Name: Date:

Partial Exam

Biophysics
Bioinformatics degree

1) (2 points) a) Estimate the root mean square velocity of the molecules of carbon dioxide in 5 m^3 at 40ºC and 3 atm.
b) If there are 10^6 molecules travelling at the most provable velocity, calculate the number of molecules having a three times the previous velocity.

a) $v^{rms} = \sqrt{(3RT/M)} = 421\, m/s$

b)

$$v^{mp} = \sqrt{(2RT/M)} = 344\, m/s$$

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

$$f(3 * v_{mp}) / f(v_{np}) = 7.29 \cdot 10^{-6} / 2.41 \cdot 10^{-3}$$

$$f(3 * v_{mp}) / f(v_{np}) * 10^6 \text{molec} = 3020 \text{molec. travelling at } 3\, v^{mp}$$

2) (1 point) For the two instantaneous configurations: A: {400, 50, 20, 10} and B: {300, 100, 50, 30}. Calculate which configuration has the greatest weight. Calculate the associate entropy of these configurations.

$$\ln W = N \ln N - \sum n_i \ln n_i$$

$$\ln W_A = 288.3 \qquad \ln W_B = 494.1 \qquad W_B > W_A$$

$$S = k_b \ln(W)$$

$$S_A = 3.98 \cdot 10^{-21} J/K \text{ or } 2397\, J/(K\, mol) \qquad S_B = 6.82 \cdot 10^{-21} J/K \text{ or } 4108\, J/(K\, mol)$$

3) (2 points) A system has energy levels at ε_0=0, ε_1=1.5, ε_2=2.2 kJ/mol. The degeneracies of the levels are 1, 3 and 5 respectively.
a) Calculate the partition function and the relative population of the energy levels at a temperature of 300K.
b) At what temperature is the population of the energy level at 1.5 kJ/mol equal to the population of the energy level at 2.2 kJ/mol.
a)

$$q=\sum_{levels\, i=1}^{3} g_i e^{-\beta e_i}=4.7 \qquad \beta=\frac{1}{k_b T} \text{ or } \frac{1}{RT}$$

$$p_{0\text{ level}}=\frac{g_0 e^{-\beta e_0}}{q}=0.21 \qquad p_{1\text{ level}}=\frac{g_1 e^{-\beta e_1}}{q}=0.35 \qquad p_{2\text{ level}}=\frac{g_2 e^{-\beta e_2}}{q}=0.43$$

b)

$$p_{1\text{ level}}=p_{2\text{ level}}$$

$$\frac{g_1 e^{-\beta e_1}}{q}=\frac{g_2 e^{-\beta e_2}}{q} \qquad T=165\,K$$

4) (1.5 point) The rate constant of a reaction is double when the temperature increases from 50ºC to 80ºC. Which is the activation energy of the reaction? If the reaction follows a first-order rate law, explain what happens with its half-live when the temperature is increased from 50ºC to 80ºC.

$$k_{50}=A\,e^{\frac{-Ea}{RT_{50}}} \qquad k_{80}=A\,e^{\frac{-Ea}{RT_{80}}} \qquad 2=e^{\frac{-Ea}{RT_{80}}}/e^{\frac{-Ea}{RT_{50}}} \qquad E_a=21922\,\text{J/mol}$$

5) (1 points) The decomposition of H_2O_2(aq) at 25ºC follows a first order kinetics. Determine the percentage of H_2O_2 decomposed in the first 10 minutes after the reaction was initiated. The kinetic constant of this reaction at 25ºC is $k= 7.3\cdot10^{-4}$ s^{-1}

$$\ln A=\ln A_0-k\,t$$

Remaining percentage of A =100*A/A_0=100 exp(-k t)= 64.5 %

Percentage of A decomposed =100-Remaining percentatge of A=35.5 %

6) (1 point) A reaction R → P has a kinetic constant of k =1.24 $cm^3\ mol^{-1}\ s^{-1}$. Calculate how many hours are required for the concentration of R to change from 0.450 mol L^{-1} to 0.033 mol L^{-1}.

The units of the kinetic constant indicates that is a second order reaction.

$$\frac{1}{A}=\frac{1}{A_0}+kt \qquad t=6.3h$$

7) (1.5 point) For the 2 NO + O_2 → 2 NO_2 reaction in gas phase the initial velocity of formation of O_2 was measured at 25°C

[O_2] (mmol L^{-1})	**[NO] (mmol L^{-1})**	**d[O_2]/dt (mol L^{-1} s^{-1})**
1.44	0.28	-6.9 x 10^{-7}
1.44	0.93	-7.5 x 10^{-6}
1.44	2.69	-6.0 x 10^{-5}
0.066	2.69	-3.0 x 10^{-6}

Find the orders of the reaction with respect to NO and O_2. Find the rate constant at 25°C

$$v=k[\mathrm{NO}]^{\alpha}[\mathrm{O_2}]^{\beta}$$

$$\alpha=\frac{\ln\frac{v_1}{v_2}}{\ln\frac{[\mathrm{NO}]_1}{[\mathrm{NO}]_2}}\approx 2 \qquad \beta=\frac{\ln\frac{v_3}{v_4}}{\ln\frac{[\mathrm{O_2}]_3}{[\mathrm{O_2}]_4}}\approx 1$$

$$v=k[\mathrm{NO}]^2[\mathrm{O_2}]$$

$$k=6112\,\mathrm{L^2\,mol^{-2}\,s^{-1}}$$

Additional data:

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}

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

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

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

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

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