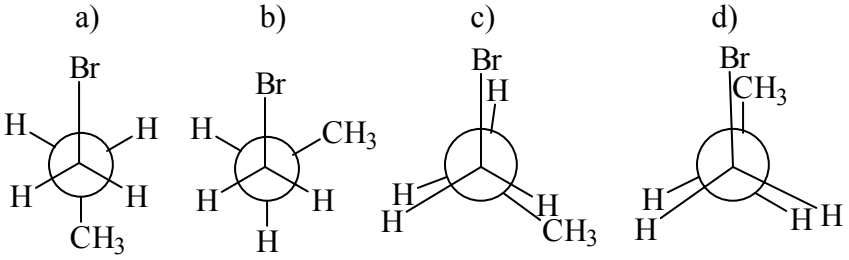
Conformational analysis

1.(14) Consider the molecule **1-bromopropane**. Sighting along C_1-C_2, **construct Newman projections** of the a) *anti* conformation, b) *gauche* conformation, c) and d) two *different* eclipsed conformations (draw four structures total). Using the information below and the fact that barrier to rotation (energy difference between E_{max} and E_{min} conformations) is **21 KJ/mol**, give the relative energies of the four conformations. **Also**, determine the contribution of a CH_3-Br eclipsing interaction.

Interaction	**Energy (KJ/mol)**
H-H *eclipse*	4.0
CH_3-H *eclipse*	6.0
Br-H *eclipse*	7.0
Br-CH_3 *gauche*	4.0
CH_3-Br *eclipse*	____?



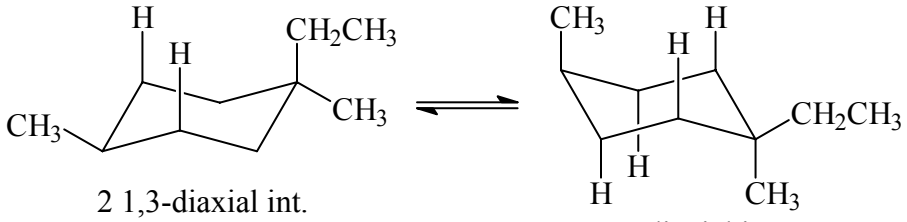
rel.E KJ/mol 0.0 4.0 17.0 21.0

Br - CH_3 eclipse = 13.0 KJ/mol

2.(14) Consider the molecule **1-ethyl-1,4-dimethylcyclohexane** where the **methyl groups are *trans* to each other**.

a) Draw the two chair conformations and determine their relative energies using the data below.

Interaction	**Energy (KJ/mol)**
Methyl - H 1,3-diaxial	3.8
Ethyl - H 1,3-diaxial	4.2



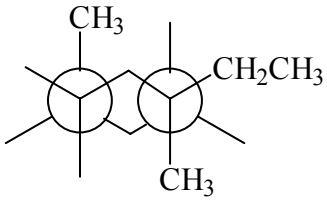
2 1,3-diaxial int.

8.4 KJ/mol

4 1,3-diaxial int.

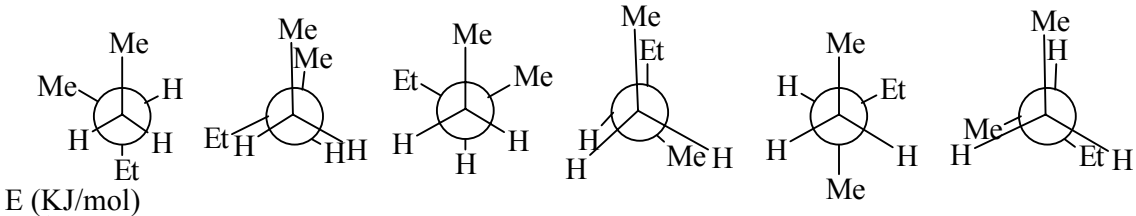
15.2 KJ/mol

b) Sighting down C_1-C_2 and C_5-C_4, draw the *Newman projection* of the *less stable* conformation.



3.(16) Consider the molecule **3-methylpentane** citing along **C_2-C_3**. Construct all six rotational conformers using Newman projections. **Also**, identify the *highest* and *lowest* energy conformations and determine the energy difference (KJ/mol) between the two. *Please be sure to draw the correct molecule!*

Interaction	Energy cost (KJ/mol)
methyl-methyl *gauche*	3.8
methyl-ethyl *gauche*	4.2
methyl-H *eclipse*	6.0
ethyl-H *eclipse*	6.4
methyl-methyl *eclipse*	11.0
methyl-ethyl *eclipse*	12.0
H-H eclipse	4.0



ΔE = 18.2 KJ/mol