SUPPLEMENTARY INFORMATION

Prediction of Greenhouse Gas Solubility in Eutectic Solvents using COSMO-RS

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1. CO_2 solubility in ESs

Table S1. Experimental data of CO_2 solubility in ChCl:Ethylene Glycol and COSMO-RS predictions at 1:2 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Ethylene Glycol	0.333	0.667	313.500	2.480	7.85E-03	44.72	8.35E-03	0.064	[1]
						5.650	1.85E-02	39.74	1.91E-02	0.031	
						10.550	3.56E-02	35.89	3.60E-02	0.009	
						19.280	6.69E-02	33.07	6.69E-02	0.001	
						27.820	9.97E-02	30.09	9.85E-02	0.012	
						38.890	1.45E-01	27.75	1.43E-01	0.016	
						50.400	1.94E-01	27.87	1.94E-01	0.000	
						59.020	2.30E-01	31.37	2.39E-01	0.039	
				ARD				33.81		2.14	

Table S2. Experimental data of CO_2 solubility in ChCl:Glycerol and COSMO-RS predictions at 1:2 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Glycerol	0.333	0.667	313.500	1.910	1.19E-02	30.40	1.23E-02	0.030	[2]
						6.220	3.90E-02	30.77	3.94E-02	0.011	
						12.390	7.71E-02	30.12	7.71E-02	0.000	
						20.120	1.25E-01	29.74	1.23E-01	0.019	
						29.780	1.75E-01	24.78	1.78E-01	0.018	
						40.020	2.37E-01	24.22	2.35E-01	0.007	
						50.400	2.94E-01	21.08	2.94E-01	0.000	
						59.910	3.31E-01	13.96	3.50E-01	0.057	
				ARD				25.64		1.78	

Table S3. Experimental data of CO_2 solubility in ChCl:Phenol and COSMO-RS predictions at 1:2 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Phenol	0.333	0.667	313.150	19.900	8.80E-02	87.49	6.51E-03	0.926	[3]
						34.600	1.26E-01	84.81	1.77E-02	0.860	
						50.100	1.60E-01	82.60	4.12E-02	0.743	
						64.500	1.86E-01	80.69	8.23E-02	0.558	
						78.000	2.14E-01	79.68	1.50E-01	0.299	
						88.700	2.37E-01	79.07	2.37E-01	0.000	
						101.700	2.51E-01	77.27	4.04E-01	0.612	
						127.400	2.75E-01	73.93	1.11E+00	3.035	
				ARD				80.69		87.90	

Table S4. Experimental data of CO_2 solubility in ChCl:Urea and COSMO-RS predictions at 1:2 molar ratio and high pressures.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Urea	0.333	0.667	313.500	125.000	3.09E-01	30.00	2.84E-01	0.080	[4]
						104.600	2.83E-01	42.14	2.83E-01	0.000	
						91.200	2.70E-01	49.62	2.81E-01	0.042	
						79.600	2.53E-01	54.70	2.77E-01	0.095	
						62.300	2.33E-01	63.17	2.62E-01	0.122	
						43.700	1.91E-01	69.71	2.26E-01	0.185	
						28.500	1.50E-01	75.54	1.76E-01	0.173	
						11.300	7.70E-02	81.61	8.55E-02	0.110	
				ARD				58.31		10.08	

Table 5. Experimental data of CO_2 solubility in ChCl:Urea and COSMO-RS predictions at 1:2 molar ratio and low pressures.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD(%)	Ref.
CO_2	ChCl	Urea	0.333	0.667	313.500	0.103	1.00E-03	82.10	[5]
						0.508	4.17E-03	80.23	
						1.058	8.43E-03	81.63	
						1.539	1.26E-02	80.97	
						2.023	1.62E-02	80.75	
				ARD				81.14	

Table S6. Experimental data of CO_2 solubility in ChCl:Urea and COSMO-RS predictions at 1:1.5 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Ref.
CO_2	ChCl	Urea	0.40	0.60	313.500	0.103	5.50E-04	71.10	[5]
						0.508	2.69E-03	70.85	
						1.058	5.36E-03	69.52	
						1.539	7.89E-03	69.86	
						2.023	1.04E-02	69.93	
				ARD				70.25	

Table S7. Experimental data of CO_2 solubility in ChCl:Urea and COSMO-RS predictions at 1:2.5 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Ref.
CO_2	ChCl	Urea	0.286	0.714	313.500	0.116	5.60E-04	78.78	[5]
						0.534	2.79E-03	76.46	
						1.003	4.89E-03	76.05	
						1.548	7.18E-03	75.54	
						2.022	9.59E-03	75.55	
				ARD				76.48	

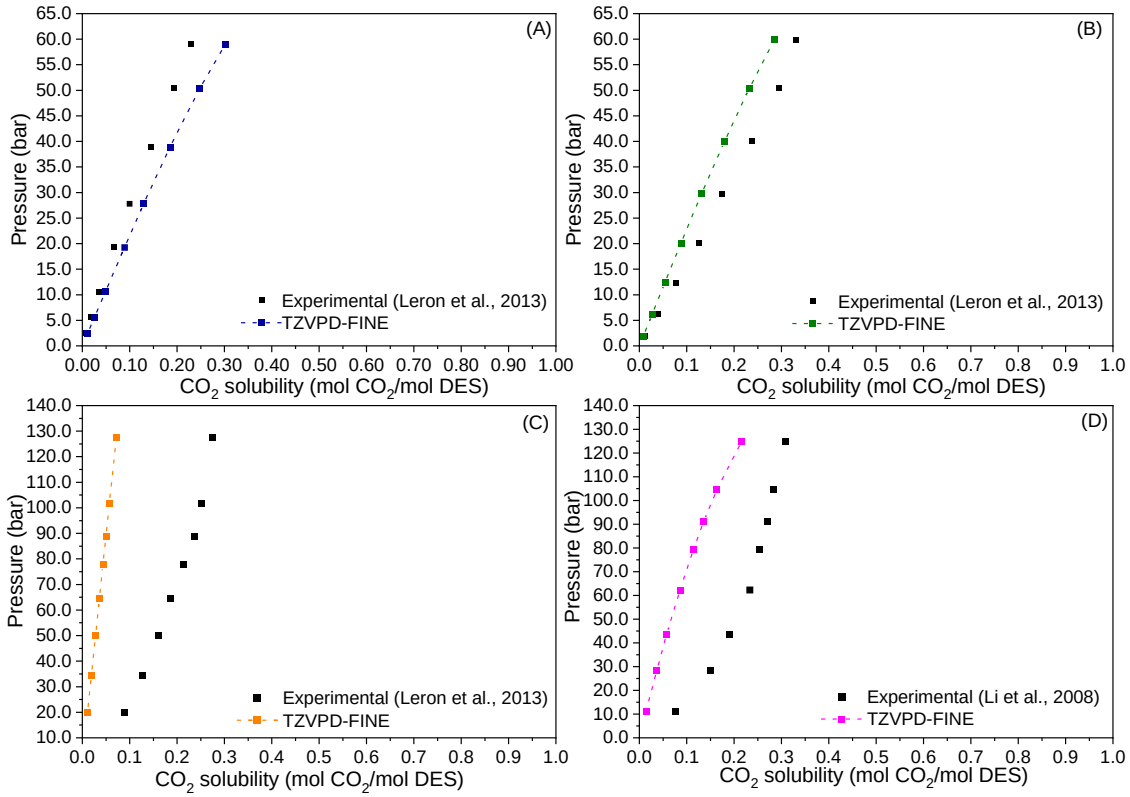

Fig. S1 Comparison of the experimental and COSMO-RS predicted CO_2 solubilities in ChCl-based ESs at 1:3 molar ratio (A) ethylene glycol, (B) glycerol, (C) phenol, and (D) urea.

Table S8. Experimental data of CO_2 solubility in ChCl:1,4 butanediol and COSMO-RS predictions at 1:3 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	1,4-butanediol	0.250	0.750	313.150	1.214	2.80E-03	193.96	2.70E-03	0.036	[6]
						2.331	5.20E-03	203.81	5.30E-03	0.020	
						3.216	7.30E-03	198.50	7.45E-03	0.021	
						4.102	9.70E-03	186.47	9.68E-03	0.002	
						5.028	1.21E-02	181.45	1.21E-02	0.000	
					ARD			192.84		1.574	

Table S9. Experimental data of CO_2 solubility in ChCl:2,3 butanediol and COSMO-RS predictions at 1:3 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	2,3-butanediol	0.250	0.750	313.150	1.193	2.90E-03	258.54	3.17E-03	0.092	[6]
						2.224	5.40E-03	259.09	6.00E-03	0.111	
						3.255	7.90E-03	259.41	8.92E-03	0.129	
						4.249	1.02E-02	263.57	1.18E-02	0.159	
						5.288	1.27E-02	263.66	1.50E-02	0.178	
		ARD						260.85		13.365	

Table S10. Experimental data of CO_2 solubility in ChCl:1,2 propanediol and COSMO-RS predictions at 1:3 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	1,2-propanediol	0.250	0.750	313.150	1.254	2.40E-03	219.81	2.32E-03	0.035	[6]
						2.178	4.40E-03	225.44	4.40E-03	0.000	
						3.176	6.70E-03	213.05	6.57E-03	0.019	
						4.205	9.30E-03	194.66	8.76E-03	0.058	
						5.154	1.15E-02	196.86	1.11E-02	0.034	
		ARD						209.96		2.917	

Table S11. Experimental data of CO_2 solubility in ChCl:Phenol and COSMO-RS predictions at 1:3 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Phenol	0.250	0.750	313.150	1.160	3.20E-03	209.84	3.32E-03	0.036	[7]
						2.181	6.40E-03	189.98	6.40E-03	0.000	
						3.173	9.50E-03	187.12	9.70E-03	0.021	
						4.115	1.24E-02	188.35	1.31E-02	0.055	
						5.068	1.56E-02	186.54	1.68E-02	0.079	
		ARD						192.37		3.83	

Table S12. Experimental data of CO_2 solubility in ChCl:Diethylene Glycol and COSMO-RS prediction at 1:3 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Diethylene Glycol	0.250	0.750	313.150	1.169	3.00E-03	215.59	3.00E-03	0.000	[7]
						2.196	5.90E-03	201.05	5.75E-03	0.025	
						3.270	9.10E-03	190.28	8.76E-03	0.037	
						4.177	1.14E-02	195.69	1.14E-02	0.000	
						5.157	1.42E-02	192.79	1.44E-02	0.011	
		ARD						199.08		1.469	

Table S13. Experimental data of CO_2 solubility in ChCl:Triethylene Glycol and COSMO-RS prediction at 1:3 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Triethylene Glycol	0.250	0.750	313.150	1.140	3.80E-03	276.82	4.37E-03	0.151	[7]
						2.208	7.80E-03	253.39	8.72E-03	0.118	
						3.182	1.11E-02	255.94	1.29E-02	0.163	
						4.149	1.54E-02	232.78	1.73E-02	0.123	
						5.106	1.94E-02	223.47	2.19E-02	0.126	
				ARD				248.48		13.606	

Table S14. Experimental data of CO_2 solubility in ChCl:Levulinic acid and COSMO-RS prediction at 1:3 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Levulinic Acid	0.250	0.750	313.150	0.808	2.70E-03	125.23	4.12E-03	0.526	[8]
						2.100	7.50E-03	110.23	1.06E-02	0.418	
						3.140	1.13E-02	108.26	1.58E-02	0.399	
						4.176	1.50E-02	108.29	2.09E-02	0.394	
						5.178	1.86E-02	107.94	2.58E-02	0.386	
				ARD				111.32		41.784	

Table S15. Experimental data of CO_2 solubility in ChCl:Furfuryl Alcohol and COSMO-RS prediction at 1:3 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Furfuryl Alcohol	0.250	0.750	313.150	0.808	2.40E-03	153.03	2.82E-03	0.176	[7]
						2.146	6.30E-03	155.38	7.35E-03	0.167	
						3.214	9.50E-03	153.17	1.08E-02	0.141	
						4.267	1.26E-02	152.97	1.42E-02	0.124	
						5.232	1.55E-02	151.75	1.71E-02	0.105	
				ARD				152.31		13.395	

Table S16. Experimental data of CO_2 solubility in ChCl:Guaiacol and COSMO-RS prediction at 1:3 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Guaiacol	0.250	0.750	313.150	0.575	1.70E-03	284.94	1.70E-03	0.000	[9]
						1.457	4.10E-03	305.00	7.65E-03	0.867	
						2.332	6.50E-03	309.48	1.21E-02	0.866	
						3.303	9.30E-03	306.09	1.70E-02	0.827	
						4.296	1.22E-02	303.41	2.19E-02	0.792	
				ARD				302.35		68.823	

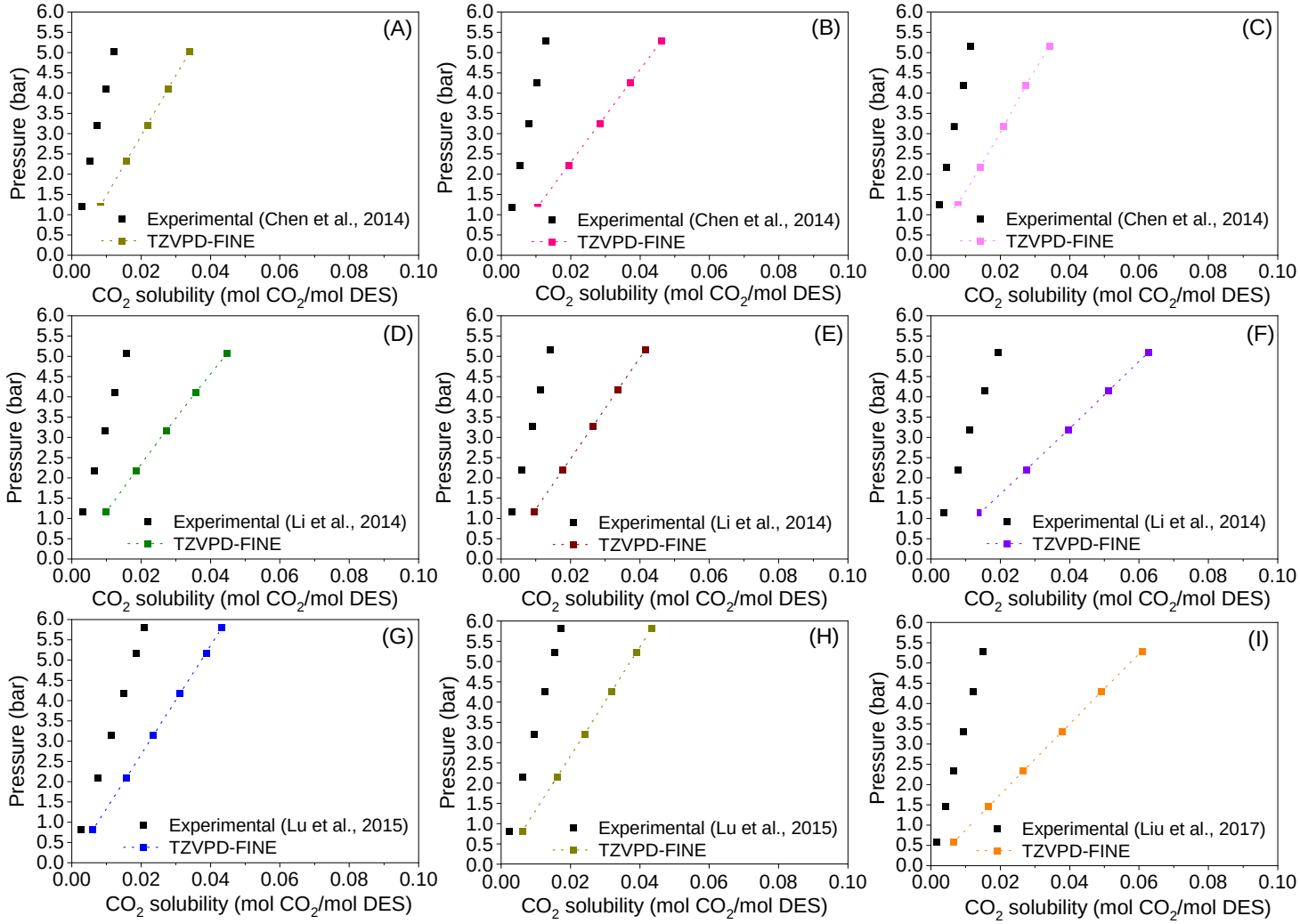

Fig. S2 Comparison between the experimental and COSMO-RS predicted CO_2 solubilities in ChCl-based ESs at 1:3 molar ratio: (A) 1,4–butanediol, (B) 2,3–butanediol, (C) 1,2–propanediol, (D) phenol, (E) diethylene glycol, (F) triethylene glycol, (G) levulinic acid, (H) furfuryl alcohol, and (I) guaiacol.

Table S17. Experimental data of CO_2 solubility in ChCl:1,4 butanediol and COSMO-RS prediction at 1:4 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	1,4-butanediol	0.20	0.80	313.150	1.195	2.60E-03	205.16	2.60E-03	0.000	[6]
						2.232	4.90E-03	202.54	4.97E-03	0.013	
						3.125	7.10E-03	192.43	7.09E-03	0.002	
						4.100	9.60E-03	183.88	9.50E-03	0.011	
						5.072	1.19E-02	183.44	1.20E-02	0.008	
					ARD			193.49		0.683	

Table S18. Experimental data of CO_2 solubility in ChCl:2,3 butanediol and COSMO-RS prediction at 1:4 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	2,3-butanediol	0.20	0.80	313.150	1.109	3.00E-03	221.40	2.93E-03	0.023	[6]
						2.172	6.10E-03	210.02	5.84E-03	0.042	
						3.180	8.70E-03	218.72	8.70E-03	0.000	
						4.149	1.18E-02	207.06	1.15E-02	0.022	
						5.110	1.45E-02	208.26	1.44E-02	0.004	
				ARD				213.09		1.825	

Table S19. Experimental data of CO_2 solubility in ChCl:1,2 propanediol and COSMO-RS prediction at 1:4 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	1,2-propanediol	0.20	0.80	313.150	1.216	2.10E-03	267.00	2.32E-03	0.107	[6]
						2.252	4.30E-03	232.49	4.40E-03	0.023	
						3.251	6.00E-03	244.56	6.49E-03	0.081	
						4.214	8.10E-03	231.40	8.58E-03	0.059	
						5.256	1.06E-02	216.46	1.09E-02	0.032	
				ARD				238.38		6.053	

Table S20. Experimental data of CO_2 solubility in ChCl:Phenol and COSMO-RS prediction at 1:4 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Phenol	0.20	0.80	313.150	1.171	3.20E-03	197.96	3.19E-03	0.003	[7]
						2.142	6.20E-03	202.99	6.47E-03	0.044	
						3.204	9.60E-03	188.18	9.85E-03	0.026	
						4.158	1.25E-02	190.45	1.33E-02	0.064	
						5.045	1.57E-02	186.52	1.69E-02	0.078	
				ARD				193.22		4.300	

Table S21. Experimental data of CO_2 solubility in ChCl:Diethylene Glycol and COSMO-RS prediction at 1:4 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Diethylene Glycol	0.20	0.80	313.150	1.165	3.00E-03	207.35	2.92E-03	0.026	[7]
						2.171	5.90E-03	191.13	5.56E-03	0.057	
						3.135	8.80E-03	181.80	8.20E-03	0.068	
						4.160	1.19E-02	176.48	1.11E-02	0.065	
						5.182	1.47E-02	178.80	1.42E-02	0.036	
				ARD				187.11		5.068	

Table S22. Experimental data of CO_2 solubility in ChCl:Triethylene Glycol and COSMO-RS prediction at 1:4 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Triethylene Glycol	0.20	0.80	313.150	1.196	4.20E-03	246.38	4.45E-03	0.060	[7]
						2.193	8.10E-03	227.77	8.39E-03	0.036	
						3.152	1.24E-02	206.39	1.24E-02	0.000	
						4.150	1.68E-02	196.43	1.68E-02	0.000	
						5.190	2.02E-02	206.95	2.16E-02	0.072	
				ARD				216.78		3.354	

Table S23. Experimental data of CO_2 solubility in ChCl:Levulinic acid and COSMO-RS prediction at 1:4 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Levulinic Acid	0.20	0.80	313.150	0.600	2.90E-03	50.85	2.97E-03	0.023	[8]
						1.769	8.50E-03	51.51	8.70E-03	0.023	
						2.824	1.35E-02	52.09	1.38E-02	0.023	
						3.801	1.85E-02	49.22	1.85E-02	0.000	
						4.851	2.31E-02	52.34	2.35E-02	0.017	
						5.659	2.73E-02	50.25	2.73E-02	0.000	
				ARD				51.04		1.435	

Table S24. Experimental data of CO_2 solubility in ChCl:Furfuryl Alcohol and COSMO-RS prediction at 1:4 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Furfuryl Alcohol	0.20	0.80	313.150	0.703	2.50E-03	104.68	2.38E-03	0.047	[8]
						1.922	6.40E-03	118.24	6.40E-03	0.000	
						2.954	9.90E-03	116.56	9.69E-03	0.021	
						4.035	1.33E-02	119.91	1.30E-02	0.020	
						5.028	1.65E-02	120.64	1.60E-02	0.029	
						5.688	1.83E-02	124.90	1.80E-02	0.019	
				ARD				119.49		2.268	

Table 25. Experimental data of CO_2 solubility in ChCl:Guaiacol and COSMO-RS prediction at 1:4 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CO_2	ChCl	Guaiacol	0.20	0.80	313.150	0.534	1.40E-03	341.63	2.88E-03	1.061	[9]
						1.425	4.40E-03	275.92	7.63E-03	0.734	
						2.359	7.20E-03	281.34	1.25E-02	0.737	
						3.355	1.03E-02	280.28	1.76E-02	0.710	
						4.318	1.32E-02	283.08	2.25E-02	0.701	
						5.429	1.65E-02	286.76	2.79E-02	0.693	
		ARD						291.50		77.625	

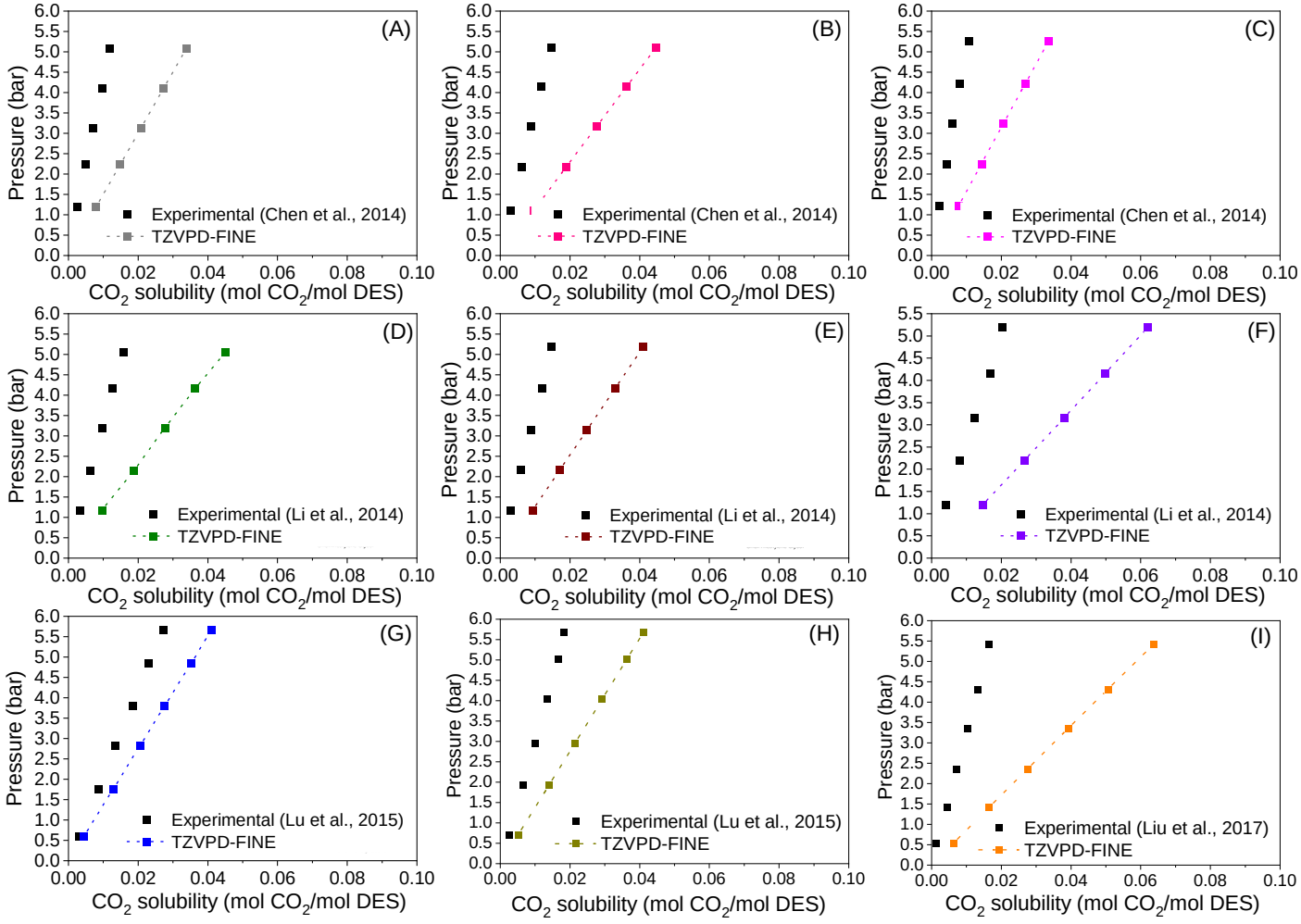

Fig. S3 Comparison between the experimental and COSMO-RS predicted CO_2 solubilities in ChCl-based ESs at 1:4 molar ratio: (A) 1,4–butanediol, (B) 2,3–butanediol, (C) 1,2–propanediol, (D) phenol, (E) diethylene glycol, (F) triethylene glycol, (G) levulinic acid, (H) furfuryl alcohol, and (I) guaiacol.

2. CH_4 solubility in ESs

Table S26. Experimental data of CH_4 solubility in ChCl:Lactic acid and COSMO-RS prediction at 1:1 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CH_4	ChCl	Lactic Acid	0.50	0.50	298.15	0.051	4.25E-03	99.27	3.90E-04	0.908	[10]
						0.929	1.09E-02	94.85	7.12E-03	0.348	
						4.944	4.08E-02	92.66	3.80E-02	0.067	
						9.946	7.81E-02	92.28	7.69E-02	0.016	
						14.930	1.16E-01	92.19	1.16E-01	0.000	
						19.928	1.55E-01	92.17	1.56E-01	0.006	
						24.922	1.94E-01	92.17	1.96E-01	0.009	
						29.910	2.34E-01	92.19	2.36E-01	0.010	
						34.929	2.77E-01	92.30	2.77E-01	0.000	
						39.922	3.18E-01	92.32	3.18E-01	0.000	
						44.933	3.60E-01	92.35	3.60E-01	0.000	
						49.933	4.03E-01	92.39	4.02E-01	0.002	
			ARD					93.10		11.386	

Table S27. Experimental data of CH_4 solubility in ChCl:Malonic acid and COSMO-RS prediction at 1:1 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CH_4	ChCl	Malonic Acid	0.50	0.50	298.15	0.050	3.79E-03	99.53	3.51E-04	0.907	[10]
						0.918	9.88E-03	96.66	6.46E-03	0.346	
						4.940	3.73E-02	95.24	3.49E-02	0.066	
						9.942	7.17E-02	95.00	7.05E-02	0.016	
						14.938	1.06E-01	94.93	1.06E-01	0.000	
						19.929	1.42E-01	94.90	1.43E-01	0.008	
						24.924	1.77E-01	94.90	1.79E-01	0.010	
						29.921	2.14E-01	94.91	2.16E-01	0.011	
						34.914	2.54E-01	94.98	2.54E-01	0.000	
						39.937	2.91E-01	94.99	2.91E-01	0.001	
						44.928	3.30E-01	95.01	3.29E-01	0.000	
						49.933	3.68E-01	95.03	3.68E-01	0.001	
			ARD					95.51		11.391	

Table S28. Experimental data of CH_4 solubility in ChCl:Phenylacetic acid and COSMO-RS prediction at 1:1 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Corrected Solubility	RD (%)	Ref.
CH_4	ChCl	Phenylacetic Acid	0.50	0.50	298.15	0.050	4.02E-03	98.47	3.86E-04	0.904	[10]
						0.916	1.05E-02	89.25	7.08E-03	0.323	
						4.946	3.96E-02	84.69	3.83E-02	0.034	
						9.943	7.64E-02	84.03	7.70E-02	0.009	
						14.938	1.14E-01	83.88	1.16E-01	0.020	
						19.917	1.52E-01	83.88	1.55E-01	0.021	
						24.923	1.90E-01	83.94	1.94E-01	0.019	
						29.921	2.30E-01	84.01	2.33E-01	0.016	
						34.936	2.72E-01	84.24	2.73E-01	0.003	
						39.932	3.13E-01	84.33	3.13E-01	0.001	
						44.935	3.54E-01	84.40	3.52E-01	0.004	
						49.920	3.96E-01	84.51	3.92E-01	0.010	
				ARD				85.80		11.367	

Table S29. Experimental data of CH_4 solubility in ChCl:Urea and COSMO-RS prediction at 1:2 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Ref.
CH_4	ChCl	Urea	0.333	0.667	313.150	0.134	7.00E-05	74.99	[5]
						0.527	2.80E-04	75.41	
						1.076	5.70E-04	75.33	
						1.536	8.10E-04	75.22	
						2.028	1.10E-03	75.90	
				ARD				75.37	

Table S30. Experimental data of CH_4 solubility in ChCl:Urea and COSMO-RS prediction at 1:1.5 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Ref.
CH_4	ChCl	Urea	0.40	0.60	313.150	0.103	6.00E-05	73.97	[5]
						0.509	2.50E-04	69.12	
						0.994	4.90E-04	69.23	
						1.505	6.90E-04	66.91	
						1.996	9.10E-04	66.72	
				ARD				69.19	

Table S31. Experimental data of CH_4 solubility in ChCl:Urea and COSMO-RS prediction at 1:2.5 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Ref.
CH_4	ChCl	Urea	0.286	0.714	313.150	0.114	4.00E-05	65.68	[5]
						0.503	2.60E-04	76.70	
						1.015	4.70E-04	73.99	
						1.520	7.20E-04	74.57	
						2.019	9.50E-04	74.39	
				ARD				73.07	

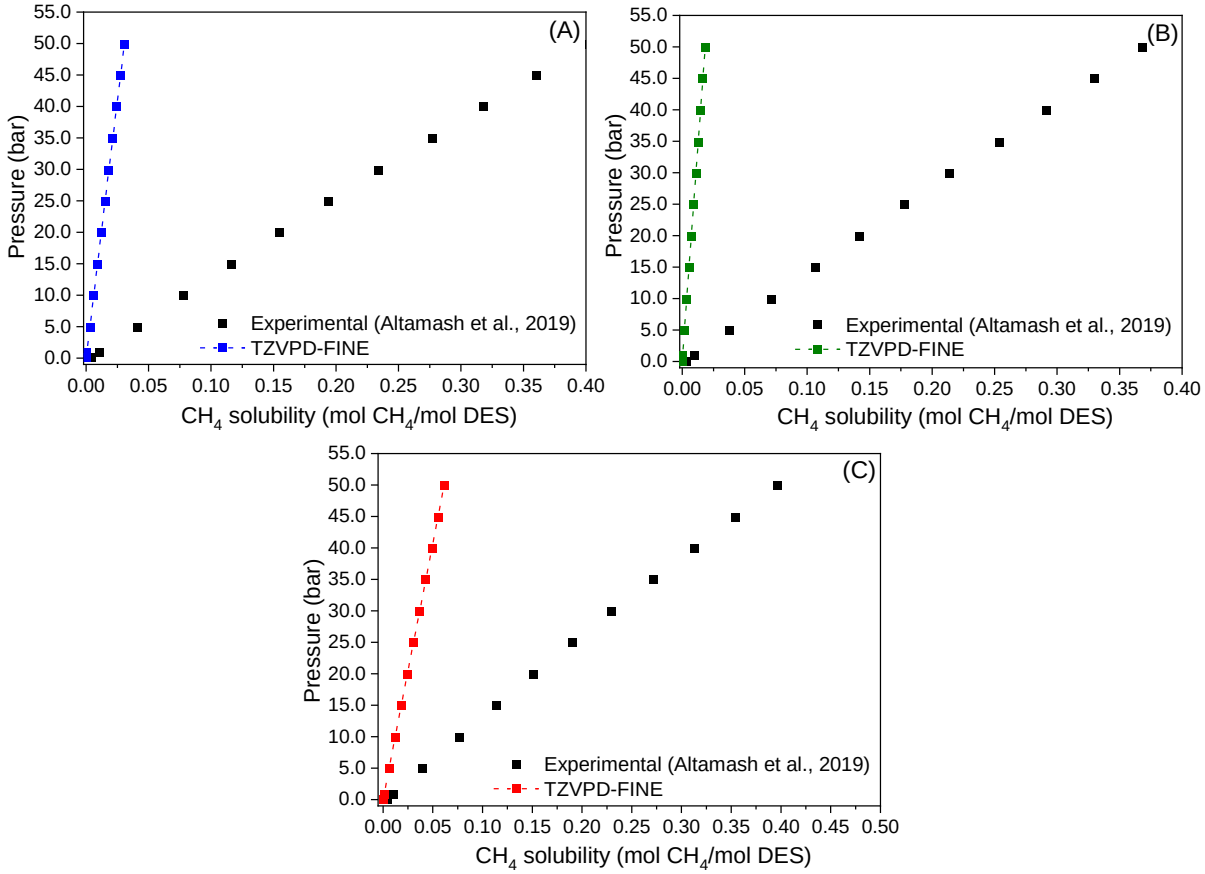

Fig. S4 Comparison between the experimental and COSMO-RS predicted CH_4 solubilities in ChCl-based ESs at 1:1 molar ratio: (A) lactic acid, (B) malonic acid, and (C) phenylacetic acid.

3. H_2S solubility in ESs

Table S32. Experimental data of H_2S solubility in ChCl:Urea and COSMO-RS prediction at 1:2 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Ref.
H_2S	ChCl	Urea	0.333	0.667	313.150	0.117	2.58E-03	60.40	[5]
						0.524	1.24E-02	47.94	
						0.994	2.35E-02	47.36	
						1.526	3.59E-02	47.27	
						2.004	4.64E-02	48.68	
					ARD			50.33	

Table S33. Experimental data of H_2S solubility in ChCl:Urea and COSMO-RS prediction at 1:1.5 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Ref.
H_2S	ChCl	Urea	0.40	0.60	313.150	0.114	3.74E-03	26.12	[5]
						0.547	1.62E-02	37.61	
						0.994	2.92E-02	37.59	
						1.500	4.23E-02	41.39	
						2.021	5.55E-02	43.61	
					ARD			37.27	

Table S34. Experimental data of H_2S solubility in ChCl:Urea and COSMO-RS prediction at 1:2.5 molar ratio.

Gas	HBA(1)	HBD(2)	x_1	x_2	T (K)	P (bar)	Experimental Solubility	RD (%)	Ref.
H_2S	ChCl	Urea	0.286	0.714	313.150	0.099	2.11E-03	51.22	[5]
						0.482	8.72E-03	77.49	
						1.014	1.84E-02	76.67	
						1.506	2.76E-02	73.77	
						1.985	3.51E-02	79.66	
					ARD			71.76	

4. References

1. R. B. Leron and M. H. Li, Thermochim Acta 551, 14 (2013).

2. R. B. Leron and M. H. Li, Journal of Chemical Thermodynamics 57, 131 (2013).

3. Y. Ji, Y. Hou, S. Ren, C. Yao, and W. Wu, Fluid Phase Equilib 429, 14 (2016).

4. X. Li, M. Hou, B. Han, X. Wang, and L. Zou, J Chem Eng Data 53, 548 (2008).

5. F. Liu, W. Chen, J. Mi, J. Y. Zhang, X. Kan, F. Y. Zhong, K. Huang, A. M. Zheng, and L. Jiang, AIChE Journal 65, 1 (2019).

6. Y. Chen, N. Ai, G. Li, H. Shan, Y. Cui, and D. Deng, J Chem Eng Data 59, 1247 (2014).

7. G. Li, D. Deng, Y. Chen, H. Shan, and N. Ai, J Chem Thermodyn 75, 58 (2014).

8. M. Lu, G. Han, Y. Jiang, X. Zhang, D. Deng, and N. Ai, J Chem Thermodyn 88, 72 (2015).

9. X. Liu, B. Gao, Y. Jiang, N. Ai, and D. Deng, J Chem Eng Data 62, 1448 (2017).

10. T. Altamash, A. I. Amhamed, S. Aparicio, and M. Atilhan, Ind Eng Chem Res 58, 8097 (2019).