UNIVERSITI SAINS MALAYSIA

First Semester Examination
Academic Year 2004/2005

October 2004

KAA 506 – Computer in Chemistry

Time : 3 hours

Please make sure this paper consists of SEVEN printed pages before answering the questions.

Answer FIVE questions.

Only the first five questions answered by the candidate will be marked.

1. Cucurbituril, see Fig. 1., a rigid molecule possessing a hydrophobic cavity, is a macrocyclic host molecule. At each entrance to the cavity, six polar carbonyl groups are located. These conditions are ideal for the complexation of organic molecules with cucurbituril. A molecular modeling study involving the complexation of organic molecules by cucurbituril is therefore proposed.

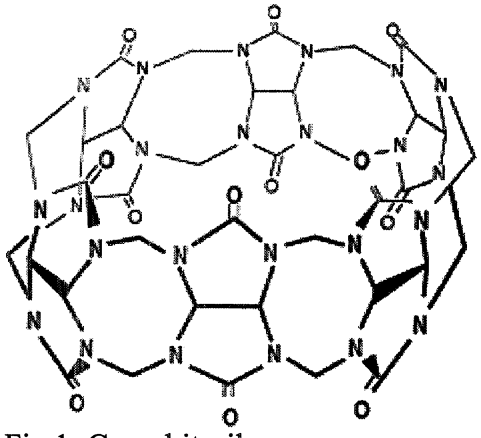


Fig.1: Cucurbituril

(i) What is the most common method of molecular modeling used to study the complexation described above and state your reasons.

(ii) State the steps involved in a molecular modeling studies.

(iii) Write the command for geometry optimization process, using the method described in (i).

(iv) Write the structure of CH_3CH_2OH in Z-matrics format.

(v) Give three examples of property calculations that can be performed.

(20 marks)

2. (a) Describe the functions and write the Excel commands involving STEYX, LINEST and STDEV.

(6 marks)

(b) Write the Excel equation for

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad \text{and} \quad y = \sqrt{\frac{15}{16\pi}\cos 2\phi}$$

(4 marks)

(c) Values in cell B8:B21 and C8:C21 correspond to the concentration of A in the integrated forms of the rate law. Write the appropriate formula involved and the corresponding Excel formula.

Table 1

	A	B	C	D	E
1	1st order d[A]/dt =k [A]		2nd order d[A]/dt=k[A]^2		
2					
3	k_1	0.01			
4	k_2	0.01			
5	Ao	1			
6		1st order	2nd order		
7	t,s	[A], M	[A],M		
8	10	0.90483742	0.909091		
9	20	0.81873075	0.833333		
10	30	0.74081822	0.769231		
11	40	0.67032005	0.714286		
12	50	0.60653066	0.666667		
13	60	0.54881164	0.625		
14	70	0.4965853	0.588235		
15	80	0.44932896	0.555556		
16	90	0.40656966	0.526316		
17	100	0.36787944	0.5		
18	110	0.33287108	0.47619		
19	120	0.30119421	0.454545		
20	130	0.27253179	0.434783		
21	140	0.24659696	0.416667		

(10 marks)

3. Develop a MATLAB function to calculate a root of a polynomial equation by Newton Raphson method. Calculate the specific volume of a pure gas, *n*-butane, at a given temperature and pressure by using the Soave-Redlich-Kwong equation of state:

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b))}$$

Given

$$a = \frac{0.4278R^2T_C^2}{P_C}$$

$$b = \frac{0.0867RT_C}{P_C}$$

where T_C and P_C are critical temperature and pressure, respectively. The variable α is an empirical function of temperature:

$$\alpha = \left[1 + S\left(1 - \sqrt{\frac{T}{Tc}}\right)\right]^2$$

The value S is a function of ω:

$$S = 0.48508 + 1.55171\omega - 0.15613\omega^2$$

Given that the physical properties of *n*-butane are :

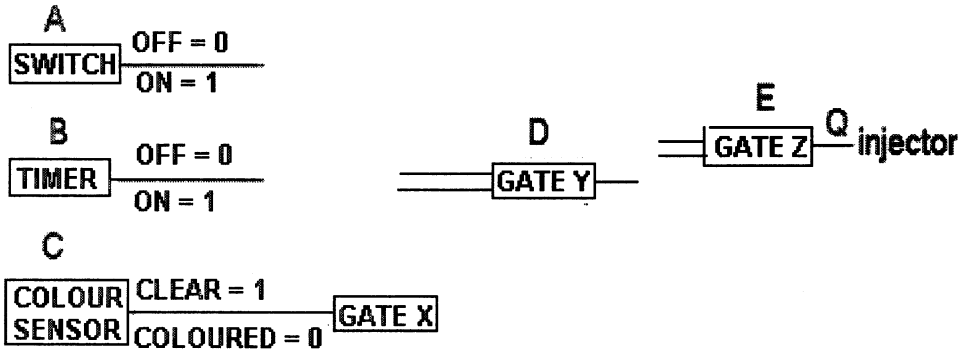
$T_C = 425.2K$ $P_C = 3797$ kPa $\omega = 0.1931$

and the gas constant R = 8.3145 J mol^{-1} K^{-1}

(20 marks)

4. A process control designer has developed a system to control the injection of chemicals into a liquid flow stream. The injection of the chemicals can be done manually, or by the use of a timer, so long as the sensor indicates that the liquid has slightly change in its colour.

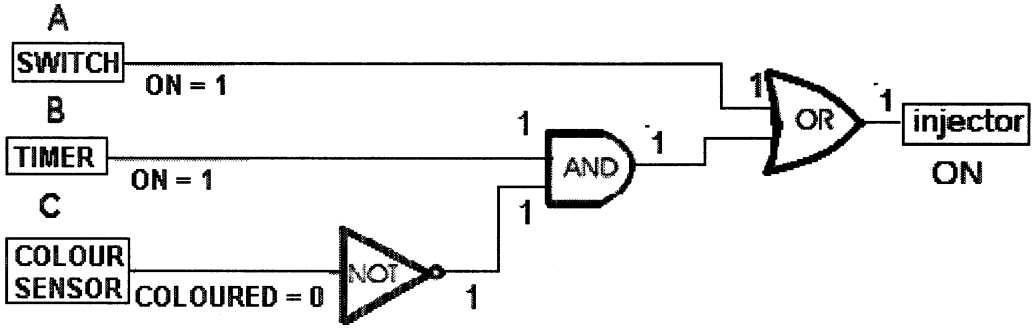
(a) Below is an incomplete logic circuit for the control system. Redraw the logic circuit using the correct logic gates. Note the output of the colour sensor is '0' (false, low, off) when the colour change. The chemical must be injected when the colour is changing.



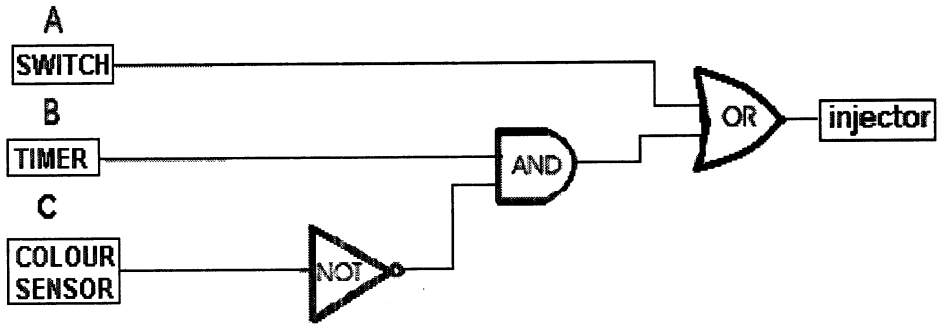
Name the logic gates you have used:

(3 marks)

(b) Below is the logic circuit showing the logic states of inputs and outputs of all the gates when the injector is ON.



On the logic circuit below, write the logic states of all inputs and outputs and state either under the following conditions,:
liquid is coloured, the manual switch is off and the timer is 'on' the injector be on or off ?



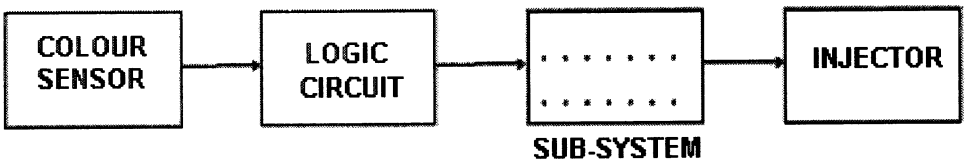
(6 marks)

(c) Complete the truth table for the logic circuit that controls the injection system

INPUTS					OUTPUTS
A	B	C	D	E	Q
0	0	0	1	0	0
0	0	1	0	0	0
0	1	0	1	1	1
0	1	1			
1	0	0			
1	0	1			
1	1	0			
1	1	1			

(8 marks)

(d) Normally a logic circuit such as the one used to control the injection cannot power the injector. In the space below name the subsystem that could be used.



(3 marks)

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5. (a) The automation of chemical analyses can give better analytical results in terms of precision and accuracy. This system can be applied online or inline for the quality or process control in products manufacturing process

(i) What is the meaning of online quality control?

(ii) What is the meaning of inline process control?

(iii) Name three analytical measurements which can be performed inline.

(9 marks)

(b) Draw a flow chart for a spectrophotometric titration of acid/ base and the determination of the equivalence point. Name all accessories required to implement the above task.

(11 marks)

6. (a) An operational amplifier can play very important roles in analytical signal conditioning before data acquisition process. Draw a circuit diagram to achieved each of the following.

(i) Amplify 50 times of 0.001 V signal.

(ii) Do a summation of 3 different sources of signal.

(iii) Differentiate an incoming signal.

(iv) Integrate an incoming signal.

. (12 marks)

(b) Give your suggestion with justification for an analytical instrument to conduct

(i) the high speed analysis in a clinical laboratory, and.

(ii) an online analysis of coloured species in a solution

(8 marks)

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