Name: Date:

Partial Exam

Biophysics
Bioinformatics degree

1) (2.0 points) Two synaptic vesicles have a volume of 20.000 nm^3 and 30.000 nm^3, respectively. In the small vesicle, there are $2\cdot10^6$ molecules of a neurotransmitter. In the big vesicle, there are only 10^6 molecules of the same neurotransmitter.
a) Considering a division of the volume of the synaptic vesicles in cubic cells of 1 nm^3, calculate the entropy associated with the movement of this neurotransmitter in both vesicles.
b) Then, consider a fusion of both vesicles forming a vesicle of 50.000 nm^3 of volume. Calculate the entropy associated with the movement of all $3\cdot10^6$ molecules of the neurotransmitter in this new generated vesicle. Compare with the sum of the previous entropies and discuss if this process is reversible or irreversible, and if this process is related with some thermodynamic law.

a) $W = Num.Cells^{Num.Molec}$

$\ln(W) = Num.Molec \ln(Num.Cells)$

$S = k_b \ln(W)$

$S_{Ves1} = 2.73\,10^{-16}\,J/K$ $\quad S_{Ves2} = 1.42\,10^{-16}\,J/K$

b) $S_{VesBig} = 4.48\,10^{-16}\,J/K$

$S_{Ves1} + S_{Ves1} = 4.15\,10^{-16}\,J/K$

Irreversible process. 2nd law.

2) (1.5 points) A container of 0.5 litres has $4\cdot10^{20}$ molecules of CO_2 at 25ºC. Another container of 40 cm^3 has $6\cdot10^{20}$ molecules of N_2 at 40ºC. If we put in contact both containers, determine the final temperature. Assume ideal gases having only kinetic energy and consider that in the mixing the average kinetic energy is distributed equally among all particles.

$v^{rms} = \sqrt{(3RT/M)} = \sqrt{(3k_B T/m)}$

$E_c = \frac{1}{2} m v^2 = \frac{3}{2} k_b T$

The energy per molecule is:

$E_c(CO_2) = 6.17\,10^{-21}\,J$ $\quad E_c(N_2) = 6.48\,10^{-21}\,J$

$Etotal = NumCO_2 * E_c(CO_2) + NumN_2 * Ec(N_2) = 6.36\,J$

$E_{final\,per\,molec.} = E_{total} / (NumCO_2 + NumN_2)$

$T_{final} = \frac{E_{final} * 2}{3 k_B} = 307\,K = 34\,C$

3) (1.5 points) It is observed that one drug could bind to its protein target in two different places (site A and site B). The energy associated to the binding of the drug when it is attached to site A is of -15.5 kJ/mol, and when it is attached to the site B is of -13.7 kJ/mol. Determine at which temperature the population of the drug binding the site A is double than the population of the drug binding the site B.

$p_i = \exp(-E_i/RT)/q$

$p_A/p_B = \exp(-E_A/RT)/\exp(-E_B/RT) = 2$

$T = 312.3\,K = 39\,C$

4) (1.5 points) In a study of the alcohol-dehydrogenase-catalyzed oxidation of ethanol, the molar concentration of ethanol decreased in a first-order reaction from 220 mmol L^{-1} to 56.0 mmol L^{-1} in $1.22 \cdot 10^4$ s at 25ºC and decreased in $6.2 \cdot 10^3$ s at 50ºC. a) Which is the rate constant of the reaction at 25ºC? Which is the rate constant of the reaction at 35ºC?

$\ln(A_t) = \ln(A_0) - k\,t$

$k_{25C} = 1.12\,10^{-4}\,s^{-1} \quad k_{50C} = 2.21\,10^{-4}\,s^{-1}$

$k = A\exp(-E_a/RT)$ Making a system with the two constants: Ea: 21667 J/mol

Again, knowing Ea and k25 we can obtain the constant at any temperature:
$k_{35C} = 1.49\,10^{-4}\,s^{-1}$

5) (1.5 points) In the first order reaction A → products, the concentration of A is [A] = 0.816 M at the initial time of the reaction, and [A]=0.632 M after 16 minutes. a) Determine the value of the rate constant b) Deduce the analytical expression of the half life for this reaction, and calculate its value. c) At which time the concentration of [A] will be 0.235 M? Which will be the concentration of [A] at 2.5 h?

$\ln(A_t) = \ln(A_0) - k\,t$
$k = 0.016\,min^{-1}$

$t_{1/2} = \ln(2)/R = 2603\,s$

$t = 4668\,s$

$[A] = 0.074\,M$

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6) (2.0 points) In the reaction 2 A + B → C at 500K, the following data were obtained

Experiment	$[A]_0$ /(mol L^{-1})	$[B]_0$/(mol L^{-1})	V_0/(10^{-3} mol L^{-1} s^{-1})
1	0.26	0.26	5.4
2	0.52	0.26	10.8
3	0.52	0.52	21.6

a) Determine the partial order of A and B, and the rate constant at 500K.
b) In other experiment, if the concentration of $[A]_0$ =0.4M and $[B]_0$ =0.004M. Determine the rate constant of pseudo-first order. Calculate the concentration of B after 1 minute.

a) $v=k[A]^{\alpha}[B]^{\beta}$

$\alpha=\ln(v_2/v_1)/\ln(A_2/A_1)=1$

$\beta=\ln(v_3/v_2)/\ln(A_3/A_2)=1$

$k=0.080\,L/(mol\,s)$

b) $k_{app}=k[A]=0.032\,s^{-1}$

$\ln(B_t)=\ln(B_0)-k_{app}t$

$B_{1\,min}=5.8\,10^{-4}\,M$

Additional data and equations:

M(H)=1 g mol^{-1}; M(C)=12 g mol^{-1}; M(O)=16 g mol^{-1}; M(N)=14 g mol^{-1}

k_B=1.3806488·10^{-23} J K^{-1}

R=8.314 J K^{-1} mol^{-1}

R=0.082 atm L K^{-1} mol^{-1}

N_A=6.022·10^{23} mol^{-1}

$$v^{mp}=\sqrt{(2RT/M)}$$

$$\bar{v}=\sqrt{(8RT/(\pi M))}$$

$$v^{rms}=\sqrt{(3RT/M)}$$

$$f(v)=4\pi\left(\frac{m}{2\pi k_B T}\right)^{3/2} v^2 e^{-mv^2/(2k_B T)}$$

$$\frac{1}{[A]_0-[B]_0}\ln\frac{[B]_0[A]}{[A]_0[B]}=kt$$