## **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<sub>3</sub>-Br eclipsing interaction.

<b>Interaction</b>	Energy (KJ/mol)
H-H eclipse	4.0
CH <sub>3</sub> -H eclipse	6.0
Br-H eclipse	7.0
Br-CH <sub>3</sub> gauche	4.0
CH <sub>3</sub> -Br eclipse	?
a)	b)
u)	0)

## 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.

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

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