Kinetics Study of Solid-State Oxidation and Reduction

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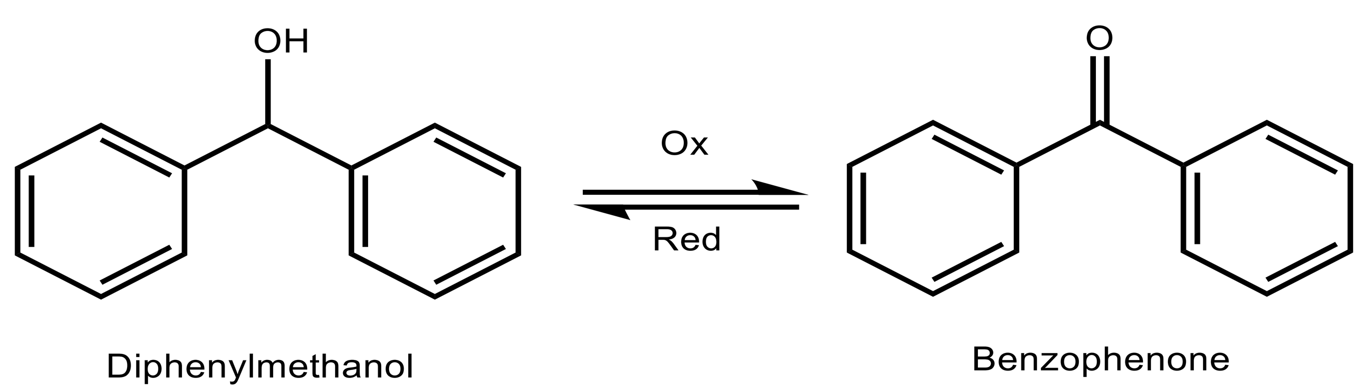
Abstract

In this research we explore the kinetics of the oxidation of diphenylmethanol to benzophenone in the solid-state, monitored via IR spectroscopy. Solvent waste is a leading factor in the financial and environmental costs of synthetic chemistry.[1] Solid-state reactions are of interest to the greater scientific community because they have the potential to significantly minimize solvent waste.



Scheme 1. Solid-state oxidation and reduction reactions between diphenylmethanol and benzophenone

Results And Discussion

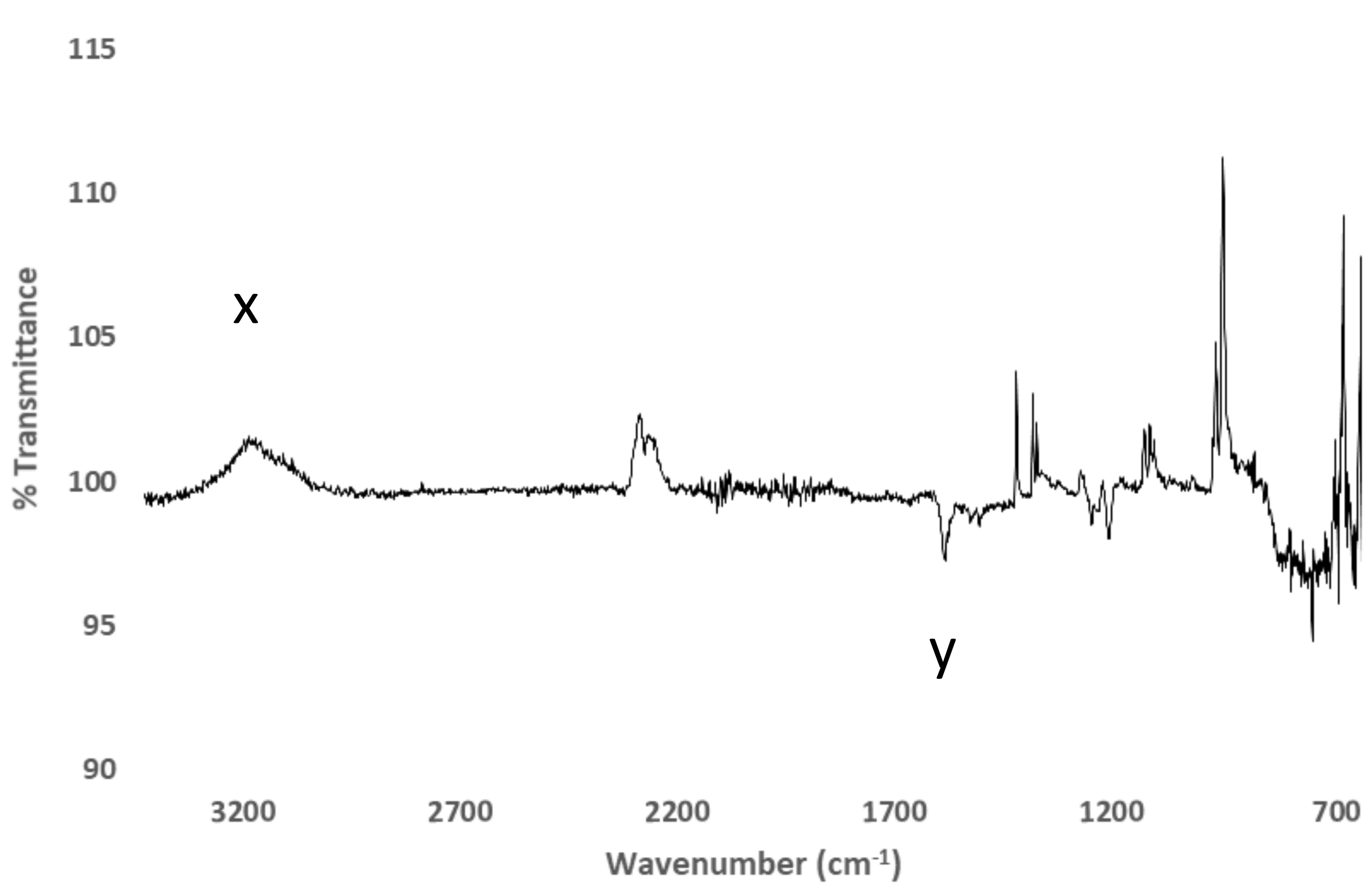


Figure 1. IR subtraction spectrum for the solid-state oxidation of diphenylmethanol to benzophenone. Increase in transmittance in the alcohol region (marked by x) and decrease in transmittance in the carbonyl region (marked by y) indicate the reaction is progressing.

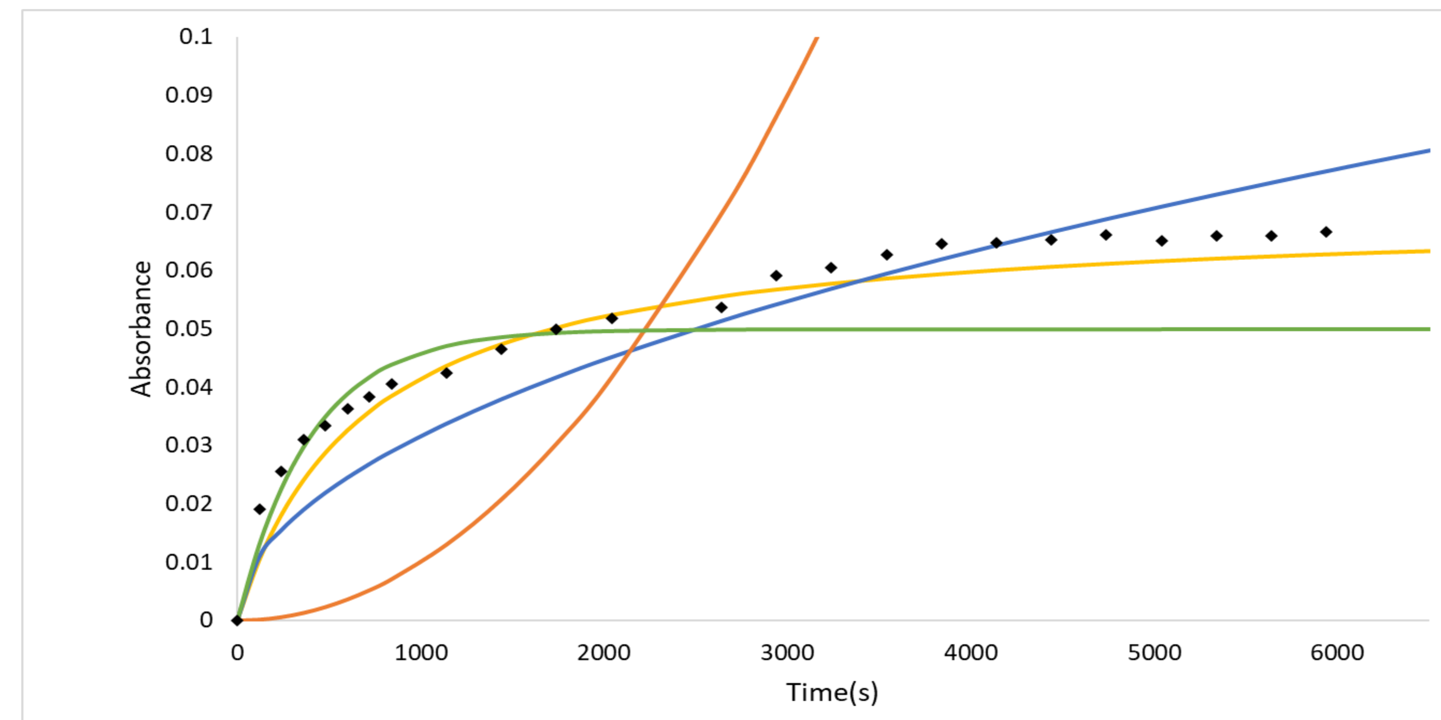


Figure 2. Change in absorbance of the carbonyl peak as a function of time (black (diamonds) plotted against first order (green), second order (yellow), 1D diffusion (blue) and nucleation (orange) rate laws.[2]

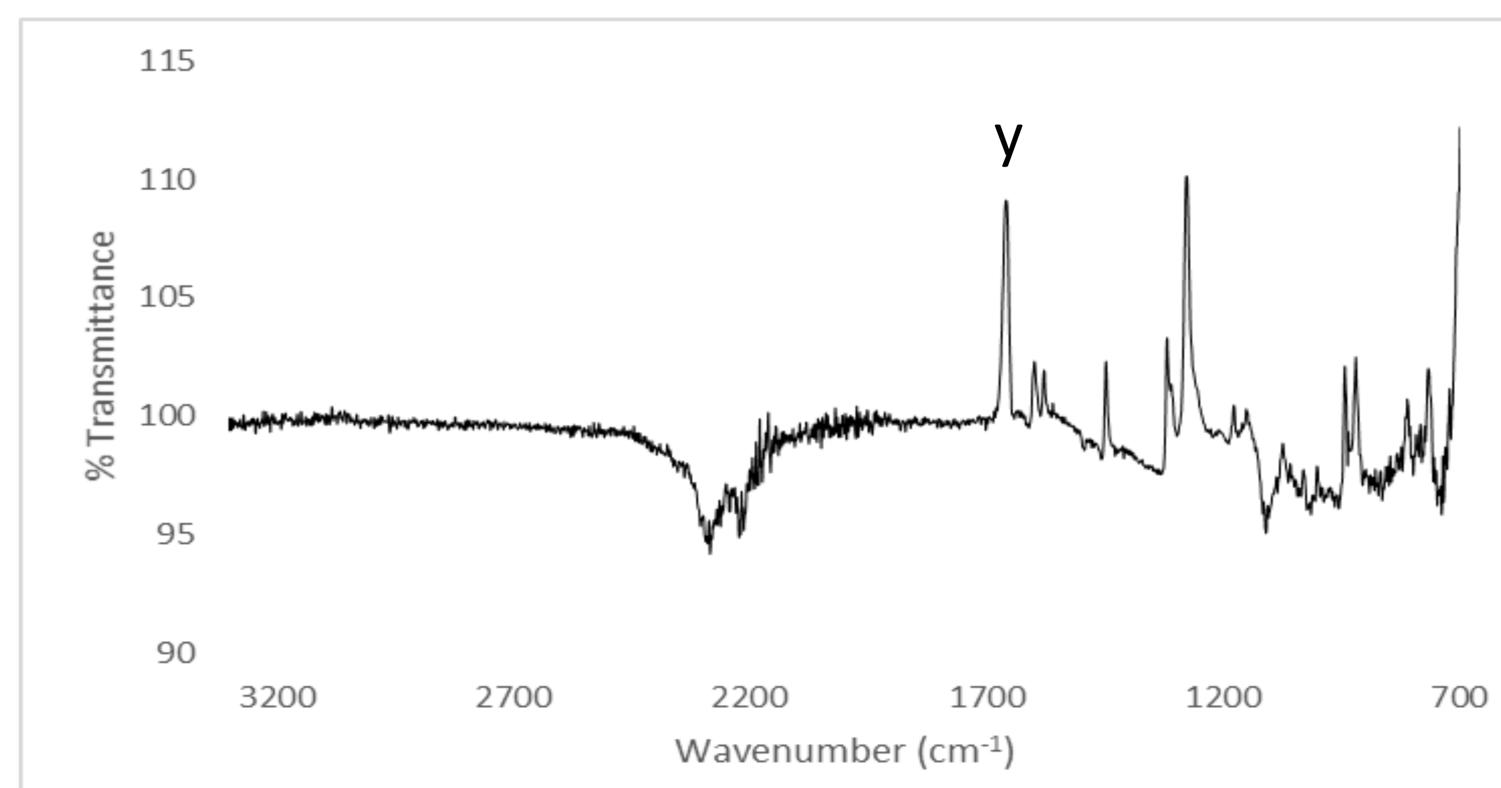


Figure 3. IR subtraction spectrum for the solid-state reduction of benzophenone. Increase in transmittance in the carbonyl region at 1656 cm^{-1} (marked by y) indicates a decrease in the amount of carbonyl present.

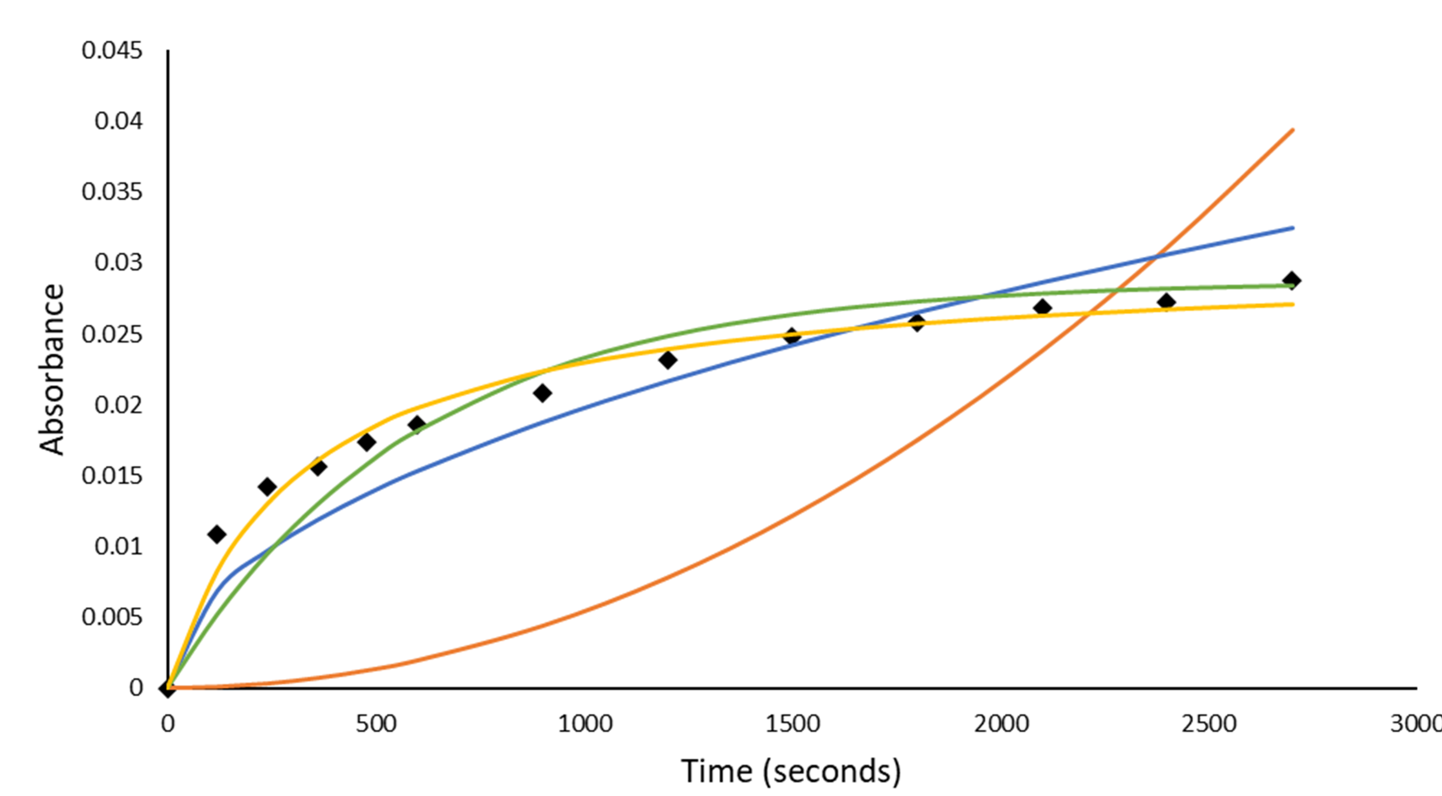


Figure 4. Change in absorbance of the carbonyl peak as a function of time (black diamonds) is plotted against first order (green), second order (yellow), 1D diffusion (blue) and nucleation (orange) rate laws.[2]

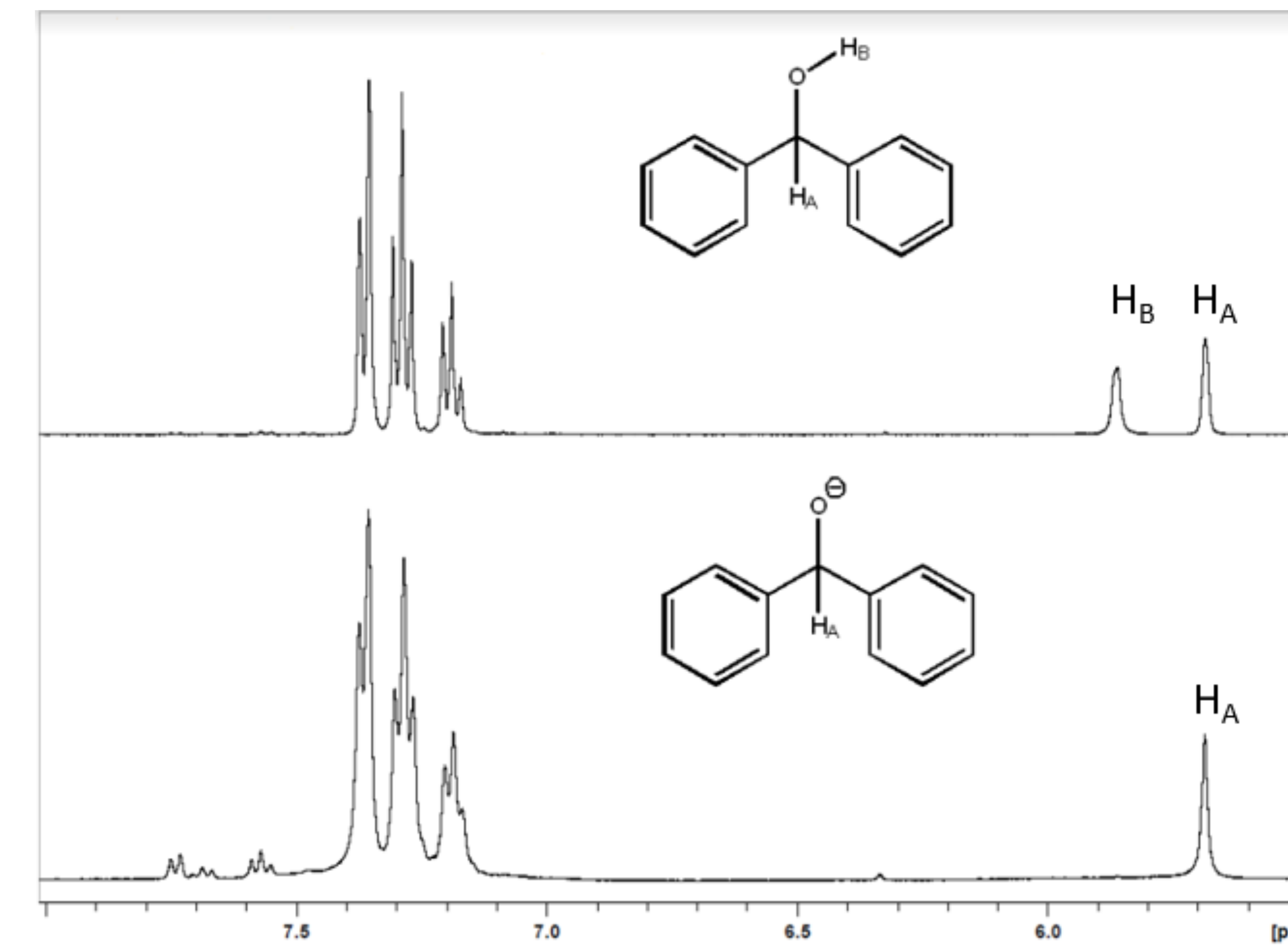


Figure 5. Stacked ^{1}H NMR spectrum (400 MHz, DMSO) of diphenylmethanol (top) and dibenzylmethylene oxide (bottom). Absence of H_B suggests the presence of dibenzylmethylene oxide.

Future Work

- Identify a reagent mixture that successfully oxidizes diphenylmethanol without creating water as a byproduct.
- Optimize reaction conditions for solid-state. reduction of benzophenone to diphenylmethanol
- Compare solid-state and traditional solvent based reaction kinetics mechanisms.

References

1. United States Environmental Protection Agency. Green Chemistry. https://www.epa.gov/greenchemistry (accessed Nov 21, 2019).
2. J. Pharmaceutical Science 2006, v.95, no.3, p 472-498, Basics and applications of solid-state kinetics-A pharmaceutical perspective

Acknowledgements

We would like to thank Caroline Pharr and John Rowley for their guidance on this project and the E.L. Weigand Foundation for funding and resources.