RAJARATA UNIVERSITY OF SRI LANKA
FACULTY OF APPLIED SCIENCES

B.Sc. (Special) Degree in Chemistry
Fourth Year - Semester I Examination – Oct/Nov 2017

CHE 4211 – Electronics and IT for Chemists

Time: Two (2) hours

Answer all **Four Questions**

1. The following formula is used in an MS Excel spreadsheet to grade students according to the marks obtained. Study the formula carefully and answer the following questions.

=IF(A3>=90,"A+",IF(A3>=80,"A".IF(A3>=75,"A",IF(A3>=65,"B+",IF(A3>=60,"B",IF (A3>=55,"B-",IF(A3>=50,"C+",IF(A3>=45,"C",IF(A3>=40,"C- ",IF(A3>=35,"D",IF(A3>=30,"D-",IF(A3>=25,"E+",IF(A3>=20,"E",IF(A3>=10,"E- ",IF(A3>=0,"F")))))))))))

a) Identify the general type of function that is employed in this formula. What is the reference cell that is being referred by the formula before deciding the final grading **(10 marks)**

b) What is the range of marks allocated for each grade? **(10 marks)**

c) Write an 'if' function to limit the grades to the following marks ranges in MS Excel.
"A-" 69-79

"A" 80-95

"A+" 96 and above

"No Distinction" any marks below 69

(16 marks)

d) Study the following calibration plot (figure1) obtained using MS Excel. It illustrates the change of absorbance of a nickel complex with increasing concentration.

Identify the following from the plot

i. The dependent variable
ii. The independent variable
iii. The gradient of the slope
iv. The correlation coefficient

(16 marks)

e) If a solution of the above iron complex with an unknown concentration shows an absorbance of 65, what would be the concentration the solution? State the assumption/s that you made in the deduction.

(10 marks)

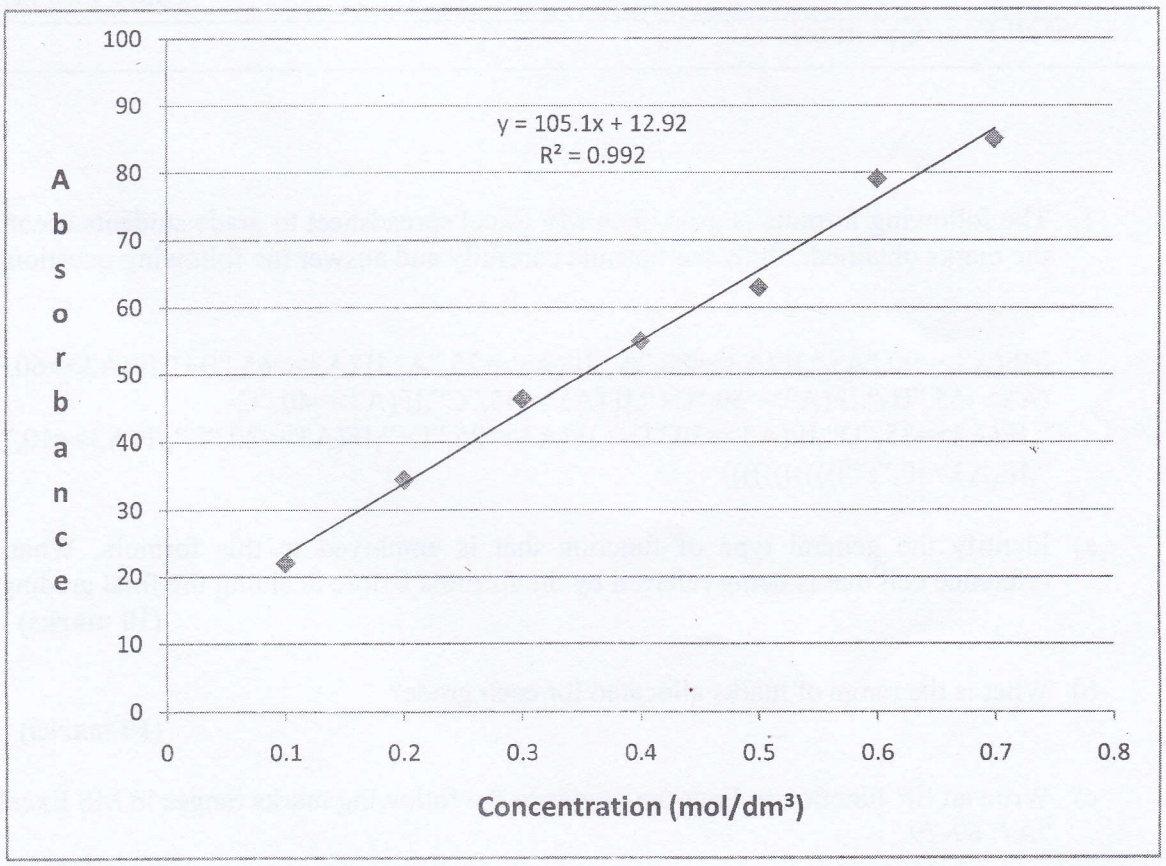

Figure1: Change of absorbance of a nickel complex with increasing concentration.

f)

i. List down four molecule editing softwares

(8 marks)

ii. Briefly explain their common features and state their native file formats

(10 marks)

g) How to draw the compound Ferrocene and similar sandwitch compounds in CambridgesoftChemdraw 7.0 software? Briefly explain

(10 marks)

h) Briefly explain what it is meant by "SMILES" and their usefulness in cheminformatics.

(10 marks)

2.

a)

i. Write a shot account on the "molecular visualization softwares" including the evolution of these softwares, applications on desktop and web-based.

(20 marks)

ii. RasMol/Raswin is a visualization program created by Roger Sayle and used to display small molecules, properties and nucleic acids.

I. Assume that you have a protein pdb file called 2VDY.pdb and it is located on "D:\rasmol\" . Write a rasmol script file that opens the pdb file, change background color as white, restrict the view to residues 195-296 in blue color, display the polar side chains in red color with ball and stick and display the possible hydrogen bonds.

(20 marks)

II. A student prepared a rasmol script file as follows

```
Zap
Load "D:\rasmol\1qlx.pdb
Select all
Select yellow
Select HIS
Color red
cpk
Echo Press any key to continue
Pause
Exit

Saved as D:\rasmol\qlx.txt
In command prompt typed as : script one.txt
```

What are the observations?

(20 marks)

b)

i. Write a shot accounton subject gateways and how these differ from search engines

(10 marks)

ii. Google scholar is a freely accessible web search engine that indexes the full text or metadata of scholarly literature across an array of publishing formats and disciplines. What are the features, specifications and limitation inGoogle scholar? Explain briefly

(10 marks)

c) Microsoft (MS) Word has a built-in equation editor. The equation editor allows you to easily define complex equations within a word document.

i. What is the different between "Professional format" and "Linear format" in the equation editor?

(10 marks)

ii. Briefly discuss the limitation of Microsoft equation editor(at least two limitations).

(10 marks)

3.

Consider a purely resistive circuit with a resistor connected to an AC generator.

i. If the instantaneous current in the resistor is given by IR(t), write down an equation for theinstantaneous voltage drop (VR(t)) across the resistor.
ii. Obtain an equation for the instantaneous current IR(t) in the resistor.
iii. Plot the IR(t) and the VR(t) as a function of time on the same graph.
iv. Draw the phase diagram for the above circuit and discuss the phase relationship betweenthe IR(t) and VR(t).
v. When calculating the average current in this circuit, explain why it is necessary to define anaverage of the square of the current instead of taking the average value of current over oneperiod.

(100 marks)

4.

Consider the following transistor circuits (figure1) with $\beta = 200$.

i. Find the Thevenin's voltage and current for the above circuit.
ii. Draw the simplified circuit with two power sources and one base resistor.
iii. Find the Q-points of the circuit.
iv. Sketch the load line.
v. Check whether Q point is independent on changing β.

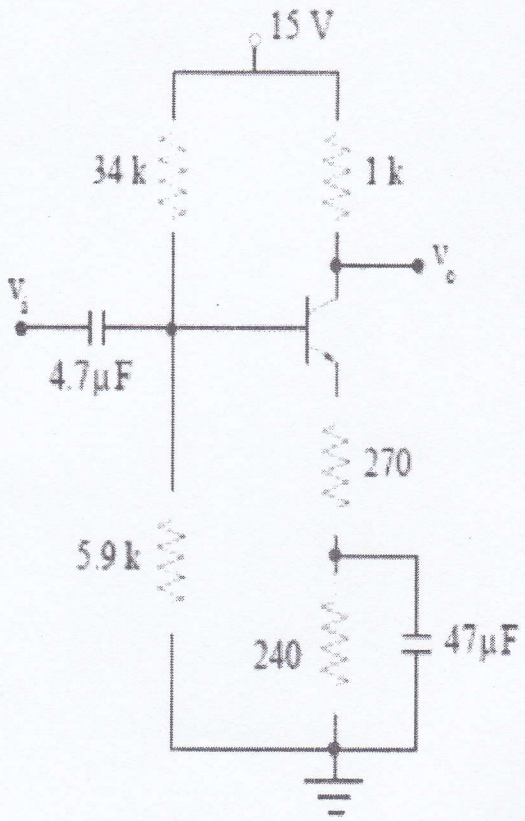

Figure1:Transistor circuitswith $\beta = 200$.

(100 marks)

----End----