

An insight into the molecular mechanism that control the solubility of CH₄ in ionic liquids

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Electronic Supplementary Information

Table S1. List of ionic liquids used in this work, together with acronym, supplier, CAS-Number and other properties.

No	Full Name	Acronym	Supplier	CAS Number	Chemical Formula	Molecular Weight	Purity Wt%
1	1-butyl-3-methylimidazolium acetate	[C ₄ C ₁ im][Ac]	Merck	284049-75-8	C ₁₀ H ₁₈ N ₂ O ₂	198.26	95
2	1-Butyl-3-methylimidazolium dimethyl phosphate	[C ₄ C ₁ im][DMP]	Iolitec	891772-94-4	C ₁₀ H ₂₁ N ₂ O ₄ P	264.26	98
3	1-Butyl-3-methylimidazolium dibutyl phosphate	[C ₄ C ₁ im][DBP]	Iolitec	663199-28-8	C ₁₆ H ₃₃ N ₂ O ₄ P	348.42	97
4	1-Butyl-3-methylimidazolium thiocyanate	[C ₄ C ₁ im][SCN]	Merck	344790-87-0	C ₉ H ₁₅ N ₃ S	197.30	95
5	1-Butyl-3-methylimidazolium methyl sulfate	[C ₄ C ₁ im][MeSO ₄]	Merck	401788-98-5	C ₉ H ₁₈ N ₂ O ₄ S	250.32	97
6	1-Butyl-3-methylimidazolium octyl sulfate	[C ₄ C ₁ im][OcSO ₄]	Merck	445473-58-5	C ₁₆ H ₃₂ N ₂ O ₄ S	348.50	95
7	1-Butyl-3-methylimidazolium trifluoroacetate	[C ₄ C ₁ im][TFA]	Iolitec	174899-94-6	C ₁₀ H ₁₅ F ₃ N ₂ O ₂	252.11	97
8	1-Butyl-3-methylimidazolium hexafluorophosphate	[C ₄ C ₁ im][PF ₆]	Iolitec	174501-64 -5	C ₈ H ₁₅ F ₆ N ₂ P	284.18	99
9	1-Butyl-3-methylimidazolium tetrafluoroborate	[C ₄ C ₁ im][BF ₄]	Iolitec	174501-65-6	C ₈ H ₁₅ BF ₄ N ₂	226.02	99
10	1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[C ₄ C ₁ im][Tf ₂ N]	Iolitec	174899-83-3	C ₁₀ H ₁₅ F ₆ N ₃ O ₄ S ₂	419.37	99
11	1,3-Dimethylimidazolium bis(trifluoromethylsulfonyl)imide	[C ₁ C ₁ im][Tf ₂ N]	Iolitec	174899-81-1	C ₇ H ₉ F ₆ N ₃ O ₄ S ₂	377.28	99
12	1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[C ₂ C ₁ im][Tf ₂ N]	Iolitec	174899-82-2	C ₈ H ₁₁ F ₆ N ₃ O ₄ S ₂	391.31	99
13	1-Hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[C ₆ C ₁ im][Tf ₂ N]	Iolitec	382150-50-7	C ₁₂ H ₁₉ F ₆ N ₃ O ₄ S ₂	447.42	99
14	1-Decyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[C ₁₀ C ₁ im][Tf ₂ N]	Iolitec	433337-23-6	C ₁₆ H ₂₇ F ₆ N ₃ O ₄ S ₂	505.53	99
15	1-Butyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)imide	[C ₄ C ₁ pip][Tf ₂ N]	Iolitec	623580-02-9	C ₁₂ H ₂₂ F ₆ N ₂ O ₄ S ₂	436.44	99
16	1-Butyl-4-methylpyridinium bis(trifluoromethylsulfonyl)imide	[C ₄ C ₁ py][Tf ₂ N]	Iolitec	475681-62-0	C ₁₂ H ₁₆ F ₆ N ₂ O ₄ S ₂	430.39	99
17	1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	[C ₄ C ₁ pyrr][Tf ₂ N]	Iolitec	223437-11-4	C ₁₁ H ₂₀ F ₆ N ₂ O ₄ S ₂	422.41	99

Table S2. Experimental, $x_{\text{CH}_4,\text{E}}$, and predicted, $x_{\text{CH}_4,\text{C}}$, mole fraction solubility of CH_4 in ionic liquids at different temperatures and pressure, P .

No.	T/K	p/MPa	$x_{\text{CH}_4,\text{E}}$	$x_{\text{CH}_4,\text{C}}$	ARD
[C ₄ C ₁ im][Ac]					
1	298.15	0.12	0.0020	0.0009	0.12
2	298.15	0.27	0.0048	0.0019	0.29
3	298.15	0.57	0.0100	0.0040	0.60
4	298.15	1.15	0.0197	0.0080	1.17
5	298.15	1.80	0.0265	0.0125	1.40
6	298.15	2.37	0.0386	0.0163	2.23
7	298.15	2.93	0.0492	0.0202	2.90
8	298.15	3.44	0.0573	0.0236	3.36
9	298.15	4.06	0.0623	0.0278	3.45
10	298.15	4.65	0.0776	0.0318	4.58
11	298.15	5.24	0.0873	0.0357	5.15
12	298.15	5.78	0.0916	0.0394	5.22
13	298.15	6.25	0.1056	0.0425	6.31
14	298.15	6.84	0.1132	0.0464	6.68
15	313.15	0.10	0.0014	0.0006	0.08
16	313.15	0.19	0.0027	0.0011	0.15
17	313.15	0.47	0.0065	0.0027	0.38
18	313.15	1.17	0.0163	0.0068	0.95
19	313.15	1.81	0.0239	0.0105	1.34
20	313.15	2.33	0.0330	0.0135	1.95
21	313.15	3.57	0.0500	0.0206	2.94
22	313.15	4.34	0.0584	0.0250	3.34
23	313.15	5.21	0.0744	0.0300	4.44
24	313.15	5.96	0.0836	0.0342	4.94
25	313.15	7.03	0.0950	0.0402	5.47
26	328.15	0.09	0.0011	0.0005	0.06
27	328.15	0.31	0.0037	0.0015	0.21
28	328.15	1.03	0.0120	0.0051	0.68
29	328.15	1.99	0.0232	0.0099	1.34
30	328.15	2.94	0.0360	0.0146	2.14
31	328.15	3.57	0.0433	0.0176	2.56
32	328.15	4.40	0.0515	0.0217	2.98
33	328.15	5.02	0.0608	0.0248	3.60
34	328.15	5.81	0.0696	0.0286	4.10
35	328.15	6.86	0.0758	0.0337	4.20
36	343.15	0.10	0.0010	0.0004	0.06
37	343.15	0.44	0.0046	0.0019	0.27
38	343.15	1.06	0.0106	0.0046	0.60
39	343.15	1.86	0.0190	0.0081	1.09
40	343.15	2.83	0.0302	0.0122	1.80
41	343.15	3.45	0.0366	0.0149	2.17
42	343.15	4.36	0.0447	0.0188	2.59

43	343.15	5.05	0.0535	0.0217	3.17
44	343.15	5.78	0.0605	0.0248	3.57
45	343.15	6.69	0.0646	0.0287	3.59
[C ₄ C _{1im}][DMP]					
1	298.15	0.12	0.0020	0.0008	0.12
2	298.15	0.27	0.0047	0.0018	0.29
3	298.15	0.57	0.0097	0.0038	0.60
4	298.15	1.15	0.0192	0.0076	1.16
5	298.15	1.80	0.0259	0.0119	1.40
6	298.15	2.37	0.0379	0.0156	2.23
7	298.15	2.93	0.0482	0.0193	2.90
8	298.15	3.44	0.0562	0.0226	3.36
9	298.15	4.06	0.0612	0.0267	3.45
10	298.15	4.65	0.0763	0.0305	4.58
11	298.15	5.24	0.0858	0.0344	5.14
12	298.15	5.78	0.0901	0.0379	5.22
13	298.15	6.25	0.1040	0.0409	6.30
14	298.15	6.84	0.1115	0.0448	6.67
15	313.15	0.10	0.0014	0.0006	0.08
16	313.15	0.19	0.0027	0.0011	0.16
17	313.15	0.47	0.0065	0.0026	0.39
18	313.15	1.17	0.0162	0.0066	0.96
19	313.15	1.81	0.0238	0.0102	1.36
20	313.15	2.33	0.0329	0.0131	1.98
21	313.15	3.57	0.0498	0.0200	2.98
22	313.15	4.34	0.0583	0.0244	3.40
23	313.15	5.21	0.0743	0.0293	4.50
24	313.15	5.96	0.0836	0.0334	5.01
25	313.15	7.03	0.0950	0.0394	5.56
26	328.15	0.09	0.0011	0.0004	0.06
27	328.15	0.31	0.0037	0.0015	0.22
28	328.15	1.03	0.0121	0.0051	0.70
29	328.15	1.99	0.0235	0.0097	1.38
30	328.15	2.94	0.0364	0.0144	2.20
31	328.15	3.57	0.0438	0.0174	2.64
32	328.15	4.40	0.0522	0.0215	3.07
33	328.15	5.02	0.0616	0.0245	3.71
34	328.15	5.81	0.0706	0.0284	4.22
35	328.15	6.86	0.0768	0.0335	4.34
36	343.15	0.10	0.0011	0.0004	0.06
37	343.15	0.44	0.0047	0.0019	0.28
38	343.15	1.06	0.0109	0.0046	0.63
39	343.15	1.86	0.0195	0.0081	1.14
40	343.15	2.83	0.0310	0.0122	1.88
41	343.15	3.45	0.0376	0.0149	2.27
42	343.15	4.36	0.0459	0.0188	2.71
43	343.15	5.05	0.0549	0.0218	3.31
44	343.15	5.78	0.0622	0.0250	3.73

45	343.15	6.69	0.0674	0.0289	3.86
[C ₄ C ₁ im][DBP]					
1	298.15	0.20	0.0048	0.0018	0.30
2	298.15	0.42	0.0103	0.0037	0.65
3	298.15	0.85	0.0195	0.0076	1.19
4	298.15	1.37	0.0310	0.0122	1.88
5	298.15	1.83	0.0417	0.0163	2.55
6	298.15	2.28	0.0552	0.0203	3.50
7	298.15	2.70	0.0604	0.0239	3.65
8	298.15	3.18	0.0712	0.0282	4.30
9	298.15	3.65	0.0805	0.0324	4.81
10	298.15	4.13	0.0916	0.0366	5.50
11	298.15	4.57	0.1050	0.0405	6.45
12	298.15	4.95	0.1087	0.0439	6.49
13	298.15	6.41	0.1404	0.0567	8.37
14	298.15	7.39	0.1609	0.0653	9.56
15	313.15	0.14	0.0032	0.0011	0.21
16	313.15	0.34	0.0069	0.0026	0.42
17	313.15	0.85	0.0169	0.0066	1.03
18	313.15	1.37	0.0277	0.0105	1.71
19	313.15	1.80	0.0349	0.0139	2.10
20	313.15	2.71	0.0576	0.0208	3.68
21	313.15	3.38	0.0662	0.0260	4.02
22	313.15	4.07	0.0779	0.0312	4.67
23	313.15	4.69	0.0971	0.0359	6.11
24	313.15	6.51	0.1238	0.0498	7.40
25	313.15	7.67	0.1453	0.0586	8.66
26	328.15	0.12	0.0022	0.0008	0.14
27	328.15	0.74	0.0136	0.0050	0.86
28	328.15	1.48	0.0257	0.0100	1.57
29	328.15	2.24	0.0395	0.0151	2.44
30	328.15	2.78	0.0476	0.0188	2.88
31	328.15	3.42	0.0593	0.0231	3.62
32	328.15	3.95	0.0677	0.0266	4.11
33	328.15	5.56	0.0880	0.0375	5.05
34	328.15	6.37	0.1067	0.0429	6.38
35	328.15	7.52	0.1262	0.0505	7.57
36	343.15	0.18	0.0031	0.0011	0.20
37	343.15	0.35	0.0051	0.0021	0.30
38	343.15	0.85	0.0161	0.0051	1.10
39	343.15	1.49	0.0229	0.0090	1.40
40	343.15	2.27	0.0393	0.0136	2.56
41	343.15	2.77	0.0422	0.0166	2.56
42	343.15	3.49	0.0531	0.0210	3.21
43	343.15	4.05	0.0615	0.0243	3.72
44	343.15	5.63	0.0845	0.0338	5.07
45	343.15	6.84	0.1031	0.0410	6.21
[C ₄ C ₁ im][SCN]					

1	298.15	0.13	0.0010	0.0005	0.06
2	298.15	0.29	0.0024	0.0010	0.14
3	298.15	0.60	0.0051	0.0021	0.30
4	298.15	1.21	0.0100	0.0042	0.58
5	298.15	1.91	0.0136	0.0066	0.70
6	298.15	2.50	0.0199	0.0087	1.12
7	298.15	3.09	0.0254	0.0107	1.47
8	298.15	3.63	0.0296	0.0126	1.70
9	298.15	4.28	0.0324	0.0149	1.75
10	298.15	4.91	0.0404	0.0171	2.33
11	298.15	5.53	0.0456	0.0193	2.63
12	298.15	6.10	0.0480	0.0213	2.67
13	298.15	6.59	0.0555	0.0231	3.24
14	298.15	7.22	0.0596	0.0253	3.44
15	313.15	0.11	0.0008	0.0003	0.04
16	313.15	0.20	0.0014	0.0006	0.08
17	313.15	0.49	0.0035	0.0015	0.20
18	313.15	1.23	0.0088	0.0038	0.50
19	313.15	1.91	0.0129	0.0058	0.71
20	313.15	2.46	0.0179	0.0075	1.04
21	313.15	3.76	0.0272	0.0115	1.57
22	313.15	4.58	0.0320	0.0140	1.79
23	313.15	5.50	0.0408	0.0169	2.39
24	313.15	6.29	0.0461	0.0194	2.67
25	313.15	7.42	0.0526	0.0229	2.97
26	328.15	0.10	0.0006	0.0003	0.03
27	328.15	0.32	0.0021	0.0009	0.12
28	328.15	1.09	0.0068	0.0030	0.38
29	328.15	2.10	0.0132	0.0057	0.75
30	328.15	3.11	0.0205	0.0085	1.20
31	328.15	3.76	0.0248	0.0103	1.44
32	328.15	4.64	0.0296	0.0128	1.68
33	328.15	5.30	0.0350	0.0146	2.04
34	328.15	6.14	0.0402	0.0169	2.32
35	328.15	7.24	0.0439	0.0200	2.39
36	343.15	0.11	0.0006	0.0003	0.04
37	343.15	0.47	0.0027	0.0012	0.16
38	343.15	1.11	0.0063	0.0028	0.35
39	343.15	1.97	0.0113	0.0049	0.64
40	343.15	2.99	0.0180	0.0074	1.06
41	343.15	3.64	0.0219	0.0091	1.28
42	343.15	4.60	0.0268	0.0115	1.53
43	343.15	5.33	0.0322	0.0134	1.88
44	343.15	6.10	0.0365	0.0153	2.12
45	343.15	7.06	0.0411	0.0177	2.34
[C ₄ C ₁ im][MeSO ₄]					
1	298.15	0.14	0.0009	0.0006	0.02
2	298.15	0.30	0.0016	0.0013	0.03

3	298.15	0.62	0.0036	0.0028	0.09
4	298.15	1.25	0.0072	0.0056	0.16
5	298.15	1.96	0.0108	0.0088	0.19
6	298.15	2.57	0.0142	0.0116	0.26
7	298.15	3.17	0.0180	0.0144	0.37
8	298.15	3.73	0.0211	0.0169	0.42
9	298.15	4.40	0.0244	0.0199	0.45
10	298.15	5.04	0.0274	0.0228	0.46
11	298.15	5.67	0.0316	0.0257	0.59
12	298.15	6.27	0.0339	0.0284	0.55
13	298.15	6.77	0.0372	0.0307	0.64
14	298.15	7.41	0.0421	0.0336	0.84
15	313.15	0.11	0.0006	0.0004	0.02
16	313.15	0.21	0.0011	0.0008	0.02
17	313.15	0.50	0.0025	0.0020	0.05
18	313.15	1.27	0.0062	0.0050	0.13
19	313.15	1.96	0.0102	0.0077	0.25
20	313.15	2.52	0.0130	0.0099	0.31
21	313.15	3.86	0.0167	0.0152	0.15
22	313.15	4.70	0.0225	0.0185	0.39
23	313.15	5.65	0.0285	0.0223	0.62
24	313.15	6.46	0.0321	0.0255	0.66
25	313.15	7.62	0.0366	0.0301	0.65
26	328.15	0.10	0.0005	0.0003	0.01
27	328.15	0.33	0.0015	0.0012	0.03
28	328.15	1.12	0.0048	0.0039	0.09
29	328.15	2.15	0.0098	0.0075	0.23
30	328.15	3.19	0.0129	0.0111	0.18
31	328.15	3.86	0.0154	0.0135	0.19
32	328.15	4.76	0.0204	0.0166	0.37
33	328.15	5.44	0.0241	0.0190	0.51
34	328.15	6.30	0.0275	0.0220	0.55
35	328.15	7.43	0.0301	0.0260	0.41
36	343.15	0.11	0.0005	0.0003	0.02
37	343.15	0.48	0.0018	0.0015	0.03
38	343.15	1.14	0.0047	0.0036	0.11
39	343.15	2.02	0.0082	0.0063	0.19
40	343.15	3.06	0.0106	0.0096	0.10
41	343.15	3.74	0.0145	0.0117	0.27
42	343.15	4.73	0.0182	0.0148	0.34
43	343.15	5.48	0.0219	0.0172	0.47
44	343.15	6.26	0.0247	0.0197	0.50
45	343.15	7.25	0.0265	0.0228	0.37
[C ₄ C ₁ im][OcSO ₄]					
1	298.15	0.13	0.0028	0.0010	0.18
2	298.15	0.27	0.0061	0.0022	0.39
3	298.15	0.57	0.0127	0.0045	0.82
4	298.15	1.16	0.0241	0.0092	1.49

5	298.15	1.82	0.0330	0.0145	1.85
6	298.15	2.38	0.0482	0.0190	2.93
7	298.15	2.95	0.0605	0.0235	3.71
8	298.15	3.46	0.0712	0.0276	4.36
9	298.15	4.08	0.0895	0.0325	5.69
10	298.15	4.68	0.1048	0.0373	6.75
11	298.15	5.27	0.1128	0.0420	7.08
12	298.15	5.82	0.1185	0.0464	7.21
13	298.15	6.29	0.1249	0.0502	7.47
14	298.15	6.88	0.1403	0.0549	8.55
15	313.15	0.10	0.0020	0.0007	0.13
16	313.15	0.19	0.0036	0.0014	0.23
17	313.15	0.47	0.0088	0.0033	0.55
18	313.15	1.18	0.0209	0.0082	1.26
19	313.15	1.82	0.0351	0.0127	2.24
20	313.15	2.34	0.0445	0.0164	2.82
21	313.15	3.59	0.0590	0.0251	3.39
22	313.15	4.36	0.0767	0.0305	4.62
23	313.15	5.24	0.0963	0.0367	5.97
24	313.15	6.00	0.1085	0.0419	6.66
25	313.15	7.07	0.1227	0.0495	7.32
26	328.15	0.09	0.0016	0.0006	0.10
27	328.15	0.31	0.0052	0.0019	0.33
28	328.15	1.04	0.0157	0.0065	0.93
29	328.15	2.00	0.0338	0.0124	2.14
30	328.15	2.96	0.0494	0.0184	3.10
31	328.15	3.59	0.0541	0.0223	3.18
32	328.15	4.42	0.0690	0.0275	4.15
33	328.15	5.05	0.0817	0.0314	5.03
34	328.15	5.85	0.0937	0.0364	5.73
35	328.15	6.90	0.1013	0.0429	5.83
36	343.15	0.10	0.0016	0.0006	0.10
37	343.15	0.45	0.0065	0.0025	0.40
38	343.15	1.06	0.0163	0.0060	1.03
39	343.15	1.87	0.0278	0.0105	1.73
40	343.15	2.85	0.0362	0.0159	2.02
41	343.15	3.47	0.0495	0.0195	3.00
42	343.15	4.39	0.0616	0.0246	3.71
43	343.15	5.08	0.0742	0.0285	4.57
44	343.15	5.82	0.0840	0.0326	5.14
45	343.15	6.73	0.0897	0.0377	5.20
[C ₄ C ₁ im][TFA]					
1	298.15	0.19	0.0022	0.0008	0.13
2	298.15	0.39	0.0044	0.0017	0.27
3	298.15	0.78	0.0094	0.0035	0.59
4	298.15	1.23	0.0146	0.0055	0.91
5	298.15	1.61	0.0161	0.0072	0.89
6	298.15	2.00	0.0224	0.0089	1.35

7	298.15	2.35	0.0272	0.0105	1.67
8	298.15	2.77	0.0318	0.0123	1.95
9	298.15	3.17	0.0352	0.0142	2.10
10	298.15	3.57	0.0448	0.0160	2.88
11	298.15	3.94	0.0481	0.0177	3.04
12	298.15	4.26	0.0529	0.0191	3.38
13	298.15	5.66	0.0632	0.0255	3.77
14	298.15	6.57	0.0759	0.0297	4.62
15	313.15	0.13	0.0015	0.0005	0.10
16	313.15	0.32	0.0032	0.0012	0.20
17	313.15	0.80	0.0080	0.0031	0.49
18	313.15	1.23	0.0128	0.0048	0.80
19	313.15	1.59	0.0152	0.0062	0.90
20	313.15	2.43	0.0253	0.0095	1.58
21	313.15	2.96	0.0287	0.0116	1.71
22	313.15	3.56	0.0348	0.0140	2.08
23	313.15	4.07	0.0421	0.0160	2.61
24	313.15	5.80	0.0585	0.0230	3.56
25	313.15	6.83	0.0674	0.0272	4.02
26	328.15	0.21	0.0019	0.0007	0.12
27	328.15	0.70	0.0067	0.0025	0.42
28	328.15	1.36	0.0117	0.0047	0.69
29	328.15	2.01	0.0192	0.0070	1.22
30	328.15	2.43	0.0230	0.0085	1.45
31	328.15	3.00	0.0271	0.0105	1.66
32	328.15	3.42	0.0306	0.0120	1.85
33	328.15	4.97	0.0450	0.0175	2.74
34	328.15	5.68	0.0511	0.0201	3.11
35	328.15	7.20	0.0607	0.0256	3.51
36	343.15	0.17	0.0015	0.0005	0.10
37	343.15	0.30	0.0023	0.0010	0.13
38	343.15	0.72	0.0061	0.0023	0.38
39	343.15	1.27	0.0107	0.0040	0.67
40	343.15	1.93	0.0141	0.0061	0.80
41	343.15	2.36	0.0189	0.0075	1.14
42	343.15	2.97	0.0238	0.0095	1.43
43	343.15	3.45	0.0286	0.0110	1.76
44	343.15	4.94	0.0401	0.0158	2.43
45	343.15	5.86	0.0447	0.0188	2.60
[C ₄ C ₁ im][PF ₆]					
1	298.15	0.17	0.0014	0.0005	0.08
2	298.15	0.26	0.0024	0.0008	0.15
3	298.15	0.55	0.0048	0.0017	0.31
4	298.15	1.11	0.0079	0.0034	0.44
5	298.15	1.75	0.0140	0.0054	0.86
6	298.15	2.29	0.0185	0.0071	1.14
7	298.15	2.84	0.0213	0.0088	1.26
8	298.15	3.33	0.0252	0.0103	1.49

9	298.15	3.93	0.0311	0.0122	1.89
10	298.15	4.50	0.0353	0.0141	2.12
11	298.15	5.07	0.0401	0.0159	2.42
12	298.15	5.60	0.0445	0.0176	2.68
13	298.15	6.05	0.0476	0.0191	2.84
14	298.15	6.62	0.0524	0.0210	3.14
15	313.15	0.10	0.0007	0.0003	0.04
16	313.15	0.19	0.0021	0.0005	0.16
17	313.15	0.45	0.0036	0.0013	0.24
18	313.15	1.13	0.0088	0.0032	0.56
19	313.15	1.75	0.0118	0.0050	0.68
20	313.15	2.26	0.0155	0.0064	0.90
21	313.15	3.45	0.0254	0.0099	1.55
22	313.15	4.20	0.0305	0.0121	1.83
23	313.15	5.05	0.0369	0.0146	2.23
24	313.15	5.78	0.0425	0.0168	2.57
25	313.15	6.81	0.0496	0.0199	2.96
26	328.15	0.09	0.0006	0.0002	0.04
27	328.15	0.30	0.0025	0.0008	0.17
28	328.15	1.00	0.0076	0.0027	0.49
29	328.15	1.93	0.0134	0.0051	0.83
30	328.15	2.85	0.0199	0.0076	1.22
31	328.15	3.45	0.0226	0.0093	1.33
32	328.15	4.26	0.0281	0.0115	1.66
33	328.15	4.86	0.0334	0.0132	2.02
34	328.15	5.63	0.0383	0.0153	2.30
35	328.15	6.64	0.0455	0.0181	2.74
36	343.15	0.10	0.0006	0.0002	0.04
37	343.15	0.43	0.0027	0.0011	0.17
38	343.15	1.02	0.0068	0.0026	0.43
39	343.15	1.80	0.0120	0.0045	0.75
40	343.15	2.74	0.0185	0.0069	1.16
41	343.15	3.34	0.0222	0.0085	1.37
42	343.15	4.22	0.0264	0.0107	1.57
43	343.15	4.90	0.0306	0.0125	1.81
44	343.15	5.60	0.0367	0.0143	2.24
45	343.15	6.48	0.0426	0.0166	2.59
[C ₄ C ₁ im][BF ₄]					
1	298.15	0.16	0.0012	0.0005	0.07
2	298.15	0.24	0.0024	0.0007	0.17
3	298.15	0.50	0.0043	0.0015	0.28
4	298.15	1.01	0.0063	0.0030	0.33
5	298.15	1.59	0.0125	0.0047	0.78
6	298.15	2.08	0.0163	0.0062	1.00
7	298.15	2.58	0.0190	0.0077	1.13
8	298.15	3.03	0.0230	0.0091	1.39
9	298.15	3.57	0.0272	0.0107	1.65
10	298.15	4.09	0.0308	0.0123	1.85

11	298.15	4.61	0.0340	0.0139	2.01
12	298.15	5.09	0.0392	0.0154	2.38
13	298.15	5.50	0.0424	0.0166	2.58
14	298.15	6.02	0.0459	0.0182	2.77
15	313.15	0.09	0.0006	0.0002	0.04
16	313.15	0.17	0.0021	0.0005	0.16
17	313.15	0.41	0.0035	0.0011	0.24
18	313.15	1.03	0.0069	0.0027	0.42
19	313.15	1.59	0.0107	0.0042	0.65
20	313.15	2.05	0.0140	0.0055	0.85
21	313.15	3.14	0.0225	0.0084	1.41
22	313.15	3.82	0.0267	0.0103	1.65
23	313.15	4.59	0.0322	0.0124	1.99
24	313.15	5.25	0.0369	0.0142	2.27
25	313.15	6.19	0.0421	0.0168	2.54
26	328.15	0.08	0.0005	0.0002	0.03
27	328.15	0.27	0.0024	0.0007	0.17
28	328.15	0.91	0.0058	0.0022	0.36
29	328.15	1.75	0.0121	0.0043	0.78
30	328.15	2.59	0.0174	0.0063	1.11
31	328.15	3.14	0.0179	0.0077	1.03
32	328.15	3.87	0.0239	0.0095	1.44
33	328.15	4.42	0.0275	0.0108	1.66
34	328.15	5.12	0.0313	0.0126	1.88
35	328.15	6.04	0.0373	0.0148	2.24
36	343.15	0.09	0.0005	0.0002	0.03
37	343.15	0.39	0.0022	0.0009	0.13
38	343.15	0.93	0.0055	0.0021	0.35
39	343.15	1.64	0.0097	0.0037	0.61
40	343.15	2.49	0.0148	0.0056	0.92
41	343.15	3.04	0.0175	0.0068	1.07
42	343.15	3.84	0.0222	0.0086	1.36
43	343.15	4.45	0.0243	0.0100	1.43
44	343.15	5.09	0.0279	0.0115	1.64
45	343.15	5.89	0.0336	0.0133	2.03
[C ₄ C ₁ im][Tf ₂ N]					
1	298.15	0.12	0.0019	0.0007	0.12
2	298.15	0.27	0.0045	0.0017	0.29
3	298.15	0.56	0.0093	0.0035	0.59
4	298.15	1.13	0.0170	0.0070	1.00
5	298.15	1.77	0.0284	0.0110	1.74
6	298.15	2.33	0.0373	0.0145	2.28
7	298.15	2.88	0.0446	0.0180	2.66
8	298.15	3.38	0.0526	0.0212	3.14
9	298.15	3.99	0.0633	0.0251	3.82
10	298.15	4.57	0.0720	0.0288	4.33
11	298.15	5.15	0.0814	0.0325	4.89
12	298.15	5.69	0.0901	0.0360	5.41

13	298.15	6.14	0.0968	0.0390	5.78
14	298.15	6.72	0.1062	0.0428	6.34
15	313.15	0.10	0.0014	0.0006	0.09
16	313.15	0.19	0.0035	0.0011	0.25
17	313.15	0.46	0.0070	0.0026	0.44
18	313.15	1.15	0.0171	0.0065	1.06
19	313.15	1.78	0.0246	0.0100	1.46
20	313.15	2.29	0.0319	0.0129	1.90
21	313.15	3.51	0.0505	0.0199	3.06
22	313.15	4.27	0.0609	0.0242	3.67
23	313.15	5.13	0.0734	0.0292	4.42
24	313.15	5.86	0.0841	0.0335	5.06
25	313.15	6.91	0.0985	0.0397	5.88
26	328.15	0.09	0.0012	0.0005	0.07
27	328.15	0.30	0.0045	0.0015	0.29
28	328.15	1.02	0.0141	0.0052	0.89
29	328.15	1.95	0.0260	0.0101	1.59
30	328.15	2.89	0.0384	0.0150	2.35
31	328.15	3.51	0.0451	0.0182	2.69
32	328.15	4.32	0.0557	0.0224	3.32
33	328.15	4.94	0.0649	0.0257	3.92
34	328.15	5.72	0.0746	0.0298	4.48
35	328.15	6.75	0.0883	0.0353	5.30
36	343.15	0.10	0.0012	0.0005	0.07
37	343.15	0.44	0.0053	0.0021	0.32
38	343.15	1.04	0.0129	0.0049	0.79
39	343.15	1.83	0.0227	0.0087	1.39
40	343.15	2.78	0.0346	0.0133	2.13
41	343.15	3.40	0.0418	0.0162	2.56
42	343.15	4.29	0.0512	0.0205	3.06
43	343.15	4.97	0.0591	0.0238	3.53
44	343.15	5.69	0.0693	0.0273	4.20
45	343.15	6.58	0.0812	0.0317	4.95
[C ₁ C ₁ im][Tf ₂ N]					
1	298.15	0.14	0.0010	0.0010	0.06
2	298.15	0.44	0.0042	0.0042	0.28
3	298.15	1.10	0.0097	0.0097	0.60
4	298.15	1.54	0.0122	0.0122	0.70
5	298.15	2.13	0.0181	0.0181	1.09
6	298.15	2.88	0.0240	0.0240	1.42
7	298.15	3.58	0.0314	0.0314	1.91
8	298.15	4.06	0.0355	0.0355	2.16
9	298.15	4.96	0.0414	0.0414	2.43
10	298.15	5.54	0.0497	0.0497	3.05
11	298.15	6.29	0.0539	0.0539	3.20
12	298.15	6.94	0.0582	0.0582	3.40
13	298.15	7.33	0.0603	0.0603	3.46
14	298.15	7.81	0.0717	0.0717	4.42

15	313.15	0.17	0.0015	0.0015	0.10
16	313.15	0.41	0.0026	0.0026	0.14
17	313.15	0.77	0.0065	0.0065	0.41
18	313.15	1.25	0.0099	0.0099	0.60
19	313.15	1.89	0.0152	0.0152	0.93
20	313.15	2.55	0.0191	0.0191	1.11
21	313.15	3.37	0.0266	0.0266	1.59
22	313.15	4.39	0.0336	0.0336	1.95
23	313.15	5.04	0.0394	0.0394	2.32
24	313.15	6.10	0.0516	0.0516	3.19
25	313.15	7.14	0.0572	0.0572	3.40
26	328.15	0.21	0.0020	0.0020	0.14
27	328.15	0.78	0.0062	0.0062	0.39
28	328.15	1.46	0.0103	0.0103	0.60
29	328.15	2.03	0.0143	0.0143	0.82
30	328.15	2.90	0.0217	0.0217	1.30
31	328.15	3.72	0.0267	0.0267	1.55
32	328.15	4.34	0.0347	0.0347	2.17
33	328.15	5.59	0.0427	0.0427	2.58
34	328.15	6.58	0.0494	0.0494	2.94
35	328.15	7.33	0.0563	0.0563	3.39
36	343.15	0.17	0.0008	0.0008	0.03
37	343.15	0.59	0.0037	0.0037	0.20
38	343.15	1.01	0.0078	0.0078	0.50
39	343.15	1.58	0.0105	0.0105	0.61
40	343.15	2.37	0.0159	0.0159	0.92
41	343.15	3.00	0.0212	0.0212	1.27
42	343.15	4.01	0.0273	0.0273	1.59
43	343.15	5.14	0.0388	0.0388	2.41
44	343.15	6.67	0.0483	0.0483	2.91
45	343.15	7.38	0.0527	0.0527	3.14
[C ₂ C ₁ im][Tf ₂ N]					
1	298.15	0.11	0.0010	0.0005	0.05
2	298.15	0.39	0.0049	0.0017	0.32
3	298.15	0.80	0.0094	0.0035	0.59
4	298.15	1.25	0.0128	0.0055	0.73
5	298.15	1.85	0.0207	0.0082	1.25
6	298.15	2.60	0.0284	0.0116	1.68
7	298.15	3.10	0.0353	0.0138	2.15
8	298.15	3.57	0.0407	0.0160	2.48
9	298.15	4.58	0.0499	0.0206	2.93
10	298.15	5.18	0.0598	0.0234	3.64
11	298.15	5.93	0.0674	0.0269	4.05
12	298.15	6.58	0.0736	0.0300	4.36
13	298.15	6.96	0.0791	0.0318	4.74
14	298.15	7.04	0.0819	0.0321	4.98
15	313.15	0.19	0.0022	0.0008	0.14
16	313.15	0.44	0.0038	0.0018	0.20

17	313.15	0.76	0.0082	0.0031	0.51
18	313.15	1.26	0.0129	0.0051	0.78
19	313.15	1.72	0.0178	0.0070	1.08
20	313.15	2.37	0.0234	0.0097	1.37
21	313.15	3.31	0.0335	0.0136	2.00
22	313.15	4.37	0.0446	0.0180	2.65
23	313.15	5.08	0.0543	0.0210	3.33
24	313.15	6.17	0.0645	0.0257	3.88
25	313.15	7.11	0.0740	0.0297	4.42
26	328.15	0.13	0.0012	0.0005	0.08
27	328.15	0.34	0.0038	0.0013	0.25
28	328.15	1.15	0.0111	0.0043	0.68
29	328.15	1.79	0.0164	0.0068	0.97
30	328.15	2.73	0.0258	0.0104	1.55
31	328.15	3.56	0.0335	0.0136	1.99
32	328.15	4.23	0.0418	0.0162	2.56
33	328.15	5.49	0.0533	0.0211	3.22
34	328.15	6.52	0.0626	0.0252	3.74
35	328.15	7.06	0.0685	0.0273	4.11
36	343.15	0.19	0.0023	0.0007	0.16
37	343.15	0.57	0.0047	0.0020	0.27
38	343.15	0.90	0.0088	0.0032	0.56
39	343.15	1.42	0.0125	0.0050	0.75
40	343.15	1.88	0.0154	0.0067	0.88
41	343.15	2.52	0.0223	0.0090	1.34
42	343.15	3.60	0.0315	0.0128	1.86
43	343.15	4.74	0.0406	0.0170	2.35
44	343.15	6.30	0.0582	0.0227	3.55
45	343.15	7.08	0.0644	0.0256	3.88
[C ₆ C ₁ im][Tf ₂ N]					
1	298.15	0.14	0.0031	0.0011	0.21
2	298.15	0.44	0.0088	0.0034	0.53
3	298.15	0.82	0.0168	0.0063	1.04
4	298.15	1.39	0.0270	0.0108	1.62
5	298.15	1.84	0.0346	0.0142	2.04
6	298.15	2.61	0.0493	0.0202	2.91
7	298.15	3.13	0.0651	0.0244	4.07
8	298.15	3.62	0.0713	0.0281	4.31
9	298.15	4.56	0.0854	0.0356	4.98
10	298.15	5.28	0.1085	0.0413	6.72
11	298.15	6.05	0.1184	0.0475	7.09
12	298.15	6.72	0.1248	0.0528	7.19
13	298.15	7.10	0.1314	0.0559	7.55
14	298.15	7.91	0.1414	0.0624	7.90
15	313.15	0.11	0.0023	0.0008	0.16
16	313.15	0.39	0.0068	0.0027	0.41
17	313.15	0.56	0.0104	0.0039	0.66
18	313.15	1.21	0.0212	0.0084	1.29

19	313.15	1.61	0.0293	0.0111	1.82
20	313.15	2.37	0.0403	0.0165	2.38
21	313.15	3.28	0.0565	0.0228	3.37
22	313.15	4.51	0.0761	0.0315	4.46
23	313.15	5.40	0.0985	0.0378	6.06
24	313.15	6.45	0.1137	0.0453	6.84
25	313.15	7.42	0.1298	0.0522	7.76
26	328.15	0.14	0.0021	0.0009	0.12
27	328.15	0.30	0.0058	0.0019	0.39
28	328.15	0.97	0.0156	0.0061	0.95
29	328.15	1.72	0.0266	0.0108	1.58
30	328.15	2.76	0.0427	0.0174	2.53
31	328.15	3.63	0.0566	0.0229	3.37
32	328.15	4.47	0.0746	0.0283	4.63
33	328.15	5.37	0.0853	0.0340	5.13
34	328.15	6.28	0.0995	0.0398	5.97
35	328.15	7.23	0.1144	0.0460	6.84
36	343.15	0.11	0.0024	0.0006	0.18
37	343.15	0.47	0.0073	0.0027	0.46
38	343.15	0.83	0.0124	0.0047	0.76
39	343.15	1.42	0.0210	0.0082	1.28
40	343.15	1.99	0.0284	0.0115	1.69
41	343.15	2.67	0.0375	0.0154	2.21
42	343.15	3.84	0.0540	0.0222	3.19
43	343.15	5.03	0.0713	0.0291	4.22
44	343.15	6.65	0.1006	0.0386	6.20
45	343.15	7.32	0.1061	0.0425	6.36
[C ₁₀ Cl ₁ im][Tf ₂ N]					
1	298.15	0.14	0.0053	0.0015	0.38
2	298.15	0.40	0.0119	0.0043	0.76
3	298.15	0.74	0.0194	0.0079	1.15
4	298.15	1.14	0.0314	0.0121	1.93
5	298.15	1.73	0.0458	0.0184	2.74
6	298.15	2.52	0.0654	0.0268	3.86
7	298.15	3.06	0.0855	0.0326	5.30
8	298.15	3.56	0.0967	0.0378	5.89
9	298.15	4.43	0.1168	0.0471	6.98
10	298.15	5.18	0.1431	0.0550	8.81
11	298.15	5.88	0.1552	0.0625	9.27
12	298.15	6.57	0.1664	0.0698	9.66
13	298.15	7.05	0.1768	0.0748	10.19
14	298.15	7.88	0.1848	0.0837	10.11
15	313.15	0.13	0.0044	0.0013	0.32
16	313.15	0.43	0.0111	0.0040	0.70
17	313.15	0.66	0.0151	0.0062	0.89
18	313.15	1.16	0.0270	0.0110	1.61
19	313.15	1.49	0.0386	0.0141	2.45
20	313.15	2.27	0.0531	0.0214	3.17

21	313.15	3.05	0.0697	0.0286	4.11
22	313.15	4.24	0.0967	0.0399	5.68
23	313.15	5.02	0.1247	0.0472	7.75
24	313.15	5.74	0.1353	0.0539	8.14
25	313.15	6.93	0.1616	0.0651	9.65
26	328.15	0.16	0.0034	0.0013	0.21
27	328.15	0.37	0.0086	0.0031	0.55
28	328.15	0.89	0.0187	0.0075	1.12
29	328.15	1.65	0.0344	0.0139	2.05
30	328.15	2.80	0.0592	0.0236	3.57
31	328.15	3.60	0.0742	0.0303	4.39
32	328.15	4.52	0.0997	0.0381	6.17
33	328.15	5.45	0.1151	0.0459	6.92
34	328.15	6.33	0.1342	0.0532	8.10
35	328.15	7.21	0.1515	0.0606	9.09
36	343.15	0.13	0.0025	0.0010	0.14
37	343.15	0.46	0.0102	0.0035	0.66
38	343.15	0.75	0.0157	0.0058	0.99
39	343.15	1.32	0.0249	0.0101	1.48
40	343.15	2.00	0.0375	0.0152	2.22
41	343.15	2.71	0.0517	0.0207	3.10
42	343.15	3.97	0.0745	0.0303	4.42
43	343.15	4.82	0.0887	0.0367	5.20
44	343.15	5.89	0.1173	0.0449	7.24
45	343.15	6.66	0.1269	0.0507	7.62
[C ₄ C ₁ pip][Tf ₂ N]					
1	298.15	0.13	0.0026	0.0010	0.16
2	298.15	0.49	0.0123	0.0036	0.86
3	298.15	0.99	0.0187	0.0074	1.14
4	298.15	1.54	0.0293	0.0116	1.77
5	298.15	2.02	0.0383	0.0152	2.31
6	298.15	2.49	0.0473	0.0188	2.85
7	298.15	2.93	0.0555	0.0221	3.34
8	298.15	3.45	0.0653	0.0261	3.93
9	298.15	3.95	0.0748	0.0299	4.49
10	298.15	4.45	0.0812	0.0338	4.74
11	298.15	4.91	0.0928	0.0373	5.55
12	298.15	5.31	0.1002	0.0404	5.98
13	298.15	7.08	0.1332	0.0543	7.90
14	298.15	8.22	0.1545	0.0633	9.12
15	313.15	0.17	0.0028	0.0011	0.17
16	313.15	0.40	0.0069	0.0027	0.42
17	313.15	1.00	0.0172	0.0068	1.04
18	313.15	1.54	0.0294	0.0104	1.90
19	313.15	1.98	0.0339	0.0134	2.05
20	313.15	3.05	0.0520	0.0207	3.14
21	313.15	3.69	0.0630	0.0251	3.79
22	313.15	4.44	0.0716	0.0302	4.13

23	313.15	5.07	0.0863	0.0346	5.17
24	313.15	7.25	0.1229	0.0499	7.31
25	313.15	8.55	0.1447	0.0591	8.56
26	328.15	0.16	0.0026	0.0010	0.16
27	328.15	0.89	0.0179	0.0055	1.24
28	328.15	1.70	0.0266	0.0105	1.61
29	328.15	2.51	0.0391	0.0155	2.36
30	328.15	3.04	0.0472	0.0187	2.85
31	328.15	3.74	0.0581	0.0231	3.50
32	328.15	4.27	0.0692	0.0264	4.28
33	328.15	6.22	0.0961	0.0387	5.74
34	328.15	7.11	0.1110	0.0443	6.67
35	328.15	8.52	0.1311	0.0533	7.78
36	343.15	0.11	0.0016	0.0006	0.10
37	343.15	0.38	0.0084	0.0021	0.63
38	343.15	0.90	0.0129	0.0051	0.78
39	343.15	1.58	0.0226	0.0089	1.37
40	343.15	2.40	0.0313	0.0136	1.77
41	343.15	2.93	0.0419	0.0166	2.53
42	343.15	3.70	0.0528	0.0210	3.18
43	343.15	4.29	0.0581	0.0243	3.38
44	343.15	6.17	0.0877	0.0352	5.25
45	343.15	7.51	0.1063	0.0429	6.34
[C ₄ C ₁ py][Tf ₂ N]					
1	298.15	0.11	0.0021	0.0008	0.14
2	298.15	0.36	0.0071	0.0026	0.44
3	298.15	0.94	0.0188	0.0069	1.19
4	298.15	1.42	0.0260	0.0104	1.55
5	298.15	2.03	0.0362	0.0149	2.13
6	298.15	2.62	0.0471	0.0193	2.78
7	298.15	3.17	0.0566	0.0234	3.32
8	298.15	3.81	0.0745	0.0282	4.64
9	298.15	4.44	0.0862	0.0329	5.33
10	298.15	5.06	0.0976	0.0376	6.00
11	298.15	5.64	0.1056	0.0420	6.36
12	298.15	6.14	0.1117	0.0459	6.58
13	298.15	6.61	0.1203	0.0494	7.09
14	298.15	7.42	0.1434	0.0557	8.77
15	313.15	0.14	0.0026	0.0009	0.16
16	313.15	0.36	0.0070	0.0023	0.46
17	313.15	0.85	0.0142	0.0056	0.86
18	313.15	1.53	0.0247	0.0101	1.46
19	313.15	2.09	0.0371	0.0138	2.33
20	313.15	2.71	0.0436	0.0179	2.57
21	313.15	3.29	0.0527	0.0218	3.10
22	313.15	4.20	0.0680	0.0279	4.01
23	313.15	4.71	0.0751	0.0313	4.38
24	313.15	6.65	0.1142	0.0445	6.96

25	313.15	7.70	0.1284	0.0517	7.67
26	328.15	0.19	0.0032	0.0011	0.20
27	328.15	0.70	0.0116	0.0042	0.74
28	328.15	1.38	0.0207	0.0082	1.25
29	328.15	2.39	0.0353	0.0143	2.10
30	328.15	3.09	0.0458	0.0186	2.72
31	328.15	3.94	0.0576	0.0237	3.39
32	328.15	4.43	0.0698	0.0267	4.32
33	328.15	5.60	0.0854	0.0339	5.15
34	328.15	6.48	0.0980	0.0392	5.87
35	328.15	7.93	0.1192	0.0482	7.10
36	343.15	0.14	0.0027	0.0008	0.19
37	343.15	0.47	0.0070	0.0026	0.44
38	343.15	0.92	0.0123	0.0050	0.73
39	343.15	1.47	0.0206	0.0081	1.25
40	343.15	2.19	0.0297	0.0120	1.77
41	343.15	2.85	0.0380	0.0157	2.23
42	343.15	3.71	0.0543	0.0205	3.38
43	343.15	4.34	0.0606	0.0240	3.66
44	343.15	6.27	0.0866	0.0348	5.19
45	343.15	7.54	0.1048	0.0419	6.29
[C ₄ C ₁ pyrr][Tf ₂ N]					
1	298.15	0.17	0.0038	0.0012	0.26
2	298.15	0.49	0.0089	0.0033	0.56
3	298.15	0.99	0.0171	0.0066	1.04
4	298.15	1.51	0.0258	0.0102	1.56
5	298.15	1.94	0.0321	0.0131	1.90
6	298.15	2.38	0.0392	0.0161	2.31
7	298.15	2.78	0.0454	0.0188	2.66
8	298.15	3.28	0.0550	0.0223	3.27
9	298.15	3.74	0.0628	0.0255	3.73
10	298.15	4.20	0.0715	0.0287	4.28
11	298.15	4.63	0.0752	0.0316	4.36
12	298.15	4.98	0.0809	0.0341	4.68
13	298.15	6.82	0.1124	0.0471	6.52
14	298.15	7.98	0.1314	0.0554	7.60
15	313.15	0.16	0.0024	0.0010	0.14
16	313.15	0.40	0.0072	0.0025	0.47
17	313.15	1.02	0.0157	0.0062	0.95
18	313.15	1.51	0.0228	0.0092	1.36
19	313.15	1.91	0.0308	0.0117	1.91
20	313.15	2.98	0.0453	0.0183	2.70
21	313.15	3.52	0.0523	0.0217	3.06
22	313.15	4.23	0.0622	0.0261	3.61
23	313.15	4.80	0.0707	0.0297	4.11
24	313.15	7.04	0.1020	0.0439	5.81
25	313.15	8.31	0.1262	0.0520	7.41
26	328.15	0.16	0.0026	0.0009	0.17

27	328.15	0.92	0.0130	0.0051	0.78
28	328.15	1.70	0.0241	0.0095	1.46
29	328.15	2.45	0.0341	0.0137	2.03
30	328.15	2.89	0.0394	0.0162	2.31
31	328.15	3.58	0.0482	0.0201	2.81
32	328.15	4.04	0.0551	0.0227	3.24
33	328.15	5.05	0.0713	0.0285	4.28
34	328.15	5.91	0.0833	0.0334	4.99
35	328.15	7.28	0.1024	0.0414	6.10
36	343.15	0.12	0.0022	0.0006	0.16
37	343.15	0.35	0.0049	0.0018	0.31
38	343.15	0.83	0.0105	0.0043	0.62
39	343.15	1.47	0.0187	0.0076	1.12
40	343.15	2.23	0.0282	0.0115	1.67
41	343.15	2.72	0.0346	0.0141	2.05
42	343.15	3.43	0.0467	0.0178	2.90
43	343.15	3.98	0.0516	0.0206	3.10
44	343.15	5.91	0.0773	0.0308	4.65
45	343.15	7.23	0.0939	0.0378	5.61

Table S3. Predicted volume of cation and anion of ionic liquids using COSMO-RS

	$V_{m,COSMO}/nm^3$		
	Cation	Anion	Ionic Liquid
[C ₄ C ₁ im][Ac]	0.1997	0.0724	0.2721
[C ₄ C ₁ im][BF ₄]	0.1996	0.0729	0.2725
[C ₄ C ₁ im][Tf ₂ N]	0.1995	0.2206	0.4201
[C ₄ C ₁ im][DMP]	0.1997	0.1319	0.3316
[C ₄ C ₁ im][DBP]	0.1997	0.2621	0.4618
[C ₄ C ₁ im][PF ₆]	0.1995	0.1037	0.3032
[C ₄ C ₁ im][SCN]	0.1996	0.0695	0.2691
[C ₄ C ₁ im][MeSO ₄]	0.1997	0.1041	0.3037
[C ₄ C ₁ im][OcSO ₄]	0.1996	0.2573	0.4570
[C ₄ C ₁ im][TFA]	0.1997	0.0957	0.2954
[C ₄ C ₁ pip][Tf ₂ N]	0.2323	0.2207	0.4529
[C ₄ C ₁ pyrr][Tf ₂ N]	0.2155	0.2207	0.4362
[C ₄ C ₁ py][Tf ₂ N]	0.2173	0.2206	0.4379
[C ₁ C ₁ im][Tf ₂ N]	0.1339	0.2205	0.3544
[C ₂ C ₁ im][Tf ₂ N]	0.1554	0.2206	0.3760
[C ₆ C ₁ im][Tf ₂ N]	0.2436	0.2206	0.4642
[C ₁₀ C ₁ im][Tf ₂ N]	0.3312	0.2206	0.5518

Table S4. Excess enthalpy of (ionic liquids + CH₄) binary system at different temperatures predicted using COSMO-RS. The value is at $x_{\text{CH}_4} = 0.01$ and given in J·mol⁻¹

Ionic liquid + CH ₄	T/K	Methane				Cation				Anion			
		$H_{\text{E,INT}}$	$H_{\text{E,MF}}$	$H_{\text{E,HB}}$	$H_{\text{E,vdW}}$	$H_{\text{E,INT}}$	$H_{\text{E,MF}}$	$H_{\text{E,HB}}$	$H_{\text{E,vdW}}$	$H_{\text{E,INT}}$	$H_{\text{E,MF}}$	$H_{\text{E,HB}}$	$H_{\text{E,vdW}}$
[C ₄ C ₁ im][Ac]	298.15	34.44	34.19	0	0.25	-44.01	-45.41	1.74	-0.56	3.69	1.88	1.72	0.08
[C ₄ C ₁ im][BF ₄]	298.15	51.24	47.23	0	4.01	-41.81	-40.36	2.73	-4.58	18.84	16.32	2.72	-0.20
[C ₄ C ₁ im][Tf ₂ N]	298.15	46.62	32.13	0	14.49	-13.63	-5.46	1.09	-9.30	3.14	1.77	1.09	0.10
[C ₄ C ₁ im][DMP]	298.15	34.13	33.51	0	0.62	-30.63	-31.85	1.85	-0.85	-0.03	-1.77	1.83	0.04
[C ₄ C ₁ im][DBP]	298.15	24.79	23.89	0	0.9	-11.78	-12.14	1.23	-0.96	-2.17	-3.50	1.22	0.15
[C ₄ C ₁ im][PF ₆]	298.15	55.50	46.83	0	8.67	-27.69	-19.52	1.10	-9.39	19.14	18.37	1.10	-0.33
[C ₄ C ₁ im][SCN]	298.15	44.74	45.66	0	-0.92	-40.50	-43.96	1.88	1.18	16.36	14.11	1.86	0.39
[C ₄ C ₁ im][MeSO ₄]	298.15	41.99	40.71	0	1.28	-35.80	-37.27	2.45	-1.31	7.17	4.64	2.43	0.11
[C ₄ C ₁ im][OcSO ₄]	298.15	29.03	27.61	0	1.42	-10.52	-10.91	1.52	-1.24	-0.09	-1.83	1.52	0.22
[C ₄ C ₁ im][TFA]	298.15	43.63	36.54	0	7.10	-32.53	-26.61	1.12	-7.21	9.05	7.95	1.11	-0.01
[C ₄ C ₁ pip][Tf ₂ N]	298.15	46.08	31.75	0	14.33	-16.91	-8.73	0.70	-8.89	4.12	3.23	0.70	0.03
[C ₄ C ₁ pyrr][Tf ₂ N]	298.15	48.13	33.29	0	14.85	-15.72	-7.43	0.74	-9.05	3.92	2.97	0.74	0.04
[C ₄ C ₁ py][Tf ₂ N]	298.15	44.25	30.56	0	13.69	-16.29	-7.87	0.93	-9.26	3.69	2.56	0.93	0.05
[C ₁ C ₁ im][Tf ₂ N]	298.15	57.40	39.76	0	17.65	-6.86	1.69	1.33	-9.88	1.54	-0.19	1.34	0.20
[C ₂ C ₁ im][Tf ₂ N]	298.15	53.01	36.66	0	16.35	-11.22	-2.61	1.19	-9.86	2.86	1.33	1.21	0.14
[C ₆ C ₁ im][Tf ₂ N]	298.15	42.23	29.10	0	13.13	-14.16	-6.35	0.99	-8.77	2.99	1.74	1.00	0.07
[C ₁₀ C ₁ im][Tf ₂ N]	298.15	35.76	24.66	0	11.10	-14.07	-7.34	0.85	-7.65	2.69	1.64	0.85	0.05
[C ₄ C ₁ im][Ac]	313.15	36.01	35.66	0	0.35	-44.11	-45.75	1.99	-0.60	4.58	2.54	1.97	0.07
[C ₄ C ₁ im][BF ₄]	313.15	53.37	49.08	0	4.29	-41.84	-40.31	2.87	-4.80	19.95	17.29	2.86	-0.19
[C ₄ C ₁ im][Tf ₂ N]	313.15	47.74	33.29	0	14.45	-13.58	-5.56	1.13	-9.20	3.00	1.64	1.14	0.03
[C ₄ C ₁ im][DMP]	313.15	35.94	35.21	0	0.73	-30.80	-32.23	2.08	-0.89	0.82	-1.15	2.06	0.03
[C ₄ C ₁ im][DBP]	313.15	26.39	25.40	0	1.00	-11.93	-12.48	1.42	-0.98	-1.86	-3.35	1.42	0.12
[C ₄ C ₁ im][PF ₆]	313.15	57.14	48.21	0	8.93	-27.60	-19.31	1.13	-9.53	19.51	18.68	1.13	-0.31
[C ₄ C ₁ im][SCN]	313.15	46.54	47.48	0	-0.94	-40.30	-43.98	2.05	1.22	17.43	15.03	2.03	0.37
[C ₄ C ₁ im][MeSO ₄]	313.15	44.01	42.59	0	1.42	-35.92	-37.52	2.64	-1.40	8.18	5.47	2.62	0.09
[C ₄ C ₁ im][OcSO ₄]	313.15	30.68	29.16	0	1.52	-10.66	-11.18	1.67	-1.27	0.07	-1.76	1.66	0.17

[C ₄ C ₁ im][TFA]	313.15	45.39	38.17	0	7.22	-32.64	-26.95	1.34	-7.21	9.80	8.49	1.32	-0.01
[C ₄ C ₁ pip][Tf ₂ N]	313.15	46.94	32.66	0	14.28	-16.96	-8.88	0.71	-8.80	3.95	3.11	0.71	-0.03
[C ₄ C ₁ pyrr][Tf ₂ N]	313.15	49.03	34.23	0	14.79	-15.78	-7.59	0.75	-8.94	3.75	2.85	0.75	-0.02
[C ₄ C ₁ py][Tf ₂ N]	313.15	45.28	31.62	0	13.66	-16.27	-7.97	0.96	-9.16	3.56	2.44	0.96	-0.01
[C ₁ C ₁ im][Tf ₂ N]	313.15	58.66	41.12	0	17.54	-6.57	1.74	1.41	-9.72	1.43	-0.33	1.42	0.11
[C ₂ C ₁ im][Tf ₂ N]	313.15	54.21	37.93	0	16.27	-10.99	-2.61	1.26	-9.71	2.73	1.19	1.27	0.07
[C ₆ C ₁ im][Tf ₂ N]	313.15	43.29	30.18	0	13.10	-14.22	-6.53	1.03	-8.70	2.86	1.62	1.04	0.01
[C ₁₀ C ₁ im][Tf ₂ N]	313.15	36.67	25.58	0	11.09	-14.29	-7.63	0.87	-7.60	2.57	1.53	0.88	0.00
[C ₄ C ₁ im][Ac]	328.15	37.64	37.20	0	0.44	-44.28	-46.15	2.22	-0.64	5.48	3.21	2.20	0.07
[C ₄ C ₁ im][BF ₄]	328.15	55.40	50.85	0	4.54	-41.88	-40.25	2.97	-5.01	20.99	18.22	2.95	-0.18
[C ₄ C ₁ im][Tf ₂ N]	328.15	48.75	34.37	0	14.38	-13.56	-5.68	1.16	-9.09	2.82	1.49	1.17	-0.03
[C ₄ C ₁ im][DMP]	328.15	37.76	36.93	0	0.84	-31.02	-32.63	2.29	-0.94	1.63	-0.53	2.27	0.01
[C ₄ C ₁ im][DBP]	328.15	28.00	26.91	0	1.09	-12.11	-12.82	1.60	-1.00	-1.57	-3.21	1.59	0.09
[C ₄ C ₁ im][PF ₆]	328.15	58.65	49.50	0	9.15	-27.52	-19.14	1.15	-9.64	19.75	18.88	1.14	-0.28
[C ₄ C ₁ im][SCN]	328.15	48.30	49.27	0	-0.96	-40.15	-44.02	2.19	1.26	18.45	15.93	2.17	0.35
[C ₄ C ₁ im][MeSO ₄]	328.15	45.98	44.43	0	1.55	-36.07	-37.76	2.79	-1.48	9.13	6.29	2.77	0.07
[C ₄ C ₁ im][OcSO ₄]	328.15	32.28	30.66	0	1.62	-10.82	-11.42	1.78	-1.30	0.19	-1.71	1.78	0.13
[C ₄ C ₁ im][TFA]	328.15	47.12	39.79	0	7.33	-32.77	-27.30	1.53	-7.21	10.53	9.01	1.52	0.00
[C ₄ C ₁ pip][Tf ₂ N]	328.15	47.72	33.50	0	14.22	-17.03	-9.04	0.71	-8.70	3.74	2.96	0.71	-0.09
[C ₄ C ₁ pyrr][Tf ₂ N]	328.15	49.82	35.11	0	14.72	-15.84	-7.77	0.75	-8.84	3.53	2.69	0.75	-0.09
[C ₄ C ₁ py][Tf ₂ N]	328.15	46.21	32.60	0	13.61	-16.27	-8.08	0.97	-9.05	3.37	2.28	0.98	-0.06
[C ₁ C ₁ im][Tf ₂ N]	328.15	59.80	42.40	0	17.40	-6.34	1.75	1.47	-9.56	1.24	-0.52	1.48	0.03
[C ₂ C ₁ im][Tf ₂ N]	328.15	55.29	39.11	0	16.18	-10.83	-2.63	1.30	-9.56	2.55	1.02	1.31	0.00
[C ₆ C ₁ im][Tf ₂ N]	328.15	44.24	31.18	0	13.06	-14.31	-6.73	1.06	-8.61	2.69	1.48	1.06	-0.04
[C ₁₀ C ₁ im][Tf ₂ N]	328.15	37.49	26.43	0	11.06	-14.50	-7.91	0.88	-7.54	2.42	1.41	0.88	-0.04
[C ₄ C ₁ im][Ac]	343.15	39.49	38.96	0	0.52	-44.52	-46.59	2.43	-0.68	6.37	3.90	2.41	0.06
[C ₄ C ₁ im][BF ₄]	343.15	57.55	52.77	0	4.79	-41.96	-40.18	3.02	-5.19	21.93	19.11	3.00	-0.17
[C ₄ C ₁ im][Tf ₂ N]	343.15	49.81	35.47	0	14.34	-13.56	-5.82	1.17	-8.97	2.58	1.29	1.18	-0.09
[C ₄ C ₁ im][DMP]	343.15	39.71	38.78	0	0.94	-31.27	-33.05	2.47	-0.99	2.41	0.08	2.45	-0.01
[C ₄ C ₁ im][DBP]	343.15	29.65	28.47	0	1.17	-12.32	-13.17	1.74	-1.02	-1.33	-3.09	1.74	0.06
[C ₄ C ₁ im][PF ₆]	343.15	60.25	50.89	0	9.36	-27.46	-19.00	1.14	-9.71	19.87	18.98	1.14	-0.25
[C ₄ C ₁ im][SCN]	343.15	50.24	51.22	0	-0.98	-40.06	-44.06	2.30	1.29	19.40	16.80	2.28	0.33

[C ₄ C ₁ im][MeSO ₄]	343.15	48.06	46.39	0	1.67	-36.27	-38.00	2.90	-1.55	10.01	7.09	2.88	0.05
[C ₄ C ₁ im][OcSO ₄]	343.15	33.89	32.18	0	1.71	-11.00	-11.69	1.87	-1.33	0.25	-1.68	1.86	0.08
[C ₄ C ₁ im][TFA]	343.15	48.99	41.56	0	7.43	-32.93	-27.66	1.71	-7.19	11.23	9.53	1.69	0.00
[C ₄ C ₁ pip][Tf ₂ N]	343.15	48.54	34.37	0	14.17	-17.11	-9.22	0.70	-8.59	3.48	2.77	0.70	-0.16
[C ₄ C ₁ pyrr][Tf ₂ N]	343.15	50.68	36.02	0	14.66	-15.92	-7.94	0.74	-8.73	3.28	2.51	0.74	-0.15
[C ₄ C ₁ py][Tf ₂ N]	343.15	47.18	33.59	0	13.59	-16.30	-8.21	0.97	-8.94	3.13	2.10	0.97	-0.12
[C ₁ C ₁ im][Tf ₂ N]	343.15	61.07	43.74	0	17.32	-6.18	1.73	1.50	-9.40	0.98	-0.74	1.50	-0.05
[C ₂ C ₁ im][Tf ₂ N]	343.15	56.47	40.35	0	16.12	-10.70	-2.68	1.32	-9.41	2.30	0.82	1.33	-0.07
[C ₆ C ₁ im][Tf ₂ N]	343.15	45.22	32.19	0	13.03	-14.41	-6.93	1.06	-8.52	2.47	1.30	1.06	-0.09
[C ₁₀ C ₁ im][Tf ₂ N]	343.15	38.31	27.27	0	11.04	-14.72	-8.20	0.87	-7.48	2.23	1.27	0.88	-0.08

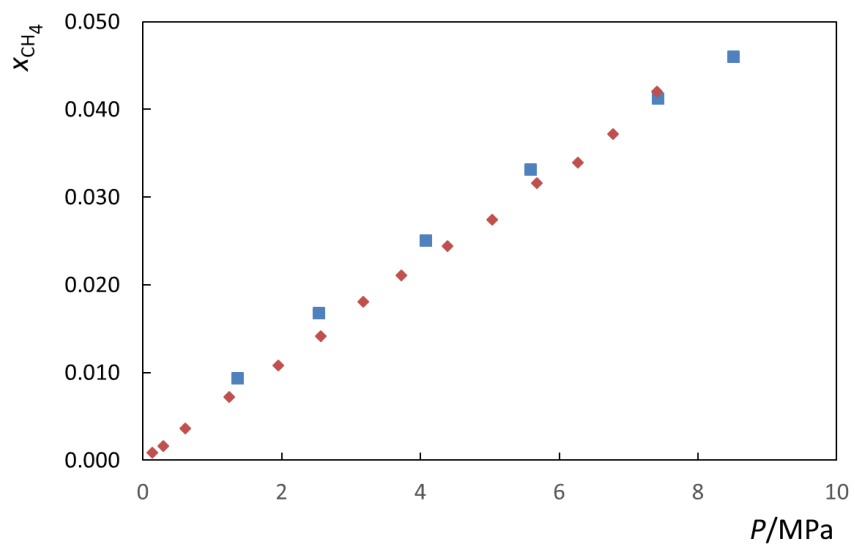


Figure S1. Solubility of CH_4 in ionic liquid $[C_4C_{1im}][MeSO_4]$. Symbols: (■), The data from reference ¹ at temperature 293.15 K; (◆), the data from this work at 298.15 K.

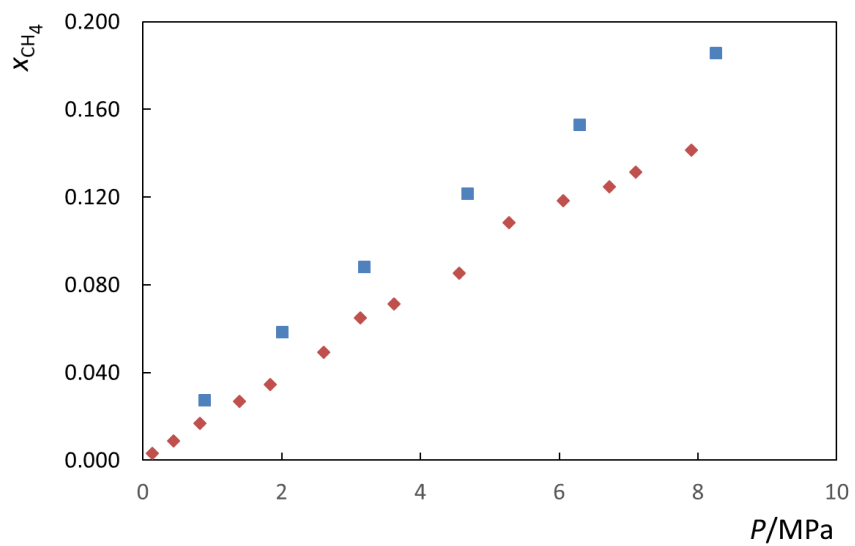


Figure S2. Solubility of CH₄ in ionic liquid [C₄C₁im][Tf₂N]. Symbols: (■), The data from reference ² at temperature 293.15 K; (◆), the data from this work at 298.15 K.

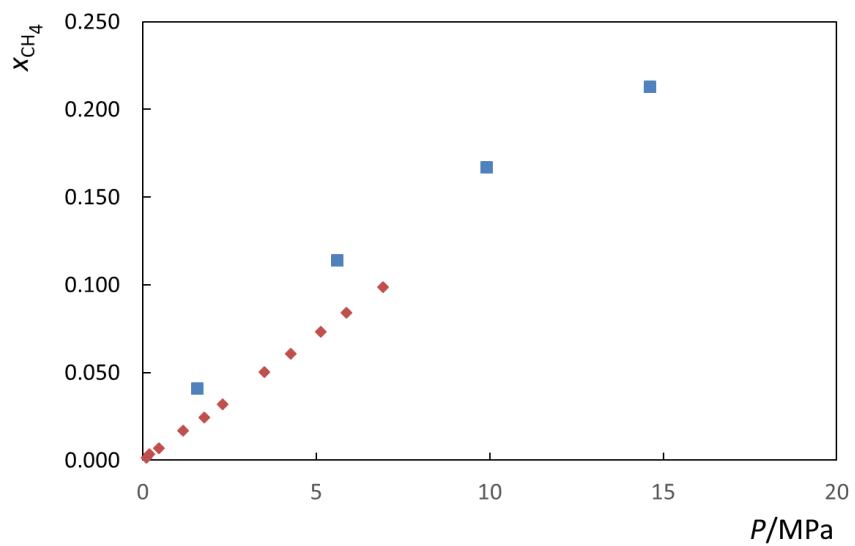


Figure S3. Solubility of CH₄ in ionic liquid [C₄C₁im][Tf₂N]. Symbols: (■), The data from reference ³ at temperature 313.15 K; (◆), the data from this work at 313.15 K.

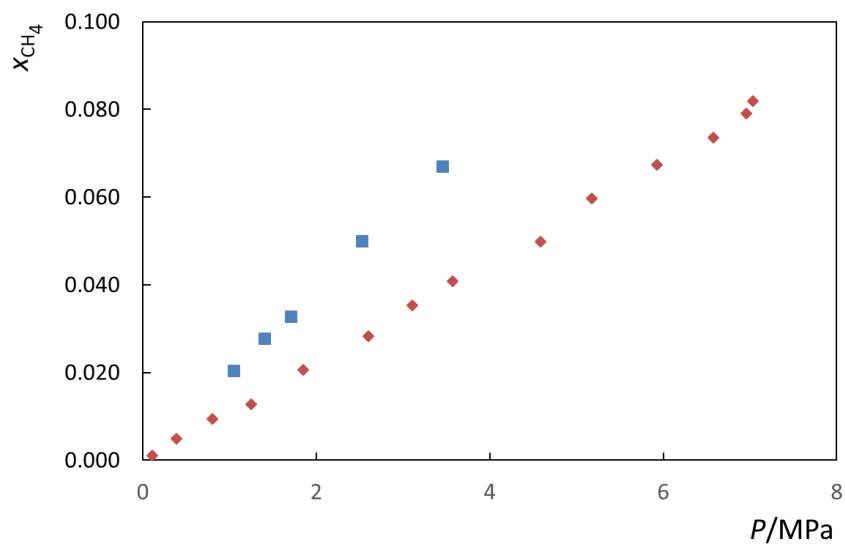


Figure S4. Solubility of CH₄ in ionic liquid [C₄C₁im][Tf₂N]. Symbols: (■), The data from reference⁴ at temperature 313.15 K; (◆), the data from this work at 313.15 K.

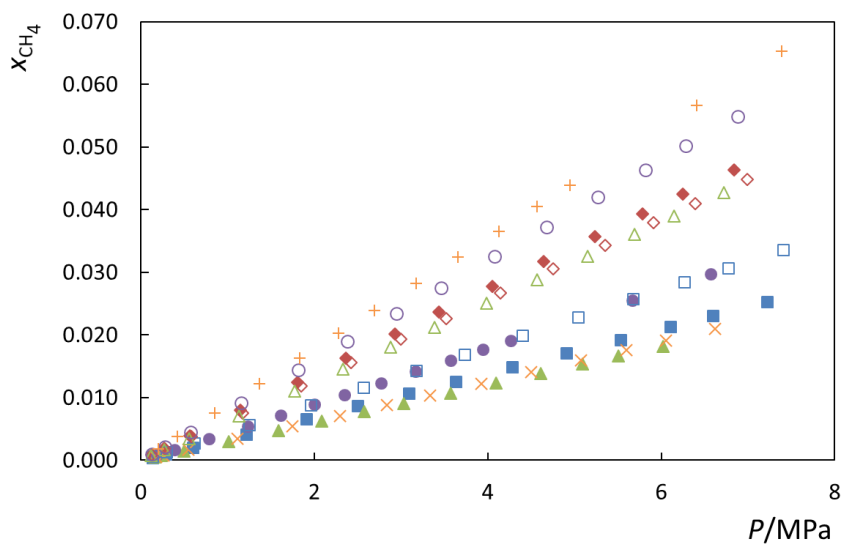


Figure S5. Predicted solubility of CH_4 , x_{CH_4} , in ionic liquid with different anion as function of pressure, P , at temperature 298.15 K using COSMO-RS. Symbols: (■), $[\text{C}_4\text{C}_{1\text{im}}][\text{SCN}]$; (◆), $[\text{C}_4\text{C}_{1\text{im}}][\text{Ac}]$; (▲), $[\text{C}_4\text{C}_{1\text{im}}][\text{BF}_4]$; (●), $[\text{C}_4\text{C}_{1\text{im}}][\text{TFA}]$; (×), $[\text{C}_4\text{C}_{1\text{im}}][\text{PF}_6]$; (□), $[\text{C}_4\text{C}_{1\text{im}}][\text{MeSO}_4]$; (◊), $[\text{C}_4\text{C}_{1\text{im}}][\text{DMP}]$; (△), $[\text{C}_4\text{C}_{1\text{im}}][\text{Tf}_2\text{N}]$; (○), $[\text{C}_4\text{C}_{1\text{im}}][\text{OcSO}_4]$, and (+), $[\text{C}_4\text{C}_{1\text{im}}][\text{DBP}]$.

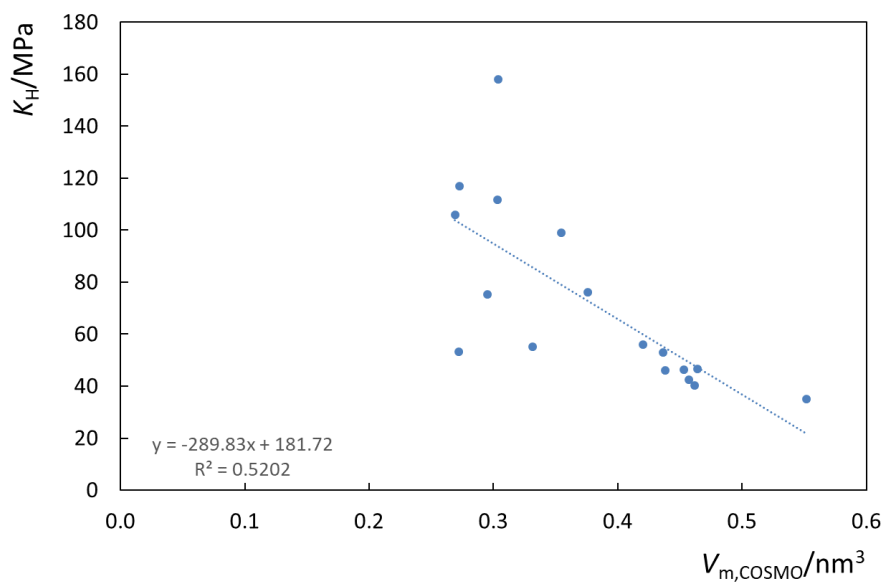


Figure S6. Plot of predicted volume of ionic liquid using COSMO-RS, $V_{m,COSMO}$, against experimentally calculated Henry's law constant, K_H , of CH_4 in ionic liquids at temperature 298.15 K.

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