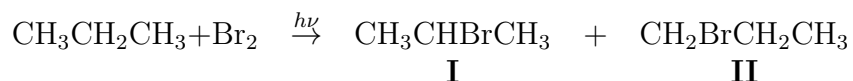


**Problem set 3**

1. The photochemical monobromination of propane results in a mixture of two isomers:



We assume that the reaction is subject to the thermodynamic control. The degeneracy of each state (isomer) is equal to the number of propane's hydrogen atoms that can be replaced with a bromine atom to form the respective isomer.

It was found that, at the room temperature ( $T=298\text{ K}$ ), the two isomers are formed in the following relative amounts: 97 % of 2-bromopropane (I) and 3 % of 1-bromopropane (II). Estimate the energy difference between the two isomers. Express it as  $\Delta E = E_{II} - E_I$ . Comment on the result obtained based on your organic chemistry knowledge.

2. Based on the Boltzmann law, sketch an approximate plot of the probability density of chloride counter-ions that form the so-called "ion cloud" around a sodium cation in aqueous solution. To make the picture more realistic, assume that the vdW radii of the sodium and chloride ions are  $1.9\text{ \AA}$  and  $2.9\text{ \AA}$ , respectively. Note that both the Pauli repulsion and the Coulombic attraction need to be considered. Although no accurate calculations are required to make a detailed plot, for those who want to try, please assume the relative (dimensionless) dielectric constant of water of 80.

The value of the universal gas constant is  $R = 8,3145\text{ J}/(\text{mol}\cdot\text{K})$ ,  $1\text{ kcal} = 4184\text{ J}$ .