Problem set 3

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

$$\underset{}{CH_3CH_2CH_3}+Br_2 \xrightarrow{h\nu} \underset{\textbf{I}}{CH_3CHBrCH_3} + \underset{\textbf{II}}{CH_2BrCH_2CH_3}$$

   We assume that the reaction is subject to the thermodynamic control. The degeneration of each state (isomer) is equal to the number of propape'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 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 Å and 2.9 Å, 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 $R = 8,3145$ J/(mol*K), 1 kcal = 4184 J.