CHEM 241-601

Problems from Wade chapters 3 and 4

1. Consider the molecule *trans* 1-bromo-4-methylcyclohexane and **draw the two flip chair conformations**. The energy difference between the two flip conformations is 9.6 KJ/mole. **Circle the more stable conformation**. If the energy of one methyl-H 1,3-diaxial interaction is 3.8 KJ/mol, what is the value of one bromine-H 1,3-diaxial interaction?
What is *more* spacially (sterically) demanding, a Br atom or a CH_3 group? _________

2. Free radical bromination of alkanes can be problematic because mixtures of products can result when more than one kind of C-H bond is present in the substrate. This is the case with the bromination of **propane** where **1-bromopropane (A)** and **2-bromopropane (B)** can form.

Using the general mechanism for the propagation steps i) and ii) shown below and the list of bond dissociation energies, determine ΔH_1, ΔH_2, and ΔH_{rxn} for each reaction (formation of **A** and **B**).

$$CH_3CH_2CH_3 + Br_2 \text{ ----------> } \underset{\textbf{A}}{CH_3CH_2CH_2Br} + \underset{\textbf{B}}{(CH_3)_2CHBr} + HBr$$

General reaction: $RH + X_2$ ------------> $RX + HX$

ΔH^{o} (KJ/mol)

A **B**

i) $R\text{-}H + X^{\cdot}$ -----------------> $R^{\cdot} + H\text{-}X$ $\Delta H_{I} =$

ii) $R^{\cdot} + X_2$ -------------------> $R\text{-}X + X^{\cdot}$ $\Delta H_{ii} =$

$\Delta H_{rxn} =$

a) Which product is more likely to form, 1-bromopropane or 2-bromopropane? Explain.

b) Which step is the rate-determining step, i) or ii)? Explain.

c) Draw a reaction profile for the 2 steps in the reaction you chose in part b). Draw it as close to scale as you can.

Bond	**BDE (KJ/mol)**
Br-Br	193
H-Br	366
$CH_3CH_2CH_2$-H	420
$(CH_3)_2CH$-H	401
$CH_3CH_2CH_2$-Br	285
$(CH_3)_2CH$-Br	274