CHM 201
CH 5 problem

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**).

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

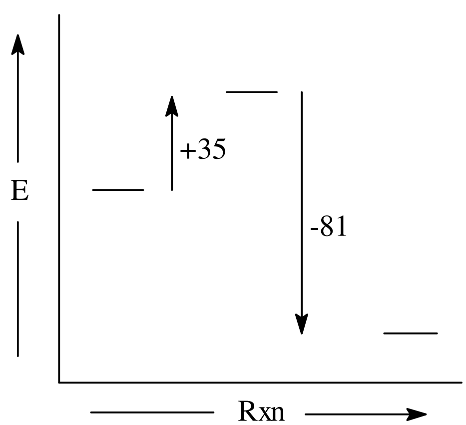
General reaction: $RH + X_2$ ------------> $RX + HX$

		ΔH^o (KJ/mol) **A**	**B**
i)	$R\text{-}H + X^\cdot$ -----------------> $R^\cdot + H\text{-}X$	420-366=+54	401-366=+35
ii)	$R^\cdot + X_2$ -------------------> $R\text{-}X + X^\cdot$	193-285=-92	193-274=-81
	ΔH_{rxn}	**-38KJ/mol**	**-46KJ/mol**

a) Which product is more likely to form, 1-bromopropane or 2-bromopropane? Explain.
   2-bromopropane (B) because the first propogation step has a lower ΔH_i, therefore a lower E_{act}.

b) Which step is the rate-determining step, i) or ii)? Explain.
   In both reactions, step i) is rate determining. This is because the Eact is highest for the first step (due to the ΔH_i being higher – Hammonds Postulate).

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. Draw a smooth line for the reaction pathway.



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