RAJARATA UNIVERSITY OF SRI LANKA
FACULTY OF APPLIED SCIENCES

B.Sc. (General) Degree in Applied Sciences
First Year– Semester II Examination – November/December 2016

CHE 1106 MATHEMATICAL METHODS FOR CHEMISTRY

Answer **All** questions.   Time: One hour

The use of a non-programmable calculator is permitted.

$1 \text{ Pa} = 10^5 \text{ N m}^{-2}$
Avogadro Number $(N_A) = 6.023 \times 10^{23} \text{ mol}^{-1}$
Universal Gas Constant $(R) = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$

1. (i) One mol of a gas occupies a volume of $25 \times 10^{-3} \text{ m}^3$ at a pressure of 1×10^5 Pa.
   Calculate the temperature of the gas using the van der Waals equation.

$$\left(P + \frac{an^2}{V^2}\right)(v - nb) = nRT$$

a and b are constants of $0.10 \text{ Pa m}^6 \text{ mol}^{-1}$ and $4.0 \times 10^{-5} \text{ m}^3 \text{ mol}^{-1}$ respectively.

(ii) Simplify the following:

$$\frac{\sqrt[3]{ab^3}\,(ac^4)^2}{a^{\frac{4}{3}}\,b}$$

(iii) For the reaction, $aA + bB \rightarrow cC + dD$ write an expression for the logarithm of equilibrium constant (k)

(iv) For a reaction, the activation energy (E_a) is 52.0 kJ mol^{-1} and pre exponential factor A is 1.00. What is the rate constant (k) of the reaction when the temperature is 241 K?

$$k = A\,e^{\frac{-Ea}{RT}}$$

2. (a) Find the integrals of the following:

      i. $\int (2x + 6x^2)dx$

      ii. $\int \frac{x^2 + 2x^3 - 4x^4}{x^3} dx$

      iii. $\int 6\sin(3x)\, dx$

(b) A curve of gradient $4x^5$ passes through the points $(1, 2)$. What is the full equation?

(c) The ideal gas equation is $PV = nRT$ find:

      i. $\left(\frac{\partial V}{\partial T}\right)_p$ ii $\left(\frac{\partial T}{\partial p}\right)_v$

3.   (a) Convert the following

      i. $60°$ into radians

      ii. $\frac{3\pi}{8}$ radians into degrees

  b)   The position of certain bands in the infra-red spectrum of SO_2 can be used to determine the angle θ of the O—S—O bond. The analysis leads to the equation

$$\sin^2 \frac{\theta}{2} = 0.769$$

Find the value of θ in degrees.

  c)   A carbon – carbon bond has a length of 154 pm. If the bond is positioned at an angle of $30°$ to a surface as shown in the picture. What is the projected length of the bond in meters?