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CO_2 Catalytic Reduction: Synthesis of Cyclic Carbonates Catalyzed by 2-aminoacetyl chloride hydrobromide immobilized in Cellulose Nanocrystals

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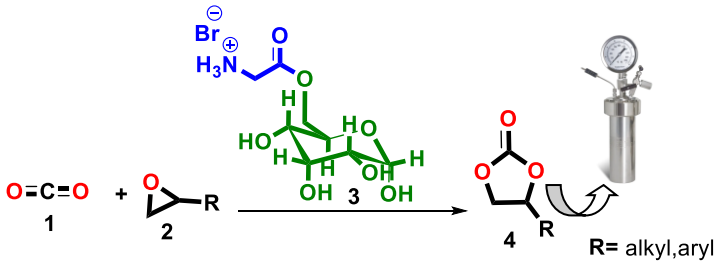
The development of civilization has historically been linked to the use of fossil fuels. The intense exploitation of natural resources through anthropogenic actions has contributed to ever-increasing concentrations of greenhouse gases in the atmosphere (e.g., CO_2), causing climate changes. Within this context, an alternative for CO_2 mitigation is to use it as a synthon for the construction of organic molecules with higher added value (e.g., carbonates, carbamates, methane, light olefins). In the present work, the cycloaddition of CO_2 to epoxides for the formation of cyclic carbonates was evaluated, using cellulose nanocrystals (CNC) immobilized with 2-aminoacetyl chloride hydrobromide. CNC were prepared via 45-minute hydrolysis of eucalyptus bleached cellulose Kraft pulp, using 64% sulfuric acid at 45°C. The reaction was stopped with cold distilled water. The solution was dialyzed for 4 days, sonicated and the resulting CNC suspension was stored at 4°C. CNC were functionalized with 2-aminoacetyl chloride hydrobromide using a 24-hour reflux system in toluene and pyridine. The modified CNC was washed with acetone, dried at 40°C for 72 hours, and chemically characterized using MEV-EDS, XRD, FTIR with KBr, and TGA [**1**]. The synthesized catalyst, immobilized CNC (**3**)**,** was used in the catalytic tests of CO_2 (**1**) cycloaddition to epoxides (**2**) (**Scheme 1**). The catalytic results demonstrated that when using the immobilized CNC, there were conversions between 76-100% of the substrates into their carbonates (**4**). When 1-2 mol% of 2-aminoacetyl chloride hydrobromide was used as a catalyst, only 6-7% of styrene oxide, respectively, was converted into styrene carbonate. However, the reaction using only the CNC in the system with CO_2 and styrene oxide, styrene carbonate was not formed. The results using the immobilized CNC are exciting because they demonstrate the importance of using the combination of two organic materials (cellulose and an amino acid derivative) so that the cycloaddition reaction of CO_2 to epoxides can occur selectively for the formation of the respective carbonates.

Scheme 1- Synthesis of cylic carbonates from CO_2 with various epoxides [a,b,c]



[a]**Reaction Conditions: 1:** CO_2 pressure (8 bar); **2:** 5 mmol; **3:** 30 wt% with respect to substrate; 24h at 120°C; [b]Conversion determined by ^1H NMR spectroscopy analysis of crude reaction mixture ($CDCl_3$, 500 MHz); [c] The synthesis made within a Parr reactor model.

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References: [**1**] Z. Wu *et al*., Cellulose, **25**, 4905–4918, (2018); [**2**] W. Bezerra *et al*., Molecular Catalysis, **530** 112632, (2022).