RAJARATA UNIVERSITY OF SRI LANKA
FACULTY OF APPLIED SCIENCES

B.Sc. (Special) Degree in Chemistry
Third Year– Semester I Examination – November/ December 2016

CHE 3120 – CALCULATIONS IN CHEMISTRY

Answer ALL questions **Time: One (1) hour**

The use of a non-programmable calculator is permitted

1. Give the following complex numbers in the form of a + ib,

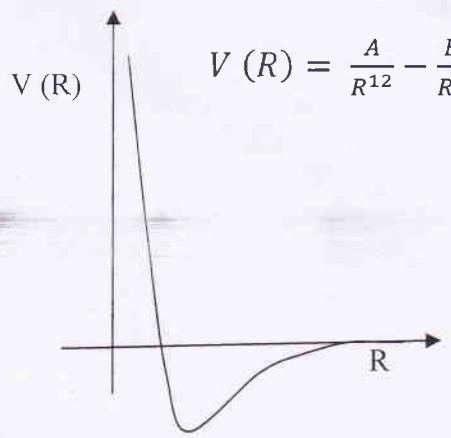
   (a) $(2 + i)\,(1 - i)$

   (b) $(-4 - 4i) - 5i$

   (c) $(1 + 2i)\,(1 - 2i)$

   (d) $\frac{1-2i}{2+3i}$

2. The Lennard-Jones potential describes the potential energy between two atoms separated by a distance R. The equation and graph of this function is shown below, where A and B are constants. The two particles are at their equilibrium separation when the potential is at a minimum (V is at a minimum). By differentiating this equation with respect to R find the equilibrium separation.



$$V(R) = \frac{A}{R^{12}} - \frac{B}{R^{6}}$$

3.

(a) The Maxwell Boltzmann Distribution is a probability distribution of finding particles at certain speed v in 3 dimensions. It has the form of

$$f(v) = Av^2 e^{-Bv^2}$$

Where A and B are constants. Using the chain rule and product rule find the $\frac{\partial f(v)}{\partial v}$

(b) For Y = 2 ln z + sin zx find $\frac{(\partial Y)}{(\partial x)_z}$ & $\frac{(\partial Y)}{(\partial z)_x}$

(c) The ideal gas equation is PV = nRT. Find $\frac{(\partial V)}{(\partial T)_p}$ & $\frac{(\partial T)}{(\partial P)_V}$

4. Find the integrals of the following:

(a) $I = \int 9e^{3z}\, dz$

(b) $I = \int (5\ \cos -x) + \sin(3x)\, dx$

(c) $I = \int_0^{\pi} \sin x\ dx$

(d) In a reaction mixture at a fixed temperature the concentration of a reactant [A] varies with time according to the differential equation:

$$\frac{d[A]}{dt} = -2kA^2$$

Integrate the equation with the boundary limits that when t = 0 and [A] = $[A]_0$ to get the following equation.

$$\frac{1}{[A]} - \frac{1}{[A]_0} = 2kt$$