



UNIVERSITY OF KELANIYA - SRI LANKA

FACULTY OF SCIENCE

**Bachelor of Science Honors in Applied Chemistry Degree Examination
Nov. 2022**

**Academic Year 2020/2021– Semester I
APCH 11612 – Computer Skills for Chemists**

(Part I- Practical Exam)

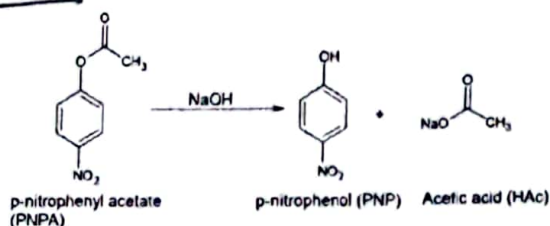
Number of Questions: Two (02)
Number of pages: Two (02)

Time: One (01) hour thirty (30) minutes
Answer all questions

Save all your data files (answer sheet, excel and chem sketch) in the folder labelled as exam with index no as the file name.

Download the answer sheet to paste relevant graphs or data, and save in the exam folder.

- (1) Hydrolysis is one of the ways organic pollutants can be degraded abiotically. In this experiment the base hydrolysis of p-nitrophenyl Acetate (PNPA) to p-nitrophenol (PNP) and acetic acid (HAc) was studied. The concentration of PNPA was determined by UV-Visible spectroscopy by measuring the absorbance at 275 nm.



- (i) The absorbance of the standard solutions of PNPA with the following concentrations was measured at 275 nm in order to construct a calibration curve as shown in table 1. Using MS excel,
- (a) Plot the calibration curve of Average absorbance vs. concentration of PNPA. ($y = mx$)
 - (b) Display the linear regression equation with R^2 in the calibration curve.
 - (c) Mark error bars on the graph as standard deviation. (30 marks)

Table 1

Concentration of PNPA/ M	Absorbance in trial 1	Absorbance in trial 2	Absorbance in trial 3
0.05	0.13	0.09	0.12
0.10	0.26	0.26	0.24
0.15	0.39	0.35	0.41
0.20	0.52	0.41	0.53
0.25	0.65	0.67	0.68
0.3	0.78	0.78	0.73
0.35	0.91	0.91	0.93

- (ii) The degradation of PNPA with time was recorded as absorbance of the reaction mixture at 275 nm at specified time intervals in the following table 2. Using the above calibration curve, calculate the concentrations of the PNPA (at the specified time intervals as $[A]_t$) according to Beer's law ($A = \epsilon cl$ where $l = 1\text{cm}$, A is absorbance, c is concentration and ϵ is extinction coefficient)

Table 2

t/s	Absorbance of reaction mixture at 275 nm	Concentration of PNPA $[A]_t$
0	0.082	
14	0.078	
39	0.071	
60	0.067	
80	0.062	
110	0.055	
140	0.049	
170	0.044	
210	0.038	

(10 marks)

- (iii) (a) Find the initial concentration of the PNPA (i.e. $[A]_0$ at $t = 0$ s) according to table 2 calculations.
 (b) Find the order of the reaction plotting following integrated rate laws ($A = \text{concentration}$). Display linear regression equation and the R^2 for each of the curve fitting.
 (c) Calculate the rate constant (k) for the reaction according to rate law in (b) above.

Order	Rate law	Integrated Rate Law	Linear plot	Slope
0 th	rate = k	$[A]_0 - [A]_t = kt$	$[A]_t - [A]_0$ vs. t	$-k$
1 st	rate = $k[A]$	$\ln \frac{[A]_t}{[A]_0} = -kt$	$\ln([A]_t / [A]_0)$ vs. t	$-k$
2 nd	rate = $k[A]^2$	$\frac{1}{[A]_t} - \frac{1}{[A]_0} = kt$	$1/[A]_t - 1/[A]_0$ vs. t	k

(30 marks)

- 2/ The mechanism for base hydrolysis of ester is given below. Use Chems sketch software to draw the mechanism. (30 marks)

