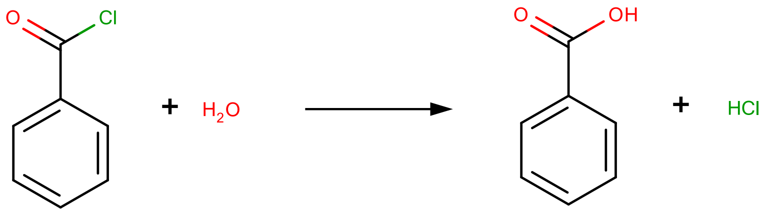
KINETICS OF BENZOYL CHLORIDE HYDROLYSIS

INTRODUCTION

Acid chlorides (R–COCl) are derivatives of carboxylic acids (R–COOH), in which the –OH group in the (–COOH) functional group was substituted with a chlorine atom –Cl. They are the most reactive derivatives of carboxylic acids. As a result of acid chloride hydrolysis, a corresponding carboxylic acid, and hydrogen chloride are formed.

In the case of benzoyl chloride (PhCOCl) the reaction proceeds according to the following equation:



(1)

$$A + B \rightarrow \text{products} \quad (2)$$

Assuming the ideal mixing of the reagents and the constant volume of the reaction mixture, changes in the concentrations of the substrates in time may be described using a 2nd order kinetic equation:

$$-\frac{dc}{dt} = k \cdot c_A \cdot c_B \quad (3)$$

It results from the reaction stoichiometry (equation 2) that the concentration of substrate A decreases to the value $c_A = a - x$, then the concentration of substrate B decreases to the value $c_B = b - x$, equation (3) may be written as:

$$-\frac{dc_A}{dt} = -\frac{dc_B}{dt} = k \cdot (a - x) \cdot (b - x) \quad (4)$$

where:

c_A – concentration of substrate A,
c_B – concentration of substrate B,
a – initial concentration of substrate A (e.g. water),
b – initial concentration of substrate B (e.g. PhCOCl),
x – temporary concentration of the product,
t – time,
k – reaction rate constant,

Since the loss of substrate concentration equals the increase in the concentration of the product:

$$-\frac{dc_A}{dt} = \frac{dx}{dt} \quad (5)$$

the kinetic equation takes the form:

$$\frac{dx}{dt} = k \cdot (a - x) \cdot (b - x) \tag{6}$$

After the separation of the variables and integration within the limits of integration resulting from the boundary condition $x = 0$ for t = 0, equation (6) takes the form:

$$\frac{1}{(a - b)} ln \frac{b(a - x)}{a(b - x)} = k \cdot t \tag{7}$$

The equation below should be constant and equal to the searched constant process rate:

$$\frac{1}{t} \cdot \frac{1}{(a - b)} ln \frac{b(a - x)}{a(b - x)} = const = k \cdot \tag{8}$$

PURPOSE OF EXERCISE

The objective of this task is to determine the reaction rate constant for benzoyl chloride hydrolysis at various initial concentrations of the reagents.

APPARATUS

- thermostat (np. U-1.),
- magnetic stirrer and a magnetic stirring bar (dipole),
- conductometer (CC-501),

LAB GLASS

- a thermostatic reaction vessel,
- beakers 50 cm^3, 100 cm^3,
- glass pipettes (1, 5 i 10 cm^3),
- measuring flasks 10 ml - 3 pieces.

CHEMICALS

- Distilled water,
- Acetone - AC (Cz.D.A),
- 5M solution of benzoyl chloride (PhCOCl) in acetone (AC).

EXPERIMENT PROCEDURES

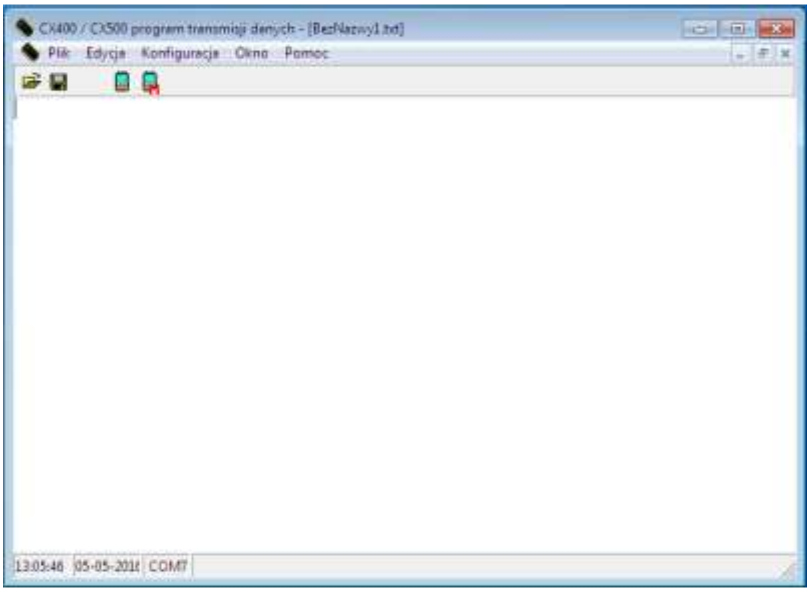
- All measurements should be performed at a constant temperature of 35 ºC,
- Prepare diluted solutions of water in acetone in 10 ml volumetric flasks,

- Run 3 reactions of benzoyl chloride hydrolysis in prepared solutions, changing the amounts of the reagents according to the table given below:

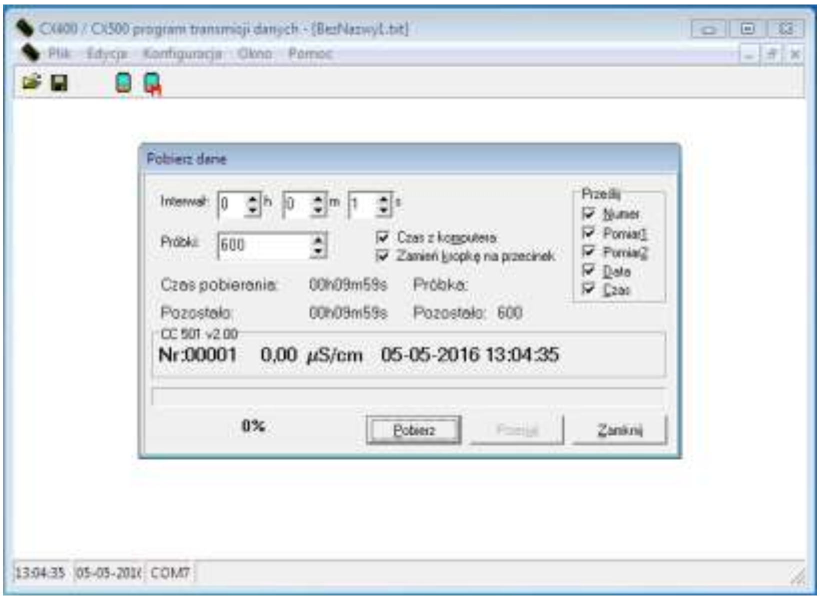
Table 1.

No.	Solution H_2O : AC		Amount of PhCOCl
	Water [cm^3]	AC [cm^3]	[cm^3]
1	5	to 10	0.40
2	4	to 10	0.40
3	3	to 10	0.80

- Turn on the CC-501 conductometer,
- After pouring respective amounts of the substrates (water and acetone) into the volumetric vessel turn on the mixing function and next immerse the conductometer probe,
- Heat the mixture to a temperature of 35°C,
- On the computer screen start the S4i5-pc. application (Fig. 1),



- From the menu "File" select the option "Download data",
- Set the value of the interval at 1 s and the number of samples at 3000,



- After the temperature stabilizes push the "Download" button,
- After pushing the "Download" button the values of electrolytic conductivity (σ) measured by the conductometer will be recorded (measurement sampling). Simultaneously the measured values σ will be displayed in the "Download data" window and entered successively in the form of text data in the NoName.txt. file,
- After approx. 30 seconds from the beginning of sampling, supplement the water-acetone solution with a respective amount (according to Table 1) of 5M PhCOCl solution in acetone. After adding PhCOCl the value of conductivity of the solution will start to increase,
- Wait until the completion of the reaction, i.e. stabilization of conductivity. Turn off the recording of measurements by pushing the "Stop" button,
- In the menu "File" record data in the folder "Measurements",
- Prepare the system for the next reaction, i.e. **wash the vessel, electrodes, and thermometer with acetone,**
- After completion of the measurements submit the files with recorded measurement data by e-mail.

CAUTION!

- after removing the mixing element (dipole) pour the spent solution into the vessel labeled "Liquid waste",

PREPARATION OF RESULTS

- Import the results to a spreadsheet,
- Remember when separating the data to take into consideration the order to magnitude initially recorded using symbols µS/cm, mS/cm, etc. All numerical data have to be expressed in the same units (e.g. µS/cm or mS/cm),
- Assume the moment, in which the water-acetone mixture was supplemented with the PhCOCl solution, as the reaction onset time,
- Plot the dependence of conductivity (σ) on time (t),

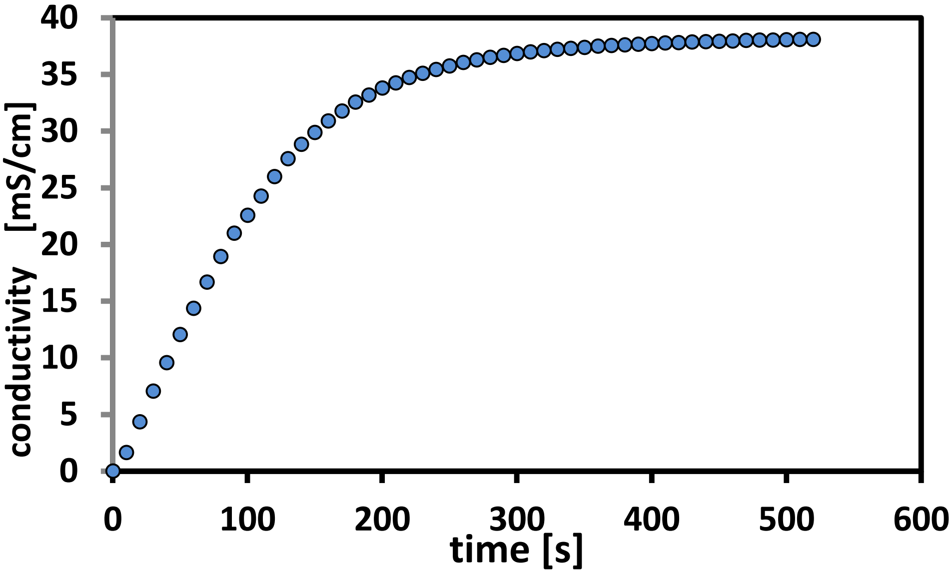


Fig3. Example of the measurement plot

- Calculate the initial concentration of water (*a*), PhCOCl (*b*), and the instantaneous concentration of product (*x*), i.e. HCl, from formula (9):

$$x = \frac{\sigma_t - \sigma_o}{\sigma_{max}} \cdot b \qquad (9)$$

where:

σ_t – the value of conductivity at a given time point (in time *t*),
σ_o – initial value of conductivity (water-acetone solution before adding PhCOCl at a constant temperature),
σ_{max} – the final value of conductivity (after the completion of the reaction),
b – initial concentration of benzoyl chloride solution,

- Calculate reaction rate constants *k* using equation (8),
- Calculate mean values of reaction rate constant ($\bar{k}$) for individual concentrations and standard deviation $\bar{k}$.

No.	The initial concentration of water *a* [mol·dm^{-3}]	The initial concentration of *PhCOCl* *b* [mol·dm^{-3}]	Mean values of reaction rate constant $\bar{k}$ [dm^{3}mol^{-1} s^{-1}]	Standard deviation of the mean $\bar{k}$ [dm^{3}mol^{-1} s^{-1}]
1				
2				
3				

Template of the table and draft of the study

…………………………….. *Faculty* ………………………………. *Field of study* *Full-time/ part-time studies*	……………………………………………… *Name and surname*	…………………………………... *Date:*
Group no.: ………………… *Team no.:* …………………	……..…………… *Exercise no.:*	……………………………………. *Instructor:*

…………………………….. *Wydział* ………………………………. *Kierunek* *Studia stacjonarne/niestacjonarne*	……………………………………………… *Imię i Nazwisko studenta*	…………………………………... *Data wykonywania ćwiczenia:*
Nr grupy: …………………... *Nr zespołu:* …………………..	……..…………… *Nr ćwiczenia:*	……………………………………. *Nazwisko Prowadzącego:*

1. Temat ćwiczenia
2. Cel ćwiczenia:
3. Wstęp teoretyczny:
4. Pomiary:
5. Obliczenia:
6. Wykresy:
7. Wnioski

1. Exercise title:
2. The aim of the exercise:
3. Theoretical introduction:
4. Results:
5. Calculations:
6. Graphs:
7. Conclusions: