

Table 1. Best suitable molecular parameters for describing both the pure IL and the high pressure VLE of the binary systems CO₂ + [C₄mim][N(CN)₂] and N₂O + [C₄mim][N(CN)₂]. Average absolute deviations are included for each set.

m_i	$\sigma_{ii}(\text{Å})$	<i>IL density %AAD</i>				<i>%AAD CO₂</i>	<i>%AAD N₂O</i>	Set
						(293.42 K and 363.19 K)	(283.15 K and 347.64 K)	
4.549	4.064	415.00	3450	2250	0.07	33.0	55.5	A.I
4.666	4.030	415.00	3450	2250	0.07	31.4	52.5	A.II
4.752	4.010	425.00	3450	2250	0.15	29.5	52.9	A.III
5.250	3.888	415.00	3450	2250	0.96	30.5	32.6	A.IV
5.500	3.807	399.09	3450	2250	0.11	32.5	21.8	A.V
6.200	3.656	395.15	3450	2250	0.12	278.2	23.4	A.VI
4.997	3.934	394.08	4250	3850	0.03	33.3	39.6	A.VII
5.478	3.788	380.00	4250	2650	1.36	36.9	21.8	A.VIII
5.500	3.813	400.37	4250	3850	0.03	29.6	21.2	A.IX
5.207	3.879	391.87	4450	3950	0.02	34.4	36.4	A.X
5.566	3.794	392.77	4450	3950	0.02	30.5	17.6	A.XI
6.200	3.666	404.80	4450	3950	0.05	312.4	23.1	A.XII
5.700	3.748	386.62	3850	2850	0.79	45.6	15.2	A.XIII
5.700	3.754	383.83	3850	2450	0.15	38.6	16.6	A.XIV
5.700	3.754	384.28	3850	2450	0.19	39.2	12.1	A.XV
5.506	3.812	404.09	3850	2650	0.04	32.5	24.6	A.XVI
5.172	3.901	425.00	3850	2450	0.19	28.2	38.6	A.XVII
4.919	3.967	425.00	3850	2250	0.18	26.9	45.9	A.XVII I

Table 2. Best suitable molecular parameters for describing both the pure IL and the binary systems CO₂ + [C₄mim][SCN] and N₂O + [C₄mim][SCN] considering only one association point on the IL (A). Average absolute deviations are included for each set.

IL %AAD

%A

2450	0.10
3050	0.10
3250	0.10
3850	0.09
3450	0.10
3650	0.09
3050	0.13
3050	0.10
3050	0.11
2650	0.11
3050	0.13
2650	0.11
2850	0.10

Table 3. Best suitable molecular parameters for describing both the pure IL and the binary systems CO₂ + [C₄mim][SCN] and N₂O + [C₄mim][SCN] considering two association points on the IL (A+B). Average absolute deviations are included for each set.

m_i	$\sigma_{ii}(\text{Å})$	ϵ_{ii}/k_B (K)	ϵ_{ii}^{HB}/k_B (K)	K_{ii}^{HB} (Å ³)	IL %AAD	%AAD CO ₂	%AAD N ₂ O	Set
						(293.12 K and 382.73 K)	(323.15 K and 382.73 K)	
5.500	3.761	423.60	3450	2250	0.08	33.5	7.5	C.I
5.500	3.756	412.15	3450	2850	0.10	29.1	7.9	C.II
5.500	3.748	395.73	3450	3850	0.17	29.2	14.0	C.III
5.500	3.752	402.88	3450	3850	0.13	30.0	14.0	C.IV

5.500	3.761	420.80	3450	3250	0.08	36.4	14.1	C.V
5.500	3.749	399.19	3450	2650	0.17	31.5	17.1	C.VI
4.702	3.964	425.00	3450	3850	0.10	64.6	36.2	C.VII
4.648	3.980	425.00	3450	3650	0.09	70.8	50.1	C.VIII
4.308	4.081	425.00	3450	2850	0.09	79.6	55.1	C.IX
5.500	3.750	407.39	3450	2250	0.23	31.5	15.0	C.X
5.500	3.761	421.79	3450	2850	0.08	34.8	14.1	C.XI
5.196	3.830	415.60	3450	2250	0.05	43.7	23.6	C.XII

Table 4. Best suitable molecular parameters for describing both the pure IL and the binary systems $N_2O + [C_4mim][Ac]$. Average absolute deviations are included for each set.

m_i	$\sigma_{ii}(\text{\AA})$	ϵ_{ii}/k_B (K)	ϵ_{ii}^{HB}/k_B (K)	K_{ii}^{HB} (\AA^3)	IL %AAD	%AAD N_2O	Set
					(283 K and 347 K)		
5.596	3.759	399.14	4250	3850	0.041	23.2	D.I
5.540	3.771	396.84	4450	3850	0.037	25.8	D.II
5.561	3.767	399.07	4250	3850	0.041	24.7	D.III
5.469	3.787	396.58	4450	3950	0.037	30.3	D.IV
5.356	3.813	396.31	4450	3950	0.037	34.0	D.V
5.338	3.818	396.27	4450	3950	0.037	34.7	D.VI
5.288	3.830	396.15	4450	3950	0.037	36.8	D.VII
5.252	3.838	396.05	4450	3950	0.037	37.6	D.VIII
5.320	3.822	396.22	4450	3950	0.037	37.7	D.IX
5.260	3.837	396.07	4450	3950	0.037	39.7	D.X

5.254	3.838	396.06	4450	3950	0.037	39.9	D.XI
5.800	3.702	396.37	3550	2650	0.586	16.9	D.XII
5.800	3.710	399.69	3450	2650	0.116	18.7	D.XIII
5.800	3.713	395.86	4250	3850	0.044	20.0	D.XIV
5.796	3.715	399.48	4250	3850	0.041	20.1	D.XV
5.800	3.715	399.65	4250	3850	0.041	20.1	D.XVI
5.794	3.716	399.47	4250	3850	0.041	20.3	D.XVII
5.787	3.717	399.46	4250	3850	0.041	20.4	D.XVIII
5.780	3.719	399.45	4250	3850	0.041	20.8	D.XIX
5.776	3.720	399.44	4250	3850	0.041	20.9	D.XXI
5.754	3.724	399.41	4250	3850	0.041	21.6	D.XXII
5.872	3.699	397.45	4450	3950	0.037	17.7	D.XXIII
