Kinetic Study of the Reaction between Ethanol and Chloroacetyl Chloride in Chloroform

A Laboratory Experiment using Fourier Transform Infrared Spectroscopy

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In this work, we study the reaction between chloroacetyl chloride and ethanol using chloroform as a solvent.

Calculating the Reaction Rate

As is well-known (*1*), the rate of a reaction is given by the following equation.

$$v = -\left(\frac{1}{a}\right)\frac{d[A]}{dt} = K[A]^n[B]^m \ldots [N]^z \quad (1)$$

where [A] is the concentration of any of the reactants; a is the stoichiometric coefficient of A; K is the rate constant; and the letters $n, m, \ldots z$ indicate the orders with respect to the reactants.

To calculate v, the change of the concentration with time is needed. There are different methods (*2*) to determine the concentrations of the products (or reactants) at time t.

The Use of FTIR Absorption

The method used in this experiment is the measurement of the intensity of an IR absorption band belonging to one of the reaction components. This component (product or reactant) is the control species.

The concentration at each time can be obtained from the integrated intensity using Lambert–Beer's equation.

$$A = \varepsilon c L \quad (2)$$

There are some important limitations to consider in the use of dispersive infrared spectroscopy. One of the most important is the time needed to scan the spectrum because the concentration changes continuously during the scan. The use of FTIR spectroscopy makes it possible to obtain spectra quickly, so the reaction can be considered as not advancing during the scan.

The Experiment

- ***Caution***: Chloroacetyl chloride is ***corrosive***. Chloroacetyl chloride is also a ***lachrymator***. It must be handled with care, in a fume hood if possible.

The experiment described in this paper was done in three steps.

- Determine the experimental conditions: concentration range, control species, bands to be measured, and the times at which the spectra will be obtained.
- Measure the control band area, and calculate the concentration changes of the control species.
- Determine the reaction order and interpret the results obtained.

Determining the Experimental Conditions

Chloroacetyl chloride makes the most convenient control species due to its carbonyl stretching band. This is shown by a study of the IR spectra of ethanol, chloroacetyl chloride (reactants), and ethyl chloroacetate (product). Use of the trans isomer band alone would be more preferable. Because the concentration of each isomer (trans and gauche) (*3*) in chloroacetyl chloride is not known accurately, the sum of the two-carbonyl band area must be taken as a measure of the concentration.

Table 1. Reactant Concentrations, Band Area of Control Species (t = 0), and Temperature for Each Reaction

Expt	[EtOH] (mol L^{-1})	[$ClCH_2$–COCl] (mol L^{-1})	A_0 (cm^{-1})	T (°C)
1	0.2553	0.0410	24.601	20
2	0.2553	0.0692	41.546	20
3	0.5136	0.0434	26.041	20
4	0.0742	0.0463	27.781	25
5	0.1065	0.0527	31.652	25
6	0.1386	0.0527	31.652	25
7	0.2553	0.0834	40.068	25
8	0.2553	0.0363	21.755	25
9	0.0355	0.0506	30.139	25

The range of concentrations used for ethanol and chloroacetyl chloride, as well as the temperature at which each experiment was carried out are shown in Table 1. The concentration range of chloroacetyl chloride was chosen to minimize the errors in measuring absorbance. Of course, a

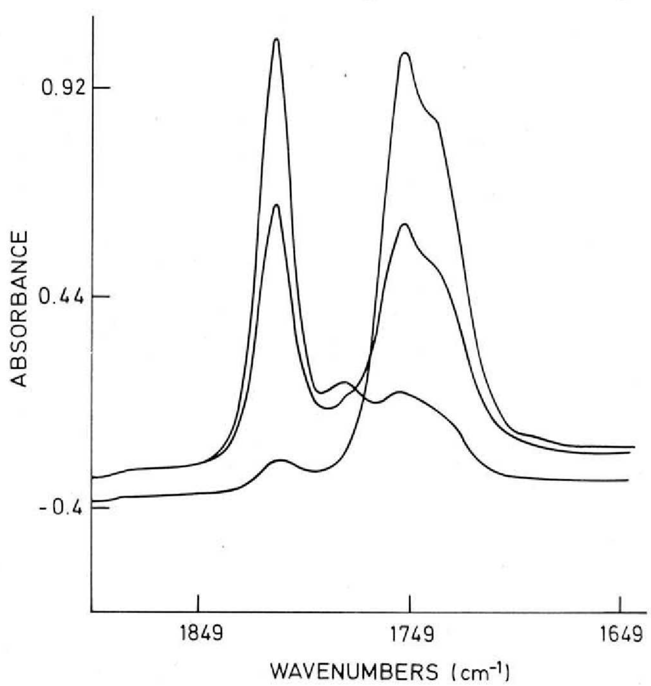

Figure 1. Time evolution of the reaction between ethanol (0.255 M) and chloroacetyl chloride (0.069 M).