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Functionalization of HMTA and investigation of its catalytic activity in the reaction of CO_2 and epoxide

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In recent years, the conversion of carbon dioxide (CO_2) into valuable compounds has gained significant attention as a way to decrease the green housegas CO_2 [1]. In this study, we focused on the functionalization of hexamethylenetetramine (HMTA) with a halogen and then investigate its catalytic activity for converting CO_2 to cyclic carbonates.

HMTA was converted to $HMTA^+X^-$ where X = I, Cl, Br at mild reaction conditions. The synthesized $HMTA^+X^-$ was used as a catalyst in CO_2 conversion with styrene oxide, aiming to produce styrene carbonate [2], which holds great potential as a green solvent and a useful reactant for generating biodegradable polymers [3]. The reaction conditions, including temperature, catalyst loading, and reaction time were accurately optimized through DOE to achieve the highest yields. The results demonstrated that $HMTA^+X^-$ exhibited remarkable catalytic activity and under optimized conditions, we could achieve a yield of >99% for the formation of styrene carbonate.

In conclusion, our study presents a successful synthesis of a novel HMTA derivative. We investigate its catalytic activity for CO_2 conversion into styrene carbonate, highlighting its potential for sustainable CO_2 utilization. These results contribute to the development of metal-free catalysts and provide insights into the efficient transformation of CO_2 into value-added chemicals [4].

Keywords: HMTA, Carbon dioxide, Carbon Conversion, Catalysis.

References

[1] Pescarmona, Paolo P., and Masoumeh Taherimehr. "Challenges in the catalytic synthesis of cyclic and polymeric carbonates from epoxides and CO 2." *Catalysis Science & Technology* 2, no. 11 (2012): 2169-2187.
[2] Yan, T., Liu, H., Zeng, Z.X. and Pan, W.G., 2023. Recent progress of catalysts for synthesis of cyclic carbonates from CO2 and epoxides. *Journal of CO2 Utilization*, *68*, p.102355.
[3] Taherimehr, Masoumeh. "Study of metal acetylacetonates as catalyst in the reaction of CO2 and styrene oxide to produce styrene carbonate." *Applied Chemistry* 16, no. 61 (2021): 113-124.
[4] Qu, Ye, Yanglin Chen, and Jianmin Sun. "Conversion of CO2 with epoxides to cyclic carbonates catalyzed by amino acid ionic liquids at room temperature." *Journal of CO2 Utilization* 56 (2022): 101840.