

Nucleophilic substitution



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Experimental: Theoretical: Discussion [6] The experimental findings obtained are largely consistent with theory. The activation energy obtained in Part C, 138.6 kJ/mol is not too far below the theoretical activation energy of 148.526 kJ/mol [6], while Part A confirms the theory that k is dependent on the initial concentration of reactants, since it is a first order reaction. This is clearly depicted in Figure 3, where the alteration of the amount of *t*-butyl chloride being added to the reaction vessel clearly produced a different rate constant.

The findings from Part B of the experiment proved that the reaction followed the S_N1 mechanism, reaction rate to increase due to the usage of polar solvents to stabilize the carbocation being produced during this mechanism in the slow, rate-determining step [5]. However, there were errors in the experiment, which led to the results being slightly off from theory, such as the lower than expected value for the activation energy. One major source of error was the fact that *t*-butyl chloride reacts with water. Since there is water present in the air, this actually reduces the concentration of the *t*-butyl chloride solution.

If a sample was left exposed for longer, more would react, lowering the concentration further. The following equation shows the reaction with water: $[3] + H_2O \rightarrow [3] + HCl$ Another source of error would be the hydrophilic nature of acetone. This means that acetone, being polar, is attracted to water, another polar compound. As a result of this, the acetone has water molecules clumped around it in the acetone/water mixture, which inhibits the reaction slightly, as the *t*-butyl chloride molecules, being bulkier, find it harder to access the acetone.

While the reaction was ongoing, it was noticed that there was usually a temperature rise that accompanied it. This is another source of error, since the increase in temperature would contribute to an increased rate, which would in turn show up on the measurements taken due to the increase in conductivity of the mixture in the reaction vessel. Lastly, the room imperative experiment (run 7 from the Procedure section) did not have a water bath, making it a biased trial.

If the experiment were to be repeated, there should be a room temperature water bath for that particular run, to make the experiments uniform and fair. Conclusion The introduction to the experiment stated that the kinetics of the nucleophilic substitution reaction were to be studied and found to be affected by changes in concentration of t-butyl chloride, the percentage composition of the acetone/water solution (solvent polarity) and the temperature at which the reaction was to be carried out.

The results from this experiment were successful in proving that changes to these three conditions varied the rate constant (k), thus they affected the kinetics of the reaction. Upon research it was found that econometric analysis could also be carried out on other reactions such as the hydrolysis of urea (which is highly important for plants to be able to absorb nitrogen from urea)[7], and to study titrations of acids and bases, where the conductivity starts to fall as a base is added to an acid, until it reaches a minimum at the neutralization point, before rising again when more base or acid is added [8].

For the hydrolysis of urea, it initially reacts with water to produce ammonia gas, carbonic acid, water and carbon dioxide. For the plants to obtain the nutrients, the water must react with the ammonia to produce ammonium ions that can be absorbed. $\text{NH}_3 + \text{H}_2\text{O} \rightleftharpoons \text{NH}_4^+ + \text{OH}^-$ The rate of production of the ammonium ion can be studied using contemporary, allowing us to deduce the rate at which plants are obtaining nutrients from the urea, and to note how much ammonia is escaping as gas as opposed to being converted to an ion.