CO₂ Activation throughout C-N, C-O and C-C Bond Formation

Ala'a F. Eftaiha,^{*a} Abdussalam K. Qaroush,^{*b} Ibrahim K. Okashah,^c Fatima Alsoubani,^a Jonas

Futter,^d Carsten Troll,^d Bernhard Rieger,^d and Khaleel I. Assaf,^{*c}

^aDepartment of Chemistry, The Hashemite University, P.O. Box 150459, Zarqa 13115, Jordan. E-mail: <u>alaa.eftaiha@hu.edu.jo</u> ^bDepartment of Chemistry, Faculty of Science, The University of Jordan, Amman 11942, Jordan. E-mail: <u>a.qaroush@ju.edu.jo</u>

^cDepartment of Chemistry, Faculty of Science, Al-Balqa Applied University, Al-Salt 19117, Jordan. E-mail: khaleel.assaf@bau.edu.jo

^dWACKER-Lehrstuhl für Makromolekulare Chemie, Technische Universität München, Lichtenbergstraße 4, 85747, Garching bei München, Germany

Electronic Supporting Information

	A. O	B. OH	C. NH ₂
	(⊂ C=O)	(⊂CH-OH)	(⊂CH-NH₂)
Physical appearance	Colorless liquid	Colorless, viscous liquid	Clear to yellowish liquid
Density (g/mL)	0.9478	0.9624	0.8647
Boiling point (°C)	155.6	161.8	134.5
р <i>К</i> а	n.a.	16	10.64

Scheme S1. The chemical structure and the corresponding physical properties of: A. cyclohexanone (\subset C=O), B. cyclohexanol (\subset CH-OH) and C. cyclohexylamine (\subset CH-NH₂).



Figure S1. DEPT-135 spectrum of \subset C=O/DBU mixture after bubbling CO₂. The peaks labeled in *red* designate the enol and carboxylate carbons.



Figure S2. ¹H NMR spectrum of \subseteq C=O/DBU mixture after bubbling CO₂.



Figure S3. ¹H NMR spectrum of \subseteq CH-OH/DBU mixture after bubbling CO₂.



Figure S4. The ATR-FTIR spectra of \subseteq CH-NH₂ (*black*), \subseteq CH-NH₂ /DBU before (*red*) and after (*blue*) bubbling CO₂



Figure S5. ¹³C NMR spectra of DMSO- d_6 solutions of: **A.** \subseteq C=O/DBU, **B.** \subseteq CH-OH/DBU and **C.** \subseteq CH-NH₂/DBU after bubbling CO₂.

Element	% Expected	% Found
С	64.43	63.04
Н	10.81	9.77
N	11.56	11.11

Table S1. CHN results of [\subseteq CH-NH-C(=O)O]⁻[\subseteq CH-NH₃]⁺ obtained from EA.