Supporting Information for

How the presence of CO_2 absorption promoters and composition of the choline chloride/amine/molecular solvent mixtures influence its thermophysical properties and ability to absorb carbon dioxide

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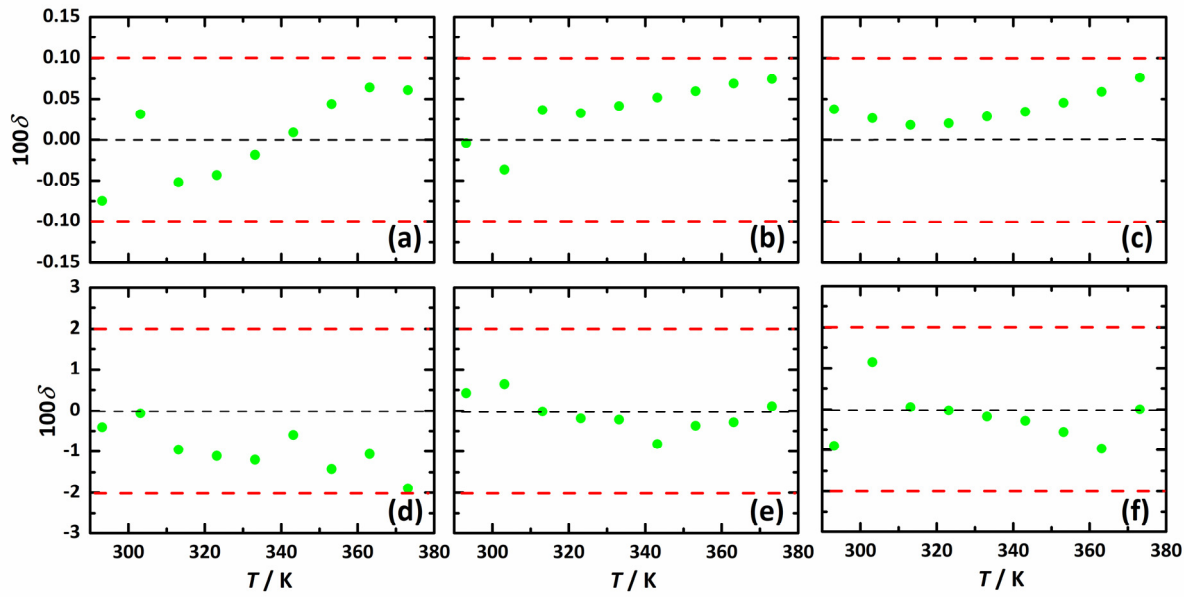

Figure S1. Relative deviation ($\delta = (Y^{exp} - Y^{fit})/ Y^{fit}$) of experimentally obtained data (Y^{exp}) from the fit (Y^{fit}) of density (a-c) and viscosity (d-f) for the calibration standards N7.5 (a, d), N26 (b, e) and N415 (c, f) within the temperature range of T = (293.15 to 373.15) K. Fit data (Y^{fit}) were obtained by fitting the density and viscosity data provided by the supplier for the delivered oil batches with eqs. 3 and 8, respectively. Black dash line indicates zero; red dash lines correspond to the estimated uncertainties, see manuscript.

Table S1. Remaining Water Content (w_{H_2O})[a] in the Mixtures of Row-I and Row-II[b]

Series I		Series II	
System	w_{H_2O} (ppm)	System	w_{H_2O} (ppm)
I-MEA/EG	809 ± 34	II-MEA/EG	735 ± 13
I-DEA/EG	567±28	II-MEA/EG/TMG	678 ± 22
I-EDA/EG	765 ± 41	II-MEA/EG/DBU	548 ± 31
I-TEA/EG	602 ± 17	II-MEA/EG/PP	604 ± 24
I-MEA/DMSO	378 ± 35		

[a]An average of 7-9 measurements with a standard deviation; mass fraction ($w_{H_2O} = m_{H_2O}/m_{sample}$).[b] Standard uncertainty for mole fraction estimation is$u(x_i)$ = 0.001.

Table S2. CO_2 absorption capacity (m_{CO_2}) of the15 and 30 wt.% aqueous MEA solution and NH_3 absorption capacity of the DES composed of NH_4SCN and glycerol mixed in a mole ratio of 2:3 at temperatures (T) and P = 0.1 MPa.[a]

Absorption capacity[b]	m_{gas}	P	T	Ref.	m_{CO_2}[c,d]	Average[c,d]
15% aqueous MEA solution + CO_2						
504.6 g_{CO_2}/kg_{MEA}	1.719	101.3	298.15	1f	1.73	
0.742 mol_{CO_2}/mol_{MEA}(2.5 N)[e]	1.82	100	298.15	2g		
0.673 mol_{CO_2}/mol_{MEA}(2.5 N)[e]	1.65	100	313.15	2g	1.62	
30% aqueous MEA solution + CO_2						
453.0 ±16.3 g_{CO_2}/kg_{MEA}	3.1 ± 0.1	101.3	298.15	1f	1) 3.07	
0.663 mol_{CO_2}/mol_{MEA}	3.25	100	298.15	2g	2) 3.04	3.05 ± 0.02
0.694mol_{CO_2}/mol_{MEA}	3.39	100	298.15	3g	3) 3.05	
0.603 mol_{CO_2}/mol_{MEA}	2.96	100	313.15	2g	1) 2.99	
0.646 mol_{CO_2}/mol_{MEA}	3.17	110	313.15	3g	2) 3.00	2.99 ± 0.01
0.594 mol_{CO_2}/mol_{MEA}	2.92	101.3	313.15	4g	3) 2.98	
[NH_4SCN:Gly = 2:3] + NH_3						
10.36mol_{NH_3}/kg_{DES}	10.36	101.3	313.15	5f	1) 10.41	
10.35 mol_{NH_3}/kg_{DES}	10.35	100.0	313.15	6f	2) 10.36 3) 10.38	10.38 ± 0.03

[a]Units are $mol_{gas}/kg_{solution}$for m_{CO_2}; K for T; MPa for P; for the data obtained in the present work, standard uncertainties are $u(P)$ = 100 Pa for P, $u(T)$ = 0.02 K for T and $u(100w_{MEA})$ = 0.01 for $100w_{MEA}$. [b]Units provided in the original papers; [c]This work. [d]The relative expanded uncertainty for absorption capacity is $U_r(m_{CO_2})$ = 0.05 (0.95 level of confidence)for the data obtained in the present work. [e]The actual mass fraction is 15.25 wt %. [f]Results of gravimetric measurements. [g]Results of volumetric measurements.

Table S3. Density (ρ) of the mixtures composed of MEA (1), EG (2) and ChCl (3) with $x_1 = 0.667$, $x_2 = 0.222$, and $x_3 = 0.111$ for Series I and $x_1 = 0.222$, $x_2 = 0.667$, and $x_3 = 0.111$ additionally containing 5 wt.% of such additives as TMG, H_2O, DBU and PP for Series II at Temperatures (T) and P = 0.1 MPa.[a]

T / K	283.15	288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15	338.15	343.15	348.15	353.15
System	**Series I: $x_1 = 0.667$, $x_2 = 0.222$, and $x_3 = 0.111$**														
I-MEA/EG			1.10139	1.09812	1.09485	1.0916	1.08835	1.08508	1.08183	1.07858	1.07536	1.07207	1.06882	1.06556	1.06225
I-DEA/EG	1.11275	1.10852	1.10544	1.10242	1.09938	1.09631	1.09329	1.09024	1.08716	1.08409	1.08099	1.07787	1.07471	1.07053	1.06733
I-EDA/EG	1.01614	1.01166	1.00759	1.00357	0.99955	0.99554	0.99152	0.98749	0.98347	0.97945	0.97544	0.9714	0.96738	0.96335	0.95965
I-TEA/EG	1.07216	1.06745	1.06345	1.06057	1.05654	1.05264	1.04875	1.04488	1.04103	1.03718	1.03334	1.0295	1.02565	1.02179	1.01795
I-MEA/DMSO	1.06064	1.05684	1.05332	1.04982	1.04631	1.04282	1.03932	1.03581	1.03231	1.02881	1.02531	1.0218	1.01828	1.01476	--
I-MEA/H_2O	1.13142	1.12876	1.12602	1.12332	1.12058	1.11778	1.11497	1.11215	1.10937	1.10613	1.10323	1.10032	1.09741	1.09445	1.09151
System	**Series II: $x_1 = 0.222$, $x_2 = 0.667$, and $x_3 = 0.111$ + 5 wt.% of additives**														
II-MEA/EG			1.10139	1.09812	1.09485	1.0916	1.08835	1.08508	1.08183	1.07858	1.07536	1.07207	1.06882	1.06556	1.06225
II-MEA/EG/TMG	1.10345	1.09994	1.09649	1.09307	1.08967	1.08624	1.08282	1.07939	1.07639	1.07377	1.07039	1.06701	1.06354	1.06009	1.05659
II-MEA/EG/H_2O	1.10481	1.10147	1.09826	1.09501	1.09176	1.08851	1.08525	1.08198	1.0787	1.07543	1.07217	1.06888	1.06558	1.06229	1.05893
II-MEA/EG/DBU	1.10655	1.10273	1.09933	1.09597	1.09261	1.08926	1.08587	1.08249	1.07912	1.07579	1.07245	1.06913	1.06581	1.06248	1.05914
II-MEA/EG/PP	1.10541	1.10116	1.09786	1.09459	1.0913	1.08799	1.08469	1.08139	1.07806	1.07478	1.07146	1.06817	1.0649	1.06155	1.05818

[a]Standard uncertainties are $u(x_i) = 0.001$, $u(T) = 0.01$ K and $u(P) = 10$ kPa. The relative expanded uncertainty is $U_r(\rho) = 0.001$ (0.95 level of confidence).

Table S4. Density (ρ) of the mixtures composed of MEA (1), EG (2) and ChCl (3) with $x_1 = 0.667$, $x_2 = 0.222$, and $x_3 = 0.111$ for Series I and $x_1 = 0.222$, $x_2 = 0.667$, and $x_3 = 0.111$ additionally containing 5 wt.% of such additives as TMG, H_2O, DBU and PP for Series II at Temperatures (T) and P = 0.1 MPa after complete CO_2 saturation.[a]

T / K	283.15	288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15	338.15
System	**Series I: $x_1 = 0.667$, $x_2 = 0.222$, and $x_3 = 0.111$**											
I-MEA/EG			1.21982	1.21782	1.21488	1.21188	1.20896	1.20615				
I-DEA/EG		1.2275	1.2244	1.2213	1.2181	1.2148	1.2117	1.2085	1.2069			
I-TEA/EG	1.21062	1.20777	1.20484	1.20195	1.19902	1.19602	1.19302	1.19				
I-MEA/DMSO	1.23118	1.22809	1.22484	1.22158	1.2183	1.21491	1.21172	1.20863	1.20541	1.20211		
I-MEA/H_2O	1.23857	1.23583	1.2329	1.22993	1.22688	1.224	1.22132	1.21853	1.21583	1.2131	1.21034	1.20766
System	**Series II: $x_1 = 0.222$, $x_2 = 0.667$, and $x_3 = 0.111$ + 5 wt.% of additives**											
II-MEA/EG			1.16141	1.15832	1.15525	1.15214	1.14904	1.14588				
II-MEA/EG/TMG	1.16498	1.16227	1.15915	1.15605	1.15291	1.14975	1.14653					
II-MEA/EG/H_2O	1.1658	1.16283	1.1598	1.15671	1.15362	1.15046	1.14689					
II-MEA/EG/DBU	1.16785	1.16369	1.16054	1.15924	1.15623	1.15313	1.15001	1.14685				
II-MEA/EG/PP	1.17944	1.17575	1.17272	1.16966	1.16656	1.16344	1.16029	1.15679				

[a]Standard uncertainties are $u(x_i) = 0.001$, $u(T) = 0.01$ K and $u(P) = 10$ kPa. The relative expanded uncertainty is $U_r(\rho) = 0.001$ (0.95 level of confidence).

Table S5. Viscosity (η) of the mixtures composed of MEA (1), EG (2) and ChCl (3) with $x_1 = 0.667$, $x_2 = 0.222$, and $x_3 = 0.111$ for Series I and $x_1 = 0.222$, $x_2 = 0.667$, and $x_3 = 0.111$ additionally containing 5 wt.% of such additives as TMG, H_2O, DBU and PP for Series II at Temperatures (T) and P = 0.1 MPa.[a]

T / K	283.15	288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15	338.15	343.15	348.15	353.15
System	**Series I: $x_1 = 0.667$, $x_2 = 0.222$, and $x_3 = 0.111$**														
I-MEA/EG			55.2	42.3	33.1	26.1	20.9	17.0	14.0	11.6	9.81	8.32	7.14	6.18	5.40
I-DEA/EG	852	576	395	276	197	144	107	80.8	62.1	48.4	38.4	30.7	24.9	20.5	17.0
I-EDA/EG	36.6	27.9	21.4	16.8	13.4	10.9	8.91	7.46	6.25	5.36	4.59	4.01	3.52	3.10	2.70
I-TEA/EG	39.6	30.6	23.7	18.6	15.0	12.3	10.1	8.51	7.17	6.19	5.32	4.68	4.11	3.64	3.23
I-MEA/DMSO	81.7	60.2	44.7	34.1	26.6	21.0	16.8	13.7	11.3	9.40	7.88	6.76	5.81	5.04	
I-MEA/H_2O	860	574	394	277	200	147	110	84.5	65.8	52.1	41.9	33.9	27.9	23.2	19.5
System	**Series II: $x_1 = 0.222$, $x_2 = 0.667$, and $x_3 = 0.111$ + 5 wt.% of additives**														
II-MEA/EG			37.0	29.7	24.1	19.8	16.4	13.7	11.6	9.89	8.53	7.38	6.46	5.69	5.01
II-MEA/EG/TMG	70.8	53.9	41.4	32.6	26.1	21.1	17.3	14.3	12.3	10.4	8.87	7.62	6.61	5.78	5.05
II-MEA/EG/H_2O	45.2	35.8	28.3	22.7	18.5	15.2	12.6	10.7	9.00	7.76	6.67	5.84	5.12	4.52	3.99
II-MEA/EG/DBU	74.4	56.9	43.8	34.6	27.8	22.5	18.4	15.3	12.8	10.8	9.26	7.96	6.91	6.05	5.29
II-MEA/EG/PP	79.5	60.9	46.8	36.9	29.5	23.8	19.4	16.0	13.4	11.3	9.62	8.24	7.13	6.22	5.47

[a]Standard uncertainties are $u(x_i) = 0.001$, $u(T) = 0.01$ K and $u(P) = 10$ kPa. The relative expanded uncertainty is $U_r(\eta) = 0.02$ (0.95 level of confidence).

Table S6. Viscosity (η) of the mixtures composed of MEA (1), EG (2) and ChCl (3) with $x_1 = 0.667$, $x_2 = 0.222$, and $x_3 = 0.111$ for Series I and $x_1 = 0.222$, $x_2 = 0.667$, and $x_3 = 0.111$ additionally containing 5 wt.% of such additives as TMG, H_2O, DBU and PP for Series II at Temperatures (T) and P = 0.1 MPa after complete CO_2 saturation.[a]

T / K	283.15	288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15	338.15
System	**Series I: $x_1 = 0.667$, $x_2 = 0.222$, and $x_3 = 0.111$**											
I-MEA/EG			4384	2865	1938	1325	917	662				
I-DEA/EG		12724	7892	5021	3293	2211	1503	1066	799			
I-TEA/EG	20111	12192	6878	4300	2762	1826	1224	857	602	438		
I-MEA/DMSO	17085	9639	5955	3742	2477	1665	1135	808	576	425	316	239
I-MEA/H_2O	5201	3170	1968	1385	998	735	552	423	329			
System	**Series II: $x_1 = 0.222$, $x_2 = 0.667$, and $x_3 = 0.111$ + 5 wt.% of additives**											
II-MEA/EG			111	85.4	66.7	52.6	42.0	33.9				
II-MEA/EG/TMG	246	180	133	101	78.3	61.3	48.6					
II-MEA/EG/H_2O	138	104	78.4	60.7	47.9	38.2	30.9					
II-MEA/EG/DBU	257	188	138	105	81.5	63.7	50.5	40.7				
II-MEA/EG/PP	371	268	196	147	112	86.9	68.2	54.6				

[a]Standard uncertainties are $u(x_i) = 0.001$, $u(T) = 0.01$ K and $u(P) = 10$ kPa. The relative expanded uncertainty is $U_r(\eta) = 0.02$ (0.95 level of confidence).

Table S7. Absorption capacity, m_{CO_2}, and amine efficiency, c_{CO_2}, for the mixtures composed of MEA (1), EG (2) and ChCl (3) with $x_1 = 0.667$, $x_2 = 0.222$, and $x_3 = 0.111$ for Series I and $x_1 = 0.222$, $x_2 = 0.667$, and $x_3 = 0.111$ additionally containing 5 wt.% of such additives as TMG, H_2O, DBU and PP for Series II at T = 313.15 K and pressure P = 0.1 MPa[a]

Series I			Series II		
System	m_{CO_2} [b]	c_{CO_2} [b]	System	m_{CO_2} [b]	c_{CO_2} [b]
I-MEA/EG	4.62	0.485	II-MEA/EG	1.77	0.560
I-DEA/EG	3.25	0.484	II-MEA/EG/TMG	1.83	0.610
I-EDA/EG	6.41	0.667	II-MEA/EG/H_2O	1.73	0.574
I-TEA/EG	0.411	0.0794	II-MEA/EG/DBU	1.84	0.614
I-MEA/DMSO	4.89	0.539	II-MEA/EG/PP	2.20	0.731
I-MEA/H_2O	5.59	0.505			

[a]Standard uncertainties are $u(P)$ = 100 Pa for P, $u(T)$ = 0.02 K for T and $u(x_i)$ = 0.001 for x_i; the relative expanded uncertainties for CO_2absorbing capacity and efficiency are $U_r(m_{CO_2})$ = 0.05 and $U_r(c_{CO_2})$ = 0.05 (0.95 level of confidence), respectively. [b]Units are $\mathrm{mol}_{CO_2} \times \mathrm{kg}^{-1}_{\mathrm{solution}}$ for m_{CO_2} and $\mathrm{mol}_{CO_2} \times \mathrm{mol}^{-1}_{\mathrm{MEA}}$ for c_{CO_2}.

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