EASTERN UNIVERSITY, SRI LANKA

THIRD YEAR SECOND SEMESTER EXAMINATION IN SCIENCE

2008/2009 (Sept./ Nov. 2010)

CH 304 QUANTUM CHEMISTRY AND INDUSTRIAL CHEMISTRY & METALLURGY

Answer all questions Time: 01 hour

Planck constant (h) = 6.626×10^{-34} J s Boltzmann constant (k) = 1.38×10^{-23} J K^{-1}

Speed of Light (c) = 3×10^{8} m s^{-1}

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1. (a) Write the down the Schrödinger equation in one dimesional box and explain the terms involved in it.

(10 marks)

(b) How is the wave function interpreted in terms of the probability?

(05 marks)

(c) For a particle of mass 9.1×10^{-31} kg in a certain one – dimensional box, transition from n = 3 to n = 2 transition occurs at $\nu = 4.0 \times 10^{14}$ s^{-1}.

(i) Find the length of the box (20 marks)

(ii) At what value of n does the energy of the particle reach ½ kT at 300K?

(20 marks)

(iii) Show that the frequency of the transition from n = 3 to n = 2 is 5/3 times frequency of the n = 2 to n = 1 transition.

(15 marks)

(d) Predict the wavelength (in nm) of the lowest-energy electronic transition in the following polymethine ion:

$(CH_3)_2N^+ = CH - CH = CH - CH = CH - N(CH_3)_2$

Assume that all the C-C and C-N bonds lengths equal 1.40 $\mathring{A}$. Note that N^+ and N contribute 1 and 2 π-electrons, respectively.

(30 marks)

Turn over

2. (a) What is Ellingham diagram?

(b) Aluminum is used for extraction of metals, such as chromium from their respective oxides. What is the principal reason for using this metal (Al) as the reducing agent?

Explain using the information given below.

$4/3Al_{(s)} + O_{2(g)} \longrightarrow 2/3\ Al_2O_{3(s)}$ $\quad \Delta G = -827\ kJmol^{-1}$

$4/3\ Cr_{(s)} + O_{2\,(g)} \longrightarrow 2/3\ Cr_2O_{3\,(s)}$ $\quad \Delta G = -540\ kJmol^{-1}$

(30 marks)

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

(40 marks)

(d) Explain briefly the hydration of Portland cement.

(30 marks)

End of Paper