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# EXAM I COURSE
# TFY4310 MOLECULAR BIOPHYSICS

## Suggested Solutions

**Exercise 1.** [total: 32 pts]

Justify **eight** (8) of the following sentences [4 pts each]:

1. The C–C single bonds are shorter and stronger in $H_2C$=CH–CH=$CH_2$ than in $H_2C$=CH–$CH_2$–CH=$CH_2$.

   **Answer:** $H_2C$=CH–CH=$CH_2$ is a conjugated molecule, that is, the single and double bonds alternate. In $H_2C$=CH–$CH_2$–CH=$CH_2$ there are two single bonds between the double bonds. For the conjugated molecule, the quantum mechanical solution suggests that the $\pi$ orbitals that form the double bonds partially overlap over the single bonds, providing the single bond with a double bond character. That is, the single bond in a conjugated system presenting a stronger and shorter bond that equivalent single bonds in non-conjugated systems.

2. Mean-field theories based on the Poisson-Boltzmann equation, do not account for the attractive forces that may arise between surfaces with equal charge sign (for example, DNA condensation in the presence of trivalent ions).

   **Answer:** Charged surfaces in solution will have their counterion condensed at the surface, in a phenomenon call ion condensation. The effect of ion condensation on a surface or particle is a reduced double-layer repulsion. There is however another counterion effect between similarly charged surfaces that gives rise to attraction. This is contrary to the Poisson-Boltzmann equation that predicts a repulsion at all separations between equally charged surfaces. This additional electrostatic force arises from the correlation of the counterions in each double layer, that may form a highly polarizable layer at each interface whose fluctuations in density give rise to an attractive van der Waals-like force with another double-layer. These effects, known as *ion-correlation* or *charge fluctuations force* become significant at small distances ($< 4$ nm), and increase with the surface charge density and valency of the counterions. Mean-field theories do not take the counterions into account explicitly, they only take into account their average effect in the system, and therefore this force is not included in the Poisson-Boltzmann equation.

3. The hydrogen bond is best described as a Coulombic interaction, than as a (point) dipole-dipole interaction.

   **Answer:** Since water is a dipolar molecules it is often tempting to describe the interaction between two water molecules as a dipole-dipole interaction. However this approximation does not account for the orientation of the water molecules in respect to each other. The dipole-dipole approximation predicts a maximum interaction when the dipoles are aligned according to the figure below, while the two water molecules orient according to the diagram on the right-hand side.

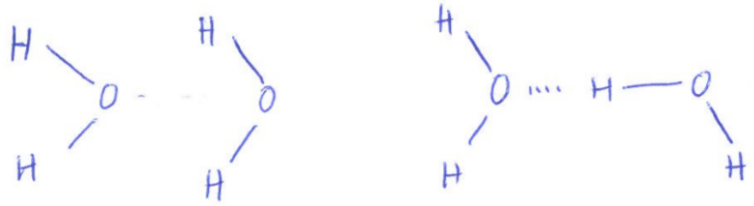


Figure 1: Drawing showing the orientation of two water molecules which would be most favorable taking into account a dipole-dipole type of interaction (left-hand side), and the orientation of two water molecules that interact via a hydrogen bond (right-hand side).

   Of course, one should realize that the dipole-dipole interaction is based on electrostatic arguments (one solves the Coulomb potential for the discrete charges) but assumes that the distance between dipoles is much larger than the distance between the charges in the dipole. This is not the case in the hydrogen bond since the length of the bond is equivalent to the dimensions of the water molecule.

4. The formation of surfactant micelles is entropically driven.

   **Answer:** The main driving force for the formation of surfactant micelles is the hydrophobic interaction between the non-polar surfactant tails.

   Hydrophobic interactions arise from the so-called hydrophobic effect. A water molecule in a water solution forms in average around 3.5 H-bonds with the neighboring water molecules. When a non-polar molecule is placed in water the closest water molecules will arrange around the non-polar molecules (which whom they cannot form H-bonds) to avoid the disruption of the H-bonds. In this process the water molecules form cage-like stuctures (clathrates), which decreases the water mixing entropy. Forcing two apolar molecules together decreases the entropy of the apolar molecules but also decreases the apolar area that is exposed to the water, allowing for the release of some of the structured water. This leads to a large increase in the water mixing entropy, which is the dominant effect in surfactant micellar formation.

5. When applying the freely-rotating statistical polymer chain model, a suitable value for the $\theta$ angle is 109.4°.

   **Answer:** The freely-rotating statistical chain model is based on the freely-jointed chain model, which uses a random walk to relate the dimensions of a polymer chain with the number of segments and their length. In addition, an angular component is introduced, to account for the fact that there are some restriction to the value that the angle between consecutive bonds can adopt.

The majority of the polymers have a backbone composed of [$CH_2$] monomers. The carbon in the monomer is $sp^3$ hybridized, which means that the bonding orbitals in the carbon, for these molecules, are four $sp^3$ orbitals that are orthogonal and therefore have a 104 °. Therefore, the sigma bonds between the carbon and the two hydrogen and the two adjacent carbons will be roughly this angle.

6. Brownian dynamic techniques are more suitable to follow the folding of a protein than Monte Carlo simulations.

   **Answer:** Monte Carlo simulations are based on the generation of random numbers to describe, for example, particle position or probabilities of a specific move type. Therefore these are (usually) only suitable to probe systems in equilibrium, such as the more probable equilibrium conformation of a protein under specific conditions. Brownian dynamic techniques, on the other hand, are based on the resolution of Newton's equation of motion and are, therefore, more suitable to follow the dynamics of protein folding.

7. Spin-spin ($T_2$) relaxation does not involve the flipping of spins between levels.

   **Answer:** In a typical 1D-NMR experiment we can define two relaxation times: The spin-lattice relaxation ($T_1$) occurs when the radio frequency pulse is turned off and the magnetization that was centered in the $xy$-plane returns to the $x$-axis. During this period the spins return to their fundamental state, that is, it involves the flipping of spins between levels; The spin-spin relaxation ($T_2$), on the other hand, occurs because different spins will have slightly different precessing frequencies due to differences in their chemical environment. This leads to the unbundling of the spins in the $xy$-plane that leads to a decrease in the magnetization in the $xy$-plane, but no changes in the magnetization in the $z$-axis, $M_z$; that is, there is no variation in the spin level population.

8. COSY and NOESY are complementary techniques in the study of biomacromolecular conformation.

   **Answer:** COSY and NOESY are 2-D NMR methodologies. COSY employs the coupling of spins mediated through the covalent bonds (generally up to three bonds) and so, it gives information about the primary structure of the biomacromolecules. NOESY, on the other hand, explores the nuclear Overhauser effect which relies on dipole coupling. Such coupling has a $r^{-3}$ dependence and so it is only present when the nuclei are close in space (up to 5 Å). Since this signal is not mediated by the covalent bonds it provides information about the secondary and high order level structures.

   Together, COSY and NOESY are very useful in the study of biomacromolecule conformation.

9. Infra-red and Raman spectroscopies are complementary techniques.

   **Answer:** Both Infra-red (IR) and Raman spectroscopies probe the vibrational modes of molecules and are based on the excitation of vibrational modes as a consequence of the absorption of electromagnetic radiation of the correct wavelength by the molecule. The difference between the techniques arises from the fact that the selection rules are different. In the case of IR spectroscopy one of the selection rules states that the transition dipole moment, which lies along the direction of the changing dipole moment, needs to be different than zero. In Raman spectroscopy a vibrational mode is only observable in the spectrum if there is a change in the polarizability of the molecule.

Some vibrational modes will therefore be IR-active and Raman inactive, while some other will show a particular vibration mode in the Raman spectrum but not in the IR spectrum. The $CO_2$ molecule is a typical example. Being a symmetric molecule with no permanent dipole moment, the symmetric stretching mode will be IR-inactive but Raman active. On the other hand the asymmetric stretching mode will be IR active and Raman-inactive.

10. The Maxwell model is useful in predicting the response of a polymer during stress relaxation where a constant strain is imposed $\gamma = \gamma_0$.

**Answer:** The Maxwell model has been proposed to explain the time-dependent mechanical behavior of viscous materials. It consists of a spring with elastic modulus $K$, and a dashpot with viscosity $\eta$, in series. The constitutive equation is

$$\eta \frac{\mathrm{d}\gamma}{\mathrm{d}t} = \frac{\eta}{K}\frac{\mathrm{d}\tau}{\mathrm{d}t} + \tau, \tag{1}$$

where $\gamma$ and $\tau$ are the strain and the stress, respectively.

If a constant strain $\gamma = \gamma_0$ is imposed Eq. (1) becomes

$$\frac{\eta}{K}\frac{\mathrm{d}\tau}{\mathrm{d}t} + \tau = 0.$$

The solution of this equation is

$$\tau = \tau_0 \mathrm{e}^{-\frac{K}{\eta}t}, \tag{2}$$

where $\tau_0$ is the initial stress.

The quantity $\lambda = \eta/K$, the relaxation time, is a measure of the rate at which stress decays.

**Comment 1:** According to Eq. (2) the Maxwell model predicts that the stress relaxes completely over a long period of time. This, in fact, is not normally the case for a real polymer. However, we can say that the Maxwell model describes the stress relaxation of a polymer in first approximation.

**Comment 2:** A qualitative answer with a schematics of the variation of strain and stress with time would have also been accepted as correct.

11. In dilute macromolecule solutions, shear thinning occurs when the shear rate (rate of deformation) is faster than rate of orientation of the macromolecules.

**Answer:** Viscosity in a solution results from the friction that arises between shear lines when the solution flows. In a macromolecular solution an increase in viscosity (from that of the pure solvent) is due to the fact that molecules have sufficiently large dimensions to cross adjacent shear lines. When the solution is deformed, for simplicity lets us imagine that is flowing, the macromolecules will align in the direction of the deformation, but Brownian motions of the polymers and solvent will act to randomize the orientation of the molecules. If the shear rate is larger than the rate of orientation of the macromolecules, these will not have opportunity to relax their orientation and will remain aligned in solution, in the direction of the flow. This will decrease the friction between shear lines, leading to a decrease in the viscosity.

## **Exercise 2.** [total: 39 pts]

Chromatin is the complex of DNA and eight proteins (histone octamer) found in all eukaryotic cells. The fundamental repeating unit of chromatin is the nucleosome particle. The

properties of DNA and protein in nucleosomes, in water, were determined using a range of techniques.

Data obtained from dynamic light scattering, and plotted on a graph of the $\ln(g^{(1)}(q,\tau))$ versus $\tau$, was found to be linear with a slope: $-1.381\times10^4$ s$^{-1}$. The scattering angle was 90° and the wavelength of the light through the medium was 500 nm. The temperature was 20 °C.

In the same solution velocity sedimentation performed at 18,100 revolutions per minute, obtained the following data:

| Time (minutes) | Boundary position $r$ (cm) |
|---|---|
| 0 | 4.460 |
| 80 | 4.593 |
| 160 | 4.713 |
| 240 | 4.844 |

Gel electrophoresis showed that the DNA molecule associated with a single nucleosome protein complex is 200 base pairs in length. The average molecular weight of a DNA base pair is 600 g mol$^{-1}$.

1. Calculate the translational diffusion coefficient of the nucleosomes.

   **Answer:** To calculate the translational friction coefficient we use the data obtained from the dynamic light scattering measurements. It is mentioned that the graph of the $\ln(g^{(1)}(q,\tau))$ versus $\tau$, was found to be linear with a slope: $-1.381\times10^4$ s$^{-1}$. Using
   $$g^{(1)}(q,\tau) = \exp(-q^2 D_{\mathrm{T}}\tau)$$
   we see that slope $= -q^2 D_{\mathrm{T}}$. Knowing that the scattering angle was 90° and the wavelength of the light through the medium was 500 nm we calculate $q$ according to
   $$q = \frac{4\pi}{\lambda}\sin\left(\frac{\theta}{2}\right) = 1.777\times10^7 \text{ m}^{-1}$$
   The translational diffusion coefficient is then:
   $$D_{\mathrm{T}} = 1.381\times10^4/q^2 = 4.373\times10^{-11} \text{ m}^2\text{s}^{-1}$$

2. What is the molecular weight of the nucleosome particle? Assume that the specific partial volume of the nucleosome particle is 0.66 cm$^3$/g.

   **Answer:** To calculate the molecular weight of the nucleosome particles we can use the Svedberg equation. For this we need to know the sedimentation coefficient and the friction coefficient. For the former let us use the data from the sedimentation centrifugation where we can obtain the sedimentation coefficient by evaluating the slope of a plot of $\ln(r)$ versus $t$. To improve the quality of the data let us calculate the slope using three different sets of points (*e.g.*, consecutive points) and take the average:

   | $t_2 - t_1$ (m) | $\ln(r_2/r_1)$ | slope (min$^{-1}$) |
   |---|---|---|
   | 80 | 0.0294 | $3.675\times10^{-4}$ |
   | 80 | 0.0259 | $3.238\times10^{-4}$ |
   | 80 | 0.0274 | $3.425\times10^{-4}$ |

   The average of the slope is:
   $$s\omega^2 = 3.446\times10^{-4} \text{ min}^{-1}$$

Knowing that $\omega^2 = (18,100 \times 2\pi)^2) = 1.293 \times 10^{10}$ min$^{-2}$, we obtain:

$$s = \frac{3.446 \times 10^{-4}}{1.293 \times 10^{10}} = 2.66 \times 10^{-14} \text{ min} = 1.60 \times 10^{-12} \text{ s} = 16.0 \text{ S}$$

Then take the usual relationship for s:

$$s = \frac{M_1\,(1 - \overline{V}_1^{(S)}\rho)}{N_{\text{Av}} f} = \frac{M_1\,(1 - \overline{V}_1^{(S)}\rho) D_{\text{T}}}{N_{\text{Av}} k_B T}$$

so,

$$M_1 = \frac{N_A k_B T s}{D_{\text{T}}(1 - \overline{V}_1^{(S)}\rho)} = 262.2 \text{ kg/mol} = 2.622 \times 10^5 \text{ g/mol}.$$

3. Assuming the nucleosome particle to be spherical, calculate its Stokes (hydrodynamic) radius.

   **Answer:** We can calculate the Stokes radius of the nucleosome particles using:

$$D_{\text{T}} = \frac{k_B T}{6\pi\eta R_H} \quad \Rightarrow \quad R_H = \frac{k_B T}{6\pi\eta D_{\text{T}}} = 4.91 \times 10^{-7} \text{ cm} = 4.91 \text{ nm}.$$

4. Each base pair in DNA is separated from the adjacent base pairs by about $3.4 \times 10^{-10}$ m. Calculate the length of the DNA in the nucleosome and comment this result in view of the result obtained in question 2.3.

   **Answer:** The length (equivalent to the contour length), $L$ is calculated simply by:

$$L = 200\,[\text{or } 199] \times 3.4 \times 10^{-10} = 6.8 \times 10^{-8} \text{ m} = 68 \text{ nm}$$

   We can see that this value is larger than that of the hydrodynamic radius of the DNA/protein complex, indicating that the DNA is somewhat folded in the complex.

   **Note:** Some students have calculated the length using the statistical chain model for a freely-jointed chain. Unfortunately this model is only valid for Gaussian chains, which is not the case for the stiff short DNA molecules that the question refers to. In addition, the model provides the end-to-end distance which is, indeed, a measure of size but it is not strictly speaking the length of a molecule.

5. The rotational coefficient of the DNA molecules can be studied using transient electrically-induced birefringence (TEB). Describe briefly the main modules of the TEB instrumentation and the experimental procedure. What is the observable and how is the rotational friction coefficient calculated from the obtained data?

   **Answer:** Transient electrically-induced birefringence (TEB) is used to measure the rotational diffusion coefficient of macromolecules. The methodology is such that the macromolecules of interest are aligned using an electric field. The electric field is switched off and the relaxation of the molecules back to a random orientation is followed using a suitable property: birefringence, in this case. Birefringence is a property that arises when a sample has different optical properties (refractive index) in different directions. A macromolecule solution normally shows no birefringence but can be made optically anisotropic if the macromolecules are forced into an anisotropic arrangement such as an alignment. When asymmetrical biomolecules are aligned along a common axis, the refractive index of the solution will be different for light polarised along this axis and an axis normal to it.

   The main components of the TBE experimental procedure are depicted in figure 2. In short, a laser is used to illuminate the sample, placed in the Kerr sample holder. A polarizer placed between these two orients the light according to a specific plane. The

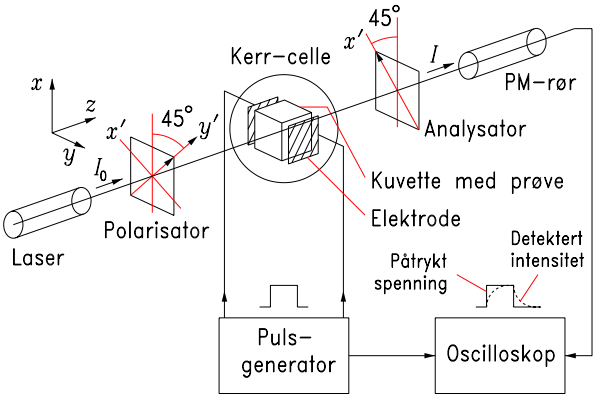


Figure 2: Drawing of the measuring set-up for measuring electrically induced birefringence.

analyzer, placed after the sample is oriented 90° relatively to the polarizer. Thus the intensity $I$ coming out of the analyzer will be zero when there is no birefringence in the Kerr cell. When the sample is birefringent, on the other hand, there will be a phase shift in the polarized light which is detected, amplified and analyzed.

Experimentally, the macromolecule solution is placed in the Kerr cell, and the electric field in turned on. When the intensity is stationary the electric field is turned off. This gives rise to a exponential decay of the detected intensity, according to

$$I(t) = \frac{I_0}{4}\delta_0^2 \exp(-12 D_R t)$$

where $I_0$ is the intensity detected prior to the switching off of the field. The rotational diffusion coefficient, $D_R$ can be determined from, for example, the slope of the plot $\ln I(t)$ versus $t$.

6. How are the proteins and DNA packed in the nucleosome? To answer this question, assume that the histone octamer forms a unhydrated spherical complex with specific volume 0.74 $\mathrm{cm}^3/\mathrm{g}$.

   i Calculate the radius of this hypothetical protein sphere.

   **Answer:** To calculate the radius of the protein sphere we use the given information on the specific volume. The molecular weight of the protein octamer is equal to the molecular weight of the nucleosome ($2.622 \times 10^5$ g/mol, from question 2.2) minus the molecular weight of the DNA ($200 \times 600 = 1.2 \times 10^5$ g/mol), that is $1.422 \times 10^5$ g/mol.

   The volume occupied by the protein octamer can be calculated according to

   $$v_1 = \frac{V_1^{(S)} M_1}{N_{\mathrm{Av}}} = \frac{0.74 \times 1.422 \times 10^5}{6.022 \times 10^{23}} = 1.747 \times 10^{-19}\ \mathrm{cm}^3$$

   and the radius according to:

   $$R_{\mathrm{prot}} = \left(\frac{3v_1}{4\pi}\right)^{1/3} = \left(\frac{3 \times 1.747 \times 10^{-19}}{4\pi}\right)^{1/3} = 3.47 \times 10^{-7}\ \mathrm{cm} = 3.47\ \mathrm{nm}\,.$$

   ii Contrast matching experiments performed with a small-angle neutron scattering equipment allow to determine that the DNA in the nucleosome was organized as a toroid (donut) with an inner radius of around 3.5 nm and an outer radius of

roughly 4.9 nm. Discuss the overall structure of the nucleosome. Discuss qualitatively what is meant with contrast matching and how this is done experimentally.

**Answer:** Taking into account the calculated values one can conclude that the nucleosome is composed of a protein core (with the radius of about 3.5 nm) and DNA wrapped around it.

Scattering techniques detect variations in the sample media. In case of small-angle neutron scattering (SANS), neutrons are scattered by the nuclei of atoms, and the scattering length of various nuclei and molecules are tabulated. While in the X-ray scattering lengths of atoms are simply proportional to the atomic number, neutron scattering lengths vary irregularly with the type of nucleus and different isotopes of the same atom (or nucleus) can have very different scattering lengths. In particular, the scattering length of the hydrogen's nucleus (a proton) is very different than that of deuterium. By mixing different proportions of water and deuterated water, it is possible to match the (average) scattering length of the protein octamer, effectively making it invisible and allowing to study the structure of the DNA solely. It is equally possible to contrast match the solvent to the DNA and obtain detailed structural information of the proteins.

**Exercise 3.** [total: 29 pts]

Consider a solution of spherical and negatively charged hydrogel particles.

1. Discuss the (three) different terms that contribute to the swelling behavior of the hydrogel particles. Name, for each of the three terms, a solution property and a property of the particle that are expected to influence the swelling behavior.

   **Answer:** The three terms that contribute to the swelling behavior of charged hydrogel particles are the mixing, the elastic and ionic contributions.

   The first originates from the fact that the systems want to increase its entropy, that is the polymer chains within the gel particle want to mix with the solvent. The characteristics of the polymer and the quality of the solvent ($\chi$ (Flory) parameter) will affect the mixing component, as well as the temperature of the medium.

   The elastic term describes the deformation of the network upon swelling. Polyelectrolyte (particle) characteristics that affect this contribution in particle swelling are, for example, flexibility of the polyeletrolytes and the number of cross-links in the network. Temperature would be a solution property.

   If the polymer in the network is charged, then the counterions will be drawn into the polyelectrolyte network which will increase the osmotic pressure inside the gel and, concomitantly, induce its swelling. The electrostatic term is thus dependent on the difference on ion concentration in and out of the gel. Properties that will influence the swelling behavior of the gel particles are the ionic strength of the solution and the charge density of the polyelectrolytes in the network, for example.

2. Explain the concepts of Stern layer and diffuse electric double-layer.

   **Answer:** The Stern layer (also called Helmholtz layer) refers to the fact that when a charged surface (say a charged nanoparticle) is placed in solution its counterions do not simply spread uniformly in solution (as one would expect from a pure mixing entropy

point of view) but instead, a reasonably large number of counterions will be found within a few Å of the surface. From this "layer" on, the concentration of counterions will decrease until it reaches the bulk ion concentration. This second layer, often called ion cloud, is named the diffuse electric double-layer.

3. What is the influence of ionic strength on the (i) swelling behavior of the gel particles and (ii) the stability of the particles in solution? Justify.

   **Answer:** (i) An increase in the ionic strength of a solution with negatively charged hydrogel particles will lead to the deswelling of the particles. As discussed above the electrostatic term in gel swelling is dependent on the difference of ions in and out of the network. Increasing the concentration of ions in the solution will decrease the mentioned difference, leading to a decrease in osmotic pressure and concomitant deswelling (shrinking) of the gel.

   (ii) Charged particles in solution are stabilized (do not associate and precipitate out of solution) due to the electrostatic repulsions between the particles. Increasing the ionic strength will screen the electrostatic repulsions between the charged particles, which will lead to a reduced stability of the particles in solution.

4. Let us imagine that the particles have collapse into a rigid and (overall) neutral spherical structure. Under these circumstances the excluded volume is defined by surface contact between solute molecules and the reduced osmotic pressure, $\Pi/c$, can be written according to:

$$\frac{\Pi}{c} = RT \left(\frac{1}{M_{\rm w}} + B\,c\right),$$

   where the second virial coefficient $B$ is defined in terms of the excluded volume $u$ as

$$B = \frac{1}{2}\frac{N_{\rm Av}u}{M_{\rm w}^2}.$$

   A plot of $\Pi/c$ versus $c$ for an aqueous solution of these particles at 25 °C shows a linear behavior, where the intercept and the slope of the line are 35.5 N m kg$^{-1}$ and 0.182 N m$^4$ kg$^{-2}$, respectively.

   i. Evaluate the molecular weight and the excluded volume of the particles.

      **Answer:** The form of $\Pi/c$ as a function of $c$ suggests that the plot of $\Pi/c$ versus $c$ should be a straight line, with the intercept and slope equal to:

$$\text{intercept} = \left(\frac{\Pi}{c}\right)_0 = \frac{RT}{M_{\rm w}}, \qquad \text{slope} = RTB.$$

      Calculation of the molecular weight:

      $M_{\rm w} = RT(\Pi/c)_0^{-1} = (8.314)(298)/35.6 = 69.6\,\text{kg mole}^{-1}$, where $R$ is the constant, equal to $K_{\rm B}N_{\rm Av}$.

      The mass per particle is obtained by dividing by $N_{\rm Av}$:

      $M = 69.6/(6.02\times10^{23}) = 1.16\times10^{-22}\,\text{kg molecule}^{-1}$.

      Calculation of $B$ by dividing the slope by $RT$:

      $B = 0.182/((8.314)(298)) = 7.35\times10^{-5}\,\text{m}^3\,\text{kg}^{-2}\,\text{mole}$.

      The excluded volume can be calculated with the expression above:

$$u = \frac{2BM_{\rm w}^2}{N_{\rm Av}} = \frac{2(7.35\times10^{-5})(69.6)^2}{6.02\times10^{23}} = 1.18\times10^{-24}\,\text{m}^3\,\text{molecule}^{-1}.$$

ii. How do you expect the osmotic pressure to change when the particles are charged?

**Answer:**

When the particles are charged, the average distance between the particles increases which increases the osmotic pressure of the solution.

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The following formulas and data may or may not be of use in answering the preceding questions. You do not need to derive any of the formulas but all parameters must be defined, if used.

Electron charge: $e = 1.602 \times 10^{-19}$ C

Avogadro constant: $N_{\mathrm{Av}} = 6.022 \times 10^{23}$ mol$^{-1}$

Boltzmann constant: $k_{\mathrm{B}} = 1.380 \times 10^{-23}$ m$^2$ kg s$^{-2}$ K$^{-1}$

Properties of water at 20 °C:
$\varepsilon = 78.4; \quad \eta = 0.01$ g cm$^{-1}$s$^{-1}$; $\quad \rho = 1.02$ g/cm$^3$

Temperature: $[\mathrm{K}] = [^\circ\mathrm{C}] + 273.15$

Atomic orbitals: H: $1s^1$ ; C: $1s^2 2s^2 2p_x^1 2p_y^1$ ; O: $1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$

Atomic weights: $\mathrm{A}_r(\mathrm{H}) = 1.0$ ; $\mathrm{A}_r(\mathrm{C}) = 12.0$

Thermodynamics $\quad G = H - TS \qquad A = U - TS \qquad \vec{F} = -\vec{\nabla} A$

$$S = k_{\mathrm{B}} \ln W$$

Statistical chain molecules $\left\langle R_{\mathrm{ee}}^2 \right\rangle = Q^2 n$

$$\left\langle R_{\mathrm{ee}}^2 \right\rangle = Q^2 n \left( \frac{1 - \cos\theta}{1 + \cos\theta} \right)$$

$$\left\langle R_{\mathrm{ee}}^2 \right\rangle = Q^2 n \left( \frac{1 - \cos\theta}{1 + \cos\theta} \right) \left( \frac{1 + \langle \cos\phi \rangle}{1 - \langle \cos\phi \rangle} \right)$$

Coulomb potential $\quad V(r) = \dfrac{z_1 z_2 \, e^2}{4\pi\epsilon_0 \epsilon r}$

Screened Coulomb potential

$$V(r) = \frac{z_1 z_2 \, e^2}{4\pi\epsilon_0 \epsilon r} \exp\left( -\frac{r}{\lambda_{\mathrm{D}}} \right)$$

Debye screening length $\quad \lambda_{\mathrm{D}}^2 = \dfrac{\epsilon k_{\mathrm{B}} T}{\sum_i (eZ_i)^2 \, n_{i\infty}}$

Friction coefficients $\vec{F} = -f\vec{v}, \qquad \vec{M} = -\xi\vec{\omega}$

Stokes formula $f = 6\pi\eta R_h, \qquad \xi = 8\pi\eta R_h^3$

For long chains and the random walk model $\left\langle R_{\mathrm{ee}}^2 \right\rangle = 6\left\langle R_G^2 \right\rangle$

Hydrodynamic volume $v_{\mathrm{h},1} = \left(\overline{V}_1^{(S)} + \delta\overline{V}_0^{(S)}\right)\frac{M_1}{N_{\mathrm{Av}}}$

Specific volume (per mass) $V_1^{(S)} = v_1\left(\frac{N_{\mathrm{Av}}}{M_1}\right)$

Fick's laws $\frac{\partial c}{\partial t} = -\vec{\nabla}\cdot\vec{J}, \qquad \vec{J} = -D_{\mathrm{T}}\vec{\nabla}c, \qquad \frac{\partial c}{\partial t} = D_{\mathrm{T}}\frac{\partial^2 c}{\partial x^2}$

Nernst-Einstein relations $fD_{\mathrm{T}} = k_{\mathrm{B}}T, \qquad \xi D_{\mathrm{R}} = k_{\mathrm{B}}T$

Lamm-equation $\frac{\partial c(r,t)}{\partial t} = D_{\mathrm{T}}\left(\frac{\partial^2 c(r,t)}{\partial r^2} + \frac{1}{r}\frac{\partial c(r,t)}{\partial r}\right) - s\omega^2\left(r\frac{\partial c(r,t)}{\partial r} + 2c(r,t)\right)$

Sedimentation centrifugation: $s = \frac{\ln\left(c_0/c_{\mathrm{p}}(t)\right)}{2\omega^2 t}; \quad s = \frac{\ln\left(r_2/r_1\right)}{\omega^2(t_2 - t_1)}$

Svedberg equation $s = \left(1 - \overline{V}_1^{(S)}\rho\right)\frac{M_1}{N_{\mathrm{Av}}f}$

Equilibrium centrifugation: $m_1(r) = m_1(r_{\mathrm{m}})\exp\left\{\frac{M_1(1 - \overline{V}_1^{(\mathrm{S})}\rho)\omega^2(r^2 - r_{\mathrm{m}}^2)}{2RT}\right\}$

Electrically-induce birefringence:

$$I(t) = \frac{I_0}{4}\delta_0^2\exp(-12D_R t)$$

Nuclear spin $\vec{m} = \gamma\vec{L}, \qquad (\vec{m})^2 = \gamma^2\hbar^2\ell(\ell+1), \qquad m_{\mathrm{z}} = m_\ell\,\gamma\,\hbar$

Gyromagnetic ratio

| Nucleus | $^{1}$H | $^{2}$H | $^{13}$C | $^{14}$N | $^{19}$F | $^{31}$P |
|---|---|---|---|---|---|---|
| $\gamma\left(10^7\frac{\mathrm{rad/s}}{\mathrm{T}}\right)$ | 26.753 | 4.107 | 6.728 | 1.934 | 25.179 | 10.840 |

Small-angle scattering:

$$q = \frac{4\pi}{\lambda}\sin\left(\frac{\theta}{2}\right)$$

Guinier approximation: $I_s(q) = I_0\exp\left(-\frac{1}{3}q^2R_G^2\right)$

Discrete identical

homogeneous particles: $\langle I_s(q)\rangle = Nb^2(0)P(q)S(q)$

Static light scattering:
RGD regime $\dfrac{\langle I_{\mathrm{S}}(q)\rangle}{I_0} = cM\kappa\dfrac{1}{R^2},$

Large systems $\dfrac{\kappa c}{R_\theta} = \dfrac{1}{M}\left[1+\dfrac{16\pi^2}{3\lambda^2}R_{\mathrm{G}}^2\sin^2\dfrac{\theta}{2}\right]\cdot[1+2B_2c],$

Dynamic light scattering:
Siegert relation: $g^{(2)}(q,\tau) = 1+[g^{(1)}(q,\tau)]^2$

$g^{(1)}(q,\tau) = \exp(-q^2D_T\tau)$

Constitutive equation of the Maxwell model:

$$\tau + \frac{\eta}{K}\dot{\tau} = \eta\dot{\gamma} \Rightarrow \tau + \lambda\dot{\tau} = \eta\dot{\gamma}$$