FACULTY OF SCIENCE

| DEPARTMENT OF CHEMISTRY |  |
| :---: | :---: |
| MODULE: | CEM2A20 / CEM 02A2 (Intermediate Physical Chemistry) |
| CAMPUS: | APK |
| EXAM | Supplimentary Exam - 2019 |
|  |  |

DATE: June 2019
ASSESSOR:
MODERATOR:
DURATION: 3 Hours

TIME:
Dr. S. Sitha
Prof. R. Meijboom
Total Marks: 100

NUMBER OF PAGES: 4 Pages (Including this page and a periodic table)
INSTRUCTIONS: Answer all the questions. Using of a non-graphing scientific calculator is allowed.

## Important Equations \& Physical Constants:

| Trigonometric identities: | $\operatorname{Sin}^{2} \theta=\frac{1-\cos 2 \theta}{2}$ | $\sin 2 \theta=2 \sin \theta \cdot \cos \theta$ <br> $2 \operatorname{Sin} \theta \cdot \operatorname{Sin} \phi=\operatorname{Cos}(\theta-\phi)-\operatorname{Cos}(\theta+\phi)$ |
| :--- | :--- | :--- |


| Planck's Constant | h | $6.626 \times 10^{-34} \mathrm{~J} \cdot \mathrm{~S}$, | $6.626 \times 10^{-34} \mathrm{~kg} \cdot \mathrm{~m}^{2} \cdot \mathrm{~S}^{-1}$ |
| :--- | :--- | :--- | :--- |
| Universal Gas Constant | R | $8.314 \mathrm{~J} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}$, | $1.986 \mathrm{cal} \cdot \mathrm{K}^{-1} \cdot \mathrm{~mol}^{-1}$, |
|  |  | $0.082 \mathrm{~L} \cdot \mathrm{~atm} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}$, |  |

## Question 1:

(10 marks)
Consider a system containing 63.998 grams of $\mathrm{O}_{2}$ (an ideal gas). This system then undergoes an isothermal reversible expansion process at $25^{\circ} \mathrm{C}$. During this process the volume changed from 15.0 litres to 50.0 L . Calculate the change in internal energy, work-done, heat exchanged and change in entropy during the process.

## Question 2:

(23 marks)
Consider a system containing 20.0 L of gaseous $\mathrm{N}_{2}$ (an ideal gas) is at 10 atm pressure and $25^{\circ} \mathrm{C}$ of temperature. The system undergoes an adiabatic reversible expansion process until the pressure got reduced to 1 atm . Calculate the workdone.

## Question 3:

(6 marks)
In a thermal fuel cell, a combustion reaction of propane is happening at standard temperature condition. Calculate change in the standard Gibbs' free energy for the reaction using the data shown below.
$\Delta_{\mathrm{i}} \mathrm{G}^{0}$ of $\mathrm{CO}_{2}(\mathrm{~g})=-394.36 \mathrm{~kJ} . \mathrm{mol}^{-1}$
$\Delta_{\mathrm{t}} \mathrm{G}^{0}$ of $\mathrm{H}_{2} \mathrm{O}(\mathrm{l})=-237.13 \mathrm{~kJ} . \mathrm{mol}^{-1}$
$\Delta_{\mathrm{f}} \mathrm{G}^{0}$ of $\mathrm{C}_{3} \mathrm{H}_{8}(\mathrm{~g})=-23.49 \mathrm{~kJ} . \mathrm{mol}^{-1}$

## Question 4:

(7 marks)
When ammonia gas reacts with gaseous oxygen it produces gaseous nitric oxide and water vapor. If the change in internal energy for the reaction is 9080.0 J and the change in the entropy for the reaction is $35.7 \mathrm{JK}^{-1}$ at $27^{\circ} \mathrm{C}$, using Gibb's free energy equation, predict whether at $27^{\circ} \mathrm{C}$, the reaction is spontaneous or not.

## Question 5:

(4 marks)
Calculate the change in Gibb's Free energy for the following reaction and predict whether the reaction is spontaneous under standard conditions or not?

$$
4 \mathrm{KClO}_{3(\mathrm{~s})} \rightarrow 3 \mathrm{KClO}_{4(\mathrm{~s})}+\mathrm{KCl}_{(\mathrm{s})}
$$

Given:

|  | $\Delta H_{f}^{0}(\mathrm{~kJ} / \mathrm{mol})$ | $S^{0}(\mathrm{~J} / \mathrm{mol} . \mathrm{K})$ |
| :--- | :--- | :--- |
| $\mathrm{KClO}_{3(\mathrm{~s})}$ | -397.7 | 143.1 |
| $\mathrm{KClO}_{4(\mathrm{~s})}$ | -432.8 | 151.0 |
| $\mathrm{KCl}_{(\mathrm{s})}$ | -436.7 | 82.6 |

## Question 6:

A quantum mechanical particle is confined to move in one dimension between $x$ $=0$ and $x=L$.
(a) Write the mathematical expression for the wave function of the above particle in its ground state.
(b) Determine the value of the normalization constant, ' $\boldsymbol{A}$ ' and write the final normalized wave function.
(c) Using the normalized wave function as found in the part 2(a), find the probability that the particle will be found between $x=0$ and $x=L / 3$.

## Question 7:

(8 marks)
Show that the function $e^{-3 i k x}$ is eigenfunction of one dimensional kinetic energy operator. What is the eigen value?

## Question 8:

(25 marks)
(a) In a gaseous reaction, the time for half change ( $\mathrm{t}_{1 / 2}$ ) for various initial partial pressures $(P)$ are recorded as follows:

| $\mathbf{P}(\mathbf{m m ~ o f ~ H g})$ | 500 | 600 | 800 | 1000 |
| :---: | :--- | :--- | :--- | :--- |
| $\mathbf{t}_{1 / 2}(\mathrm{mins})$ | 268 | 223 | 168 | 134 |

What is the trend for $\mathrm{t}_{1 / 2}$ with respect to the increase in the initial partial pressures? Based on the trend, assign whether the reaction is either $0^{\text {th }}$ order or $1^{\mathrm{ST}}$ order or $2^{\mathrm{ND}}$ order and explain the reason behind your choice. Then using the appropriate $\mathrm{t}_{1 / 2}$ equation for the above assigned order, calculate the values of ' $k$ ' at various partial pressures and confirm the above order of the reaction.
(b) For a first order reaction, the values of $\mathrm{k}, \mathrm{A}$ and $\mathrm{E}_{\mathrm{a}}$ are $1.155 \times 10^{-3} \mathrm{sec}^{-1}$, $4.0 \times 10^{13} \mathrm{sec}^{-1}$ and $98.6 \mathrm{~kJ} \mathrm{~mol}^{-1}$, respectively. Calculate the value of temperature.
(c) Show that in the case of a first order reaction, the time taken for the completion of $99.9 \%$ of the reaction is approximately 10 times of the halflife of the reaction.


