

Supplementary information for

Design and thermophysical characterization of Betaine hydrochloride-based Deep Eutectic Solvents as a new platform for CO₂ capturing

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Table S1: Influence of varying molar ratio of HBA and HBDs on the freezing point (T_f) of DES.

HBA: HBD₁:HBD₂	Ratio	T_f (°C)	Remarks
BHC: U	1:1	Do not form DES	-
	1:2	Do not form DES	-
	1:3	80	-
	1:4	35	-
	1:5	50	-
	1:6	60	-
BHC: U: EG	1:4:0.5	32	Become solid after 24h
	1:4:1.0	30	Become solid after 24h
	1:4:1.5	28	Become solid after 24h
	1:4:2.0	26	Clear and stable
	1:4:2.5	18	Clear and stable
BHC: U: DEG	1:4:0.5	31	Become solid after 24h
	1:4:1.0	26	Become solid after 24h
	1:4:1.5	22	Become solid after 24h
	1:4:2.0	18	Become solid after 24h
	1:4:2.5	15	Clear and stable
BHC: U: TEG	1:4:0.5	28	Become solid after 24h
	1:4:1.0	24	Become solid after 24h
	1:4:1.5	19	Become solid after 24h
	1:4:2.0	16	Become solid after 24h
	1:4:2.5	10	Clear and stable
BHC: U: GLY	1:4:0.5	25	Become solid after 24h
	1:4:1.0	22	Become solid after 24h
	1:4:1.5	15	Become solid after 24h
	1:4:2.0	10	Clear and stable
	1:4:2.5	> 0	Clear and stable

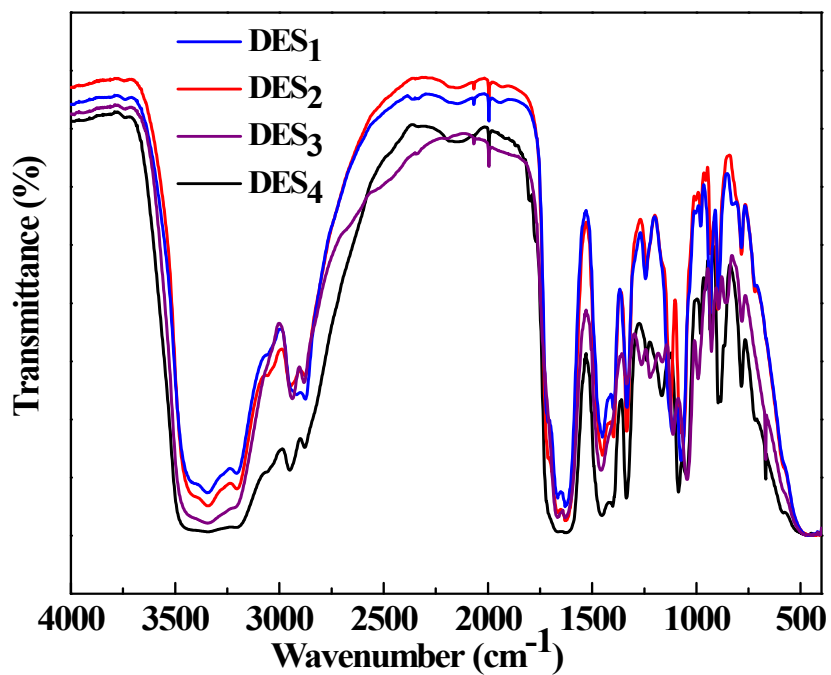
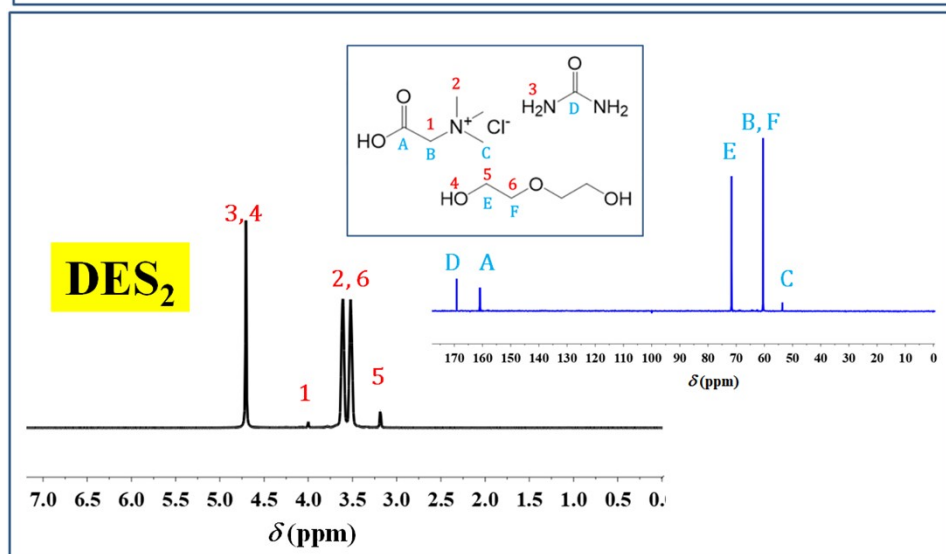
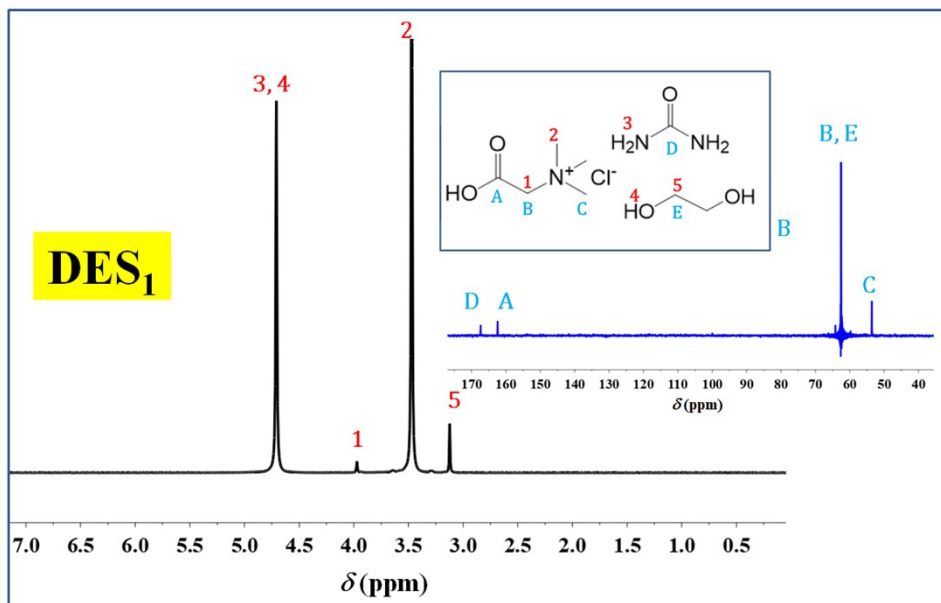


Fig. S1: FT-IR spectra of prepared DESs. Blue, Red, Purple, and Black lines represent: DES₁, DES₂, DES₃, and DES₄ respectively.



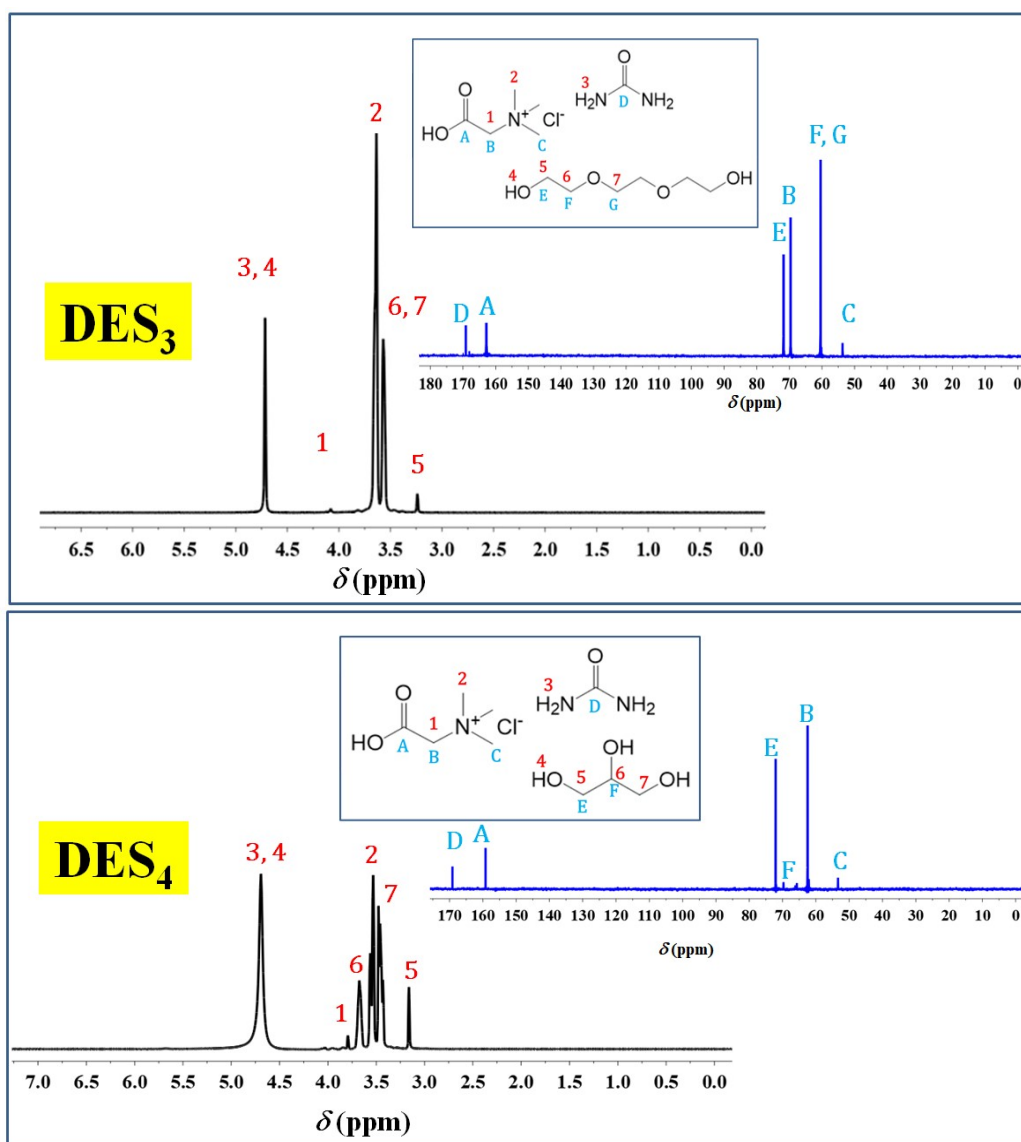


Fig. S2: Spectroscopic data of ¹H (black color spectrum) and ¹³C-NMR (blue color spectrum) of the prepared DESs.

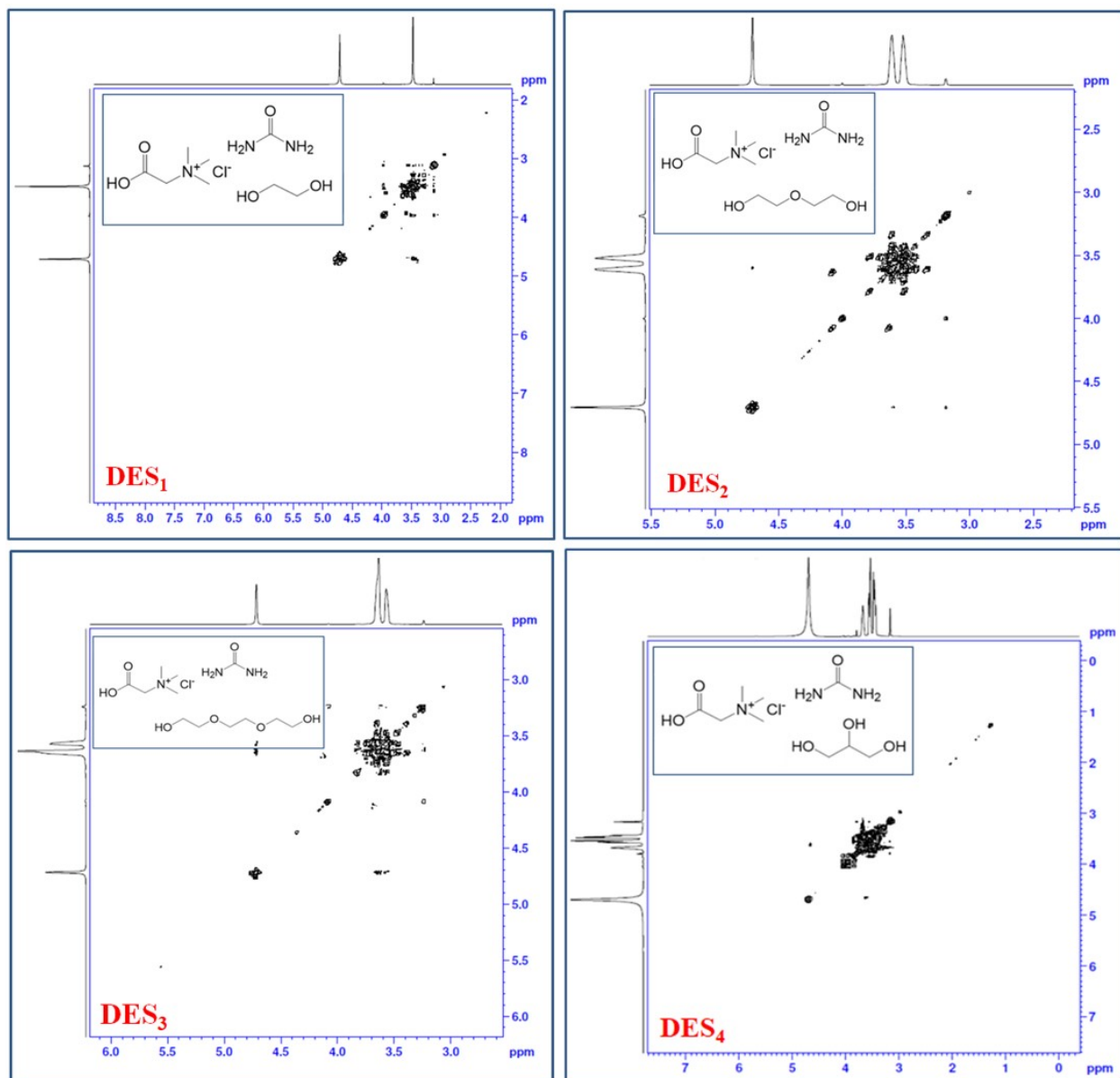


Fig. S3: The Experimental 2D-NOESY spectra of the prepared DESs.

Table S2: The experimental and evaluated thermophysical properties such as density (ρ) thermal expansion coefficient (α_p), speed of sound (u), isentropic compressibility (κ_s), viscosity (η), electrical conductivity (κ), the prepared DESs at the temperature, T (K) = (303.15 - 333.15) and pressure, p=101 kPa.^a

T (K)	ρ (g.cm ⁻³)				$\alpha_p \times 10^{-4}$ (K ⁻¹)			
	DES ₁	DES ₂	DES ₃	DES ₄	DES ₁	DES ₂	DES ₃	DES ₄
303.15	1.2038	1.2100	1.2184	1.2640	4.97	5.03	5.09	6.28
308.15	1.2005	1.2064	1.2153	1.2601	4.99	5.05	5.10	6.30
313.15	1.1979	1.2031	1.2121	1.2561	5.00	5.06	5.11	6.32
318.15	1.1942	1.2001	1.2090	1.2522	5.01	5.07	5.12	6.34
323.15	1.1913	1.1972	1.2059	1.2481	5.02	5.08	5.14	6.36
328.15	1.1887	1.1942	1.2027	1.2444	5.04	5.10	5.15	6.38
333.15	1.1854	1.1912	1.1997	1.2411	5.05	5.11	5.16	6.40
u (m.s ⁻¹)					κ_s (TPa ⁻¹)			
303.15	1874.29	1855.13	1849.14	1954.89	236.4	240.1	240.0	207.0
308.15	1864.85	1844.23	1838.45	1945.65	239.5	243.7	243.4	209.6
313.15	1855.53	1834.63	1827.56	1936.45	242.4	246.9	247.0	212.3
318.15	1846.20	1824.58	1817.45	1925.26	245.6	250.2	250.4	215.4
323.15	1836.86	1814.63	1807.46	1914.23	248.7	253.6	253.8	218.6
328.15	1827.65	1804.87	1796.14	1903.56	251.8	257.0	257.7	221.7
333.15	1818.17	1794.25	1785.45	1894.23	255.1	260.7	261.4	224.5
η (mPa.s)					κ (mS. cm ⁻¹)			
303.15	149.46	489.02	812.19	1017.02	3.17	0.97	0.51	0.22
308.15	96.66	312.37	539.82	715.48	3.74	1.21	0.65	0.31
313.15	70.10	212.55	342.41	448.82	4.31	1.51	0.87	0.44
318.15	54.27	140.21	218.59	282.30	5.01	1.88	1.12	0.62
323.15	41.56	100.66	142.43	189.68	5.76	2.27	1.48	0.88
328.15	32.55	74.99	101.46	121.10	6.62	2.68	1.88	1.31
333.15	27.45	55.06	73.04	85.41	7.48	3.32	2.39	1.88

^aRelative uncertainties (u) expressed in terms of temperature as $u(T)$ for ρ and $u = \pm 0.01$ K; $u(T)$ for η and $^{nD} = \pm 0.02$ K; for $u(\rho) = \pm 1.1$ kg. m⁻³; for $u(u) = \pm 0.5$ m. s⁻¹; for $u(\kappa_s) = \pm 0.5$ TPa⁻¹; for $u(\eta) = \pm 1.0$ %; for $u(\kappa) = \pm 1.0$ %; for $u(^{nD}) = \pm 0.0004$ and for $u(p) = \pm 1.0$ kPa.

Table S3. Experimental values of refractive index (n_D), Molar volume (V_m), Molar refractions (R_m) and Free volume (f_m) for synthesized DES at Temp.(T = 303.15-333.15 K) and pressure, p=101 kPa.^a

T (K)	n_D	V_m cm ³ .mol ⁻¹	R_m cm ³ .mol ⁻¹	f_m cm ³ .mol ⁻¹	n_D	V_m cm ³ .mol ⁻¹	R_m cm ³ .mol ⁻¹	f_m cm ³ .mol ⁻¹
DES₁					DES₂			
303.15	1.4882	456.07	131.45	324.63	1.4844	544.76	155.96	388.80
308.15	1.4862	457.31	131.34	325.97	1.4822	546.36	155.82	390.55
313.15	1.4836	458.34	131.04	327.30	1.4801	547.90	155.67	392.22
318.15	1.4812	459.73	130.88	328.85	1.4781	549.24	155.50	393.74
323.15	1.4785	460.84	130.57	330.28	1.4758	550.57	155.23	395.34
328.15	1.4761	461.85	130.29	331.56	1.4735	551.94	154.98	396.97
333.15	1.4736	463.14	130.06	333.07	1.4718	553.34	154.89	398.45
DES₃					DES₄			
303.15	1.4827	631.40	180.23	451.17	1.5018	493.75	145.66	348.09
308.15	1.4804	633.02	179.95	453.06	1.4994	495.25	145.51	349.74
313.15	1.4781	634.64	179.68	454.96	1.4971	496.85	145.41	351.44
318.15	1.4758	636.27	179.40	456.88	1.4947	498.37	145.26	353.11
323.15	1.4734	637.91	179.08	458.83	1.4922	500.01	145.11	354.90
328.15	1.4712	639.61	178.84	460.77	1.4898	501.49	144.94	356.55
333.15	1.4693	641.21	178.67	462.54	1.4873	502.83	144.69	358.14

^aRelative uncertainties (u) expressed in terms of temperature as $u(T) n_D = \pm 0.02$ K; for $u(n_D) = \pm 0.0004$ and for $u(p) = \pm 1.0$ kPa.