

Can IR Light Increase the Reaction Rate of Organic Reactions? A case Study Using the Base-Catalyzed Hydrolysis of N-Methylformanilide

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Abstract

The impact of infrared (IR) light on the base-catalyzed hydrolysis of N-methylformanilide was investigated at room temperature to explore the possibility of enhancing the reaction rate. A solution containing 10 mM N-methylformanilide and a 1 M sodium hydroxide solution was prepared in a 1:1 mixture of isopropanol and water as the solvent. The experimental data revealed that the conversion percentage of the reactant versus time followed first-order kinetics. The reaction rate constants were determined to be $6.6 \times 10^{-5} \text{ s}^{-1}$ and $2.1 \times 10^{-4} \text{ s}^{-1}$ in the presence and absence of IR light, respectively. Remarkably, the rate of reaction in the presence of IR light was found to be three times faster compared to that without IR light. This initial outcome unequivocally establishes the enhanced reaction rate associated with the presence of IR light. This observation suggests the potential application of IR light in organic and biochemical reactions, such as selectively breaking specific bonds in DNA or proteins.

Infrared spectroscopy is a study of interaction of infrared radiation with chemicals by absorption, which is used to identify functional groups in chemicals [1]. These absorptions occur when the vibrational frequency of a molecular bond matches the frequency of the infrared radiation. Since the vibrational frequency of a particular bond is characteristic, infrared spectroscopy is typically used to determine the existence of bonds in a molecule. This characteristic absorption, however, has not been used in an organic reaction to selectively break a specific bond. The feasibility of facilitating bond breaking through the absorption of radiation is questionable, as the effect of infrared (IR) light on the reaction appears to be insignificant. This is due to the fact that the energy carried by mid-infrared light used in infrared spectroscopy (ranging from $4,000$ to 400 cm^{-1}) is considerably lower than the energy required to break a bond [1]. For instance, the C=O and C-N bonds in amides possess energies of approximately 750 kJ/mol and 300 kJ/mol , respectively. However, the corresponding absorption wavenumbers for these bonds are 1650 cm^{-1} and 1400 cm^{-1} , which correspond to energy values of only 20 kJ/mol and 17 kJ/mol , respectively. This stark difference in energy demonstrates that the effect of infrared light on bond breaking is trivial in this context.

In order to assess the potential impact of energy absorption on the reaction rate, we conducted an investigation on the hydrolysis of chemicals, utilizing N-methylformanilide (N-MFA) as a representative compound [1]. Our study involved comparing the reaction kinetics in the presence and absence of infrared (IR) light. It is hypothesized that the absorption of IR light will promote the stretching of both the C=O and C-N bonds, thereby po-

tentially influencing the hydrolysis process and its corresponding kinetics.

Sodium hydroxide was employed as a base to initiate the hydrolysis of N-methylformanilide, leading to the formation of N-methylaniline (N-MA). The distinct UV spectra exhibited by N-methylformanilide and N-methylaniline enable us to effectively track the changes in product concentration throughout the course of the reaction.

Due to the low solubility of N-methylformanilide in water (4.3 mg/L at 25°C), the reactions were conducted in a 1:1 mixture of isopropanol and water. To mitigate the potential influence of temperature on the reaction rate, a water bath was employed to maintain a constant temperature of 25°C throughout the experiment, as the absorption of IR light can raise the solution's temperature. This precautionary measure ensured that any observed changes in the reaction rate could be attributed solely to the presence or absence of IR light, rather than variations in temperature.

To ensure similar temperatures between two vials, 3 mL of a 10 mM N-methylformanilide solution was added to both vials, which were positioned in close proximity within the water bath. To isolate the effect of infrared light, a cardboard divider was inserted between the vials, allowing only one vial to be exposed to the light. Next, 3 mL of a 1 M sodium hydroxide solution was added to each vial. Throughout the experiment, data points were obtained by extracting 100 μL of solution from each vial at regular intervals.

Data collection for this experiment spanned a 4-hour interval, employing the following methodology. At every hour mark, a 100 μL aliquot was extracted from each reaction vial and subsequently diluted with 1.0 mL of the solvent in a scintillation vial. Subsequently, a further dilution was performed by adding the solvent to reach a final volume of 2.0 mL in a new scintillation vial, with 100 μL of the diluted solution being used. The con-

tents of this vial were then transferred to a cuvette to facilitate measurement using a UV-Vis spectroscopy instrument.

The molar absorptivity coefficients for N-methylformanilide and N-methylaniline were calculated using Beer's Law to be 30.01 $\text{cm}^{-1}\text{M}^{-1}$ for N-methylformanilide at 234 nm and 25.61 $\text{cm}^{-1}\text{M}^{-1}$ for N-methylaniline at 242 nm (Figure 1).

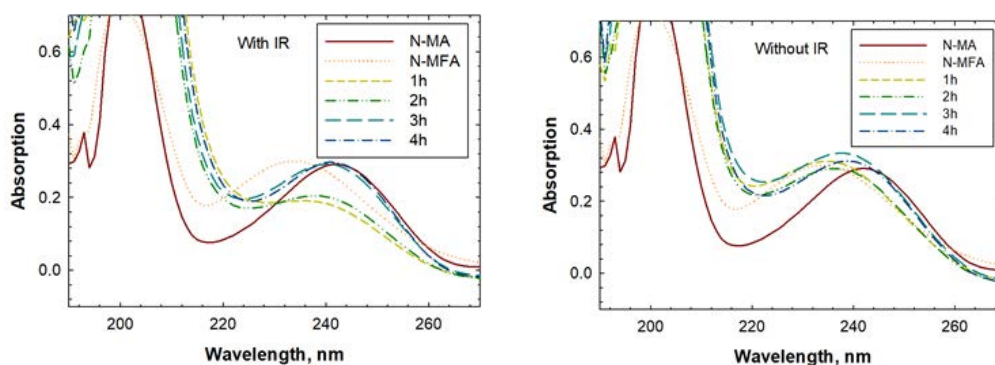


Figure 1: Uv-Visible Absorbance Of N-Methylformanilide During the Hydrolysis for Different Durations of Time in the Presence (Left) And Absence (Right) of Ir Light.

Figure 1 illustrates the observed changes in absorbance peaks at 234 nm and 242 nm, indicating the progress of the hydrolysis reaction in the presence and absence of IR light. These spectral alterations suggest the conversion of N-methylformanilide to N-methylaniline. Throughout the hydrolysis, the peak at 234 nm

gradually diminished and eventually vanished completely, while the peak at 242 nm grew in prominence, becoming the dominant peak at the conclusion of the reaction. Given this, the absorbance at 242 nm served as the basis for calculating the kinetics of the hydrolysis process.

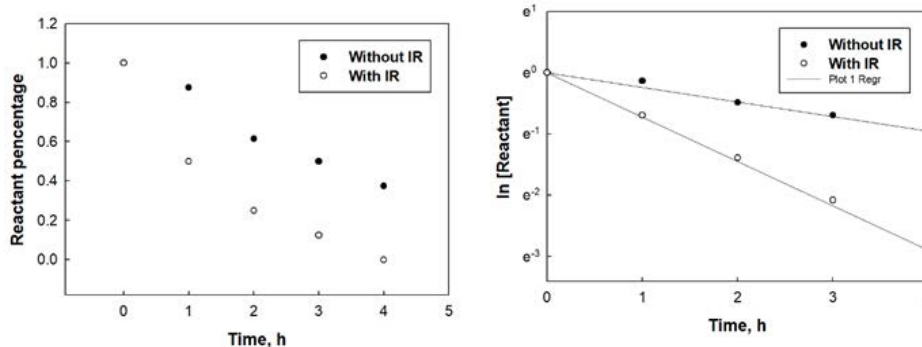


Figure 2: Uv-visible Absorbance of n-ma During the Hydrolysis of n-mfa in the Presence and Absence of ir Light. Graph of $\ln[n\text{-ma}]$ vs. Time Plotted for the First Order Models at 242 nm.

To ascertain the reaction order, various reaction models including zero order, first order, and second order were applied. Figure 2 illustrates that the relationship between the conversion percentage of the product and time aligns well with the first-order reaction model $[\ln(\text{N-MA}) = kt]$, suggesting that the reaction follows first-order kinetics. Subsequently, the reaction rate constants were determined to be $6.6 \times 10^{-5} \text{ s}^{-1}$ and $2.1 \times 10^{-4} \text{ s}^{-1}$ in the presence and absence of IR light, respectively. Notably, the rate of the reaction in the presence of IR light was found to be three times faster compared to the absence of IR light.

in the reaction rate when IR light is present. Although the rate increase observed was not substantial, it signifies the potential for such enhancement. In our experiments, we utilized a broad band of mid-infrared light, exposing both the C=O and C-N bonds to irradiation. In future investigations, it is crucial to explore whether a specific IR wavelength can selectively facilitate the breaking of a single bond. Achieving such selectivity would not only have implications for conventional organic reactions but also for biological systems, such as the targeted cleavage of specific bonds in DNA or proteins [1].

Our preliminary findings have clearly demonstrated an increase

Additionally, an important avenue for study is the effect of re-

actions under near-infrared light, specifically within the range of approximately 14,000–4,000 cm^{-1} . It is anticipated that near-infrared light, with its higher energy compared to mid-infrared irradiation, could further enhance the reaction yield. This represents a promising area of research warranting further exploration [2-4].

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