Solvent-less Substitution Reactions

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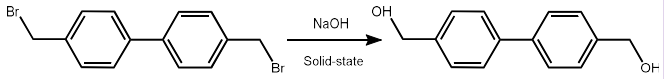
Abstract

Most chemical reactions include the use of solvents. These solvents are often hazardous and proper disposal is very costly. This investigation explores a solid-state substitution reaction from the starting material 4,4'-Bis(bromomethyl)biphenyl. Substitution reactions are commonly used to introduce different functional groups into molecules for use in various applications. This project is significant as it contributes to the green chemistry movement that began in the 1990s, which aims to prevent the generation of hazardous wastes and materials.[1]



Scheme 1. Solid-state S_N2 substitution reaction.

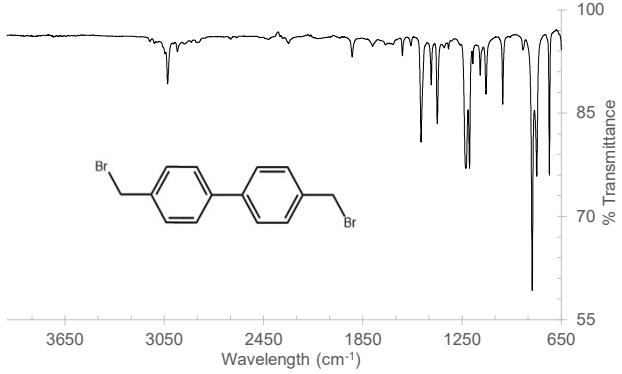


Figure 1. FT-IR spectrum of the starting material 4,4'-bis(bromomethyl)biphenyl.

Results & Discussion

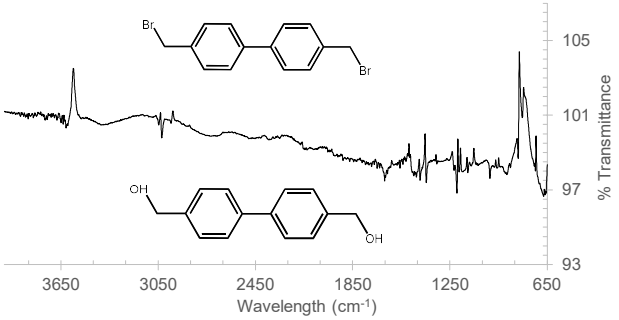


Figure 2. FT-IR subtraction spectra (60 minutes) for the solid-state reaction between 4,4'-bis(bromomethyl)biphenyl and NaOH at 20° Celsius.

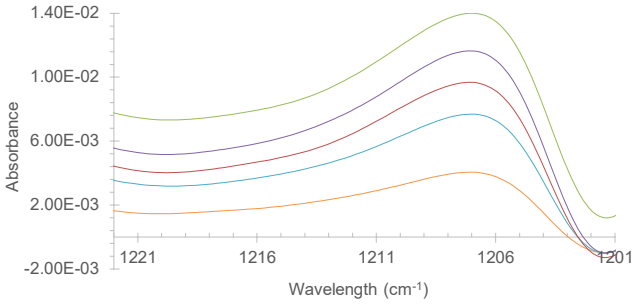


Figure 3. FT-IR spectra monitoring the growth of the peak at 1207 cm^{-1} for the solid-state reaction between 4,4'-bis(bromomethyl)biphenyl and NaOH at 20° C at 0 minutes (orange), 2 minutes (blue), 6 minutes (red), 25 minutes (purple), and 60 minutes (green).

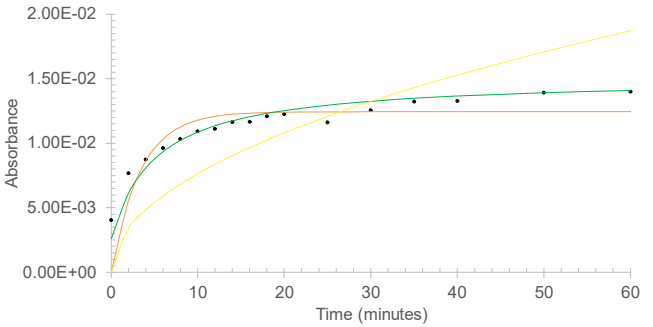


Figure 4. Absorbance as a function of time as seen by growth of the peak at 1207 cm^{-1} for the solid-state reaction of 4,4'-bis(bromomethyl)biphenyl and NaOH at 20°(black) plotted against first order (orange), second order (green) and D1 Diffusion (yellow) rate laws.

Conclusion

- A solid-state reaction between NaOH and 4,4'-Bis(bromomethyl)biphenyl at 20° Celsius was observed.
- Significant peak for C-O stretching was observed at 1207 cm^{-1}
- Equilibrium reached after ≈ 60 minutes.

Future Aims

- Conducting the reaction at different temperatures will allow for rate constants to be determined and an Arrhenius plot to be made for this system.
- Comparison of reaction rates, mechanisms, and activation energies between solventless and traditional solvent-based reactions will be carried out.
- Extending this study to included multiple reactions will allow for a broader view of the mechanisms and feasibility of solid-state reactions.

References

(1) Environmental Protection Agency. (n.d.). Green Chemistry. EPA. (Accessed March 14, 2022). https://www.epa.gov/greenchemistry

Acknowledgements

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