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EXAM I COURSE
TFY4310 MOLECULAR BIOPHYSICS

Wednesday, 10 December 2014
Time: kl. 09.00 - 13.00

Exercise 1.

Justify **nine** (9) of the following sentences:

1. The angle between hydrogen atoms in a water molecule is 104.5 °.
2. Ice is less dense than liquid water.
3. Hydrophobic interactions are entropic in nature.
4. The model describing the chain with hindered rotations is more realistic than the freely-jointed chain model.
5. When a rubber is stretched by a dead load and is heated its extension decreases.
6. According to the Flory-Huggins theory, the entropy of mixing decreases with the length of the polymer chain.
7. In sedimentation velocity, a high rotor speed maximises resolution.
8. Rotational friction coefficient is more sensitive to the shape of a molecule than the translational friction coefficient.
9. The ^{1}H-NMR spectrum of CH_3–CH_2–Br possesses a quadruplet (intensities of 1:3:3:1) and a triplet (intensities of 1:2:1) at the chemical shifts of 3.5 and 1.7 ppm (in relation to TMS), respectively.
10. The extinction coefficient (ε) of a molecule depends on the wavelength.
11. The CO_2 molecule has four modes of vibration but only three will contribute to bands in the infra-red spectrum.
12. Static light scattering allows to determine the molecular weight of a macromolecule even using concentrated samples.

Exercise 2.

1. A protein has been studied using small-angle X-ray scattering, where X-rays of $\lambda = 0.154$ nm were used, and the following data recorded:

θ (mrad)	$\ln I_s$
1.41	70.76
2.50	70.71
3.40	70.66
4.00	70.61

   Calculate the radius of inertia (gyration). If the particles are spherical, what is their diameter?

2. A few other studies were performed with the same protein sample. Sedimentation velocity measurements yield a sedimentation coefficient of 18.1 S (10^{-13} s). Data obtained from dynamic light scattering, and plotted on a graph of the $\ln(g^{(1)}(q,\tau))$ versus τ, was found to be linear with a slope: -8.368×10^3. The scattering angle was 90° and the wavelength of the light through the medium was 500 nm. The temperature was 20 °C. Assume that the solution has a viscosity of 1.0×10^{-3} Ns/m^2 and a density of 1.0 g/cm^3 and that the protein has a specific partial volume of 0.73 cm^3/g.

   Calculate the molecular weight and the hydrodynamic radius of the protein.

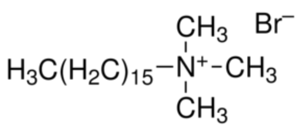
3. Assuming that the protein is a sphere, calculate the required hydration.

4. Calculate f/f_0. Assuming that the protein is a prolate ellipsoid with no hydration, estimate the axial ratio of the protein.

5. A 2D COSY ^{1}H NMR spectrum was made to the protein in question. A particular amino acid of the protein showed the following peaks in the 1D ^{1}H NMR spectrum: NH = 8.4 for both protons, αH = 4.3, βH = 2.1 and 1.9, γH = 2.3 for both. At which 2D coordinates do you expect COSY interaction? (*Hint:* the structure of the amino-acid is the following: $H_2NC_\alpha H(COO^-)C_\beta H_2C_\gamma H_2$).

Exercise 3.

Cetyltrimethylammonium bromide (CTAB) surfactant (see structure below) forms spherical micelles in solution, at relatively low surfactant concentrations.



1. Make a schematic drawing of a spherical micelle.

2. Name the main intermolecular forces involved in the stabilisation and destabilisation of a surfactant micelle in solution.

3. The addition of salt leads to the transition from a sphere to a long cylinder-like (rod-like) micelles. Why?

4. Which of the following computer simulation techniques would you use to follow this sphere-to-rod transition? Justify.

   - Molecular dynamics
   - Brownian dynamics
   - Monte Carlo simulations

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: $k_{\mathrm{B}} = 1.38 \times 10^{-23}$ m^2 kg s^{-2} K^{-1}

Standard gravity: $g = 9.80665$ m/s^2

Values for dielectric constants at 25°C: $\epsilon(\text{water}) = 78.4$; $\epsilon(\text{ethanol}) = 19.9$; $\epsilon(\text{chloroform}) = 4.81$

Temperature: [K] = [°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 $G = H - TS \qquad A = U - TS \qquad \vec{F} = -\vec{\nabla} A$

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

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 $V(r) = \frac{z_1 z_2\, e^2}{4\pi\epsilon_0 \epsilon r}$

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

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 $\left\langle R_{\mathrm{ee}}^2 \right\rangle = 6 \left\langle R_G^2 \right\rangle$

Fluid dynamic volume $v_{\mathrm{h},i} = \left(\overline{V}_i^{(S)} + \delta\overline{V}_0^{(S)}\right) \frac{M_1}{N_{\mathrm{Av}}}$

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 $f D_{\mathrm{T}} = k_{\mathrm{B}} T, \qquad \xi D_{\mathrm{R}} = k_{\mathrm{B}} T$

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: $s = \frac{\ln\{c_0/c_{\mathrm{p}}(t)\}}{2\omega^2 t}$

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

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

Perrin shape parameters for ellipsoids of revolution

Axial ratio	prolate	oblate
1	1.000	1.000
2	1.044	1.042
4	1.182	1.165
6	1.314	1.277
8	1.433	1.374
10	1.543	1.458

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:

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

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

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

Large systems $\frac{\kappa c}{R_\theta} = \frac{1}{M}\left[1 + \frac{16\pi^2}{3\lambda^2}R_\mathrm{G}^2 \sin^2\frac{\theta}{2}\right]\cdot[1 + 2B_2 c],$

with :

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

$$R_{G,\mathrm{sphere}} = \sqrt{3/5}R_s$$

Dynamic light scattering:

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

$$g^{(1)}(q,\tau) = \exp(-q^2 D_0 \tau)$$