Supporting Information for

Comparison of Solvation Effects on CO_2 Capture with Aqueous Amine Solutions and Amine-Functionalized Ionic Liquids

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Table S1. Cartesian Coordinates for the Transition State Optimized at the SMD/IEF-PCM/B3LYP/6-311++G(d,p) Level in Figure 1a: MEA + CO_2.

Atom	Coordinates (Å)		
N	−0.006800	1.126662	−0.594860
C	1.646799	−0.125133	0.077052
O	1.724464	0.198239	1.208409
O	1.934790	−0.708619	−0.907346
C	−1.235351	1.026535	0.214351
C	−2.028578	−0.234796	−0.087160
O	−1.363543	−1.451646	0.293987
H	−0.210940	0.969548	−1.579953
H	−2.956925	−0.205181	0.486079

H	−2.287865	−0.271682	−1.151438
H	−0.703601	−1.667803	−0.375359
H	0.393651	2.057385	−0.507688
H	−0.950147	1.046285	1.270010
H	−1.899474	1.881389	0.036512

Table S2. Cartesian Coordinates for the Transition State Optimized at the SMD/IEF-PCM/B3LYP/6-311++G(d,p) Level in Figure 1b: Gly^{-} + CO_2.

Atom	Coordinates (Å)		
C	−0.670745	0.461645	0.151732
H	−0.497624	1.246547	−0.589871
H	−0.562815	0.930692	1.132817
C	−2.134267	0.003669	0.004383
O	−3.008370	0.908394	0.149159
O	−2.371408	−1.208479	−0.250399
N	0.358242	−0.565967	0.002174
H	0.282078	−1.258711	0.742628
H	0.226967	−1.066038	−0.874189
C	2.483871	0.123634	−0.021935
O	2.350111	1.266424	−0.265736
O	3.025986	−0.894390	0.213017

Table S3. Cartesian Coordinates for the Transition State Optimized at the SMD/IEF-PCM/B3LYP/6-311++G(d,p) Level in Figure 1c: 2-CNpyr$^-$ + CO_2.

Atom	Coordinates (Å)		
C	2.274275	−0.384233	0.053809
N	−0.015133	−0.496420	−0.071660
C	0.490490	−1.746957	−0.036316
C	1.893566	−1.735245	0.039264
C	1.073743	0.349091	−0.015394
H	−0.166663	−2.606727	−0.063469
H	2.545339	−2.597068	0.080089
H	3.272288	0.027462	0.106704
C	−2.199780	−0.077297	0.019166
O	−2.605259	−1.179424	−0.031047
O	−2.205037	1.096032	0.087670
C	0.944204	1.749630	−0.028318
N	0.868336	2.912640	−0.038279

Table S4. Conversion from IRC to C–N Distance in Figure 1 (a) MEA + CO_2, (b) Gly$^-$ + CO_2, and (c) 2-CNpyr$^-$ + CO_2.

IRC (amu$^{1/2}$Bohr)	C–N distance (Å)		
	(a)	(b)	(c)
−5.0	2.9	2.9	2.8
−2.5	2.6	2.6	2.6
0	2.2	2.2	2.2
2.5	1.7	1.8	1.8
5.0	–	1.6	1.5

Table S5. Dipole Moments of Reactants, Transition States, and Products in Figures 3-5. [a]

Reaction	μ (Debye)		
	Rea	TS	Pro
(a) MEA + CO_2	3.51	5.00	9.18
(b) Gly^- + CO_2	12.6	9.46	4.16
(c) 2-$CNpyr^-$ + CO_2	4.06	3.55	8.64

[a] Calculated at CCSD(T)/6-311++G(d,p) in vacuum.