

Electronic Supplementary Information (ESI)

An Efficient Atom-Economical Chemoselective CO₂ Cycloaddition using Lanthanum Oxide/Tetrabutyl Ammonium Bromide

Abdussalam K. Qaroush,^{a*} Fatima A. Alsoubani,^b Ala'a M. Al-Khateeb,^b Enas Nabih,^b Esraa Al-Ramahi,^b Mohammad F. Khanfar,^c Khaleel I. Assaf,^d Ala'a F. Eftaiha^{*b}

^a Department of Chemistry, Faculty of Science, The University of Jordan, Amman 11942, Jordan.

^b Department of Chemistry, The Hashemite University, P.O. Box 150459, Zarqa 13115, Jordan.

^c Pharmaceutical and Chemical Engineering Department, German Jordanian University, P.O. Box 35247 Amman 11180, Jordan.

^d Department of Life Sciences and Chemistry, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany.

Corresponding author E-mails:

A.K.Q: a.qaroush@ju.edu.jo

A.F.E: alaa.eftaiha@hu.edu.jo

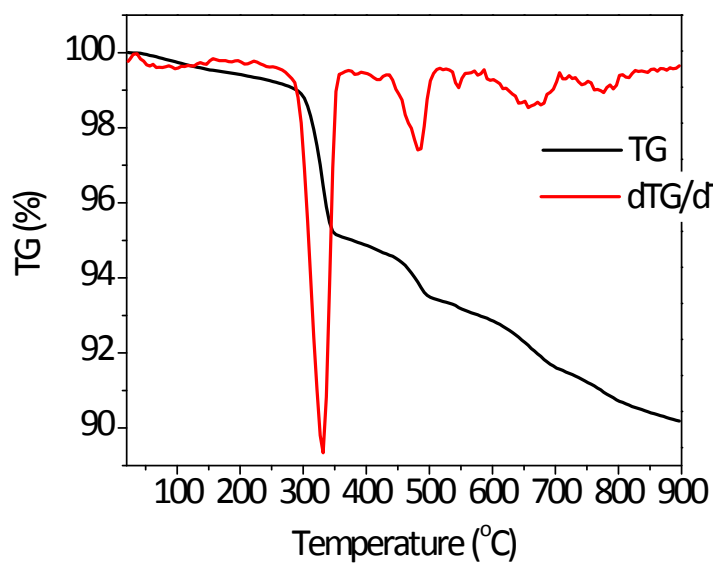


Figure S1. Thermogravimetric pattern of La_2O_3 .

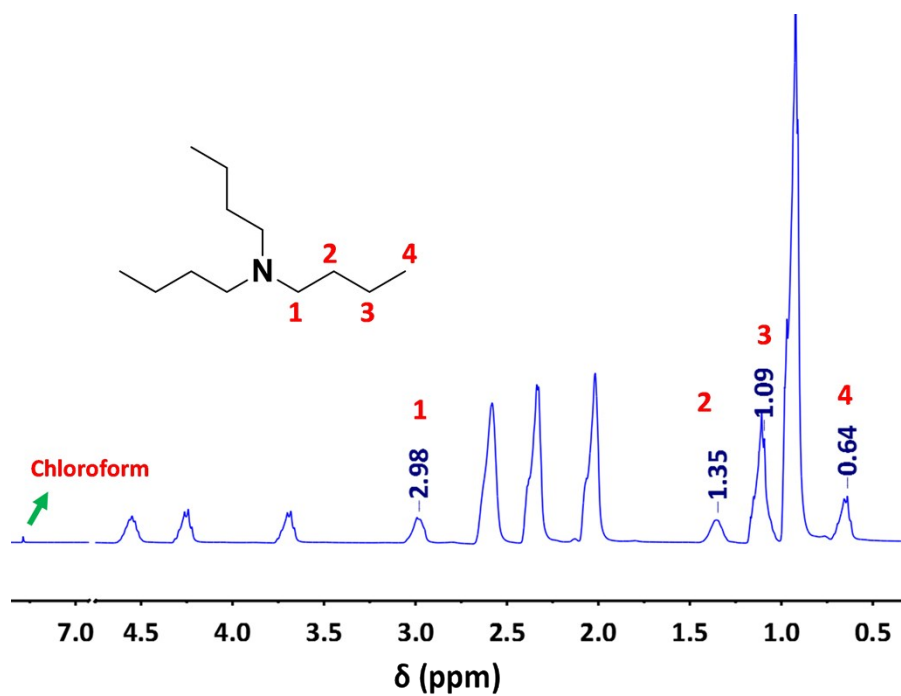


Figure S2. Partial ^1H -NMR spectrum of a reaction mixture indicating the formation of tributylamine (TBA) as a decomposition product of TBAB.

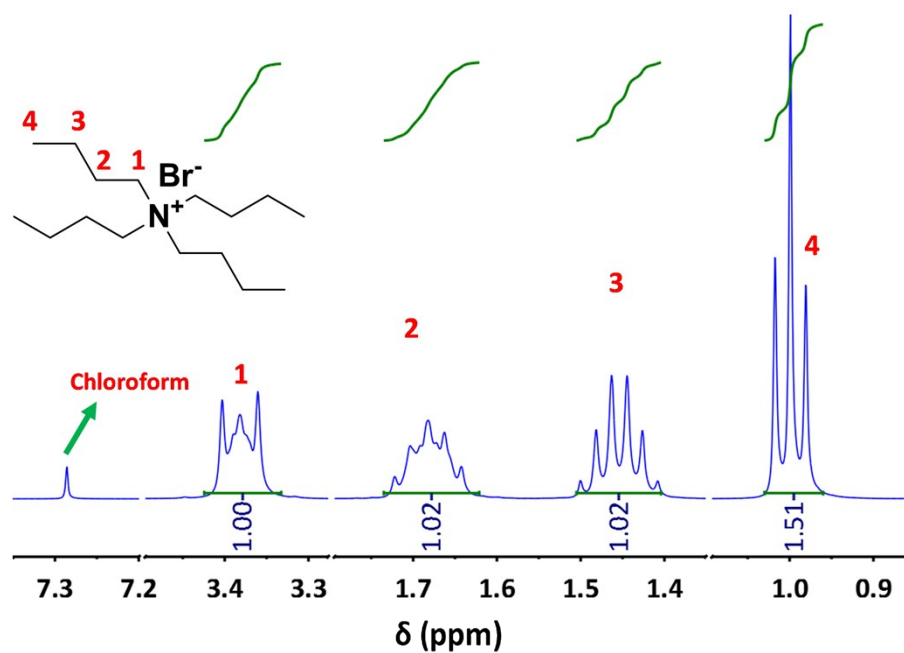


Figure S3. Partial ^1H -NMR spectrum of tetrabutylammonium bromide (TBAB).

Table S1. Turnover numbers (TONs) and turnover frequencies (TOFs) of the investigated binary catalytic system

<i>Time (h)</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>6</i>	<i>9</i>	<i>24</i>
TON (mol PC/mol La_2O_3)	18.6	36.2	38.5	55.5	66.3	69.8
TOF (mol PC/mol $\text{La}_2\text{O}_3 \cdot \text{h}$)	18.6	18.1	12.8	9.2	7.4	2.9

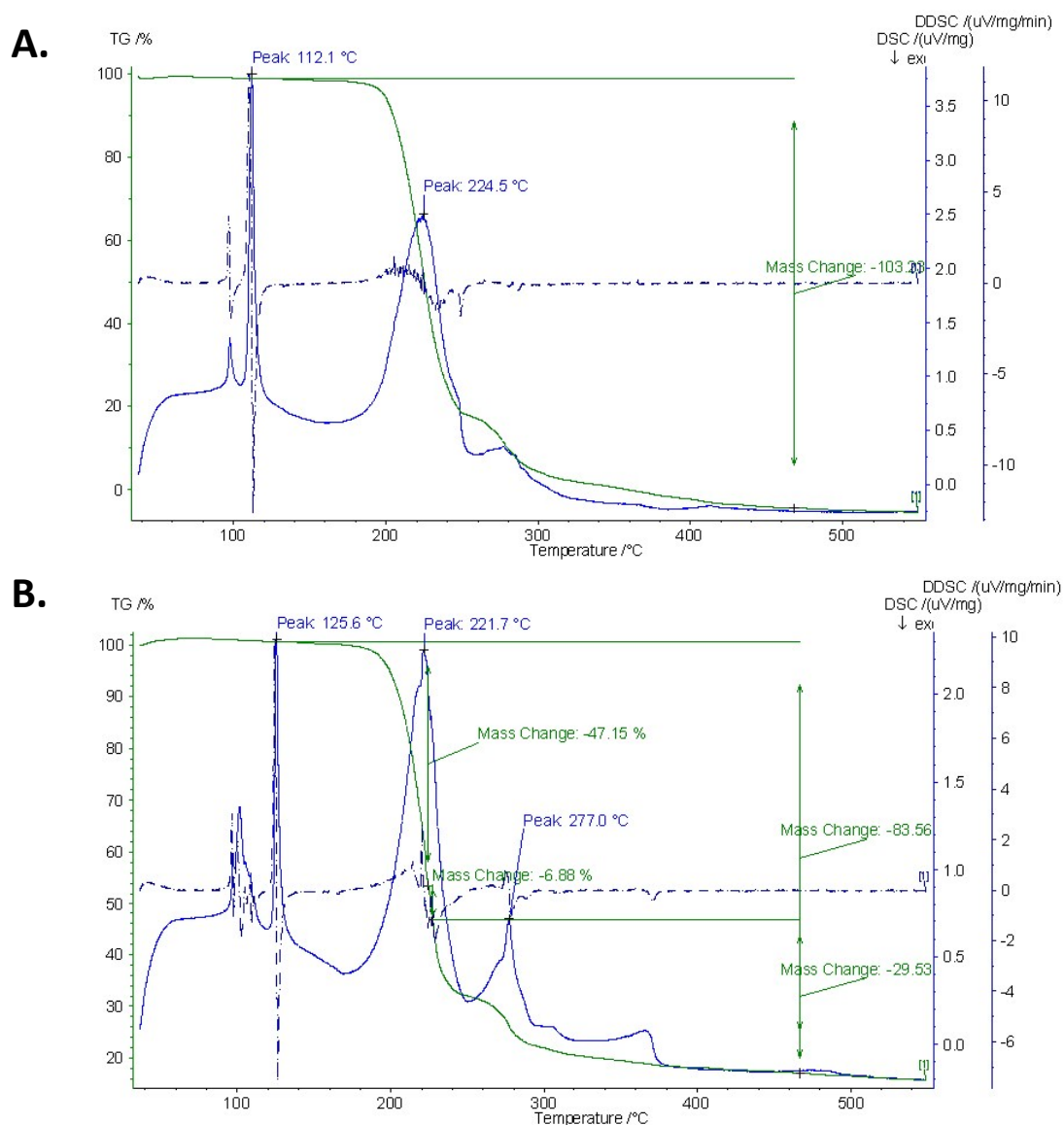


Figure S4. Thermogravimetric patterns of: **A.** TBAB. **B.** La₂O₃/TBAB (1:4). Upon addition of the La-precursor, TBAB decomposition was further suppressed (Decomposition temperature (T_d) increased from 112.1 to 126 °C).

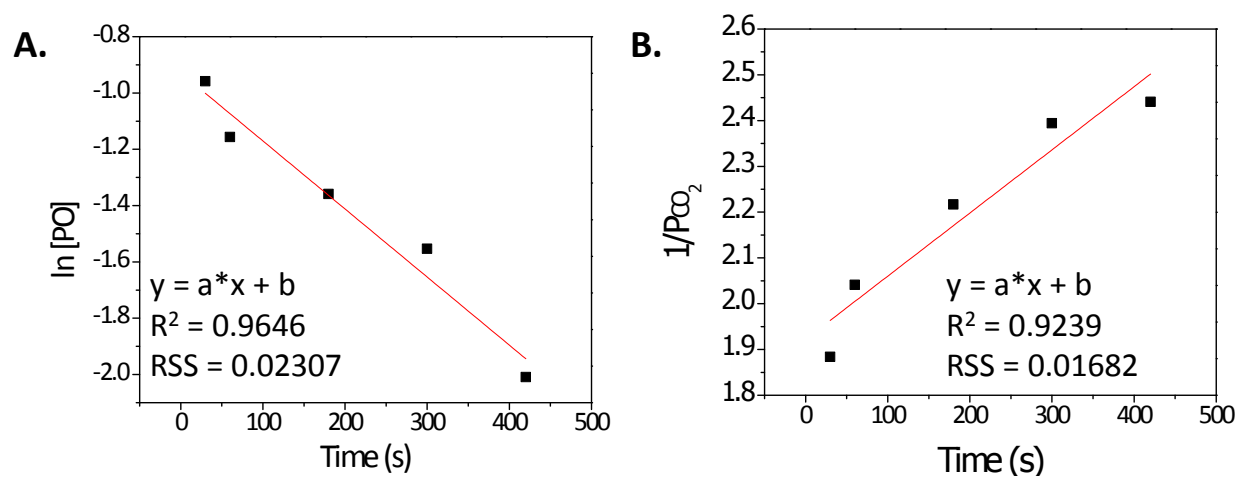


Figure S5. Plots of: **A.** $\ln [\text{PO}]$ versus time and **B.** $1/\text{PCO}_2$ against time for the cycloaddition reaction.

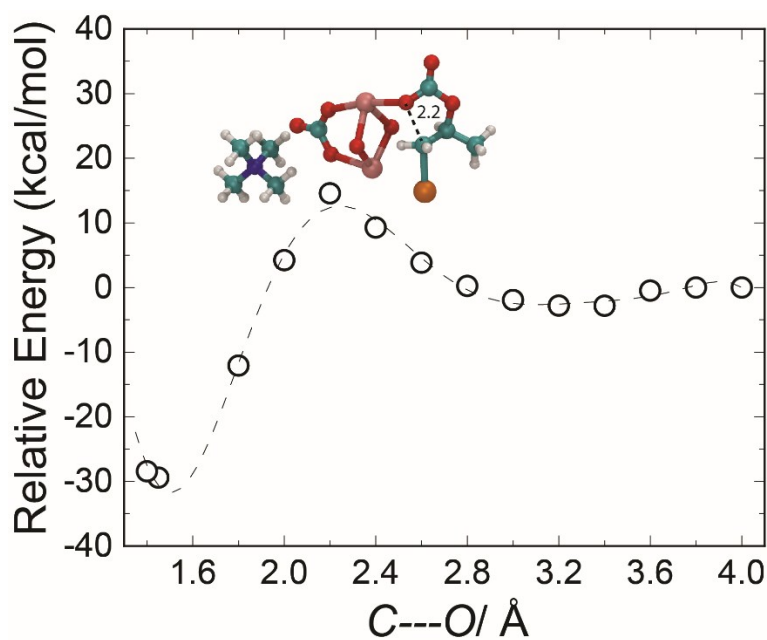


Figure S6. Energy profile for the ring-closing as a function of C---O bond distance.