CHEM 361A - Lecture 6 Activity

Statistical Mechanics

In Class

1. In this problem we will see that as the number of atoms in the system increases the probabilities of each macrostate determines that only one state will be observed.

   (a) Starting with our system with four energy levels with a total energy of three (from page 5 in the slides), determine

      i. The number of microstates in each of the three macrostates if there are 10 identical particles.

      ii. The probability of the system to be in each of the macrostates

   (b) Use the answers from Homework Problem 3 to answer these questions. In terms of the probability of each system to be in a given macrostate:

      i. When N is small (N=3), which macrostate is the most likely for the system to be in? Is it still reasonably possible for the other macrostates to be observed?

      ii. As N increases, which macrostate is the most likely for the system to be in? Is it still reasonably possible for the other macrostates to be observed?

2. We are now going to examine Ligand-Receptor Binding in the context of statistical mechanics and partition functions. Pretend that there is one receptor site in solution with L ligands. To apply a statistical mechanics framework, the region that the ligands can occupy is divided into Ω different sites that only one ligand can occupy. Assume that $\Omega \gg L$. Figure 1 shows examples of this setup.

   (a) How many microstates exist for the case where no ligands interact with the receptor? Use $\frac{\Omega!}{(\Omega-L)!} \approx \Omega^L$ to simplify your expression. This setup will assume two states: non-receptor sites with ligands, and non-receptor sites without ligands. Don't worry about the receptor site right now.

   (b) How many microstates exist for the remaining ligands when 1 ligand interacts with the receptor. Use $\frac{\Omega!}{(\Omega-(L-1))!} \approx \Omega^{L-1}$ to simplify your expression. This setup still assumes that there are two states: non-receptor sites with ligands, and non-receptor sites without ligands. Take the lost ligand to the receptor site into account.

   (c) If the energy of each ligand in solution is $\epsilon_{solution}$ and the energy of a ligand in the receptor is ϵ_{bound}, what is the energy of a microstate with all free ligands, and what is the energy of a microstate with one ligand bound to the receptor? Express $\epsilon_{bound} - \epsilon_{solution} = \Delta\epsilon$.

   (d) What is the partition function, q, for this system?

   (e) What is the probability of finding the system with one ligand bound to the receptor?

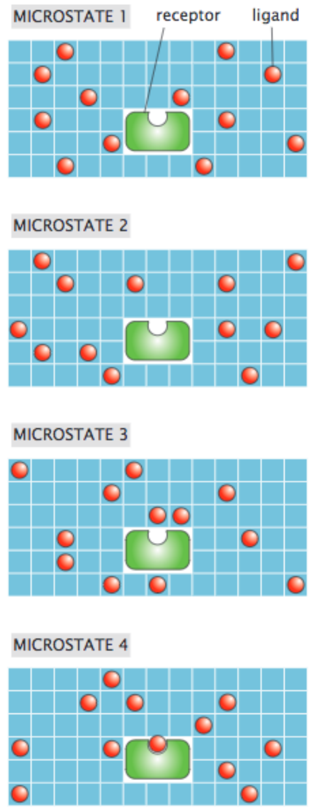

Figure 1: Examples of the ligand-receptor system with L ligands and one receptor. The region that the ligands are not interacting with the receptor is divided into Ω sites. Only one ligand can occupy each site. The first three microstates show examples where there is no ligand-receptor interaction, while microstate 4 has the receptor interacting with a ligand.

Homework

3. For the four level system with total energy 3, determine the number of microstates in each of the three macrostates if there are 50 ($W_1 = 19600$; $W_2 = 2450$; $W_3 = 50$), 100 ($W_1 = 161700$; $W_2 = 9900$; $W_3 = 100$), and 150 ($W_1 = 551300$; $W_2 = 22350$; $W_3 = 150$) identical particles. What is the probability of these systems to be in each of its macrostates? Feel free to use a software package like Excel to do these calculations. (P50: $W_1 = 0.887$; $W_2 = 0.111$; $W_3 = 0.002$, P100: $W_1 = 0.942$; $W_2 = 0.058$; $W_3 = 0.001$, P150: $W_1 = 0.961$; $W_2 = 0.039$; $W_3 = 0.000$)

4. You have a two level system and two particles that occupy this system. The energy of the lower level is ϵ_1 and the energy of the higher level is ϵ_2

   (a) There are three possible macrostates for this system.

      i. What are the energies for the three macrostates? ($2\epsilon_1$; $\epsilon_1 + \epsilon_2$; $2\epsilon_2$)

ii. What are the number of microstates in each macrostate? (1; 2; 1)

(b) What is the partition function for this system? ($q = e^{-\frac{2\epsilon_1}{k_B T}} + 2e^{-\frac{\epsilon_1+\epsilon_2}{k_B T}} + e^{-\frac{2\epsilon_2}{k_B T}}$)

(c) Write an expression that determines the probability of finding both particles in the higher energy level? (prob both in highler level $= e^{-\frac{2\epsilon_2}{k_B T}}/q$)

(d) If $\epsilon_1 = 1 \times 10^{-22}$ J and $\epsilon_2 = 2 \times 10^{-22}$ J, what is the probability of finding both particles in the higher energy level at $T = 298$ K? (0.245)

(e) If $\epsilon_1 = 1 \times 10^{-22}$ J and $\epsilon_2 = 1 \times 10^{-20}$ J, what is the probability of finding both particles in the higher energy level at $T = 298$ K? (0.0068)