BE 100. BIOENGINEERING FUNDAMENTALS
FALL 2024

PROBLEM SET 1

Due by 4 PM on October 3, 2024 (Thursday)

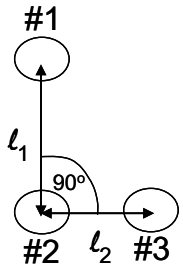
You will need to upload a pdf of your handwritten work under Assignment 1 in the Assignments tab of Bruin Learn.

1. (*Material from Lecture 2*) Draw the structure of isoleucine and label all the non-hydrogen atoms appropriately as α, β, etc at pH 7.

2. You put a hot cup of water on the table, and come back 8 hours later. When you measure the temperature throughout the cup after the 8 hours, are you investigating an equilibrium or kinetic phenomenon?

3. (*Material from Lecture 2*) What are the single-letter and three-letter abbreviations for glutamine?

4. (*Need to cover a little more material in Lecture 2.*) Using the potential described in lecture (comprised of electrostatic, van der Waals, and excluded-volume interactions), derive an expression for the contribution to the internal energy of the system due to the interactions between the three atoms shown below. The partial charges on atoms 1, 2, and 3 are Q_1, Q_2, and Q_3, respectively. The van der Waals interaction parameters between atoms 1 and 2, between atoms 1 and 3, and between atoms 2 and 3 are β_{12}, β_{13}, and β_{23}, respectively. The excluded-volume interaction parameters between atoms 1 and 2, between atoms 1 and 3, and between atoms 2 and 3 are δ_{12}, δ_{13}, and δ_{23}, respectively.



5. Short answers

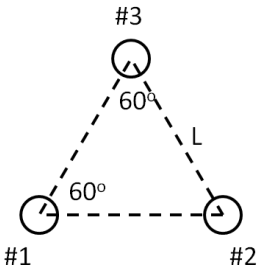
   a. Describe molecularly what is captured in the internal energy.

   b. You decide to study ice cream after it has melted and reached room temperature. Are you investigating an equilibrium or kinetic phenomenon?

   c. Consider the excluded-volume portion of the Lennard-Jones 6-12 potential. Assuming you know the parameter δ between two atoms, derive an expression for the excluded-volume force felt by one atom due to the other atom a distance ℓ away.

   d. (*Material from Lecture 2*) In molecular modeling, what is a distinct set of dihedral (χ) angles for an amino acid called?

   e. (*Need to cover a little more material in Lecture 2.*) Use the Lennard-Jones potential to derive an expression for the contribution to the internal energy of the system due to the van der Waals and excluded-volume interactions between the atoms shown below. The van der Waals interaction parameters between atoms 1 and 2, between atoms 1 and 3, and between atoms 2 and 3 are β_{12}, β_{13}, and β_{23}, respectively. The excluded-volume interaction parameters between atoms 1 and 2, between atoms 1 and 3, and between atoms 2 and 3 are δ_{12}, δ_{13}, and δ_{23}, respectively. If the β parameters increased, would the internal energy increase or decrease? Why?

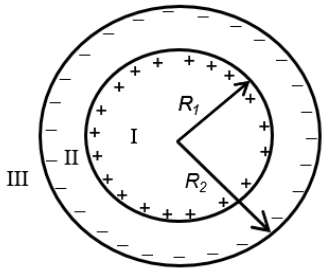


   f. (*Material from Lecture 2*) Let's say you have the x-ray crystallographic structure of the wild type of a particular protein. Why are the energetics of the covalent bonds not considered in computing the protein energy during the minimization procedure to find the lowest energy structure for a mutant being considered?

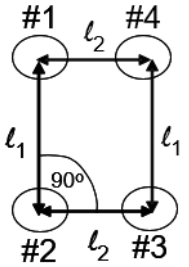
6. Given the following expression for a hypothetical potential energy function (P) as a function of r, θ, and ϕ coordinates, derive an expression for the force.

$$P = 2r^{1/2} + 5\theta^2\phi^3$$

7. (*Material from Lecture 2*) Derive expressions for $d\psi/dr$ at $r=R_1^+$ and at $r=R_2^+$ in the figure below. Note that the positive charge of +3e (where e is the electronic charge) is smeared uniformly on the spherical surface at $r=R_1$ and the negative charge of -4e is smeared uniformly on the spherical surface at $r=R_2$. There are no salt ions in Regions I and II. There are salt ions present in Region III, but you do not know their concentrations. The dielectric constants in the regions are known as ε_I, ε_{II}, and ε_{III}.

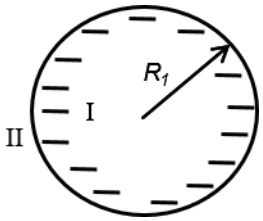


8. (*Need a little more material from Lecture 2.*). Using the Lennard-Jones potential, derive an expression for the contribution to the internal energy of the system due to the van der Waals and excluded-volume interactions between the four atoms shown below. The van der Waals interaction parameters between atoms 1 and 2, between atoms 1 and 3, between atoms 1 and 4, between atoms 2 and 3, between atoms 2 and 4, and between atoms 3 and 4 are β_{12}, β_{13}, β_{14}, β_{23}, β_{24}, and β_{34}, respectively. The excluded-volume interaction parameters between atoms 1 and 2, between atoms 1 and 3, between atoms 1 and 4, between atoms 2 and 3, between atoms 2 and 4, and between atoms 3 and 4 are δ_{12}, δ_{13}, δ_{14}, δ_{23}, δ_{24}, and δ_{34}, respectively.



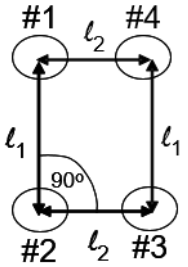
9. (*Material from Lecture 2*) Derive an expression for $d\psi/dr$ at $r=R_1^+$ in the figure below. Note that the negative charge of -3e (where e is the electronic charge) is smeared on the surface area of the cylinder at $r=R_1$. There are no ions in Region I. There are salt ions present in Region II, but you do not know their concentrations and their distribution in three-dimensional space. The dielectric constants in the regions are known as ε_I and ε_{II}. Neglect the electric fields associated with the end caps of the cylinder since the length of the cylinder (L) is much, much greater than its radius. The electric field coming out of

the end caps is much smaller than the electric field coming out of the surface area. Just focus on what is happening due to the charges on the surface area. Note that $d\psi/dz = 0$ since $L >> R$. Note also that $d\psi/d\theta = 0$ since the charges are symmetric relative to the z-axis, i.e., the charges are axisymmetric. Based on the derived expression, is the electric field pointing away or toward the surface area of the cylinder? Is this consistent with the convention used for the directionality of the electric field?



10. (*Material from Lecture 2*) What are the single-letter and three-letter abbreviations for lysine?

11. (*Need a little more material from Lecture 2.*) Using the Lennard-Jones potential, derive an expression for the force felt by atom 1 due to atom 3 in the figure below. The van der Waals interaction parameters between atoms 1 and 2, between atoms 1 and 3, between atoms 1 and 4, between atoms 2 and 3, between atoms 2 and 4, and between atoms 3 and 4 are β_{12}, β_{13}, β_{14}, β_{23}, β_{24}, and β_{34}, respectively. The excluded-volume interaction parameters between atoms 1 and 2, between atoms 1 and 3, between atoms 1 and 4, between atoms 2 and 3, between atoms 2 and 4, and between atoms 3 and 4 are δ_{12}, δ_{13}, δ_{14}, δ_{23}, δ_{24}, and δ_{34}, respectively.



12. Short answers

a. Let's consider a gas made up of two types of molecules as our system. A chemical reaction occurs that changes the covalent chemical bonds in the molecules. Will the internal energy change? Yes or No.

b. What is the name of the induced dipole-induced dipole interaction?

c. (*Material from Lecture 2*) List the names of the amino acids that have aromatic side chains.

d. Describe molecularly what is captured in the internal energy.

13. Short answers

a. (*Material from Lecture 2*) What is the radius of a water molecule? Please do not forget the units.

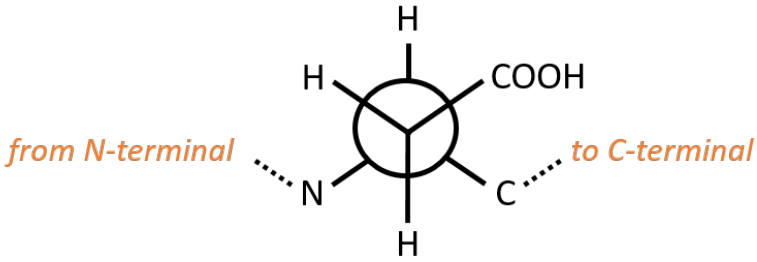
b. You take 0.05 grams of sodium chloride salt and pour it in water inside a beaker. You then mix the solution and come back 1 day later. When you measure the concentration of sodium ions throughout the solution, are you investigating an equilibrium or kinetic phenomenon?

c. (*Material from Lecture 2*) Inside the protein, what diffracts the incoming x-ray beams in x-ray crystallography?

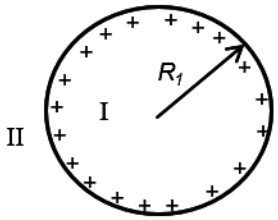
d. (*Material from Lecture 2*) True or False. The beta sheet is part of the secondary structure of a protein.

e. (*Material from Lecture 2*) What color is typically associated with oxygen atoms in structures generated by programs to visualize proteins?

f. (*Material from Lecture 2*) Please draw the dihedral angle in the image below. Please also name the amino acid.



14. (*Material from Lecture 2*) Derive an expression for $d\psi/dr$ at $r=R_1^+$. Note that the positive charge of +5e (where e is the electronic charge) is smeared on the spherical surface at $r=R_1$. There are no ions in Region I. There are salt ions present in Region II, but you do not know their concentrations. The dielectric constants in the regions are known as ε_I and ε_{II}.



15. Short answers

    a. You are monitoring the concentration of product made in a reaction and see it increasing as you take measurements at t = 0, 2, 4, and 6 minutes. Are you investigating an equilibrium or kinetic phenomenon?

    b. You add dye to a beaker and measure how the concentration of the dye at an outermost position of the beaker increases over time. Are you investigating an equilibrium or kinetic phenomenon?