EASETRN UNIVERSITY, SRI LANKA

THIRD EXAMINATION IN SCIENCE – PROPER

SECOND SEMESTER 2004/2005 (OCTOBER 2006)

CH 304 QUANTUM CHEMISTRY & METALLURGY AND INDUSTRIAL CHEMISTRY

Time allowed: **ONE Hour**

Candidate must NOT start writing their answers until told to do so

You may find the following data useful

Avogadro constant (N_A): 6.023×10^{23} mol^{-1}

Electron charge (e): 1.602×10^{-19} C

Faraday constant (F): 9.648×10^{4} $Cmol^{-1}$

Gas constant (R): 8.314 $JK^{-1}mol^{-1}$

Planck's constant (h): 6.626×10^{-34} Js

Rest mass of electron (m_e): 9.1×10^{-31} kg

Velocity of light (c): 3×10^{8} ms^{-1}

The use of a non –programmable calculator is permitted

1. (a) (i) Starting from the one-dimensional wave equation $\frac{\partial^2 u}{\partial x^2} = \frac{1}{\upsilon^2}\frac{\partial^2 u}{\partial t^2}$ for the standing wave system and substituting $u(x,t) = \psi(x)\cos(\varpi t)$, $\varpi = 2\pi\nu$ and $\nu\lambda = \upsilon$, show that

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{4\pi^2}{\lambda^2}\psi(x) = 0$$

(20 marks)

(ii) Using the derivation obtained in (i), derive the following time independent Schrodinger equation for a particle moving in a one - dimensional box with the help of de Broglie relation and the relation of momentum $p = \sqrt{2m(E-V)}$

$$\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi(x) = 0$$

(10 marks)

(b) (i) Calculate the probability that a particle restricted to move in a one – dimensional box of length 'a' is found to be the distance between '0' and 'a/4' . The wave function (ψ) of the particle given by $\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)$

(20 marks)

(ii) What is the probability of the particle beyond the distance 'a/4'?

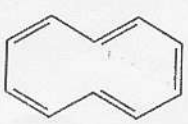
(10 marks)

(c) (i) Write the general expression for the energy levels of a particle of mass 'm' moving in a two - dimensional square box of length 'a' and identify all terms in it.

(10 marks)

(ii) The π electrons of a 10 - Annulene may be modeled as electrons in a two-dimensional square box. If the edge length of the box is 1000 pm and the π-system contains 10 electrons, what is the energy of the HOMO - LUMO transition? (1 pm = 10^{-12} m)

(30 marks)



10 - Annulene

2. (i) Metals can be extracted from their ores through several processes. Give a short account on refining of metals (physical and chemical methods).

(35 marks)

(ii) Briefly explain the dry process of manufacture of Portland cement.

(35 marks)

(iii) Briefly explain the important steps in Glass forming process.

(30 marks)

End