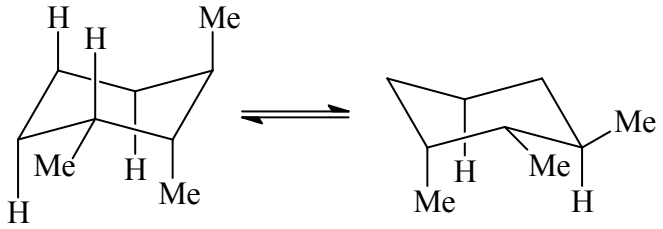
CHM 241 Problem set

1. Consider the molecule **1,2,3-trimethylcyclohexane** where the methyl groups on C_1 and C_2 are ***trans*** and groups on C_2 and C_3 are ***cis.*** Draw the two chair conformations and using the data below (you may not need all of it), determine the relative energies of both and thus the barrier to flipping between the two (in KJ/mol). Barrier = 3.8 KJ/mol

Interaction	**Energy (KJ/mol)**
$CH_3 - CH_3$ gauche	3.8
$CH_3 - H$ 1,3-diaxial	3.8
$CH_3 - CH_3$ 1,3-diaxial	15.4



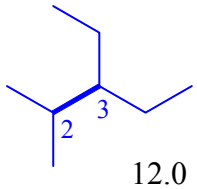
4 1,3-diaxial = 15.2 — 2 Me-H 1,3-diaxial = 7.6

1 gauche Me-Me = 3.8 — 2 gauche Me-Me = 7.6

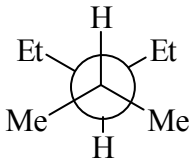
19.0 KJ/mol — **15.2 KJ/mol**

2. Construct Newman projections of **all six** of the unique rotational conformations of **2-methyl-3-ethylpentane** citing along **C_2-C_3**. Using the table below (*you will not need all of the values*), **determine the relative energies (KJ/mol) of the highest and lowest energy conformations and the barrier to rotation**. Me = methyl; Et = ethyl

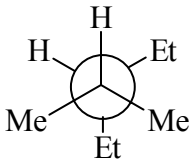
Interaction	energy (kJ/mol)
ECLIPSING	
H-H	4.0
H-Me	6.0
H-Et	7.0
Me-Me	15.0
Me-Et	16.0
Et-Et	18.0
GAUCHE	
Me-Me	3.8
Me-Et	4.0
Et-Et	4.5



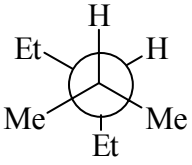
8.0



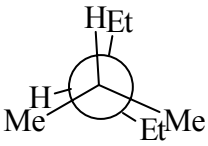
12.0



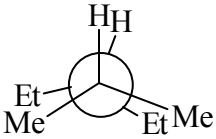
12.0



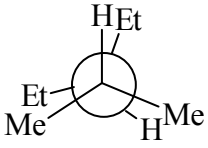
29.0



36.0



29.0



Barrier = 28 KJ/mol