

Supporting Information

“Isomer Populations in Liquids for 1-Isopropyl-3-methylimidazolium Bromide and Its Iodide, and Their Conformational Changes Accompanying the Crystallizing and Melting Processes”

Takatsugu Endo, Keiko Nishikawa*

1. Atom coordinates of the [*i*-C₃mim]⁺ ion isomers calculated at the B3LYP/6-311+G(d,p) level of theory

Asym				
Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	6	1.672108	1.156265	-0.30207
2	6	0.538716	-0.68885	0.119347
3	6	0.349103	1.420203	-0.48217
4	1	0.306888	-1.70675	0.380639
5	1	-0.14896	2.327741	-0.77838
6	1	2.537382	1.787094	-0.41597
7	6	3.020301	-0.88872	0.363259
8	1	3.538131	-0.40019	1.188022
9	1	2.781645	-1.91292	0.642444
10	1	3.651634	-0.89313	-0.52481
11	7	1.770932	-0.1688	0.074733
12	6	-1.84022	0.125171	-0.23726
13	1	-2.15475	0.839522	-1.00119
14	6	-2.41373	0.538975	1.119712
15	1	-3.5041	0.525203	1.069439
16	1	-2.10275	-0.15354	1.906189
17	1	-2.10316	1.547468	1.399935
18	7	-0.34493	0.255252	-0.21798
19	6	-2.26132	-1.27679	-0.66931
20	1	-3.34455	-1.29071	-0.7991
21	1	-1.80726	-1.56292	-1.62024
22	1	-2.02191	-2.02961	0.086656
Rotational constants (GHz)		3.380846	1.027135	0.905195

Sym

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.1133	1.257606	0.00021
2	6	-1.47426	1.232869	0.000155
3	6	-0.75211	-0.84926	-0.00023
4	7	0.32105	-0.05422	-1.8E-05
5	1	0.565309	2.092429	0.00013
6	1	-2.19148	2.036201	0.000263
7	1	-0.73267	-1.92653	-0.00017
8	7	-1.85689	-0.09441	-0.0002
9	6	1.745121	-0.52324	-6.9E-05
10	1	1.668071	-1.6131	-0.00025
11	6	2.447315	-0.06821	-1.2793
12	1	2.547248	1.019281	-1.31845
13	1	3.45261	-0.49252	-1.30421
14	1	1.915235	-0.4039	-2.17157
15	6	2.447239	-0.06864	1.279365
16	1	1.91545	-0.40521	2.17148
17	1	3.452777	-0.4924	1.303864
18	1	2.54653	1.018876	1.319215
19	6	-3.24171	-0.58928	0.000041
20	1	-3.22856	-1.67729	-0.00238
21	1	-3.75396	-0.23523	0.894123
22	1	-3.75552	-0.23138	-0.8916
Rotational Constants (GHz)		3.837107	0.938915	0.910076

2. Vibrational frequencies for two rotational isomers of the [*i*-C₃mim]⁺ ion calculated at the B3LYP/6-311+G(d,p) level of theory

Asym			Sym		
ν_{cal} (cm ⁻¹)	I_{IR} (km mol ⁻¹)	I_{Raman} (Å ⁴ amu ⁻¹)	ν_{cal} (cm ⁻¹)	I_{IR} (km mol ⁻¹)	I_{Raman} (Å ⁴ amu ⁻¹)
22.0	0.28	1.92	43.3	0.11	1.72
71.6	0.17	0.29	73.2	0.17	0.19
122.1	1.04	1.55	127.4	0.84	2.28
181.9	0.55	0.50	191.2	0.01	0.13
233.0	1.80	0.93	228.9	1.47	0.63
240.5	0.08	0.04	232.4	0.75	0.32
271.8	0.11	0.06	265.5	0.02	0.18
322.4	0.09	1.23	298.9	0.26	1.80
366.6	0.39	0.34	374.9	0.21	0.56
420.1	0.28	0.79	411.3	0.44	0.02
476.2	1.04	3.59	481.3	1.44	4.69
589.8	2.20	4.72	610.9	1.25	3.23
632.4	9.82	0.17	633.3	10.11	0.18
665.9	17.26	0.13	669.1	19.26	0.20
694.4	9.44	2.44	685.0	10.78	2.67
753.2	29.40	0.15	750.6	26.84	0.16
837.0	32.14	0.28	836.8	32.98	0.20
880.6	0.07	0.79	879.9	0.05	0.82
883.1	1.39	8.66	883.6	2.14	8.57
946.3	1.37	0.36	944.8	0.93	0.36
956.9	0.08	1.70	955.9	0.11	1.82
1017.3	1.73	2.53	1024.0	1.57	4.53
1037.7	0.41	7.42	1037.0	0.81	7.21
1099.4	3.21	3.66	1092.5	2.39	3.98
1122.8	7.45	2.98	1100.3	1.57	1.20
1128.3	7.12	5.72	1125.0	13.32	2.85
1144.7	19.56	3.14	1147.1	2.94	0.77
1149.0	4.44	0.70	1151.0	3.47	2.86
1159.4	81.05	0.94	1169.1	124.13	1.72
1194.2	38.90	1.37	1196.4	22.15	2.40
1282.4	7.66	1.35	1280.8	6.12	2.17
1323.6	6.86	15.90	1316.9	2.10	9.07
1348.8	19.73	13.54	1344.2	1.69	3.88

1353.2	7.16	5.96	1365.0	4.60	22.72
1406.3	2.66	8.93	1409.6	2.78	26.86
1416.5	14.61	1.09	1416.4	12.15	0.44
1433.4	3.70	5.02	1436.3	3.40	1.32
1445.0	11.84	21.73	1452.5	32.02	15.83
1462.8	2.79	10.50	1460.8	3.10	1.68
1483.8	5.51	5.13	1482.4	0.16	8.86
1484.4	11.07	13.03	1484.9	16.13	8.48
1491.7	4.58	3.04	1490.3	4.08	3.09
1505.2	24.81	3.95	1504.8	15.28	9.57
1508.6	4.45	5.85	1507.8	9.90	2.20
1510.7	10.48	13.58	1510.8	11.85	13.10
1589.7	57.03	1.75	1583.8	66.45	2.44
1601.8	21.36	5.58	1602.1	27.92	4.07
3039.2	5.66	5.66	3042.6	5.27	1.37
3041.8	3.42	273.17	3045.0	2.03	287.69
3068.4	3.97	178.43	3068.8	4.07	180.09
3074.4	1.11	60.94	3069.8	2.91	53.66
3107.9	4.14	19.46	3111.8	3.25	14.26
3115.3	18.48	52.06	3117.9	19.30	52.46
3120.3	6.53	41.51	3120.8	6.00	24.45
3124.9	7.73	127.46	3124.4	9.40	145.98
3148.2	0.32	43.77	3148.7	0.33	45.42
3164.1	0.49	43.77	3164.2	0.49	45.42
3273.6	15.23	41.30	3276.1	19.71	35.60
3288.1	37.37	8.63	3278.2	22.73	38.73
3292.6	0.06	120.07	3295.9	9.37	90.42
