NORWEGIAN UNIVERSITY OF SCIENCE AND TECHNOLOGY DEPARTMENT OF PHYSICS

Contact during the exam:

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EXAM I COURSE TFY 4310 MOLECULAR BIOPHYSICS

Tuesday 15. desember 2009 Time: kl. 0900 – 1300.

During the exam, the student may use:

Simple calculator according to current NTNU rules and regulations,

K. Rottmann: Matematisk formelsamling (Norwegian or German version),

Aylward & Findlay: SI Chemical data,

Øgrim & Lian: Størrelser og enheter i fysikk og teknikk,

Note: In addition you will find selected formulas and data at the end of this text.

EXERCISE 1

a) The electrostatic potential set up by a point charge on a macromolecule in aqueous solution is influenced by added salt to the aqueous solution. Describe qualitatitively the effect of adding salt to an aqueous solution on the electrostatic potential of a point charge. Show that the electrostatic potential of point charges in aqueous solution can be described by the Poisson-Boltzmann equation:

$$\varepsilon \nabla^2 V(\vec{r}) = -\sum_{i=1}^N e Z_i n_{i\infty} \exp\left\{-\frac{e Z_i V(\vec{r})}{k_B T}\right\}$$
 (1)

Define all parameters included in deriving equation 1.

b) Assume that the potential energy in the electrostatic field is much less than k_BT , and show that eq. 1 can be approximated by:

$$\nabla^2 V(\vec{r}) = \frac{1}{\lambda_D^2} V(\vec{r}) \tag{2}$$

Derive the expression for λ_D . What is the parameter λ_D , what is the property that this parameter describes, and how can you select various values for this parameter experimentally?

EXERCISE 2

- a) Make (a) schematic illustration(s) and describe the molecular organisaton of the cell membrane of red blood cells, and spectrin in particular. Briefly describe the molecular properties of isolated spectrin in aqueous solution that can be determined employing an absorption spectrophotometer, and an Ostwald capillary viscometer, respectively.
- b) The Lamm-equation:

$$\frac{\partial c(r,t)}{\partial t} = D_T \left(\frac{\partial^2 c(r,t)}{\partial^2 r} + \frac{1}{r} \frac{\partial c(r,t)}{\partial r} \right) - s\omega^2 \left(r \frac{\partial c(r,t)}{\partial r} + 2c(r,t) \right)$$
(3)

is used as a basis for analysing molecular parameters obtained by sedimentation (centrifugation) of biopolymers. Define the parameters in equation 3. Make a schematic illustration that shows snapshots of the concentration profile of a biopolymer that is analysed by sedimentation (assume homogeneous biopolymer concentration as the initial condition). Derive mathematical expressions to be used to analyse the time-dependence of information in the concentration profile for the plateau zone, and moving boundary zone, respectively.

c) Describe briefly the two phenomena primary and secondary charge effect that may occur when characterizating biopolymers employing sedimentation.

EXERCISE 3

- a) The mathematic description of scattering by photons-, neutrons and electrons has a lot of common features why? Describe briefly the mechanism for scattering of light, X-rays and neutrons, respectively, when biopolymer properties are determined employing these sources.
- b) Make a schematic drawing and describe briefly the various parts of an instrument for determination of static and dynamic light scattering properties of biopolymers in solution. The equation:

$$\frac{\kappa c}{R_{\theta}} = \frac{1}{M} \left[1 + \frac{16\pi^2}{3\lambda_1^2} R_G^2 \sin^2 \frac{\theta}{2} \right] \cdot \left[1 + 2B_2 c \right] \tag{4}$$

is used for the analyses of experimental data determined by static light scattering. Define the various parameters in equation 4. Describe which molecular parameter(s) that can be experimentally determined by static light scattering and outline how experimental data is analyzed employing equation 4 for determination of this/these molecular parameter(s).

c) Describe why dust particles in the solution represent a special challenge when determining molecular parameter(s) of biopolymers in solution employing static light scattering.

Formulas and data.

The following formulas and data may or may not be of use in answering the preceding questions. The symbols are those employed in the lecture notes. You do not need to derive these formulas, but all parameters need to be defined, if used.

Maxwell's equations: $\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$ $\vec{\nabla} \times \vec{H} = \vec{j} + \frac{\partial \vec{D}}{\partial t}$

 $\vec{\nabla} \cdot \vec{B} = 0 \qquad \qquad \vec{\nabla} \cdot \vec{D} = \rho$

Poisson's equation: $\nabla^2 V(\vec{r}) = -\rho(\vec{r})/\varepsilon$

Electromagnetism: $\vec{D} = \varepsilon_0 \vec{E} + \vec{P} = \varepsilon_r \varepsilon_0 \vec{E} + \vec{P} = \varepsilon \vec{E}$,

 $\vec{B} = \mu_0 \vec{H} + \mu_0 \vec{M} = \mu_r \mu_0 \vec{H} = \mu \vec{H}$

 $c^2 = 1/(\mu \varepsilon)$ $n = c_0/c$ $n^2 = \varepsilon_r \mu_r$ $\vec{p}_{ind} = \alpha \vec{E}$

Electron charge: 1.602 10⁻¹⁹ As

Water at 20 °C $\eta = 1.0 \ 10^{\text{-3}} \ \text{Ns/m}^2 \qquad \qquad \epsilon_r \!\!=\!\! 80$

Thermodynamics: G = H - TS A = U - TS $\vec{F} = -\vec{\nabla}A$ $S = k_B \ln W$

Statististical chain molecule: $P_{eq}(\vec{r}_{e-e}) = \left(\frac{3}{2\pi(N-1)Q^2}\right)^{3/2} \exp\left\{-\frac{3r_{e-e}^2}{2(N-1)Q^2}\right\}$

 $\langle r_{e-e}^2 \rangle = (N-1)Q^2$

Friction coefficients:

 $\vec{F} = f_T \cdot \vec{v} \qquad \qquad \vec{M} = f_R \cdot \vec{\omega}$

 $F_{T'} = f_T / f_{0,T}$ $F_{R'} = f_R / f_{0,R}$

Stokes formula $f_{0,T} = 6\pi\eta R$ $f_{0,R} = 8\pi\eta R^3$

Volume of rotational ellipsoide: $V = \frac{4}{3}\pi ab^2$

Fluiddynamic volum $v_{h,i} = m_i \left(\overline{V}_i^{(S)} + \delta \cdot V_0^{(S)} \right)$

Fick's laws: $\frac{\partial c}{\partial t} = -\vec{\nabla} \cdot \vec{J} \qquad \qquad \vec{J} = -D_T \vec{\nabla} c \qquad \qquad \frac{\partial c}{\partial t} = D_T \frac{\partial^2 c}{\partial x^2}$

Nernst-Einstein relations: $f_T D_T = k_B T$ $f_R D_R = k_B T$

Nuclear spin $\vec{m} = \gamma \vec{L}$ $(\vec{m})^2 = \gamma^2 \hbar^2 l(l+1)$ $m_z = m_l \gamma \hbar$

Scattering from molecules:

$$I(\vec{\Delta}k,t) \propto \left[P^*\left(\frac{\vec{\Delta}k}{2\pi},t\right)\right]^2 \cdot \left[\Xi^*\left(\frac{\vec{\Delta}k}{2\pi},t\right)\right]^2$$

Structure factor

Form factor

Fourier transform of continuous helix:

$$H(\vec{R}) = \frac{1}{P} \cdot \sum_{n=-\infty}^{\infty} J_n(\chi) \exp\{in(\psi + \pi/2)\} \delta(w - n/P)$$

where
$$\chi = 2\pi r_0 R$$

Light scattering

$$\frac{\kappa c}{R_{\theta}} = \frac{1}{M} \left[1 + \frac{q^2}{3} R_G^2 \right] \cdot \left[1 + 2B_2 c \right]$$

$$q^2 = \frac{16\pi^2}{\lambda_1^2} \sin^2\left(\theta/2\right)$$

$$R_{\theta} = \frac{I(\theta) r^2}{I_0}$$

$$\kappa = \frac{4\pi^2 n_L^2 \left(d\tilde{n}/dc\right)^2}{N_A \lambda_0^4}$$