Construct Newman projections for all of the unique rotational conformations of **3,4-dimethylhexane** (focus down C<sub>3</sub>-C<sub>4</sub>). Identify the lowest ( $E_{min}$ ) and highest ( $E_{max}$ ) energy conformations and determine the barrier to rotation in KJ/mol (difference between  $E_{max}$  and  $E_{min}$ ). Use the data provided (Me = methyl; Et = ethyl). How many unique conformations are there?

| Interaction                  | energy cost (K         | (J/mol)  |   |  |  |
|------------------------------|------------------------|--|---|--|--|
| Me-Me gauch                  | e 38                   | <u>10, 11101</u>   |   |  |  |
| Me-Et gauche                 | 4 1                    |  |   |  |  |
| Et-Et gauche                 | 4 5                    |  |   |  |  |
| H-H eclipse                  | 4.0                    |  |   |  |  |
| Me-H eclipse                 | 6.0                    |  |   |  |  |
| Et-H eclipse                 | 7.0                    |  |   |  |  |
| Me-Me eclipse                | e 11.0                 |  |   |  |  |
| Me-Et eclinse                | 12.0                   |  |   |  |  |
| Et-Et eclinse                | 13.0                   |  |   |  |  |
| Et Et tempse                 | 10.0                   |  |   |  |  |
| $Me \underbrace{Et}_{Et} Me$ | Et Me<br>Et Me<br>25.0 | There are 2 p<br>which stereo<br>$Et \rightarrow Me$<br>12.4<br>E = 19.8  KJ/m | Et<br>Et<br>Et<br>Me M<br>28.0<br>highest | of conformers<br>(see CH 9). E<br>Et<br>Et<br>Et<br>Me<br>12.4 | depending on<br>Either series is corre<br>Et<br>Me<br>Et Me<br>25.0 KJ/mol |
| Me                           | Et                     | Et Me  | Et<br>Et                                  | Et   | Et   |

Me

Me

12.7

 $\Delta E = 16.7 \text{ KJ/mol}$ 

Me

Ме

8.3

lowest

Me

25.0

highest

Me

Et

25.0 KJ/mol

highest

Me

Ėt

12.0

Et Me

23.0

Consider the molecule **1,2,4-trimethylcyclohexane** where the methyl groups are all *cis*. The *less stable* conformation has an energy of approximately **26.8 KJ/mol**. Draw the two chair conformations of this compound and determine the energy of the more stable conformation using the data below. How much steric strain (KJ/mol) does a methyl – methyl 1,3-diaxial interaction contribute to the less stable conformation? *Also*, draw a Newman projection of the *more stable* conformation sighting along  $C_{1,2}$  and  $C_{5,4}$ .

