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Partial Exam

Biophysics
Bioinformatics degree

1) (1.5 points) A small CO_2 fire extinguisher with a total volume of 3 litres contains 2 kg of CO_2 molecules at 23ºC.
a) Determine the most probable velocity of the CO_2 molecules and their average kinetic energy (per molecule).
b) Determine the relation of probabilities associated to find a CO_2 molecule travelling at 500 m/s with respect to find a CO_2 molecule travelling at the most probable velocity.
c) Draw a qualitative plot of the distribution of the velocities of CO_2 molecules at 23ºC and at 90ºC, indicating in the plot the approximated position of the most probable velocity and the root mean square velocity at both temperatures.

a) $v^{mp} = \sqrt{(2RT/M)} = \sqrt{(2k_B T/m)} = 334 \, \text{m/s}$

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

$E_c = \frac{1}{2} m (v^{rms})^2 = \frac{3}{2} k_b T = 6.13\text{E-}21 \, \text{J}$

b)

$f(v = 500 \, \text{m/s}) = 4\pi \left(\frac{m}{2\pi k_B T}\right)^{3/2} v^2 e^{-mv^2/(2k_B T)} = 0.0016 \, \text{s/m}$
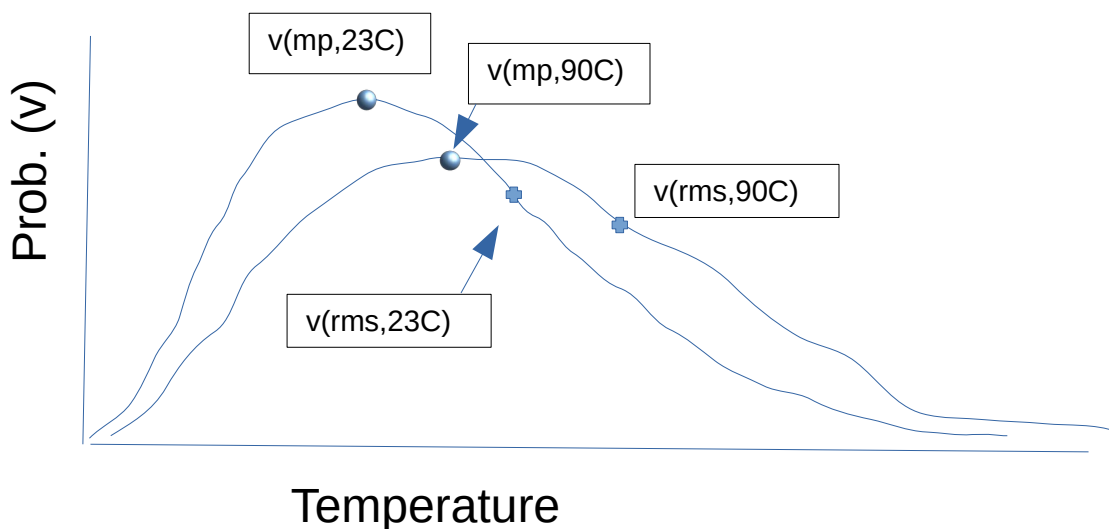
$f(v^{mp} = 334 \, \text{m/s}) = 4\pi \left(\frac{m}{2\pi k_B T}\right)^{3/2} v^2 e^{-mv^2/(2k_B T)} = 0.0025 \, \text{s/m}$

$f(v = 500 \, \text{m/s})/f(v^{mp} = 334 \, \text{m/s}) = 0.65$

c) -For each temperature: v(rms) > v(mp)
- v(mp,90C) > v(mp,23c)
- v(rms,90C) > v(rms,23C)

2) (2.0 points) In a can of tonic water (brand A) of 33 cl, there are 22 mg of caffeine molecule. In a bottle of tonic water of 1 litre of brand B, there are 26 mg of caffeine.
a) Calculate the entropy associated with the translational movement of the caffeine molecules in any of the both drinks assuming in both cases a volume cell division of 1 ml.
b) Consider the mixing of both drinks. Calculate the entropy associated with the movement of all caffeine molecules. Consider a complete additivity of the volumes. Compare the sum of the entropies with the entropy of the caffeine in the mixture and discuss if this process is reversible or irreversible.

Data: Caffeine ($C_8H_{10}N_4O_2$) M:194.19 g·mol^{-1} Density: 1.23 g/cm^3 Melting Point: 237ºC

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

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

$Num.Molec(Brand\,A) = 6.82E19\,molecules \quad Num.Molec(Brand\,B) = 8.06E19\,molecules$

$Num.Cells(Brand\,A) = 330 \quad Num.Cells(Brand\,B) = 1000$

$S = k_b \ln(W)$

$S_{Brand\,A} = 0.00546\,J/K \quad S_{Brand\,B} = 0.00769\,J/K$

b) $S_{BOTH\,DRINKS} = 0.01478\,J/K$

$S_{Brand\,A} + S_{Brand\,B} = 0.013152\,J/K$

It's a irreversible process. 2nd law.

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3) (1.5 points)   The conformational variability of a macromolecule could be studied at certain conditions with a three-level system. It has been determined that the energy of the most stable levels (e_0 and e_1) are 0 kJ/mol and 1.2 kJ/mol, respectively. An experiment determined the population of the most stable level to be p_0=0.54 (that is 54%) at 75ºC. Calculate the energy and population of the last level (level 2). Comment what happens with the population of the last level if the temperature is increased.

$$p_i = g_i \exp\left(-E_i/(RT)\right)/q \quad \text{with all } g_i=1$$

$$q = \sum_j g_j \exp\left(-E_j/(RT)\right)/q$$

$$q = 1/p_0 = 1/0.54 = 1.85$$

$$p_1 = \exp\left(-1200\,\text{J/mol}/(RT)\right)/q = 0.357$$

$$p_2 = 1 - p_0 - p_1 = 0.103$$

Isolate E_2 from $p_2 = \left(-E_2/(RT)\right)/q$ E_2 = 4788 J/mol

If the temperature is increased the population of the last level will increase. In the limit, the population of the tree levels will be 1/3.

4) (1.5 points) For the second order reaction R $\rightarrow$ products, the initial concentration of the reactant was [R]$_0$ = 0.55 M. After 11 minutes, the concentration of this reactant was determined to be [R]=0.24M.
a) Determine the value of the rate constant.
b) Using the integrated expression of the velocity, deduce the analytical expression of the half life for this reaction, and calculate its value.
c) At which time the concentration of [R] will be 0.12 M?
d) Which will be the concentration of [R] at 7.5 h?

a) $1/A_t = 1/A_0 + kt$

$k = 0.213 \, M^{-1} min^{-1} = 0.00355 \, M^{-1} s^{-1}$

b) $1/A_t = 1/A_0 + kt \quad 2/A_0 = 1/A_0 + kt_{half} \quad t_{half} = \dfrac{1}{A_0 k}$

$t_{half} = \dfrac{1}{A_0 k} = 8.516 \, min$

c) $t = (1/A_t - 1/A_0)/k = 30.5 \, min$

d) $A_{7.5h} = 1/(1/A_0 + kt_{450 \, min}) = 0.010 \, M$

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5) (1.5 points) For a second order reaction in which the initial concentration of the reactant is 0.033 M, the rate constant increases three times when the temperature increases from 30ºC to 90ºC. Which is the activation energy of the reaction? If the half live of the reaction at 30ºC is 30 minutes, at which temperature the half live will be 10 minutes?

$$k = A \exp\left(-E_a/RT\right)$$

$$k_{30C} = A \exp\left(-E_a/RT_{30C}\right) \quad k_{90C} = A \exp\left(-E_a/RT_{90C}\right)$$

$$k_{90C}/k_{30C} = 3$$

$$3 = \exp\left(-E_a/RT_{90C} + E_a/RT_{30C}\right) \quad \text{Ea= 16759 J/mol}$$

$$t_{half} = \frac{1}{A_0 k}$$

$$k_{30C} = \frac{1}{A_0 t_{half}} = 1.01 \, M^{-1} min^{-1}$$

$$k_T = \frac{1}{A_0 t_{half \, 10 \, min}} = 3.03 \, M^{-1} min^{-1}$$

$$A = k_{30C}/\exp\left(-E_a/RT_{30C}\right) = 780 \, M^{-1} min^{-1}$$

Isolate T from $k_T = A \exp\left(-E_a/RT\right)$ T= 363 K = 90 C

6) (2.0 points) In the reaction A + B → P + Q   at 37ºC, the following data were obtained

Experiment	$[A]_0/(mol\ L^{-1})$	$[B]_0/(mol\ L^{-1})$	$v_0/(mol\ L^{-1}s^{-1})$
1	0.12	0.14	$1.20 \cdot 10^{-4}$
2	0.09	0.14	$9.00 \cdot 10^{-5}$
3	0.16	0.14	$1.60 \cdot 10^{-4}$
4	0.09	0.42	$8.10 \cdot 10^{-4}$

a) Determine the partial order of A and B, and the rate constant at 37ºC.
b) In other experiment, it was prepared the following concentrations for [A]₀ =0.01M and   [B]₀ =0.70M. Determine the rate constant of pseudo-first order. Calculate the concentration of A after 1 minute.

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

$$\alpha=\frac{\ln\dfrac{v_1}{v_2}}{\ln\dfrac{[A]_1}{[A]_2}}\approx 1 \quad \beta=\frac{\ln\dfrac{v_2}{v_4}}{\ln\dfrac{[B]_2}{[B]_4}}\approx 2$$

$$v=k[A][B]^2$$

$$k_{37C}=0.051\,L^2\,mol^{-2}s^{-1}$$

b) $k_{app}=k[B]^2=2.5E\text{-}2\ s^{-1}$

$$\ln(A_t)=\ln(A_0)-k_{app}t$$

A_t=2.23E-3 M

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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}

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

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

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

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

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