Name: Date:

# Partial Exam

**Biophysics**
*Bioinformatics degree*

**1)** (1 point) We have a methane ($CH_4$) gas in a container. A sensor determines that the average kinetic energy of methane molecules is 6.4 x $10^{-21}$ J. Determine the temperature and the most probable velocity of the gas molecules in this container.

**2)** (1.5 points) We have a system of 3 levels at 20ºC with the corresponding energies ($e_0$=1 kJ/mol, $e_1$=2 kJ/mol and $e_2$=3 kJ/mol).
a) Calculate the energy of the following configurations: {9, 6, 1}, {10, 4, 2}, {11, 2, 3} and {12, 0, 4}.
b) Calculate the *weight* and the entropy of the previous configurations. Discuss which configuration is the most probable.

**3)** (1.5 points) Consider a three-level system with energy levels: 0, 2 kJ/mol and 3 kJ/mol. Calculate the population corresponding to these energy levels at T=60ºC. Comment what happens with the population of highest level (3 kJ/mol) if the temperature is increased. And what happens with this level (3 kJ/mol) if the most stable level (0 kJ/mol) were degenerated with multiplicity of 2.

**4)** (1 point) Starting from the differential form of the reaction rate of a second order reaction $-d[A]/dt=k[A]^2$ obtain the expression for the integrated form of the velocity and the expression for the half live.

**5)** (1 point) a) In the collision theory, it is supposed that an activated complex is in equilibrium with the reactants. Indicate if this sentence is true or false. If it is false indicate why.
b) The Boltzmann distribution gives the numbers of molecules in each state of a system at any temperature. Indicate if this sentence is true or false. If it is false indicate why.

**6)** (1 point) The half-live of pyruvic acid in the presence of an aminotransferase enzyme (which converts it to alanine) was found to be 221 s. How long will it take for the concentration of pyruvic acid to fall to 1/64 of its initial value in this first-order reaction?

**7)** (1.5 point) The following kinetic data ($v_0$ is the initial rate) were obtained for the reaction 2 ICl(g) + $H_2 \rightarrow I_2$ (g) + 2 HCl(g):

| **Experiment** | **$[ICl]_0$/ (mmol dm$^{-3}$)** | **$[H_2]_0$/ (mmol dm$^{-3}$)** | **$v_0$/ (mol dm$^{-3}$ s$^{-1}$)** |
|---|---|---|---|
| 1 | 1.5 | 1.5 | 3.7 x $10^{-7}$ |
| 2 | 3.0 | 1.5 | 7.4 x $10^{-7}$ |
| 3 | 3.0 | 4.5 | 22 x $10^{-7}$ |
| 4 | 4.7 | 2.7 | ? |

a) Write the rate law for the reaction.
b) Determine the value of the rate constant.
c) Use the data to predict the reaction rate for experiment 4.

**8)** (1.5 point) The Arrhenius parameters for the reaction of decomposition of cyclo-butane $C_4H_8(g) \rightarrow 2\ C_2H_4(g)$ are $\log(A/s^{-1})=15.6$ and $E_a$= 261 kJ mol$^{-1}$. What is the half-live of this first-order reaction at 20ºC and 500ºC?

**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$^{-1}$
$k_B=1.3806488\cdot10^{-23}$ J K$^{-1}$
R=8.314 J K$^{-1}$ mol$^{-1}$
R=0.082 atm L K$^{-1}$ mol$^{-1}$
$N_A=6.022\cdot10^{23}$ mol$^{-1}$

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

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

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

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

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