Ion pair geometries

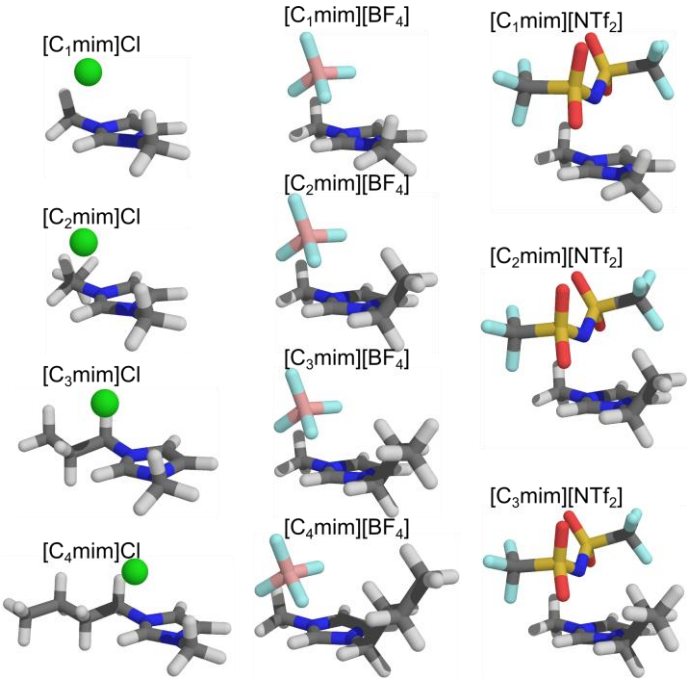

Figure S1. Lowest energy ion pairs.

Table S1. Chloride ion pair structures.

	Atom	X	Y	Z
[C1mim]Cl	C	0.0141	0.0030	0.0001
	N	0.0075	-0.0005	1.3818
	C	1.2736	-0.0034	1.8045
	N	2.0806	-0.1464	0.7509
	C	1.3087	-0.0891	-0.3944
	C	-1.1070	0.4051	2.2287
	C	3.5187	0.0790	0.8186
	Cl	1.5577	2.6211	2.1484
	H	1.5868	-0.0014	2.8356
	H	1.7497	-0.1291	-1.3777
	H	-0.8991	0.0600	-0.5707
	H	-2.0403	0.1404	1.7316
	H	-1.0421	-0.1190	3.1832
	H	-1.0257	1.4851	2.3886
	H	3.9302	-0.4707	1.6661
	H	3.9736	-0.2826	-0.1038
	H	3.6805	1.1535	0.9536
[C2mim]Cl	N	0.0110	0.0035	0.0092
	C	0.0206	-0.0004	1.3430
	N	1.2842	-0.0360	1.7708

	C	2.1051	-0.1931	0.6691
	C	1.3090	-0.1683	-0.4297
	C	1.6236	-0.3234	3.1702
	C	3.0779	-0.0169	3.4846
	C	-1.1943	-0.2454	-0.7718
	Cl	-0.5745	-2.5969	1.6884
	H	-0.8479	0.0964	1.9739
	H	3.1746	-0.2897	0.7569
	H	1.5479	-0.2460	-1.4785
	H	-1.4782	-1.2909	-0.6111
	H	-1.9900	0.4179	-0.4296
	H	-0.9803	-0.0434	-1.8214
	H	1.3695	-1.3782	3.3291
	H	0.9572	0.2859	3.7862
	H	3.2486	-0.1653	4.5537
	H	3.7562	-0.6895	2.9522
	H	3.3339	1.0179	3.2365
	N	0.0018	0.0034	0.0071
	C	0.0017	0.0072	1.3421
	N	1.2637	0.0006	1.7757
	C	2.0939	-0.1403	0.6787
	C	1.3068	-0.1422	-0.4253
	C	1.6598	-0.3062	3.1549
	C	0.6246	0.1341	4.1784
	C	1.1354	-0.1350	5.5930
	C	-1.1939	-0.2650	-0.7813
	Cl	-0.5691	-2.5612	1.8204
	H	-0.8771	0.1080	1.9549
	H	3.1639	-0.2236	0.7873
	H	1.5523	-0.2208	-1.4726
	H	-1.4612	-1.3166	-0.6349
	H	-2.0054	0.3782	-0.4382
	H	-0.9792	-0.0494	-1.8282
	H	2.6223	0.1858	3.3290
	H	1.7801	-1.3948	3.2001
	H	0.4012	1.2015	4.0519
	H	-0.2940	-0.4394	4.0110
	H	0.3874	0.1529	6.3361
	H	1.3488	-1.1999	5.7291
	H	2.0519	0.4282	5.8004
	C	0.0227	0.0052	0.0006
	N	0.0080	0.0051	1.3824
	C	1.2711	-0.0077	1.8145
	N	2.0884	0.1136	0.7672
	C	1.3215	0.0772	-0.3830
	C	-1.1179	-0.3776	2.2248

[C_3mim]Cl

[C_4mim]Cl

	C	3.5304	-0.1551	0.8104
	C	4.1402	0.1319	2.1735
	C	5.6568	-0.0594	2.1428
	C	6.2879	0.1603	3.5157
	Cl	1.5798	-2.6340	2.2369
	H	1.5654	-0.0104	2.8496
	H	1.7712	0.1095	-1.3630
	H	-0.8876	-0.0344	-0.5765
	H	-1.0607	-1.4582	2.3893
	H	-1.0476	0.1474	3.1783
	H	-2.0441	-0.0961	1.7236
	H	3.9960	0.4572	0.0313
	H	3.6476	-1.2184	0.5717
	H	3.9015	1.1590	2.4842
	H	3.7070	-0.5645	2.9025
	H	5.8811	-1.0757	1.7954
	H	6.1012	0.6311	1.4137
	H	7.3722	0.0191	3.4813
	H	6.0931	1.1749	3.8815
	H	5.8794	-0.5450	4.2467

Table S2. BF_4 ion pair structures.

	Atom	X	Y	Z
	C	0.0089	-0.0111	-0.0030
	N	0.0078	0.0146	1.3730
	C	1.2674	0.0248	1.7989
	N	2.0770	-0.0165	0.7443
	C	1.3093	-0.0306	-0.3986
	C	-1.1666	0.2216	2.2175
	C	3.5278	0.1498	0.7926
	F	1.0618	2.7125	1.1584
	B	1.5060	2.8566	2.4955
	F	0.5703	2.1842	3.3274
	F	1.6373	4.1761	2.8478
	F	2.7465	2.1688	2.6151
	H	1.5799	0.1360	2.8262
	H	1.7535	-0.0427	-1.3814
	H	-0.9071	-0.0013	-0.5723
	H	-1.9526	-0.4670	1.9045
	H	-0.8882	0.0366	3.2531
	H	-1.4815	1.2616	2.1241
	H	3.8688	-0.0607	1.8046
	H	3.9853	-0.5433	0.0852
	H	3.7676	1.1866	0.5549
m]	N	-0.0067	0.0159	0.0111

[C_1mim][BF_4]

	C	-0.0014	0.0039	1.3415
	N	1.2582	-0.0053	1.7673
	C	2.0916	0.0214	0.6710
	C	1.2966	0.0362	-0.4316
	C	1.6756	0.1153	3.1732
	C	2.5191	1.3653	3.3775
	C	-1.1890	0.1993	-0.8280
	F	0.3969	2.7234	1.0932
	B	-0.7860	2.7941	1.8707
	F	-0.5310	2.1193	3.0961
	F	-1.7965	2.0631	1.1882
	F	-1.1698	4.0951	2.0795
	H	-0.8750	0.0714	1.9728
	H	3.1655	0.0348	0.7675
	H	1.5394	0.0705	-1.4821
	H	-1.0893	-0.4284	-1.7148
	H	-2.0717	-0.0873	-0.2594
	H	-1.2713	1.2545	-1.0900
	H	2.2128	-0.7991	3.4422
	H	0.7568	0.1800	3.7568
	H	2.7396	1.4775	4.4423
	H	3.4708	1.3001	2.8411
	H	1.9650	2.2405	3.0319
$[C_3mim][BF_4]$	N	-0.0096	0.0157	0.0133
	C	-0.0040	0.0081	1.3437
	N	1.2556	0.0040	1.7696
	C	2.0889	0.0301	0.6730
	C	1.2936	0.0386	-0.4297
	C	1.6693	0.1465	3.1726
	C	2.4858	1.4188	3.3781
	C	2.7377	1.6522	4.8652
	C	-1.1929	0.1934	-0.8254
	F	0.3644	2.7284	1.0970
	B	-0.8167	2.7925	1.8785
	F	-0.5543	2.1215	3.1049
	F	-1.8232	2.0540	1.1994
	F	-1.2075	4.0914	2.0869
	H	-0.8776	0.0758	1.9750
	H	3.1626	0.0470	0.7704
	H	1.5367	0.0691	-1.4802
	H	-1.0895	-0.4320	-1.7134
	H	-2.0738	-0.0994	-0.2573
	H	-1.2814	1.2486	-1.0864
	H	2.2297	-0.7508	3.4561
	H	0.7496	0.1969	3.7586
	H	3.4402	1.3348	2.8431

	H	1.9274	2.2529	2.9436
	H	3.3493	2.5453	5.0162
	H	1.7910	1.8018	5.3938
	H	3.2606	0.8053	5.3251
$[C_4mim][BF_4]$	C	0.0054	-0.0145	0.0010
	N	0.0079	0.0126	1.3772
	C	1.2700	0.0095	1.7983
	N	2.0768	-0.0412	0.7421
	C	1.3050	-0.0495	-0.3988
	C	-1.1569	0.2541	2.2259
	C	3.5387	0.1119	0.7945
	C	3.9817	1.3883	0.0853
	C	5.4364	1.7174	0.4158
	C	5.9159	2.9673	-0.3188
	F	1.1337	2.6910	1.3897
	B	1.5727	2.7856	2.7355
	F	2.8095	2.0853	2.8287
	F	0.6317	2.0899	3.5369
	F	1.7136	4.0919	3.1301
	H	1.5858	0.1205	2.8251
	H	1.7428	-0.0742	-1.3841
	H	-0.9121	0.0026	-0.5659
	H	-1.9951	-0.3287	1.8419
	H	-0.9196	-0.0509	3.2436
	H	-1.3742	1.3229	2.2229
	H	3.9909	-0.7832	0.3550
	H	3.7993	0.1635	1.8528
	H	3.8637	1.2735	-1.0012
	H	3.3291	2.2047	0.4112
	H	5.5188	1.8717	1.4984
	H	6.0820	0.8654	0.1600
	H	6.9527	3.2046	-0.0632
	H	5.8591	2.8324	-1.4049
	H	5.2969	3.8306	-0.0539

Table S3. NTf_2 ion pair structures.

	Atom	X	Y	Z
$[C_1mim][NTf_2]$	C	0.0205	-0.0135	0.0012
	N	0.0109	-0.0021	1.4616
	C	1.1293	-0.0075	2.2653
	C	0.6975	-0.1244	3.5489
	N	-0.6761	-0.1750	3.5062
	C	-1.0648	-0.1243	2.2345
	C	-1.5383	-0.4814	4.6440
	H	0.3978	-0.9773	-0.3430

	H	0.6460	0.8064	-0.3548
	H	-1.0005	0.1044	-0.3574
	H	2.1251	0.0460	1.8540
	H	1.2388	-0.2249	4.4763
	H	-1.3470	0.2379	5.4416
	H	-1.3118	-1.4961	4.9794
	H	-2.5771	-0.4109	4.3230
	H	-2.0788	-0.2293	1.8776
	N	-0.4816	-2.8678	2.4677
	S	-1.4788	-3.4335	1.3489
	S	0.3345	-3.7656	3.5241
	O	-0.1228	-5.1274	3.7109
	O	0.5940	-2.9139	4.6821
	O	-1.7356	-2.3239	0.4295
	O	-1.2062	-4.7567	0.8302
	C	-3.0777	-3.5666	2.2818
	C	1.9826	-3.9219	2.6915
	F	-3.4485	-2.3415	2.7038
	F	-4.0373	-4.0420	1.4985
	F	-2.9473	-4.3459	3.3448
	F	1.8551	-4.5793	1.5464
	F	2.8280	-4.5732	3.4819
	F	2.4950	-2.7123	2.4317
$[C_2mim][NTf_2]$	C	0.0061	-0.0011	0.0103
	N	0.0132	-0.0045	1.3852
	C	1.2774	-0.0127	1.8030
	N	2.0811	-0.0528	0.7444
	C	1.3033	-0.0431	-0.3936
	C	-1.1521	0.2464	2.2275
	C	3.5501	0.0243	0.7846
	C	4.0547	1.1989	-0.0409
	H	3.8279	1.0775	-1.1041
	H	3.6055	2.1294	0.3132
	H	5.1398	1.2727	0.0681
	H	3.9466	-0.9296	0.4245
	H	3.8197	0.1549	1.8334
	H	1.7328	-0.0468	-1.3825
	H	-0.9119	0.0754	-0.5507
	H	-1.4485	1.2900	2.0975
	H	-1.9600	-0.4211	1.9256
	H	-0.8826	0.0544	3.2653
	H	1.6054	0.0751	2.8287
	N	1.0014	2.7359	1.5306
	S	2.0014	3.2569	2.6713
	S	0.0181	3.6715	0.6668
	C	1.0430	3.9860	-0.8443

	C	0.9225	3.1880	4.1784
	F	0.5398	1.9145	4.3852
	F	-0.1663	3.9252	4.0172
	F	1.5851	3.6071	5.2477
	O	2.9552	2.1718	2.9088
	O	2.4627	4.6245	2.5694
	O	-0.2739	4.9809	1.2125
	O	-1.0666	2.8195	0.1876
	F	1.3245	2.8327	-1.4662
	F	2.1889	4.5715	-0.5145
	F	0.3808	4.7668	-1.6898
$[C_3mim][NTf_2]$	N	-0.0114	0.0117	0.0011
	C	0.0053	0.0132	1.3304
	N	1.2694	-0.0063	1.7480
	C	2.0925	-0.0647	0.6476
	C	1.2898	-0.0457	-0.4498
	C	1.7017	-0.1917	3.1300
	C	-1.2186	-0.0827	-0.8327
	H	-2.0608	-0.1736	-0.1445
	C	-2.5359	-1.5541	-2.3764
	C	-1.1663	-1.3002	-1.7519
	H	-0.8551	-2.1674	-1.1622
	H	-0.4129	-1.1460	-2.5341
	H	-2.8937	-0.6799	-2.9322
	H	-2.4923	-2.3980	-3.0692
	H	-3.2663	-1.7940	-1.5976
	H	-0.8697	-0.0324	1.9629
	H	3.1627	-0.1568	0.7452
	H	1.5317	-0.0864	-1.4999
	H	2.4917	0.5256	3.3567
	H	2.0690	-1.2148	3.2384
	H	0.8494	-0.0228	3.7869
	H	-1.3161	0.8482	-1.4009
	N	0.3239	-2.7452	1.3427
	S	1.6171	-3.7030	1.3823
	S	-1.1730	-3.2392	1.6398
	O	2.7724	-2.8488	1.6423
	O	1.4631	-4.9552	2.0934
	O	-1.4880	-4.6122	1.3089
	O	-2.0580	-2.1597	1.1975
	C	1.8076	-4.1557	-0.4059
	C	-1.2822	-3.1210	3.4878
	F	-2.4954	-3.4693	3.8984
	F	-0.3781	-3.8874	4.0775
	F	-1.0618	-1.8470	3.8645
	F	2.8632	-4.9460	-0.5613

F	0.7235	-4.7784	-0.8523
F	1.9920	-3.0537	-1.1429

Cluster structures

Table S4. Optimised geometry of $[NMe_4][BF_4]$, 1 ion-pair.

Atom	*x*	*y*	*z*
N	-3.8322757874	1.3104721616	-0.1675080669
C	-2.3337703395	1.3666796647	-0.2249788257
C	-4.3912221301	2.6989762892	-0.2830362999
C	-4.2600383032	0.7135111252	1.1273568147
H	-4.0784141387	3.1244732065	-1.2362296518
H	-4.0009327344	3.2912096205	0.5468363393
H	-5.4790588647	2.6322830729	-0.2252663946
H	-2.0337812252	1.7957910628	-1.1818835808
H	-1.9522612374	0.3484217432	-0.1267091743
H	-1.9849425964	1.9865237476	0.6027626032
H	-3.8561071883	-0.2974239203	1.2046955460
H	-5.3506185910	0.6834102543	1.1598584821
H	-3.8800071407	1.3306605353	1.9433647845
C	-4.3403359636	0.4694318287	-1.3020127249
H	-4.0201106351	0.9205117184	-2.2421028456
H	-5.4302036098	0.4442268217	-1.2431929756
H	-3.9289793825	-0.5353956278	-1.1908223767
B	-2.7179880368	2.8811840758	-3.4625346619
F	-2.3721707590	3.4916941142	-4.6380556090
F	-2.3532556544	3.6663683158	-2.3334037266
F	-2.0919116191	1.6158615693	-3.3084373682
F	-4.1213140627	2.6639986201	-3.3853202877

Table S5. Optimised geometry of $[NMe_4][BF_4]$, 2 ion-pairs.

Atom	*x*	*y*	*z*
N	-3.8898328724	1.6031443500	-0.2027120762
C	-2.4200477733	1.7865625199	-0.4386047333
C	-4.6017978643	2.8930584385	-0.4851691921
C	-4.1251882395	1.2119360617	1.2206813232
H	-4.4211866924	3.1633315444	-1.5260676693
H	-4.2238354823	3.6470575615	0.2066760444
H	-5.6675440643	2.7364435913	-0.3047840579
H	-2.2699404880	2.0868355333	-1.4770263675
H	-1.9243339703	0.8337578530	-0.2404629743
H	-2.0641267396	2.5506240792	0.2529533575
H	-3.5883796738	0.2816856507	1.4163511604
H	-5.1970103172	1.0655709501	1.3661806862

H	-3.7576332237	2.0127855174	1.8638844934
C	-4.4033305556	0.5407370175	-1.1182524650
H	-4.2099451913	0.8528381224	-2.1451950281
H	-5.4745476689	0.4224684325	-0.9452177829
H	-3.8827566684	-0.3919388904	-0.8926435422
B	-2.8025549070	3.5711836449	-3.6890082602
F	-2.6913015365	3.8552376210	-5.0256778410
F	-3.5261580312	4.6115775803	-3.0165870901
F	-1.5402090049	3.4836610247	-3.0657662118
F	-3.4961261201	2.3629191111	-3.4535875175
H	-4.1956772737	7.6151016243	-0.8982501036
H	-4.0542245351	5.8985227104	-1.3916585880
C	-3.6988609487	6.6628586371	-0.7001178916
H	-3.8482151386	6.3625368450	0.3383710027
F	-4.5764718554	4.9656325479	1.9276274685
H	-2.5331241131	8.1697045920	-2.5551261549
H	-2.3616770870	6.4390854773	-3.0033222129
F	-2.6206264350	6.0869186763	2.3147180832
C	-1.9948880288	7.2401567217	-2.3599169233
N	-2.2294661821	6.8482124787	-0.9366775516
B	-3.3137257073	4.8782815660	2.5501495809
F	-3.4240677283	4.5938585867	3.8868312158
H	-2.2391801863	8.8429212351	-0.2462310847
H	-1.8920564390	4.8048900415	-1.3470835871
C	-1.7170739939	7.9109937350	-0.0210780787
C	-1.5155823978	5.5592334511	-0.6547486736
H	-1.9095292428	7.5983321462	1.0058701804
H	-0.9233185096	7.3880727433	-2.5054839854
H	-1.6957697047	5.2882042077	0.3860242220
F	-2.5901632855	3.8383113955	1.8772666751
H	-0.6461035352	8.0308426768	-0.1945335551
H	-0.4500105867	5.7176205893	-0.8347542939

Table S6. Optimised geometry of $[NMe_4][BF_4]$, 4 ion-pairs.

Atom	*x*	*y*	*z*
N	-0.9299646528	0.5524541378	0.1566678597
C	0.5466510653	0.3983704670	-0.0331873773
C	-1.3080475948	1.9817511953	-0.0648237145
C	-1.3128746464	0.1739798190	1.5502526788
H	-1.0274427718	2.2353980405	-1.0872742458
H	-0.7672221898	2.5800800453	0.6689693065
H	-2.3857173472	2.0601309893	0.0763388087
H	0.7974875525	0.7162937020	-1.0471469424
H	0.8019075472	-0.6528891319	0.1166896170
H	1.0504819261	1.0264370721	0.7027703902
H	-1.0450347606	-0.8717440050	1.7138966124
H	-2.3908990121	0.3140865471	1.6527772810
H	-0.7682953850	0.8228585713	2.2388835158

C	-1.6636270320	-0.3017262047	-0.8269086141
H	-1.3622246344	0.0042545366	-1.8301780590
H	-2.7342661118	-0.1420968194	-0.6921169828
H	-1.3964890214	-1.3444446364	-0.6433463876
B	0.8246519662	2.5194568374	-3.4791478940
F	1.4364254979	1.9678192877	-4.5755166208
F	0.2285230216	3.7678858754	-3.8054317831
F	1.7270245383	2.7311374512	-2.4154556327
F	-0.2177081168	1.6712757184	-3.0083006905
H	-0.6950593806	5.3261063854	-0.7632398174
H	0.4547269143	3.9833488694	-1.1348330902
C	0.2444668882	4.8409412397	-0.4946526494
H	0.2522860168	4.5587202632	0.5577540238
F	-0.8777006607	4.1179342769	2.5671292247
H	0.3710940626	6.7563365970	-2.3278967277
H	1.4483328613	5.3923739850	-2.7676201028
F	1.3025840510	4.8204054374	2.5658280048
C	1.3311664642	6.2732082705	-2.1340734842
N	1.3441351962	5.8310258541	-0.7060043035
B	0.4546896295	3.7651379709	2.9545319307
F	0.5115684341	3.5232179802	4.3037715512
H	0.1699592727	7.4562954986	-0.0535336708
H	2.7670903465	4.3180455816	-1.0575726696
C	1.1314452493	7.0037973594	0.1968608629
C	2.6468492691	5.1687234044	-0.3843766584
H	1.1416959711	6.6418447895	1.2264657711
H	2.1519895720	6.9772379728	-2.2847478810
H	2.6098886643	4.8401064594	0.6562189551
F	0.8033841034	2.6104518247	2.2075391964
H	1.9430672619	7.7156889602	0.0320167977
H	3.4478517884	5.8957660422	-0.5327102730
N	-3.2455108504	4.0178665953	-3.8482698689
C	-2.5809677722	4.1151859610	-2.5130112596
C	-4.7152743212	4.2373019395	-3.6792804617
C	-2.9904609492	2.6581823279	-4.4151903115
H	-4.8618573432	5.2377708847	-3.2687710548
H	-5.0994992902	3.4828756691	-2.9900914209
H	-5.1887171453	4.1468154570	-4.6589566945
H	-2.7616302996	5.1178602175	-2.1252066744
H	-1.5162532619	3.9417744144	-2.6673677906
H	-3.0182969464	3.3449382896	-1.8771538645
H	-1.9116313771	2.5178046818	-4.4961972313
H	-3.4661227343	2.5974040625	-5.3964451203
H	-3.4171767650	1.9212172348	-3.7324279928
C	-2.6703113832	5.0628605308	-4.7489391563
H	-2.8570858394	6.0387627633	-4.2970423603
H	-3.1600022959	4.9866969327	-5.7219953534
H	-1.5995444637	4.8734446044	-4.8426047934
B	-2.9773639618	7.8151766817	-1.4938607182

F	-2.7335226293	9.0954352366	-1.9205570947
F	-3.6938996015	7.8006837361	-0.2766058108
F	-1.7429218615	7.1221110324	-1.2778703394
F	-3.7083093036	7.0759928993	-2.4519277405
H	-5.9135778114	5.9090591590	2.3362932020
H	-5.2456876406	6.4908302514	0.7727793700
C	-5.3521767306	5.6341601926	1.4410461029
H	-5.8314863551	4.8010489910	0.9229982666
F	-5.5516976536	3.0444612050	-0.6685221987
H	-3.8467471425	6.5987932676	3.4270963284
H	-3.2064793970	7.1542640329	1.8431487051
F	-4.3878688221	1.5839867677	0.6648348344
C	-3.2709638354	6.3188192293	2.5426391208
N	-3.9830945082	5.1970110151	1.8563145688
B	-5.0896442652	1.7128577819	-0.5646500634
F	-6.1177421555	0.8105351078	-0.6474924417
H	-4.6624050594	4.3026025155	3.6445206237
H	-3.1414787641	5.6940763287	0.0010512308
C	-4.0768426413	4.0159889281	2.7684370523
C	-3.2201277471	4.8087901873	0.6306180298
H	-4.5599808717	3.2001773867	2.2270894714
H	-2.2788926006	5.9634847212	2.8280680514
H	-3.7842882825	4.0193647624	0.1344368595
F	-4.1451460943	1.5075394524	-1.6114286045
H	-3.0635238092	3.7335519271	3.0607204088
H	-2.2357792302	4.4650201180	0.9485380793

Table S7. Optimised geometry of $[NMe_4][BF_4]$, 8 ion-pairs.

Atom	*x*	*y*	*z*
N	-0.9456202337	0.4228052819	0.1055647222
C	0.5400116603	0.2914103862	0.2179727445
C	-1.2881763852	1.8159979134	-0.3118026632
C	-1.5792821552	0.1359321919	1.4273106009
H	-0.8100304149	1.9934518976	-1.2745627054
H	-0.9117796564	2.4968303946	0.4534444980
H	-2.3720126871	1.8731810537	-0.3957107690
H	0.9821899353	0.5541502379	-0.7451941884
H	0.7963156415	-0.7344234038	0.4879222461
H	0.8755473346	0.9905052894	0.9871782048
H	-1.3175880887	-0.8829376115	1.7188984221
H	-2.6596860762	0.2502343336	1.3221674377
H	-1.1885841984	0.8541171841	2.1511302726
C	-1.4630284103	-0.5311278133	-0.9238593643
H	-0.9836828870	-0.2928899624	-1.8745651031
H	-2.5439745725	-0.3985765042	-1.0009331003
H	-1.2102812727	-1.5455785723	-0.6097325925
B	0.9051983352	2.3791804467	-3.3222936513

F	1.8301543843	2.1228178700	-4.3121618285
F	0.2062707466	3.5848597265	-3.5904475847
F	1.5517190693	2.5311352402	-2.0658610303
F	-0.0378880982	1.3407406841	-3.2032169408
H	-0.7212986661	5.3149516183	-0.5862908960
H	0.4889283036	4.0578752472	-1.0449363625
C	0.2702620691	4.9040340458	-0.3923406735
H	0.3823023905	4.6206244175	0.6548846057
F	-0.9287933277	4.6698426700	3.5368224084
H	0.1259869358	6.7792739288	-2.2656960396
H	1.2891699859	5.4992830701	-2.7470399681
F	1.2024712171	4.9006511999	2.6989788898
C	1.1325893690	6.3818212248	-2.1238523448
N	1.2706889352	5.9754713781	-0.6915718698
B	0.2759905820	4.0076105131	3.2829705681
F	0.8163477323	3.4512410882	4.4329870733
H	0.0276136888	7.5388074982	-0.0118870106
H	2.7727142145	4.5310541989	-1.0465057929
C	1.0241953957	7.1488664120	0.2018624165
C	2.6444271631	5.4349821188	-0.4501655180
H	1.0977871568	6.8053203996	1.2355101336
H	1.8822674640	7.1457472488	-2.3382030922
H	2.7356920308	5.2101052907	0.6138679195
F	0.0344355355	2.9650063518	2.3358241804
H	1.7857586740	7.9037651795	-0.0039471514
H	3.3864286711	6.1818930847	-0.7373986710
N	-3.2187753444	4.0515215081	-3.7522487099
C	-2.6801452189	4.1312072715	-2.3601892811
C	-4.6817074761	4.3640634314	-3.7210107344
C	-2.9996955911	2.6670970855	-4.2730712682
H	-4.8009228005	5.3749383019	-3.3279047944
H	-5.1718454872	3.6420148139	-3.0660239251
H	-5.0704046769	4.2961271054	-4.7392790006
H	-2.8316485424	5.1478662784	-1.9965934990
H	-1.6175269897	3.8883624163	-2.4078035572
H	-3.2340252655	3.4116774323	-1.7577588367
H	-1.9276587391	2.4605437471	-4.2696067011
H	-3.4000503387	2.6114033273	-5.2876338224
H	-3.5208613203	1.9701562762	-3.6136065490
C	-2.5034492168	5.0454862139	-4.6104601375
H	-2.6721771136	6.0380277009	-4.1879558957
H	-2.9114743613	4.9826838850	-5.6213560713
H	-1.4421582731	4.7904947151	-4.6109222916
B	-3.0903304949	7.7240784061	-1.3662058636
F	-2.8743101323	9.0725601736	-1.4826668628
F	-3.8930436574	7.4128662907	-0.2456830872
F	-1.8391107364	7.0442026401	-1.1774147535
F	-3.6871581292	7.1776418799	-2.5202542944
H	-6.0523789838	5.4878143958	2.2693090578

H	-5.2576733394	6.0334883536	0.7526626964
C	-5.3449953030	5.2258110503	1.4800643517
H	-5.6364747285	4.2997370765	0.9837470930
F	-5.3063099733	3.0953062614	-0.8304221723
H	-4.2964874606	6.5439524809	3.5474142731
H	-3.5220754232	7.0719959789	2.0176658256
F	-4.3298483493	1.7029763331	0.6957856099
C	-3.5645389307	6.2899330642	2.7778029499
N	-4.0015531413	5.0246777437	2.1106450891
B	-5.0583093800	1.7329964722	-0.5305663072
F	-6.2186232094	1.0143562982	-0.4352846143
H	-4.8061147756	4.1771869718	3.8706382843
H	-2.9190134408	5.5088110258	0.3701924726
C	-4.0711794640	3.9129642626	3.1073415609
C	-3.0047712643	4.6622857139	1.0541320800
H	-4.3728818635	3.0053725411	2.5809819318
H	-2.5837593083	6.1209982090	3.2245999241
H	-3.3779116521	3.7745858214	0.5415224254
F	-4.2045168649	1.2242169010	-1.5425906570
H	-3.0824146773	3.7955633533	3.5543089326
H	-2.0548994932	4.4571023594	1.5526845973
H	3.0707687408	3.7070830812	3.9391215531
H	4.7604807441	3.8512683393	3.3323803860
C	4.0198135840	3.1910608821	3.7878074926
H	4.3953450729	2.7967700615	4.7339722211
H	2.3296721641	3.0525653273	1.7230136298
H	4.0285314847	3.2746792030	1.1708557481
N	3.7928480226	2.0412584998	2.8585018527
C	3.2919924585	2.5664072322	1.5504953358
H	1.8638452908	1.6433423234	3.6238503739
C	2.7921562602	1.0986057771	3.4455182720
H	3.1943416573	0.7202293911	4.3872329559
H	5.7878705307	2.0024935837	2.1828962096
C	5.0802878390	1.3113447765	2.6449021458
H	5.4638996090	0.9724189673	3.6066054318
H	3.1867207714	1.7282934888	0.8602561581
H	2.6538020506	0.2765350337	2.7415795901
H	4.8668888120	0.4588928501	2.0001056612
F	3.2560780353	-0.3643158557	0.5830042294
H	5.4317754468	0.1212954877	-0.2626481060
F	4.1621712726	-1.9954059426	1.9162516921
B	3.5189790000	-1.7652997721	0.6841517684
F	2.3188866791	-2.4523068296	0.6092964617
F	4.3907269433	-2.1115629620	-0.3583455005
F	6.1703470771	5.9204818392	-0.0233874202
F	6.1669003507	4.0442885616	1.3157723125
B	6.2058647671	4.5432448830	-0.0121060870
F	7.3661068769	4.0377692201	-0.6275343948
F	5.0757622510	4.0138870042	-0.6927678905

H	5.7874510683	1.8832311368	-0.3424173893
H	6.1428874949	2.9201422197	-2.4807526091
C	5.9956785354	0.9025818298	-0.7745272830
H	3.9579513145	2.2380818214	-1.7917476257
H	7.0658051579	0.6954800255	-0.7705875016
C	6.3145847195	1.9529044848	-2.9536756303
H	7.3719230693	1.6885406716	-2.9118246016
C	4.0879208706	1.2497613124	-2.2324820598
N	5.5448553542	0.9176747506	-2.1970875415
H	5.9534929729	1.9553123722	-3.9840789776
H	3.5528978570	0.4990410326	-1.6470605494
H	3.7396648272	1.2555118396	-3.2665264053
C	5.7854497263	-0.4324082696	-2.7936075608
H	6.8521638224	-0.6540845581	-2.7244764361
H	5.2083841120	-1.1648223358	-2.2259910786
H	5.4604150281	-0.4076558442	-3.8356556059
F	8.8709337829	-0.1282382622	5.8441979863
F	7.4242455280	0.3221107612	4.1147487519
B	8.7700196014	0.3736167619	4.5676412661
F	9.2208954462	1.7063534436	4.4818838467
H	9.4637951527	3.5891775155	3.0224231668
H	10.7820775500	1.5876367308	2.9294653483
C	9.7170163386	3.8429689993	1.9915460961
N	9.9614022172	2.5700972626	1.2495732624
C	11.0663975994	1.7970466988	1.8982274245
H	10.6254450318	4.4480996935	1.9556689454
H	11.9740084527	2.4032244326	1.8555287166
C	10.3211702697	2.8621308842	-0.1721744269
H	11.2345047664	3.4606338241	-0.1767629844
H	8.8896274803	4.3645346826	1.5068358406
H	8.4398472287	1.5781771079	2.3185390690
C	8.7069058609	1.7569389298	1.2759937982
H	7.9358033053	2.3357683616	0.7657347601
H	8.9178679182	0.8231683369	0.7546628144
H	9.4956320632	3.4095411325	-0.6292063387
H	10.4749682186	1.9126157288	-0.6864980315
F	9.5324099447	-0.4043396551	3.6526015103
H	11.1965352221	0.8667443702	1.3425656701
C	7.2685522059	-2.9869460219	3.2196548179
H	7.7688372318	-2.2647022151	3.8674689947
N	7.6914253637	-2.7274149678	1.8104143461
C	7.2854222843	-1.3375181715	1.4392925994
H	7.7466747511	-0.6544648675	2.1519918531
H	7.6262635452	-1.1629680846	0.4192208616
B	9.5832655828	-0.7556813849	-1.5420338257
F	8.8941181226	0.4531325413	-1.8385625099
H	6.1979119267	-1.2935319106	1.5050349162
H	6.1852248243	-2.8642114499	3.2765566971
H	7.5540953309	-4.0068141917	3.4861792468

C	9.1777407590	-2.8586703934	1.6859812301
H	9.6391440091	-2.1343673594	2.3584604760
C	7.0181124013	-3.6852792239	0.8824527476
H	9.4517824182	-2.6446454131	0.6524220563
F	8.6074433522	-1.7741621324	-1.3828076234
F	10.2364401517	-0.5725169078	-0.2987168444
F	10.4707481507	-1.0674983505	-2.5389108103
H	9.4527362087	-3.8791187171	1.9616809402
H	7.3239198419	-4.6988376127	1.1500495024
H	5.9384940144	-3.5627369244	0.9825688761
H	7.3307122620	-3.4436489397	-0.1351641667

Table S8. Optimised geometry of [C_1mim][BF_4], 1 ion-pair.

Atom	*x*	*y*	*z*
C	0.0097476009	-0.0159542135	0.0002759473
N	0.0085402828	0.0139080172	1.3761646889
C	1.2681789494	0.0266063182	1.8021044902
N	2.0777599610	-0.0173123977	0.7475981344
C	1.3101605088	-0.0355254114	-0.3952798775
C	-1.1668102510	0.2211403933	2.2192616012
C	3.5287194813	0.1490584806	0.7946611180
F	1.0600804910	2.7155498418	1.1508831427
B	1.5043656223	2.8616100723	2.4875589554
F	0.5688581989	2.1904687497	3.3207280700
F	1.6355259691	4.1817134022	2.8381245283
F	2.7450907473	2.1744699968	2.6083500585
H	1.5805853579	0.1412198765	2.8291618276
H	1.7545746443	-0.0505965718	-1.3779632044
H	-0.9064127248	-0.0088680082	-0.5688634456
H	-1.9524744776	-0.4672735355	1.9045270338
H	-0.8903535156	0.0349742583	3.2553785480
H	-1.4812794671	1.2613123871	2.1255522511
H	3.8704892318	-0.0592396301	1.8068813947
H	3.9853739238	-0.5459322612	0.0885789633
H	3.7686094650	1.1851602356	0.5540757748

Table S9. Optimised geometry of [C_1mim][BF_4], 2 ion-pairs.

Atom	*x*	*y*	*z*
C	0.0263775154	0.0871629294	0.3030337630
N	-0.0576937796	-0.0321633281	1.6725271662
C	1.1687417766	-0.1714998501	2.1665231449
N	2.0349478050	-0.1647224992	1.1585688024
C	1.3445254749	0.0038631113	-0.0203444603
C	-1.2625776361	0.0995784449	2.4856197078
C	3.4839431650	-0.2013664330	1.3255699377

F	1.2223562547	2.6678735522	1.4654003155
B	1.5249158443	2.8025244735	2.8184824081
F	0.4933038551	2.1787985717	3.5903730695
F	1.6739798142	4.1154344734	3.2056253186
F	2.7214020634	2.0717340715	3.1020937090
H	1.4210015802	-0.2667659506	3.2132370272
H	1.8476650284	0.0645749062	-0.9723931329
H	-0.8481450406	0.2341908904	-0.3109530030
H	-2.0446995833	-0.5352955435	2.0661442342
H	-1.0199365803	-0.2222509000	3.4987717700
H	-1.5676504680	1.1468185549	2.4945760453
H	3.6918012369	-0.5042813202	2.3520624637
H	3.9059475968	-0.9240988950	0.6255323039
H	3.8836472553	0.7983901666	1.1489839058
C	2.0111857751	1.2506609207	8.1800822576
N	1.3285955590	1.4228079342	6.9971717830
C	2.2011309981	1.4291431018	5.9946888806
N	3.4240883808	1.2861486995	6.4961887756
C	3.3311397926	1.1648414687	7.8649697031
C	-0.1191337684	1.4655195220	6.8209720110
C	4.6333152422	1.1524191880	5.6898335706
F	2.1516164522	-1.4098885306	6.6932509085
B	1.8477870291	-1.5444021612	5.3404855955
F	0.6505866507	-0.8143242246	5.0582177250
F	1.6988797949	-2.8572533313	4.9533335664
F	2.8784518460	-0.9200259375	4.5679502895
H	1.9562683555	1.5271064825	4.9464721978
H	4.2013823680	1.0144925798	8.4841606890
H	1.5018342593	1.1903494838	9.1288631586
H	-0.5428709845	2.1843911427	7.5240861812
H	-0.3192190487	1.7775848904	5.7954660379
H	-0.5234327361	0.4656837248	6.9865449832
H	4.3991787542	1.4824126122	4.6771898550
H	5.4165996791	1.7799970128	6.1182607725
H	4.9321324228	0.1033159950	5.6758665615

Table S10. Optimised geometry of $[C_1mim][BF_4]$, 4 ion-pairs.

Atom	*x*	*y*	*z*
C	1.0306974974	-1.1017817711	0.7009382095
N	0.8172781944	-0.9457713197	2.0520848652
C	1.9402174261	-0.5124740058	2.6234453311
N	2.8768390451	-0.4066460727	1.6841062527
C	2.3283162260	-0.7635286669	0.4711393656
C	-0.4731608571	-1.0672082428	2.7266007464
C	4.2088641496	0.1548651774	1.8839688529
F	1.1646895213	1.9629788496	1.4652366375
B	1.2652447195	2.4664091664	2.7587077767

F	0.4633179062	1.6609758203	3.6364947630
F	0.8828856215	3.7841770763	2.8635180106
F	2.6152889855	2.3115087509	3.2079930019
H	2.0666401087	-0.2778753938	3.6709118063
H	2.9024185686	-0.7331117605	-0.4412402325
H	0.2469495462	-1.4563798258	0.0486381366
H	-1.0693597039	-1.8046163914	2.1866221423
H	-0.3002904934	-1.3832451073	3.7587260384
H	-0.9634303134	-0.0922592755	2.7155733599
H	4.4436757813	0.1123100672	2.9466660709
H	4.9272257260	-0.4357503437	1.3125825217
H	4.2035673121	1.1937091269	1.5489910411
C	2.0020642864	2.0389370312	8.3164306332
N	1.3621558910	1.7575540354	7.1296704435
C	2.2078879932	1.9690801923	6.1257025616
N	3.3640888533	2.3932837660	6.6271517602
C	3.2627773747	2.4392383596	7.9994580326
C	0.0156187854	1.2199219727	6.9638349069
C	4.5645559540	2.6322014546	5.8313939984
F	3.4417171979	-0.4653810698	7.2367956097
B	3.1590046044	-0.9430105171	5.9636374397
F	1.7596244807	-0.8441968515	5.7162543814
F	3.5543329893	-2.2705588097	5.8049438256
F	3.8116789331	-0.1358616086	4.9985509959
H	1.9939284140	1.8213852757	5.0760504957
H	4.0931422352	2.7309087144	8.6227797964
H	1.5139405925	1.9197623410	9.2706983050
H	-0.6847981309	1.8268458448	7.5399849874
H	-0.2331513917	1.2652267659	5.9027208234
H	0.0042448162	0.1822728729	7.3005923238
H	4.2657432409	2.6777168397	4.7839473298
H	5.0132251502	3.5782747284	6.1382244691
H	5.2564285840	1.8018577944	5.9814148711
H	-3.0276508350	-8.3956378680	-0.4034005327
H	-3.2709757254	-6.6191574919	-0.2463610911
H	-2.9420118601	-4.3816226302	4.4227057164
C	-2.5791020306	-7.4495235139	-0.0964794244
H	-2.2181223471	-6.0110212488	4.1867515841
C	-2.2235782152	-4.9722765106	3.8514554264
H	-2.2804055789	-7.4950925069	0.9510183500
H	-2.4584129001	-4.9300844948	2.7887506627
H	-2.1074208139	-7.5476393274	-2.8878686542
N	-1.3785791692	-7.2104812186	-0.8921088683
F	-1.8264225614	-4.6815993034	0.7368647406
C	-1.2770864037	-7.2561383518	-2.2644192468
F	-0.6300281919	-7.1290028744	2.5273762214
N	-0.8916258866	-4.4105195729	4.0511215661
H	-0.9170386121	-4.0838814936	6.1764729500
C	-0.3430387826	-4.0535114261	5.2640264734

B	-1.1737987590	-3.8742412837	-0.2280706060
F	-1.4565340641	-4.3517075833	-1.5012846692
F	-1.5691725085	-2.5467229191	-0.0692061319
C	-0.2224409024	-6.7863745899	-0.3904301649
C	0.0449449802	-4.3048475885	3.1117168255
B	0.7200161059	-7.2837548773	2.9767471398
H	-0.0086224259	-6.6389497811	0.6592910414
H	-0.0815176980	-4.5396585858	2.0643119925
F	1.1023579534	-8.6015379158	2.8721005293
F	0.8204695427	-6.7802096066	4.2701811194
C	-0.0163624150	-6.8556905722	-2.5811537115
N	0.6233822418	-6.5745214160	-1.3942536699
C	0.9544688865	-3.7150128723	5.0340545454
F	0.2256007797	-3.9730090412	0.0192672136
H	0.4718274246	-6.7361454646	-3.5353425777
N	1.1678682149	-3.8713406931	3.6829561497
F	1.5219549433	-6.4783948721	2.0989091214
H	1.7382970476	-3.3604046108	5.6862600446
C	1.9699275837	-6.0369950262	-1.2281309468
C	2.4582667042	-3.7500227186	3.0083443879
H	2.2185788461	-6.0826282639	-0.1670254776
H	2.2854268103	-3.4337413779	1.9763051350
H	1.9813455402	-4.9993008735	-1.5647778163
H	2.6704049612	-6.6438217182	-1.8043280367
H	2.9484614798	-4.7250126831	3.0193405065
H	3.0545728186	-3.0127682220	3.5484494948

Table S11. Optimised geometry of $[C_1mim][BF_4]$, 8 ion-pairs.

Atom	*x*	*y*	*z*
N	-0.4957739992	0.8634963551	2.6085813936
C	0.6384260518	0.4650378311	3.1789171641
N	1.4676769730	0.0653382124	2.2164079282
C	0.8588144071	0.2291044186	0.9934555308
C	-1.6243974019	1.4668054726	3.3061345250
C	2.8620640005	-0.3082209676	2.4248442717
F	1.5783327509	3.0088859944	2.2774654005
B	1.8402253385	3.1976814786	3.6421678306
F	0.6170766809	3.0489531228	4.3541568109
F	2.4128094598	4.4118117716	3.9071134777
F	2.6975454157	2.1453541603	4.0857891219
H	0.8506444819	0.4593361502	4.2358535861
H	1.3410569127	-0.0439939731	0.0688271029
H	-1.1660528964	1.0009783887	0.5582641661
H	-2.5463147391	1.1322878183	2.8287056928
H	-1.5956870523	1.1500782849	4.3461955854
H	-1.5301568895	2.5519804602	3.2525430617
H	2.9303204789	-0.9085272328	3.3361928271

H	3.1938472587	-0.8746345412	1.5531757004
H	3.4479253634	0.6032116442	2.5444106734
C	1.4012332460	2.1717196713	9.0796564627
N	0.9133618606	2.4748188094	7.8294728427
C	1.7764788213	2.0470759627	6.9159406444
N	2.8137587086	1.4985440392	7.5375622770
C	2.5984929221	1.5558579469	8.8968139148
C	-0.4008948723	3.0181879537	7.5064954049
C	3.9166030011	0.8436310817	6.8436473322
F	0.4300357861	-0.3287206605	7.8784222124
B	0.2916199702	-0.5227721719	6.5169470956
F	-0.3734259503	0.5964027142	5.9494042713
F	-0.4088646047	-1.6858144648	6.2086941826
F	1.5750621031	-0.5794242045	5.9074756415
H	1.6487173248	2.1269973230	5.8471297777
H	3.3062175419	1.1550683937	9.6041040034
H	0.8538458865	2.4064558458	9.9780005246
H	-0.5801706740	3.9095600863	8.1091401067
H	-0.3992839001	3.2691428257	6.4461368515
H	-1.1519948907	2.2521645509	7.7012414503
H	3.8888630562	1.1706703207	5.8041547468
H	4.8578215695	1.1403353123	7.3080121438
H	3.7734981177	-0.2354640909	6.8935019315
H	-4.4208587060	-3.2857627317	-9.7132672356
H	-3.3876500080	-1.8185847497	-9.5643391277
H	-1.7055695393	-0.8165426890	-5.2541490142
C	-3.4088252671	-2.9085848601	-9.5625600878
H	-2.0247623281	-2.3970635091	-6.0371852056
C	-1.4824545040	-1.4524421737	-6.1113265293
H	-3.0026250016	-3.2862732928	-8.6237810269
H	-1.7332934014	-0.9565804625	-7.0515034121
H	-3.7997037959	-3.1504802957	-12.3704569314
N	-2.5511196656	-3.3969232396	-10.6358142086
F	-1.0669756688	-1.1199659026	-9.3989959379
C	-2.8331993198	-3.4289533674	-11.9830911168
F	-1.1845630431	-4.1488363195	-7.4918359274
N	-0.0510923258	-1.7329957318	-6.1098537909
H	0.4082729139	-1.5752750491	-4.0100233110
C	0.7629636120	-1.8116637158	-4.9997745690
B	-0.1176217175	-1.0113137195	-10.4586608815
F	-0.7473553357	-1.2846053190	-11.6605670601
F	0.4419491538	0.2602668938	-10.4382276030
C	-1.2906788546	-3.7726205983	-10.4524683156
C	0.6535159068	-2.0618332616	-7.1904106263
B	-0.0385912586	-5.0017394133	-7.5033456073
H	-0.7807102846	-3.8287617743	-9.5035447136
H	0.2849156345	-2.0973898790	-8.2027893589
F	-0.4140331097	-6.3056590942	-7.6712141221
F	0.6650245790	-4.7918538197	-6.3103626222

C	-1.7048261053	-3.8523697667	-12.6104053441
N	-0.7607661215	-4.0684515136	-11.6332320298
C	1.9908603209	-2.1879024063	-5.4448927220
F	0.8919206042	-1.9760310024	-10.2149187467
H	-1.4894221640	-4.0072120987	-13.6550276895
N	1.8996561502	-2.3222697820	-6.8139803537
F	0.7905398144	-4.5713323790	-8.5755619805
H	2.8965671659	-2.3761259778	-4.8925030419
C	0.6516438655	-4.3758106965	-11.8345931047
C	2.9288288946	-2.8284462941	-7.7119253187
H	1.0642939649	-4.6793202597	-10.8731154376
H	2.6277117906	-2.5961715613	-8.7330986052
H	1.1544481614	-3.4724354418	-12.1802955694
H	0.7402481150	-5.1838801782	-12.5614389382
H	2.9967772697	-3.9100268765	-7.5910806364
H	3.8769276567	-2.3447963372	-7.4730970684
H	-2.2775915493	-4.0531576515	-2.1059692499
H	-1.2496417378	-2.5879136881	-1.9428606241
C	-1.3505276184	-3.6467954368	-1.6985923084
H	-1.3253006899	-3.7899510072	-0.6182896442
F	-0.2077208581	-4.8851047116	1.2582357823
N	-0.2239930237	-4.3846650169	-2.2611546703
H	-0.6432118085	-4.3324136958	-4.3845564403
F	0.8742169737	-5.7891288265	3.0682063336
B	0.6341856859	-5.9519613479	1.7105683228
C	0.0283166727	-4.6245983336	-3.5939052020
F	0.0661907691	-7.1574821300	1.3992293046
C	0.7867890191	-4.8564204362	-1.5393740880
H	0.8685699179	-4.8143568670	-0.4654830920
F	1.8767042385	-5.7932771895	1.0152569303
C	1.2263648760	-5.2621624936	-3.6592918820
N	1.6747971478	-5.4014049959	-2.3649112418
H	1.7742297100	-5.6190328244	-4.5146939001
C	2.9640956982	-5.9330496244	-1.9430420627
H	2.9083432501	-6.1295767461	-0.8732006693
H	3.1622694600	-6.8552417633	-2.4906323850
H	-0.7704040767	-1.9871226079	3.8561321633
H	-1.0170174067	-3.4686909866	2.8623302399
C	-0.4390670315	-2.5528775759	2.9844533406
H	-0.5047811258	-1.9539697925	2.0726336311
H	0.9920590183	-2.9691045432	5.3373081382
N	0.9562258093	-2.9267940229	3.1974599487
C	1.5213173591	-3.1891021801	4.4234073442
F	0.9781019609	-2.1961792756	-0.6608805166
C	1.8133553853	-3.2663784169	2.2367680513
B	2.2714270198	-2.2353505077	-1.2131413387
F	2.9256196377	-1.0233408849	-0.9478918040
C	2.7612090621	-3.6875108329	4.1787875639
H	1.6436320966	-3.1758825027	1.1726177806

F	2.2055125280	-2.4837525189	-2.5831574162
N	2.9246954283	-3.7182912642	2.8117120110
H	3.5334401364	-4.0293203599	4.8483255606
F	2.9686591770	-3.2924959486	-0.5805147738
C	4.0648475022	-4.2952938789	2.1097575986
H	4.0500696443	-3.9393736796	1.0817125088
H	3.9654726173	-5.3805847104	2.1229213189
H	4.9802092978	-3.9782011806	2.6121110291
H	3.7359290743	-5.1886653773	-2.1434583207
H	-1.2566304459	5.3521308977	-1.2315853653
H	-1.9375093865	3.7410174819	-1.6446621714
C	-1.1501069353	4.4656543375	-1.8577716603
H	-4.0287023245	2.6675793078	-5.8297808625
H	-2.8804838018	4.0373409559	-5.6291555302
C	-3.0114678057	2.9569561152	-5.5616743342
H	-1.1777220567	4.7381674309	-2.9125277086
H	-2.7725564913	2.6203853964	-4.5553782951
H	0.2845475706	3.9610760493	0.5676266064
N	0.1436765406	3.8494342761	-1.5923665427
F	-1.4667067542	1.7620605912	-3.1628501655
C	0.7163375358	3.6230217279	-0.3598953108
F	-0.5334906598	4.3316454019	-4.9476257373
N	-2.0822530374	2.3175597227	-6.4852853081
H	-3.1106264196	2.6159877782	-8.3492432941
C	-2.2181276341	2.2666654369	-7.8561853468
F	-0.1978732990	0.8398712830	-1.5016549765
B	-0.6084214819	0.6953821956	-2.8213196410
C	0.9102966924	3.3025752159	-2.5322880614
F	-1.2719528568	-0.5252186374	-3.0195684983
B	0.6074129171	4.3791312302	-5.8157917204
C	-0.8838176614	1.8434685073	-6.1570600561
H	0.7141538178	3.3155720362	-3.5939397795
F	1.2911136594	5.5494457328	-5.6177138426
C	1.8633503801	2.9298464179	-0.5825668759
H	-0.4741434611	1.7895823924	-5.1600523298
F	0.1786176980	4.2055896746	-7.1240297544
N	1.9625198104	2.7448647749	-1.9431767786
C	-1.0730205850	1.7316443520	-8.3524279783
F	0.5086801140	0.7494372646	-3.6818910562
H	2.5946482643	2.5613791479	0.1178229874
F	1.4220266192	3.2602540685	-5.4481258735
N	-0.2634583708	1.4648262940	-7.2716946266
H	-0.7556611655	1.4954864514	-9.3556855372
C	2.9696916438	1.9555694564	-2.6459944217
H	2.8082362101	2.0962736891	-3.7145330452
C	1.1480768616	1.0994242042	-7.3542893447
H	1.4319664057	0.5973526048	-6.4266790697
H	2.8482739704	0.9047180929	-2.3777127112
H	3.9609932606	2.3132928278	-2.3634783174

H	1.7246075458	2.0188117776	-7.4598528332
H	1.2795667848	0.4511524597	-8.2208516661

Table S12. Optimised geometry of [C_3mim][BF_4], 1 ion-pair.

Atom	*x*	*y*	*z*
N	0.0083645172	-0.0173770953	0.0077420416
C	0.0230711892	0.0147485203	1.3378723753
N	1.2869472067	0.0062929073	1.7542049679
C	2.1085243842	-0.0581021844	0.6512900550
C	1.3061605152	-0.0725684234	-0.4459005312
C	1.7294928191	-0.1663123996	3.1466084328
C	0.8270227615	0.5431838852	4.1450780720
C	1.3797030446	0.3790359954	5.5596751762
C	-1.1866507300	-0.1796977353	-0.8165840717
F	0.4685266834	-2.6953926342	1.1489724964
B	-0.7185589302	-2.7773634033	1.9154427330
F	-0.4819100644	-2.0963028957	3.1412724507
F	-1.7340840840	-2.0590925603	1.2235272646
F	-1.0930380166	-4.0814278521	2.1242170842
H	-0.8525420964	-0.0246559397	1.9672205715
H	3.1821477079	-0.0983769696	0.7462733417
H	1.5398779670	-0.1235847761	-1.4977395978
H	-1.2853481805	-1.2320295784	-1.0848972863
H	-2.0578061227	0.1130079896	-0.2332079400
H	-1.0937391534	0.4529936982	-1.7006351542
H	2.7485017673	0.2299572400	3.1957239610
H	1.7435011127	-1.2431068577	3.3379870892
H	0.7526806446	1.6062570494	3.8830550696
H	-0.1733356739	0.1027794067	4.0968408464
H	0.7337305053	0.8764975001	6.2873692504
H	1.4357527639	-0.6798681447	5.8303198490
H	2.3828174622	0.8104752576	5.6491014528

Table S13. Optimised geometry of [C_3mim][BF_4], 2 ion-pairs.

Atom	*x*	*y*	*z*
N	-0.2351389652	0.7368086982	-0.1238170898
C	-0.2337627000	0.8496138989	1.2015042161
N	0.5946111404	-0.0635399850	1.7042230708
C	1.1276396745	-0.7980161192	0.6700604149
C	0.6034773387	-0.2971449143	-0.4795002486
C	0.9027416373	-0.2279268332	3.1273390493
C	2.2451973556	0.4039360603	3.4811340874
C	2.5424378874	0.2564587249	4.9717218739
C	-1.1074659243	1.4818123965	-1.0275318138
F	-0.4429544195	-2.9272891518	1.8410192608

B	-1.6666521369	-2.2732079374	1.9511961966
F	-1.6838190020	-1.5043048388	3.1469477616
F	-1.8544493441	-1.3865708730	0.8647049505
F	-2.7477292072	-3.1634400764	1.9829605537
H	-0.8314502979	1.5427505614	1.7797357438
H	1.7828828292	-1.6352865821	0.8499141877
H	0.7268353311	-0.5998372439	-1.5072659496
H	-1.9635376492	0.8572146755	-1.2876933736
H	-1.4606781230	2.3760935291	-0.5139868779
H	-0.5375885784	1.7488837272	-1.9188957941
H	0.8760316206	-1.3004049767	3.3378247946
H	0.0797372862	0.2311670077	3.6802520745
H	3.0393717782	-0.0682110395	2.8893675282
H	2.2258370287	1.4644573381	3.2023189510
H	3.5046658839	0.7094583427	5.2250402423
H	1.7704559276	0.7465834659	5.5741049973
H	2.5778442629	-0.7979413210	5.2649441234
N	-5.1736843027	-0.5643130757	1.3885450798
C	-4.4712209724	-0.4148023496	2.5095012800
N	-5.0476676321	0.5344825993	3.2452838310
C	-6.1361256912	1.0276416806	2.5635401512
C	-6.2143281319	0.3377295999	1.3955026805
C	-4.5881303605	0.9868442942	4.5618735472
C	-5.5359579627	0.5448284087	5.6715456083
C	-5.0650358448	1.0712406596	7.0254033057
C	-4.7966020461	-1.4150918605	0.2631094058
F	-4.1873163621	3.2397185917	2.3929276595
B	-3.0824247370	2.5740920825	1.8723430425
F	-2.4617693103	1.8227201696	2.9094999831
F	-3.4793476298	1.6798459648	0.8567919545
F	-2.1238645504	3.4553779330	1.3480342613
H	-3.5643018162	-0.9462416306	2.7730035766
H	-6.7259584062	1.8442119231	2.9485797508
H	-6.8952737829	0.4231370196	0.5636028272
H	-4.2189982943	-0.8199588149	-0.4460590559
H	-4.1840371961	-2.2365944795	0.6317811756
H	-5.7087380346	-1.7939737265	-0.2005370813
H	-4.4933618049	2.0749319012	4.5060084844
H	-3.5850996575	0.5773199706	4.6982380022
H	-6.5478519069	0.9126904772	5.4599447622
H	-5.5903859743	-0.5502936735	5.6846304271
H	-5.7380009144	0.7521357189	7.8256995663
H	-4.0615670103	0.7028393950	7.2639197167
H	-5.0298403022	2.1658646870	7.0304131269

Table S14. Optimised geometry of $[C_3mim][BF_4]$, 4 ion-pairs.

Atom	*x*	*y*	*z*

N	-5.8606765563	-2.7235160215	18.2145357808
C	-5.8129289640	-2.6116097709	16.8883685292
N	-4.9767004179	-3.5379385664	16.4169230661
C	-4.4524394768	-4.2414188089	17.4779183305
C	-5.0076493405	-3.7292177147	18.6072811907
C	-4.5957256035	-3.7442426363	15.0107912018
C	-5.5374288010	-3.0494743196	14.0399828541
C	-5.0410558031	-3.2370226281	12.6076060606
C	-6.5765387059	-1.8189972271	19.1110255023
F	-2.1278129613	-2.4907785831	16.4804986829
B	-2.7690116438	-1.2587714594	16.6212518797
F	-3.6714438450	-1.0818864971	15.5328140510
F	-3.4960304044	-1.2036875969	17.8191352772
F	-1.8473650369	-0.2003185027	16.5791742191
H	-6.3426032649	-1.8694960859	16.3026155421
H	-3.7173020403	-5.0171225985	17.3338017700
H	-4.8606314315	-3.9758455884	19.6467418689
H	-5.8743619590	-1.0760136730	19.4933830621
H	-7.3672360888	-1.3197217228	18.5518027959
H	-6.9996596775	-2.4058039789	19.9278556327
H	-4.5964052965	-4.8266172037	14.8431102281
H	-3.5757001116	-3.3656427581	14.9039036423
H	-6.5509433573	-3.4550218306	14.1488264108
H	-5.5843198768	-1.9825140465	14.2737055472
H	-5.7247431423	-2.7640662228	11.8977632968
H	-4.0534713555	-2.7809758097	12.4794089719
H	-4.9625781823	-4.2975866267	12.3425311524
N	-4.4507085761	2.4379587629	16.9345711139
C	-4.5865957689	1.7885945739	15.7794691445
N	-5.5210612432	2.3995105898	15.0582593031
C	-6.0081113788	3.4657890399	15.7734776550
C	-5.3412484970	3.4875921734	16.9564275787
C	-5.9380613284	2.0248078692	13.7055213695
C	-5.4071386287	2.9978851701	12.6580647833
C	-5.9223570450	2.6225999966	11.2705329668
C	-3.6577344017	1.9677655459	18.0639201448
F	-8.2349253188	1.4543589272	15.8153690836
B	-7.5608191464	0.3510387138	16.3192400556
F	-6.7700492025	-0.2292594643	15.2850148563
F	-6.6902010613	0.7299698215	17.3634384669
F	-8.4346468396	-0.6371068001	16.7981360929
H	-4.0708540130	0.8752620739	15.5086187214
H	-6.7906562349	4.0982878763	15.3863346732
H	-5.4261820133	4.1413829056	17.8095260311
H	-4.2612056153	1.2824364797	18.6624378965
H	-2.7800409992	1.4370825064	17.6907834693
H	-3.3577412940	2.8335311818	18.6572065286
H	-7.0313552274	1.9769630019	13.7171829050
H	-5.5724281410	1.0090597678	13.5365969439

H	-5.7095383723	4.0202646595	12.9141003033
H	-4.3133171671	2.9902661553	12.6760908707
H	-5.5399453047	3.3147393788	10.5147017130
H	-5.6034577713	1.6120555154	10.9909750630
H	-7.0168552055	2.6504465686	11.2299424449
N	0.7152051181	6.4833555434	12.7282207289
C	0.2717567706	5.4664013596	11.9926546529
N	-0.7964178174	5.8749063737	11.3083073005
C	-1.0599048395	7.1861724056	11.6332471865
C	-0.1097379613	7.5668415736	12.5275747827
C	-1.5754626140	5.0493659239	10.3812590583
C	-1.4501679064	5.5399240827	8.9429594655
C	-2.2604292608	4.6522673184	8.0003078749
C	1.7838499346	6.4041990469	13.7216991564
F	-3.3040395979	5.7020095510	12.9858892850
B	-2.5303744635	4.7964223571	13.7138289894
F	-2.0774481561	3.7673161179	12.8465268919
F	-1.4170799209	5.4388350204	14.2772576625
F	-3.2841742795	4.1908037146	14.7356973629
H	0.6800000395	4.4629821361	11.9735209736
H	-1.9110341876	7.7119472271	11.2314816196
H	0.0384437089	8.4969009239	13.0529428386
H	1.3399534320	6.1887373323	14.6952201919
H	2.4600699898	5.5967880229	13.4450698865
H	2.3096079593	7.3602005990	13.7382772779
H	-2.6101211058	5.0657782404	10.7362254475
H	-1.2061866193	4.0268656240	10.4904993773
H	-1.8029760197	6.5763805817	8.8742546173
H	-0.3930690513	5.5412940265	8.6526162676
H	-2.1839403548	5.0032365310	6.9678431237
H	-1.9026819744	3.6178958804	8.0320521339
H	-3.3199756751	4.6496161717	8.2776541501
N	-0.3842978301	2.4045001514	16.0945588684
C	-0.7301287232	1.9528131211	14.8898000490
N	0.0164022444	0.8894799849	14.6070894679
C	0.8761450980	0.6590978135	15.6531028386
C	0.6287840671	1.6138433986	16.5863538920
C	-0.0889612618	0.0678710545	13.3989576550
C	-0.7715579884	-1.2658859972	13.6821661220
C	-0.7899996109	-2.1341081986	12.4260866066
C	-0.8478560197	3.6505518121	16.6922290302
F	2.7257167332	1.6453088797	13.4590304065
B	2.0508287912	2.8146267418	13.1328440718
F	0.9471593692	2.5096589383	12.2888440309
F	1.5486613783	3.4432851179	14.2949307170
F	2.8719270375	3.7292553295	12.4545306412
H	-1.4475929439	2.4165120324	14.2239756197
H	1.5899104026	-0.1484234760	15.6299087992
H	1.0845664221	1.8054848055	17.5445501773

H	-0.1875937620	4.4629386134	16.3827206526
H	-1.8589436698	3.8631295391	16.3416226199
H	-0.8335790902	3.5357490574	17.7778166806
H	0.9281597826	-0.0562755928	13.0148614728
H	-0.6393154371	0.6601326087	12.6643743961
H	-0.2486231921	-1.7849316004	14.4937716552
H	-1.7899853389	-1.0835205481	14.0415365097
H	-1.2618863810	-3.1006243169	12.6269067299
H	-1.3472151306	-1.6492698058	11.6163492822
H	0.2251790465	-2.3272076630	12.0619459785

Table S15. Optimised geometry of $[C_3mim][BF_4]$, 8 ion-pairs.

Atom	*x*	*y*	*z*
C	4.8985234843	1.9245128526	-17.6975788243
N	5.3710091287	2.6499446836	-18.7689113303
C	4.4107933767	3.4603128096	-19.2012249695
N	3.3258155291	3.2570001828	-18.4604789673
C	3.6086313662	2.3041650612	-17.5029250211
C	6.7255762549	2.6375944009	-19.3071392213
C	2.0884703843	4.0177608120	-18.6221999739
C	1.7622277323	4.8428969632	-17.3825057204
C	0.4831729868	5.6446510300	-17.6048731338
H	0.2510507567	6.2720425674	-16.7393136753
F	5.0915868083	4.9569928881	-16.8798944364
B	5.4538561635	5.9552192158	-17.7956080255
F	4.2728964908	6.3787804803	-18.4652569906
F	6.3213544363	5.4023686341	-18.7654775731
F	6.0673464662	7.0224947987	-17.1711269690
H	4.5022953132	4.1774378324	-20.0036498212
H	2.8965387831	1.9691676149	-16.7653810711
H	5.4949734191	1.2092174558	-17.1558954296
H	7.0381179631	1.6035280858	-19.4575061183
H	6.7062264618	3.1740142516	-20.2550977623
H	7.3894383070	3.1503438026	-18.6109708968
H	1.2813387516	3.3134484984	-18.8498748368
H	2.2422409611	4.6614630625	-19.4930157674
H	1.6342030242	4.1739328615	-16.5214495261
H	2.6210457598	5.4894339540	-17.1752911730
H	0.5792041885	6.2987515735	-18.4787886740
H	-0.3742620093	4.9852216678	-17.7768002815
H	8.7416306533	7.1721328914	-21.3787867018
H	7.9593288373	5.8117536782	-22.2621230749
C	7.8537338664	6.5432255242	-21.4598149997
H	7.6726703071	6.0277640774	-20.5174578998
F	5.6473087239	4.5879402535	-21.6581319953
H	7.3641241377	8.5352514505	-23.4157535103
N	6.6991500226	7.3857140988	-21.7265518414

C	6.5653149703	8.3198875501	-22.7252994411
B	4.4216779328	4.8852106401	-22.3211823193
C	5.5740728767	7.3433600339	-21.0269596483
F	3.8858366029	3.7511510223	-22.8785405530
F	4.6415313694	5.8941235292	-23.2523346238
H	5.3765000779	6.6842147297	-20.1966160390
C	5.3177235279	8.8438990315	-22.6098684792
N	4.7210898903	8.2189004660	-21.5398855579
F	3.5348918894	5.3867525591	-21.3078672847
H	4.8090711052	9.5995824401	-23.1861222023
C	3.3318895657	8.3420831739	-21.1102779645
H	2.7340127601	7.1090710231	-22.7457686404
H	3.2217246014	7.6329932646	-20.2863840703
C	2.3645383169	8.0027883393	-22.2390203519
H	3.1900178770	9.3553060432	-20.7228679541
H	2.3457015810	8.8192591982	-22.9720210500
C	0.9651716658	7.7679824375	-21.6810286543
H	0.9758366268	6.9002313926	-21.0119119962
H	0.2473199213	7.5660477781	-22.4798246800
H	0.6044439247	8.6347462919	-21.1139500515
H	-0.4555410572	1.0949915391	-14.3700830427
H	-0.4264671609	2.3334250973	-13.1070509627
C	0.1512650106	1.5248811201	-13.5688090701
H	1.3274531428	2.7636205294	-14.8920850563
H	0.3088119296	0.7447991386	-12.8152469959
C	1.4922901909	2.0220158376	-14.0989956264
H	-0.1088336786	-0.5158269201	-8.7629223341
H	-0.2204928093	-1.5411904750	-10.1929409575
H	1.9373396332	3.6065901570	-12.6434445949
H	0.4387672641	0.0948790084	-10.3366573812
C	0.4002282872	-0.7907680102	-9.6915858580
C	2.3327450246	2.6450351030	-12.9892920786
H	2.0636516696	1.1937030453	-14.5251132334
H	3.4745527454	4.2412701637	-15.0813500081
H	2.3960528179	1.9719980135	-12.1285674812
C	4.1397468457	3.6683216689	-14.4555674399
N	3.7073990683	2.8606593013	-13.4288878453
C	1.8074028081	-1.3188991948	-9.4238533905
H	2.4406555617	-1.0393350628	-11.4847728006
H	1.8884997392	-2.6849381624	-11.1177649386
C	2.4297148825	-1.8196407377	-10.7208174021
H	1.7654027330	-2.1347713087	-8.6920711588
F	3.4626663226	-0.1767630458	-13.3091199109
H	2.4600936351	-0.5398473259	-9.0193082930
F	3.7767106746	0.9479861530	-10.3057318121
F	4.3579110688	0.6246200053	-15.2613162224
C	5.4960048748	3.5912363045	-14.4734471179
C	4.7604194248	2.3224305924	-12.8321680335
B	4.4982031698	-0.3607461561	-14.2752437924

H	6.2065723700	4.0607654533	-15.1325271653
F	5.2158644502	2.0728506975	-8.8881102864
F	4.4428988673	-1.6306845335	-14.7913558089
H	4.7291408752	1.6599391452	-11.9820878929
N	5.8587280758	2.7502916697	-13.4454722011
B	5.0011937004	0.8953713447	-9.5837952096
N	3.8300469265	-2.2055217765	-10.5303993088
H	4.7555262490	-0.8744218107	-11.9307105559
F	4.9619455452	-0.2069765226	-8.7314806456
C	4.8426419778	-1.6401448342	-11.1763934009
H	3.6955563248	-3.6826536625	-8.9672621410
F	5.7331066650	-0.1619655239	-13.5991462394
C	4.3332920752	-3.1051513517	-9.6163672665
F	6.0385713629	0.7217698457	-10.5402868444
C	7.2038816640	2.3040951278	-13.1157925217
H	7.5248424180	1.5594515689	-13.8453247398
H	7.8735503050	3.1648834076	-13.1167472627
N	5.9779775430	-2.1625848726	-10.7280757878
H	7.1707685713	1.8516683040	-12.1249359933
C	5.6862775318	-3.0767192126	-9.7411073856
H	7.1795880887	-1.1861425003	-12.0971633696
C	7.3008794665	-1.7217410641	-11.1558967074
H	6.4584510161	-3.6196318351	-9.2204640783
H	7.7123341525	-1.0515977972	-10.4016989020
H	7.9356305737	-2.5976007961	-11.2966726428
H	-1.5752508230	5.5689068896	-14.0053066545
H	-0.9669977562	7.9350822815	-12.7758095155
C	-0.5184020985	5.3000172168	-13.9020214573
H	0.3139705794	7.1414025821	-14.6837494435
H	-0.2381747434	4.6982805555	-14.7729264876
C	-0.0464310607	7.3790913621	-12.5719215599
C	0.3705920814	6.5325611771	-13.7725746782
C	1.6200180313	9.2611220662	-13.0113430864
N	1.0029540418	8.3295725472	-12.2014728958
H	-0.2033152422	6.7542955551	-11.6897025780
C	2.6228017313	9.8150539143	-12.2806195918
H	1.4123833380	6.2346967392	-13.6276187317
C	1.6182333250	8.3098415331	-11.0226937374
N	2.5950715213	9.2097856624	-11.0422056578
H	1.3854757824	7.6518195599	-10.1986478283
F	1.9928452172	5.5778851843	-11.5480762272
C	3.5315481578	9.3996436316	-9.9403126671
F	3.5942783841	6.7844041463	-12.6346231053
B	3.3825715294	5.9205292855	-11.5520464778
H	3.1556361352	8.8343732522	-9.0874635723
H	4.5052167718	9.0054516055	-10.2312494540
F	3.6732736566	6.5883101481	-10.3507922151
F	4.1323205949	4.7654220449	-11.6381064857
H	1.3150259262	9.4636029543	-14.0255546110

H	-0.4164803540	4.6734510890	-13.0082207062
H	-2.0672953140	4.9883181072	-10.4744970936
F	-0.2949028789	7.7069648729	-7.6681463601
H	3.3356221015	10.5735105449	-12.5590198383
F	0.0485498875	6.2806185031	-9.4351167260
B	0.4915609801	6.6831714449	-8.1278704100
H	3.5957974765	10.4623545461	-9.7027591208
F	0.4654007141	5.5636016707	-7.2967868086
H	0.3162833555	4.2954003642	-10.6386140385
C	0.1627819506	3.3969916204	-10.0376790416
F	1.8373360288	7.1083843178	-8.2861395244
H	2.1642170269	5.2550803539	-9.4495488317
N	1.3382771989	3.2951260522	-9.1754550520
C	2.2087885540	4.2811036739	-8.9911416523
N	3.1142706702	3.8880448336	-8.1058124688
H	4.1460536999	4.9772362872	-6.6491802797
C	4.2555558470	4.6970132781	-7.6980247091
H	4.2616067898	5.5876943631	-8.3251831979
H	5.1589483266	4.1097462485	-7.8587520761
H	-3.2206976060	3.9673082929	-9.6036694181
C	-2.2673739311	3.9663734172	-10.1375198803
H	-2.3760168971	3.3233316344	-11.0198033025
C	-1.1292502087	3.5009455179	-9.2354135613
H	-1.3622241466	2.5285553874	-8.7829889190
H	0.1590182990	2.5251189512	-10.7025245625
H	-0.9646474191	4.2192278912	-8.4288764304
C	1.6813673185	2.2447936058	-8.3498060820
C	2.8050535850	2.6147299819	-7.6841923262
H	3.4404324301	2.0696633284	-7.0062225001
H	1.1133593980	1.3300727847	-8.3266931603
H	1.1779217008	12.4406386532	-22.0039590824
H	2.2763605355	13.7345573706	-20.0545933586
C	1.9996169718	11.7201347484	-21.9315729712
H	3.5791567050	13.1752203398	-22.1390083033
H	2.1414599946	11.2781068276	-22.9216700629
C	3.0718401157	12.9816890797	-20.0509122839
C	3.2816400192	12.3855468282	-21.4384948475
C	5.0095109429	14.6282018421	-20.1440431844
N	4.2925281242	13.6149593454	-19.5458925612
H	2.8132715421	12.2091575684	-19.3230535672
C	6.1166567815	14.8289284080	-19.3824069775
H	4.1107800773	11.6765587782	-21.3741067980
C	4.9501980081	13.2040534872	-18.4680158552
N	6.0510398830	13.9354882850	-18.3376225765
H	4.6446792104	12.4035526515	-17.8136263191
F	4.8039930677	10.4772869398	-19.5010746022
C	7.0608513679	13.7154000062	-17.3079289008
F	6.3550815807	11.8517362216	-20.4583856176
B	6.2046635889	10.7472449515	-19.6243147856

H	6.5894371161	13.1557175677	-16.5009376872
H	7.8789355261	13.1347548437	-17.7340933478
F	6.6649544130	11.0732985059	-18.3220328422
F	6.8645802653	9.6388276897	-20.1046143953
H	4.6721324440	15.1158544471	-21.0439309649
H	1.6822465960	10.9221085695	-21.2510988548
H	0.5830193938	10.3063637171	-18.7173322752
F	2.9526722173	13.1906494102	-15.3963875272
H	6.9343706215	15.5231629292	-19.4888544374
F	3.0005164016	11.5913063468	-17.0463245119
B	3.4382564492	11.9551344551	-15.7370686781
H	7.4098734227	14.6831017830	-16.9453092168
F	3.0167350693	10.9523216639	-14.8514851040
H	2.8574820440	9.3613342187	-18.3580758672
C	2.5056026922	8.6792032332	-17.5797866167
F	4.8585506444	11.9747263084	-15.7630536335
H	4.9802447267	9.9633651185	-17.5038439304
N	3.5817187187	8.6141023023	-16.5976913144
C	4.6950251892	9.3310767244	-16.6775830940
N	5.4123210801	9.1215523557	-15.5822018793
H	6.6247996509	10.4505532159	-14.5273947479
C	6.7109883348	9.7244870457	-15.3371104083
H	7.0209454045	10.2297328529	-16.2514134632
H	7.4244857570	8.9383521281	-15.0862535745
H	-0.7494291766	9.8710508042	-17.6389170553
C	0.1937049396	9.5178083451	-18.0633006152
H	-0.0223284453	8.6399536862	-18.6826400685
C	1.2079483745	9.1973839123	-16.9704331458
H	0.7974443010	8.4432513580	-16.2871884791
H	2.3903878908	7.6848423434	-18.0201039193
H	1.4426181371	10.0896284231	-16.3869016418
C	3.5912118811	7.9113233901	-15.4114777570
C	4.7469140124	8.2323009447	-14.7736550898
H	5.1264678838	7.8970634384	-13.8229470182
H	2.7882013062	7.2578429216	-15.1101604138

Table S16. Optimised geometry of $[C_4mim][BF_4]$, 1 ion-pair.

Atom	*x*	*y*	*z*
C	1.7441192277	-2.0631364045	0.9142153485
N	2.1977776561	-1.1909494523	-0.0497750658
C	1.1763215839	-0.8619624323	-0.8368783624
N	0.0895449188	-1.5088600713	-0.4260588216
C	0.4201932080	-2.2635868367	0.6773790415
C	3.5179940194	-0.5653117339	-0.0778973657
C	-1.2695630050	-1.2902586354	-0.9446106341
C	-2.1830581486	-0.7277657591	0.1399948227
C	-3.5276571578	-0.2935133616	-0.4408021926

C	-4.4872164682	0.1739937180	0.6514526648
F	0.4759857050	0.9459848705	1.1182991787
B	0.6146676399	1.8869906892	0.0670861749
F	-0.2628199790	1.4845178821	-0.9809607715
F	1.9400660146	1.7821515640	-0.4309739877
F	0.3286178488	3.1605820317	0.4895007279
H	1.2062024235	-0.1256188479	-1.6259840156
H	-0.3078469388	-2.8666555494	1.1962088937
H	2.3964059190	-2.4529831921	1.6798367780
H	4.2682729592	-1.3235973981	0.1497950138
H	3.6896470125	-0.1527558677	-1.0707583421
H	3.5353781070	0.2503883404	0.6455130777
H	-1.6393055707	-2.2425868276	-1.3388866310
H	-1.1731140426	-0.5738991901	-1.7621227622
H	-2.3462129472	-1.4874209136	0.9172315317
H	-1.6765020344	0.1236216861	0.6053441110
H	-3.3555769559	0.5191537697	-1.1568296811
H	-3.9805140066	-1.1238356496	-1.0010733889
H	-5.4427701866	0.4996866720	0.2301321599
H	-4.6907613954	-0.6330641498	1.3641064063
H	-4.0594454070	1.0138310490	1.2085660913

Table S17. Optimised geometry of $[C_4mim][BF_4]$, 2 ion-pairs.

Atom	*x*	*y*	*z*
C	1.6703802080	-2.0117115837	0.8653732814
N	2.1722809618	-1.1218889288	-0.0569831673
C	1.1732432210	-0.6889158600	-0.8199797783
N	0.0502644480	-1.2847038057	-0.4322255071
C	0.3351324731	-2.1169532246	0.6282212973
C	3.5325016598	-0.5966422811	-0.1137508003
C	-1.2730491512	-0.9904036519	-0.9943947748
C	-2.2563563600	-0.5588467392	0.0876415478
C	-3.5128944286	0.0523046049	-0.5314166600
C	-4.5457442660	0.4345178541	0.5262661604
F	0.7368736384	0.8240173105	1.5613887011
B	0.7625043371	1.9295192993	0.7078647738
F	-0.2562350380	1.7692268470	-0.2864072146
F	2.0040185819	1.9413166704	0.0024366951
F	0.5788529718	3.1182972819	1.3783163332
H	1.2612746117	0.0347103554	-1.6175562183
H	-0.4276923251	-2.6945603070	1.1254681515
H	2.2981870923	-2.4737748376	1.6108131587
H	4.2372422620	-1.4285991710	-0.0706467116
H	3.6420780011	-0.0573258016	-1.0548137408
H	3.6797947908	0.0893549374	0.7219278528
H	-1.6220079898	-1.8785140207	-1.5321562836
H	-1.1138166689	-0.1904724166	-1.7211576781

H	-2.5351782132	-1.4207516205	0.7095037236
H	-1.7629934879	0.1747014558	0.7333980941
H	-3.2229297813	0.9440244113	-1.1027242874
H	-3.9572893817	-0.6514568944	-1.2490450723
H	-5.4370349013	0.8773368043	0.0716848957
H	-4.8618942720	-0.4437368872	1.0999488060
H	-4.1272124381	1.1622894068	1.2291581425
H	4.0965922837	4.5140193167	-2.2476294476
H	4.0731990953	2.9031695919	-3.0510994841
C	3.5503345735	3.5777062956	-2.3714086685
H	3.4094354416	3.0921993980	-1.4051883683
F	2.6143434675	0.8174041273	-3.0404013039
H	2.7206335969	5.2857700622	-4.4701130803
N	2.2313075037	3.8718426566	-2.9244138829
C	1.9526443482	4.7030423632	-3.9862349325
B	1.6291336518	0.6411046569	-4.0599386504
C	1.1091430473	3.2627117344	-2.5538998636
F	1.8356687945	-0.5503608401	-4.7194343728
F	1.6666305286	1.7414117683	-4.9204399553
H	1.0175548198	2.5371030074	-1.7583304506
C	0.6210857831	4.5887766561	-4.2402950035
N	0.1157311726	3.6888434463	-3.3283870375
F	0.3649091199	0.6252331837	-3.3930850237
H	0.0012770288	5.0538052899	-4.9902213947
C	-1.2479618758	3.1472437522	-3.2833196624
H	-0.8105899121	1.9765887191	-5.0223144284
H	-1.2327344812	2.3789250084	-2.5058838050
C	-1.6537203441	2.5531108695	-4.6289845876
H	-1.9261485458	3.9467074411	-2.9673329274
H	-1.8735737459	3.3570366083	-5.3447894628
C	-2.8765035404	1.6496056675	-4.4799039480
H	-2.6154159971	0.8233914067	-3.8059384260
H	-2.5400095133	0.5125183896	-6.2961360205
C	-3.3406249637	1.0907261085	-5.8231345385
H	-3.6971653923	2.2026211597	-4.0014222446
H	-3.6210322661	1.8985220712	-6.5080211512
H	-4.2074142347	0.4336008763	-5.7045215979

Table S18. Optimised geometry of $[C_4mim][BF_4]$, 4 ion-pairs.

Atom	*x*	*y*	*z*
C	-1.7547162406	-1.2799335218	10.0782424544
N	-1.3350276163	-0.3430465404	9.1610864139
C	-2.4001630824	0.1899575014	8.5692910369
N	-3.4934536250	-0.3885379246	9.0594742196
C	-3.1130388578	-1.3041044167	10.0188855568
C	0.0462210012	0.0575103352	8.9091768547
C	-4.8589139673	-0.0406394701	8.6645542263

C	-5.7279704558	0.3210141774	9.8631510421
C	-7.0172968886	1.0023902125	9.4085383780
C	-7.9402392276	1.3288079734	10.5798798159
F	-2.7986383723	1.5908698805	11.2095437195
B	-2.6743272201	2.6774360528	10.3533454592
F	-3.6801776101	2.5721900655	9.3323036680
F	-1.4168362033	2.6134758276	9.6818810269
F	-2.8058509065	3.8920774511	10.9974619549
H	-2.3894315432	0.9792537370	7.8287159588
H	-3.8351728250	-1.8757487316	10.5785028366
H	-1.0470627804	-1.8467421020	10.6641055068
H	0.6422942390	-0.8420586624	8.7496915846
H	0.0564849808	0.7061182260	8.0320121711
H	0.4143425434	0.6095708579	9.7755082119
H	-5.2767078849	-0.8856268339	8.1015642882
H	-4.7660376379	0.8077552955	7.9805754314
H	-5.9716869988	-0.5839216672	10.4376582849
H	-5.1579333063	0.9867606609	10.5188175823
H	-6.7519888346	1.9260412201	8.8776278549
H	-7.5436132623	0.3631716287	8.6854540942
H	-8.8498128897	1.8351199363	10.2430546469
H	-8.2398354364	0.4176668051	11.1095282652
H	-7.4346506195	1.9818915962	11.2986040413
H	0.7522560551	5.5428929957	8.0782936666
H	0.6672971516	4.3019640045	6.7786422268
C	0.1842220495	4.7053747933	7.6703602734
H	0.0796627516	3.9222488698	8.4216204570
F	-0.8354584049	2.0719694621	6.3903799768
H	-0.7313477405	7.0001002185	6.2738875870
N	-1.1544651789	5.1668054236	7.3171376695
C	-1.4785520142	6.2882925343	6.5872097936
B	-1.8679464750	2.2789038093	5.4344048556
C	-2.2639892772	4.4712198840	7.5447487026
F	-1.7312041288	1.3523331817	4.3998150843
F	-1.8011282104	3.5838301000	4.9513088828
H	-2.3149922352	3.5273373563	8.0659014768
C	-2.8249709629	6.2572489922	6.3909794541
N	-3.2926789717	5.1151918304	7.0033838838
F	-3.1024731410	2.0738022556	6.1054605843
H	-3.4807193884	6.9400229359	5.8743919375
C	-4.6645663577	4.5946161271	6.9733023566
H	-4.3494343751	3.8600209263	4.9869497502
H	-4.6352988014	3.6566371382	7.5322123017
C	-5.1424907369	4.3710706184	5.5421231403
H	-5.3073839023	5.2965489102	7.5147973074
H	-5.3212145005	5.3370399448	5.0494334671
C	-6.4202976323	3.5347709395	5.5176970325
H	-6.2050466661	2.5560760656	5.9665893776
H	-6.2086683895	2.8470937773	3.4697695522

C	-6.9544217159	3.3428749028	4.1002166672
H	-7.1890980055	4.0073364475	6.1446406815
H	-7.1965457198	4.3067209292	3.6387156561
H	-7.8612103163	2.7308112281	4.0952684526
H	-5.7240436916	-1.4679147506	4.9593041268
H	-4.6710775863	-1.1548459216	3.5707623819
C	-4.7471550572	-1.6965824376	4.5195130972
H	-3.6657086191	-0.2302174121	5.6843965620
C	-3.6073726752	-1.3025741414	5.4552659288
H	-4.7178976110	-2.7686992229	4.2945097580
H	-6.2770683218	-3.0043880610	9.2069562741
H	-2.0867645096	-1.0168854892	3.9576546921
H	-3.7156413634	-1.8382577992	6.4095529361
C	-2.2313600624	-1.6107588857	4.8671264512
C	-5.5911900795	-3.8382679463	9.3923584990
H	-5.0208293825	-4.2079180513	7.3443326268
H	-1.2676547728	-0.2078611224	6.1930960917
H	-4.0325800207	-2.9938037138	8.1444992033
C	-4.5336257211	-3.9572665556	8.2967250613
H	-6.1900337370	-4.7532737594	9.4543462641
C	-1.1614546709	-1.2512702585	5.8892277348
H	-5.1308424201	-3.6876648076	10.3756677504
H	-2.1385420915	-2.6689324477	4.6006204570
H	0.1697168789	0.1684207645	3.8909049601
H	-1.2177291002	-1.8949995914	6.7722003122
C	0.7417819885	-0.6207372910	4.3564516217
N	0.2008709366	-1.3865969203	5.3650524239
C	-3.4679354855	-5.0008566910	8.6342286570
H	-2.2012542299	-4.4780487424	6.9459164017
H	-3.2519634916	-5.8761451402	6.6526507501
C	-2.6428454797	-5.3657279868	7.4060125218
H	-3.9578359626	-5.8988702261	9.0351878447
F	-0.6752058654	-4.3934578900	4.9748557942
H	-2.7959576410	-4.6158586856	9.4117937387
F	-0.4889701287	-3.2889682188	8.2836222839
F	0.8511215768	-3.8149637908	3.3500262739
C	2.0167593756	-1.0599917859	4.1760346919
C	1.1123954077	-2.2595485437	5.7856610164
B	0.4455487034	-4.8337009269	4.2093157921
H	2.7831080718	-0.7520266869	3.4825944610
F	0.9622662996	-2.7482882042	9.9786473184
F	0.1436926256	-6.0043474346	3.5462967342
H	0.9750558445	-3.0002365918	6.5624459368
N	2.2303227788	-2.0710432140	5.0867008688
B	0.5466316878	-3.7780098880	9.1363278607
N	-1.5211470352	-6.2452586070	7.7597421559
H	0.0640800834	-5.2931391002	6.6709008966
F	0.0586511058	-4.8612649457	9.8645113220
C	-0.2723045834	-6.0719660854	7.3373498064

H	-2.4592021090	-7.6686012536	9.0826250189
F	1.4946175571	-5.0715341092	5.1594491484
C	-1.5527164147	-7.3333673286	8.6058126309
F	1.6102162506	-4.1921117377	8.3035828024
C	3.4075155907	-2.9282884551	5.1517284745
H	3.3565900510	-3.6519518410	4.3371405545
H	4.3003085227	-2.3053551271	5.0758219051
N	0.4955748749	-7.0166770637	7.8708978694
H	3.3972229945	-3.4567003503	6.1049866985
C	-0.2826769738	-7.8154549463	8.6777560625
H	2.2127635188	-6.4886098507	6.8391710903
C	1.9450474038	-7.0863973885	7.7101393124
H	0.1319206004	-8.6435642656	9.2305653197
H	2.4208178905	-6.6756241914	8.6020270598
H	2.2326650437	-8.1275430562	7.5557788696

Table S19. Optimised geometry of $[C_4mim][BF_4]$, 8 ion-pairs.

Atom	*x*	*y*	*z*
C	5.5437675345	1.8824736798	-17.8358440477
N	6.1606980835	2.6723663490	-18.7829141110
C	5.2342523366	3.3730430066	-19.4288820975
N	4.0430764108	3.0393711499	-18.9469031417
C	4.2090976268	2.1129413182	-17.9396541280
C	7.5911953928	2.8464911801	-18.9957099973
C	2.7925751431	3.6617805166	-19.3805682803
C	2.0489273992	4.2733626819	-18.2031505942
C	0.7906178002	5.0062583280	-18.6636682927
C	-0.1086791418	5.3684247041	-17.4879336575
F	5.2526132652	4.9086763839	-17.0136728108
B	5.6004700550	5.9648147201	-17.8696549541
F	4.4983799422	6.2101465880	-18.7313607288
F	6.6943520909	5.5637480219	-18.6742985033
F	5.9320069352	7.1036070843	-17.1638742480
H	5.4213684920	4.1074272003	-20.1968209150
H	3.3957076041	1.6910762081	-17.3733588568
H	6.0787699304	1.2294901706	-17.1657946154
H	8.0704246518	1.8667707175	-19.0101819603
H	7.7240253849	3.3499020507	-19.9534357949
H	7.9988497586	3.4701085623	-18.1994421876
H	2.1843043919	2.9002262294	-19.8794957256
H	3.0732586344	4.4190378505	-20.1156300941
H	1.7686080101	3.4805977033	-17.4953236603
H	2.7329862721	4.9573174271	-17.6872651146
H	1.0822733843	5.9076882985	-19.2192102085
H	0.2336138988	4.3769612899	-19.3702627144
H	-0.9927672559	5.9324895671	-17.8015981565
H	-0.4532590672	4.4621637150	-16.9776507058

H	0.4343613471	5.9726425830	-16.7500380546
H	9.2969392022	7.6315403441	-21.0700161155
H	8.7250743674	6.1502933140	-21.9215710296
C	8.4857158153	6.9101453800	-21.1773919215
H	8.2787108872	6.4284633232	-20.2221951729
F	6.7227394210	4.6864573451	-21.6384685322
H	7.9921081174	8.8373883744	-23.1990170826
N	7.2771429246	7.6097784765	-21.5861289106
C	7.1453264183	8.5052982696	-22.6212375469
B	5.5942306317	4.7874087893	-22.5054464313
C	6.0802333998	7.3872939426	-21.0587841192
F	5.3454519838	3.5842563808	-23.1164438032
F	5.8058124515	5.8214805751	-23.4085301859
H	5.8696520618	6.7016124315	-20.2537234196
C	5.8274287509	8.8220597882	-22.7016066943
N	5.1862424578	8.1129553170	-21.7141483096
F	4.4853286805	5.1450264889	-21.6658691308
H	5.2981518509	9.4943124709	-23.3571024233
C	3.7492022698	8.0541847101	-21.4635934362
H	3.5693483615	6.7103991853	-23.1154814833
H	3.6292879841	7.3766541203	-20.6138618138
C	2.9921347572	7.5294618340	-22.6803583777
H	3.4232043452	9.0534050110	-21.1565970186
H	2.9025068150	8.3145599344	-23.4415440644
C	1.6037174611	7.0423067691	-22.2763791230
H	1.7289465290	6.1772571033	-21.6125425690
H	1.2460343299	5.8660454212	-24.0602015508
C	0.7502758088	6.6491007356	-23.4780043000
H	1.0892930933	7.8177287141	-21.6883709466
H	0.5890683758	7.5052069176	-24.1428705235
H	-0.2295255002	6.2733905245	-23.1693721837
H	-1.9785834071	1.1951991144	-14.7331994906
H	-1.1960278941	2.4516888186	-15.7018517510
C	-1.0138951152	1.5470979850	-15.1101494033
H	-0.4504791119	2.5890239159	-13.2996997950
C	-0.0347583945	1.8276312820	-13.9749997696
H	-0.6141480005	0.7819745886	-15.7834563539
H	-1.7755013307	0.8978416096	-9.3590738489
H	1.2074348435	3.1130117936	-15.1913844863
H	0.1054810266	0.9196167729	-13.3743314352
C	1.3317620392	2.2783226556	-14.4853275738
C	-0.9460855242	0.2381453040	-9.0849158593
H	-0.7862658027	-0.7704593648	-10.9845213239
H	1.9550247810	3.6700301113	-12.9078316831
H	0.1989763895	0.6811377445	-10.8684062422
C	-0.1411151272	-0.1975119879	-10.3050361456
H	-1.3611404613	-0.6281288115	-8.5597879625
C	2.2353476535	2.6999181997	-13.3332886705
H	-0.3090391610	0.7784994593	-8.3769764419

H	1.8167936221	1.4564658051	-15.0223520282
H	3.5794752340	4.1703274631	-15.4020094535
H	2.2082002278	1.9619796831	-12.5265093933
C	4.1695406625	3.5459624586	-14.7517492117
N	3.6320596497	2.7772147079	-13.7468187608
C	1.0858459881	-1.0250503840	-9.9276987929
H	1.9087180447	-0.7931583374	-11.9249585124
H	1.1659916462	-2.3758979568	-11.6362923471
C	1.7580027934	-1.5762565442	-11.1794595340
H	0.7891606686	-1.8501086977	-9.2659816382
F	3.1289890896	-0.1720771344	-13.7782876980
H	1.8145430733	-0.4090293169	-9.3922724335
F	3.3080546324	0.9175978778	-10.6451393536
F	4.3059438151	0.6182105915	-15.5795161481
C	5.5135328721	3.3496619375	-14.7213012411
C	4.6100384162	2.1433231854	-13.1184798695
B	4.2018028695	-0.4471705024	-14.6751941794
H	6.2859420692	3.7596816674	-15.3495253532
F	4.6868971655	2.0069117406	-9.1494070291
F	3.9945840004	-1.6441344788	-15.3114083715
H	4.4890416826	1.4831492640	-12.2754304716
N	5.7632821405	2.4718650107	-13.6904083158
B	4.4795749235	0.8288978367	-9.8396644689
N	3.0920476004	-2.1047031049	-10.8851705571
H	4.2516673224	-0.9329859452	-12.2558882300
F	4.3425713064	-0.2646324454	-8.9902753925
C	4.2014692864	-1.6675247470	-11.4675073194
H	2.6905432063	-3.5023824667	-9.2965338782
F	5.3948459128	-0.4875701526	-13.8969749209
C	3.4309616559	-3.0203451568	-9.9136287770
F	5.5710267453	0.5984979661	-10.7261165492
C	7.0441887999	1.8852621233	-13.3305718773
H	7.2893027175	1.0935709569	-14.0400496564
H	7.8070958599	2.6649504955	-13.3365287476
N	5.2405326220	-2.2914022343	-10.9236925435
H	6.9483908805	1.4628073378	-12.3301941996
C	4.7845324964	-3.1364002108	-9.9378197544
H	6.6282718351	-1.4664265940	-12.2091855626
C	6.6282816997	-1.9900557563	-11.2536381546
H	5.4564266004	-3.7348104043	-9.3442582473
H	7.0425283114	-1.3442817087	-10.4796242237
H	7.1870701279	-2.9234339366	-11.3336362365
H	-2.0895599603	6.3568934133	-12.6222978663
H	-0.8041787969	8.4282637669	-11.6545811520
H	-1.6705019174	5.8508569756	-15.0544300639
C	-1.1533825263	5.8811004754	-12.9434458645
H	-0.2344396218	7.6022955505	-13.8803000848
H	-2.1479768300	4.3855709010	-14.1798112228
C	-1.3715971039	5.1524315604	-14.2640447293

C	0.0323323349	7.7267518011	-11.7371777155
C	-0.0451989635	6.9278338942	-13.0332552756
C	1.8234776003	9.3490953733	-12.5544057960
N	1.2805747237	8.4810220593	-11.6303884371
H	0.0135039172	7.0666841670	-10.8663035520
C	3.0242345257	9.7468491691	-12.0577103357
H	-0.4466951904	4.6618648905	-14.5887420422
H	0.9219457557	6.4415324393	-13.1970542157
C	2.1276531356	8.3426836228	-10.6158592366
N	3.1868850256	9.1115686846	-10.8455790062
H	1.9889171003	7.6950736218	-9.7621721156
F	2.0713466081	5.5921222870	-11.3769060787
C	4.3610523951	9.1393574039	-9.9826466918
F	3.5338714896	6.7655682405	-12.6798627210
B	3.4526508550	5.8324021394	-11.6384573006
H	4.1216640047	8.5738931914	-9.0823232846
H	5.1915765937	8.6558967228	-10.4978866726
F	4.0356297314	6.3774700695	-10.4760888888
F	4.0780126818	4.6457170991	-11.9561393834
H	1.3392335093	9.6147443977	-13.4794772635
H	-0.8861413363	5.1600132136	-12.1592129577
H	-1.7216396143	5.4548877215	-9.6095161848
F	0.9103097911	7.9651587440	-6.9717690592
H	3.7555926334	10.4165917661	-12.4794769415
F	0.6846002838	6.5111567907	-8.7347401590
B	1.4231954167	6.8273892763	-7.5424131459
H	4.6038404772	10.1741461341	-9.7364758662
F	1.3691758895	5.7289471423	-6.6873215274
H	0.4851884191	4.4440210579	-10.0194534916
C	0.3266551553	3.6354036467	-9.3032669493
F	2.7676403427	7.0289628891	-7.9575794901
H	2.6629467794	5.1386634144	-9.4455341845
N	1.5824274156	3.5134053325	-8.5654426056
C	2.6112155174	4.3358059487	-8.7298538248
N	3.5252471127	4.0629090526	-7.8117654616
H	4.8358325079	5.3199772277	-6.7851279095
C	4.8056947530	4.7430155347	-7.7104514129
H	4.8905796175	5.4125358484	-8.5650937974
H	5.5957154587	3.9918457561	-7.7420975818
H	-4.0845496888	5.1435536972	-8.8256540673
C	-3.2451793274	4.7278277970	-8.2610843922
H	-3.5761188539	3.7861857170	-7.8097857433
C	-2.0260728605	4.5053723285	-9.1511779688
H	-2.2825885028	3.8209401271	-9.9730017516
C	-0.8350010839	3.9593852518	-8.3693561414
H	-1.1318231322	3.0577083710	-7.8156292589
H	0.1576775900	2.7055565094	-9.8573301830
H	-3.0045950123	5.4215865519	-7.4499328431
H	-0.4881643565	4.6983569271	-7.6418043438

C	1.8427446348	2.6931499419	-7.4892367727
C	3.0707703589	3.0364575746	-7.0222446163
H	3.6687330693	2.6229058262	-6.2272086731
H	1.1411010912	1.9512835616	-7.1456192622
H	0.3663683315	11.5377063857	-21.1752863836
H	1.3708751776	13.4159298902	-19.6186962211
H	1.0908990485	11.5462338646	-23.5532684105
C	1.3718565481	11.1780968363	-21.4315162215
H	2.2856603388	13.0804166500	-21.8792037521
H	0.7549781166	9.8742017794	-23.0725248859
C	1.4070515424	10.7339607169	-22.8905308128
C	2.2724352257	12.8062948445	-19.7357544478
C	2.4072552581	12.2647144218	-21.1531361065
C	3.9424560576	14.6987713305	-20.0741328612
N	3.4330686065	13.6257766179	-19.3763518851
H	2.2420659860	11.9996413057	-19.0011230257
C	5.0922926392	15.0646916004	-19.4487169547
H	2.4259047269	10.4528363115	-23.1790564187
H	3.4198333313	11.8661125245	-21.2700853418
C	4.2535848386	13.3396407541	-18.3735985894
N	5.2584701555	14.2076174952	-18.3841159549
H	4.1372719895	12.5229688980	-17.6800330394
F	4.3656160782	10.5679355478	-19.4629671118
C	6.4033842564	14.1241479170	-17.4843240678
F	5.7217757060	12.1374096041	-20.4271060527
B	5.7127705807	11.0141093708	-19.5971888974
H	6.0882953968	13.5610212194	-16.6057994187
H	7.2107593684	13.5936934134	-17.9891289463
F	6.1538675519	11.3940548688	-18.2990567570
F	6.5138950739	10.0052386896	-20.0850883443
H	3.4492045716	15.1082365100	-20.9405877802
H	1.5758035457	10.3254435482	-20.7703087061
H	0.1865590985	9.7095460945	-18.5718564567
F	2.4806042070	13.0250042108	-15.2600299074
H	5.7981248769	15.8507415947	-19.6625794220
F	2.6620076437	11.4152310482	-16.8781808435
B	3.1188107856	11.8580178595	-15.5987074266
H	6.7056001224	15.1331390322	-17.2015169490
F	2.8907255149	10.8307753545	-14.6749193142
H	2.6985017693	9.1614267103	-18.2836812241
C	2.4494010323	8.4536592596	-17.4879627638
F	4.5170929952	12.0713366216	-15.7064218362
H	4.7558015500	10.0344267610	-17.4500312461
N	3.5265284642	8.5509425737	-16.5091916300
C	4.5593577690	9.3755616955	-16.6187515327
N	5.3136104436	9.2523848050	-15.5342804256
H	6.4026037255	10.6944524552	-14.4868801809
C	6.5410452733	9.9984823331	-15.3158316553
H	6.7539869466	10.5590958846	-16.2255969199

H	7.3514548955	9.2979791614	-15.1085437100
H	-2.1723506159	9.0343117786	-18.0355289095
C	-1.3844637378	8.9778274557	-17.2791828015
H	-1.5941278115	8.1133638311	-16.6378343525
C	-0.0012967791	8.8531931173	-17.9110802960
H	0.0386566418	7.9574624876	-18.5459046846
C	1.1027791797	8.7897175074	-16.8595064969
H	0.8489641365	8.0314684175	-16.1055047715
H	2.4683271603	7.4428123188	-17.9107177560
H	-1.4461861670	9.8760845256	-16.6563940606
H	1.1951493558	9.7491871428	-16.3430296221
C	3.6200220950	7.8750946767	-15.3130305252
C	4.7488269125	8.3153968290	-14.7004678190
H	5.1707623350	8.0309169261	-13.7512533914
H	2.8926304692	7.1525896545	-14.9815138616

Table S20. Optimised geometry of [C_1mim]Cl, 1 ion-pair.

Atom	*x*	*y*	*z*
C	0.011470	-0.042610	0.001800
N	0.006100	-0.000240	1.385800
C	1.278140	0.054320	1.805860
N	2.084000	-0.147480	0.753340
C	1.305800	-0.134900	-0.392610
C	-1.102660	0.429510	2.222490
C	3.514600	0.104460	0.814690
Cl	1.567660	2.548690	2.191480
H	1.591020	0.028200	2.841480
H	1.743620	-0.213870	-1.380480
H	-0.906660	-0.023680	-0.573080
H	-2.039440	0.262980	1.679920
H	-1.111950	-0.156370	3.149420
H	-0.948850	1.495920	2.448510
H	3.964090	-0.511740	1.602590
H	3.960270	-0.160990	-0.149940
H	3.650150	1.172520	1.043890

Table S21. Optimised geometry of [C_1mim]Cl, 2 ion-pairs.

Atom	*x*	*y*	*z*
C	0.016140	0.173410	0.464530
N	-0.216400	-0.193480	1.772510
C	0.954870	-0.390890	2.379130
N	1.922980	-0.233700	1.479960
C	1.362620	0.142000	0.278210
C	-1.465110	-0.007930	2.493180

C	3.339930	-0.216080	1.817600
Cl	0.868740	2.492260	3.054570
H	1.146000	-0.654020	3.431170
H	1.965560	0.352410	-0.596950
H	-0.790760	0.424210	-0.213550
H	-2.304160	-0.233590	1.825020
H	-1.483840	-0.692570	3.348730
H	-1.491980	1.035960	2.838720
H	3.455370	-0.704980	2.795780
H	3.905510	-0.746540	1.042230
H	3.658420	0.833300	1.882820
C	2.002340	1.115080	7.883280
N	1.442370	1.490900	6.681380
C	2.410770	1.647990	5.782520
N	3.581850	1.450690	6.389530
C	3.348890	1.083800	7.697440
C	0.025600	1.472320	6.343040
C	4.830860	1.265280	5.669280
Cl	2.497160	-1.235000	5.106780
H	2.219920	1.910430	4.730260
H	4.155490	0.832640	8.375690
H	1.399140	0.904780	8.758310
H	-0.540630	2.003310	7.117600
H	-0.089460	1.959990	5.364180
H	-0.292850	0.422870	6.278670
H	4.851410	1.952290	4.815720
H	5.669590	1.487760	6.338820
H	4.856460	0.222270	5.321110

Table S22. Optimised geometry of [C_1mim]Cl, 4 ion-pairs.

Atom	*x*	*y*	*z*
C	0.276660	-0.071020	0.957060
N	0.253050	-0.247390	2.323560
C	1.487240	-0.507540	2.745440
N	2.290380	-0.579800	1.683110
C	1.559030	-0.275770	0.554220
C	-0.846820	0.088320	3.217810
C	3.740570	-0.561880	1.782030
Cl	2.178890	2.311770	2.969700
H	1.748310	-0.657380	3.799520
H	2.012130	-0.234230	-0.428940
H	-0.614650	0.179500	0.394510
H	-1.784770	-0.288020	2.792780
H	-0.641260	-0.375830	4.192410

H	-0.871820	1.182230	3.319420
H	4.045570	-1.191730	2.625330
H	4.169960	-0.957920	0.854990
H	4.044140	0.480940	1.956080
C	1.982890	1.492700	8.392980
N	1.204440	1.822270	7.304110
C	1.982010	1.922150	6.225080
N	3.242520	1.715180	6.603110
C	3.269290	1.435100	7.954580
C	-0.246520	1.786030	7.256430
C	4.379650	1.715560	5.693520
Cl	1.080530	-1.101580	5.946050
H	1.685290	2.124740	5.187170
H	4.171150	1.231980	8.521940
H	1.602700	1.319250	9.394270
H	-0.644190	2.158220	8.207570
H	-0.590030	2.431280	6.439550
H	-0.553490	0.747440	7.068190
H	4.019130	2.030150	4.703510
H	5.144470	2.406760	6.067870
H	4.790670	0.698980	5.638210
H	-0.593190	-2.975130	11.032150
H	-0.238240	-1.267590	11.461960
H	0.391390	0.386850	16.250980
C	0.172370	-2.284330	11.405870
H	0.515010	-1.051510	15.148720
C	0.818540	-0.008670	15.322680
H	0.533730	-2.599250	12.395450
H	0.511260	0.621460	14.480370
H	0.378650	-1.801140	8.576930
N	1.308620	-2.284020	10.495200
C	1.280900	-2.004120	9.143730
N	2.268970	0.009470	15.418180
H	2.552610	-0.337790	17.529330
C	3.003220	-0.295380	16.545020
Cl	3.467960	0.533250	11.151940
C	2.569420	-2.490540	10.872410
C	3.069380	-0.061950	14.353680
Cl	2.376330	-2.880490	14.127980
H	2.866840	-2.692790	11.910130
H	2.805630	0.088360	13.300380
C	2.567040	-2.061470	8.704480
N	3.346280	-2.390620	9.792880
C	4.284630	-0.499480	16.138730
H	2.946420	-1.887960	7.702850
N	4.304750	-0.321960	14.772300

H	5.177400	-0.750240	16.698880
C	4.797270	-2.353660	9.839820
C	5.402410	-0.656390	13.874830
H	5.141520	-2.999430	10.655970
H	5.193680	-0.191850	12.901090
H	5.103770	-1.315000	10.029060
H	5.194690	-2.724740	8.888110
H	5.427990	-1.750230	13.772820
H	6.341180	-0.279420	14.297410

Table S23. Optimised geometry of [C_1mim]Cl, 8 ion-pairs.

Atom	*x*	*y*	*z*
C	-0.399430	0.687140	0.812810
N	-0.171060	1.027200	2.131750
C	1.084860	0.723370	2.448100
N	1.667510	0.183070	1.376760
C	0.757220	0.144570	0.333190
C	-1.093840	1.676480	3.053630
C	3.071790	-0.204950	1.333950
Cl	1.794200	3.636240	3.352000
H	1.523900	0.858700	3.432200
H	1.002970	-0.289420	-0.634590
H	-1.346030	0.832990	0.301140
H	-2.112580	1.542570	2.673090
H	-0.977010	1.196790	4.036020
H	-0.824010	2.739210	3.124380
H	3.320930	-0.733690	2.264460
H	3.221680	-0.860320	0.464930
H	3.697970	0.694580	1.249370
C	1.474010	1.654740	8.434190
N	0.738130	2.267630	7.444260
C	1.538080	2.525570	6.409900
N	2.774030	2.152080	6.732260
C	2.757380	1.587490	7.989040
C	-0.713770	2.295380	7.368150
C	3.896600	2.161180	5.802290
Cl	0.754320	-0.250320	5.532050
H	1.272790	2.965940	5.438230
H	3.652370	1.190480	8.452950
H	1.022770	1.316420	9.359230
H	-1.123740	2.549040	8.352470
H	-1.010990	3.058000	6.639840
H	-1.049230	1.303450	7.033150
H	3.612350	2.776170	4.937020

H	4.780950	2.573200	6.302890
H	4.082300	1.128190	5.479340
H	-3.695490	-4.196760	-10.220810
H	-3.029620	-2.739140	-9.392340
H	-2.179680	-0.716550	-4.342220
C	-2.823840	-3.769710	-9.710600
H	-2.654570	-2.271410	-5.127300
C	-2.028840	-1.371510	-5.211340
H	-2.540650	-4.378170	-8.840360
H	-2.277760	-0.842710	-6.141880
H	-2.560910	-2.797070	-12.358650
N	-1.690160	-3.745550	-10.626850
C	-1.666220	-3.181720	-11.883830
N	-0.624240	-1.758520	-5.253430
H	0.038140	-1.287350	-3.241070
C	0.285260	-1.719790	-4.209210
Cl	0.293810	-1.317300	-9.406250
C	-0.453340	-4.103110	-10.289980
C	-0.040050	-2.296740	-6.324990
Cl	-0.731670	-5.215460	-7.234350
H	-0.193780	-4.539730	-9.315080
H	-0.478290	-2.431480	-7.309550
C	-0.377000	-3.232740	-12.314140
N	0.355140	-3.835610	-11.315300
C	1.443060	-2.260050	-4.688660
H	0.080530	-2.889310	-13.234190
N	1.216190	-2.598840	-6.008180
H	2.389410	-2.405400	-4.176370
C	1.806450	-3.846410	-11.223510
C	2.141270	-3.244460	-6.930340
H	2.104540	-4.605300	-10.491590
H	2.023120	-2.763890	-7.912200
H	2.126520	-2.850470	-10.885230
H	2.230050	-4.095810	-12.203140
H	1.874700	-4.307940	-7.002120
H	3.159480	-3.107620	-6.549390
H	-3.230240	-3.493920	-2.778070
H	-2.097870	-2.175890	-2.285910
C	-2.329970	-3.250030	-2.202630
H	-2.496950	-3.506210	-1.149700
N	-1.226270	-4.059220	-2.708010
H	-1.830860	-4.487440	-4.768220
Cl	0.598990	-5.488400	0.937130
C	-1.090750	-4.580690	-3.979900
C	-0.134670	-4.360660	-1.998560
H	0.030210	-4.195570	-0.930440

C	0.118080	-5.207310	-4.021280
N	0.687430	-5.063370	-2.774760
H	0.579120	-5.737170	-4.848480
C	1.990060	-5.555260	-2.336720
H	1.904860	-5.799220	-1.267330
H	2.232280	-6.448640	-2.922980
H	-0.278120	-1.690900	3.665160
H	-0.693170	-3.250040	2.813030
C	-0.124950	-2.310510	2.771600
H	-0.400080	-1.759640	1.863210
H	1.831330	-2.551680	4.773070
N	1.290830	-2.649280	2.695980
C	2.126580	-2.865050	3.774840
C	1.900180	-3.057770	1.584030
Cl	2.526710	-2.104780	-1.602400
C	3.271430	-3.409030	3.274490
H	1.529460	-2.977440	0.567490
N	3.115490	-3.498930	1.903460
H	4.181160	-3.731050	3.767180
C	3.972450	-4.207070	0.963260
H	3.870630	-3.726190	-0.019290
H	3.626230	-5.249060	0.911130
H	5.009330	-4.149890	1.314560
H	2.734710	-4.761340	-2.483350
H	-1.185210	4.870300	-0.950490
H	-1.688750	3.183940	-1.392330
C	-0.944050	3.977880	-1.538640
H	-3.970610	2.571360	-5.189440
H	-2.589250	3.671290	-4.782910
C	-2.934150	2.628970	-4.836970
H	-0.860420	4.223710	-2.607730
H	-2.832930	2.146770	-3.854990
H	0.473690	4.160890	0.969230
N	0.359050	3.484820	-1.103360
C	0.932210	3.630060	0.141250
N	-2.075550	1.922910	-5.777180
H	-3.138000	2.158960	-7.642300
C	-2.229020	1.836220	-7.148710
Cl	-1.485910	0.526300	-2.272150
C	1.178380	2.780420	-1.880980
Cl	0.442430	3.911670	-4.814450
C	-0.860270	1.482340	-5.456820
H	1.010760	2.614720	-2.948520
C	2.139970	3.001590	0.097500
H	-0.491390	1.399680	-4.439750
N	2.271780	2.479030	-1.174320

C	-1.082950	1.294220	-7.648330
H	2.882140	2.908720	0.883940
N	-0.249000	1.076190	-6.568550
H	-0.785610	0.983620	-8.646790
C	3.373500	1.668370	-1.681750
H	3.539690	1.925370	-2.734630
C	1.167600	0.740640	-6.642570
H	1.442180	0.187350	-5.735470
H	3.139920	0.594510	-1.599000
H	4.274790	1.910350	-1.107110
H	1.733580	1.681740	-6.679530
H	1.323810	0.124180	-7.537760

Basis set dependence

Table S24. Basis set dependence of density matrix-based charge schemes for the $[C_1mim][BF_4]$ ion pair.

	Mulliken			Löwdin			NPA		
	CCD	ACCD	ACCT	CCD	ACCD	ACCT	CCD	ACCD	ACCT
C (C4/5)	0.11	0.63	-0.50	-0.08	0.03	0.07	0.01	0.01	-0.01
N (N1/3)	-0.39	-0.45	0.24	0.17	-0.13	0.12	-0.48	-0.48	-0.37
C (C2)	0.43	0.73	-0.45	0.06	0.12	0.08	0.48	0.46	0.42
N (N1/3)	-0.39	-0.49	0.20	0.17	-0.12	0.12	-0.48	-0.48	-0.37
C (C4/5)	0.11	0.64	-0.52	-0.08	0.05	0.07	0.01	0.01	-0.01
C (Methyl)	0.13	0.85	-0.99	-0.11	0.12	0.23	-0.31	-0.31	-0.27
C (Methyl)	0.13	0.85	-0.99	-0.11	0.11	0.25	-0.31	-0.31	-0.27
H (C2)	0.14	-0.32	0.80	0.13	0.11	-0.02	0.27	0.27	0.26
H (C4/5)	0.08	-0.36	0.63	0.10	0.09	-0.01	0.23	0.24	0.22
H (C4/5)	0.08	-0.37	0.63	0.11	0.09	-0.01	0.23	0.24	0.22
H (Methyl)	0.06	-0.18	0.31	0.08	0.06	-0.02	0.20	0.20	0.17
H (Methyl)	0.07	-0.17	0.36	0.09	0.05	-0.05	0.22	0.22	0.20
H (Methyl)	0.10	-0.01	0.37	0.10	0.06	-0.04	0.24	0.24	0.21
H (Methyl)	0.07	-0.17	0.35	0.09	0.05	-0.04	0.22	0.22	0.20
H (Methyl)	0.06	-0.18	0.31	0.09	0.06	-0.01	0.20	0.20	0.17
H (Methyl)	0.11	0.00	0.37	0.10	0.06	-0.04	0.24	0.24	0.21
F	-0.41	-0.87	-0.76	-0.12	-0.18	0.05	-0.65	-0.66	-0.61
B	0.66	2.31	1.88	-0.49	-0.14	-0.98	1.62	1.65	1.42
F	-0.42	-0.85	-0.77	-0.12	-0.17	0.10	-0.66	-0.67	-0.61
F	-0.32	-0.74	-0.71	-0.05	-0.16	0.06	-0.62	-0.63	-0.57
F	-0.42	-0.85	-0.77	-0.12	-0.18	0.07	-0.66	-0.67	-0.61

Table S25. Basis set dependence of RESP charge schemes for the $[C_1mim][BF_4]$ ion pair.

	ChelpG			Connolly			Geodesic		
	CCD	ACCD	ACCT	CCD	ACCD	ACCT	CCD	ACCD	ACCT
C (C4/5)	-0.17	-0.17	-0.17	-0.24	-0.26	-0.26	-0.23	-0.25	-0.24
N (N1/3)	0.12	0.14	0.15	0.22	0.26	0.26	0.23	0.28	0.28
C (C2)	-0.12	-0.16	-0.16	-0.18	-0.23	-0.22	-0.22	-0.27	-0.26
N (N1/3)	0.10	0.13	0.14	0.22	0.27	0.27	0.26	0.31	0.31
C (C4/5)	-0.17	-0.17	-0.17	-0.26	-0.28	-0.28	-0.27	-0.30	-0.30
C (Methyl)	-0.12	-0.13	-0.15	-0.34	-0.38	-0.39	-0.32	-0.36	-0.36
C (Methyl)	-0.05	-0.07	-0.09	-0.29	-0.33	-0.34	-0.34	-0.39	-0.39
H (C2)	-0.45	-0.44	-0.46	0.30	0.30	0.30	0.31	0.31	0.31
H (C4/5)	1.00	1.01	1.08	0.25	0.26	0.26	0.25	0.26	0.26
H (C4/5)	-0.48	-0.48	-0.50	0.25	0.26	0.25	0.24	0.25	0.24
H (Methyl)	-0.46	-0.47	-0.49	0.13	0.13	0.13	0.12	0.12	0.12
H (Methyl)	-0.48	-0.48	-0.50	0.17	0.18	0.18	0.16	0.17	0.17
H (Methyl)	0.29	0.29	0.28	0.19	0.20	0.20	0.19	0.20	0.20

H (Methyl)	0.21	0.20	0.20	0.16	0.17	0.17	0.17	0.17	0.17
H (Methyl)	0.21	0.20	0.20	0.11	0.11	0.12	0.12	0.13	0.13
H (Methyl)	0.06	0.06	0.07	0.18	0.19	0.19	0.20	0.21	0.21
F	0.11	0.11	0.12	-0.44	-0.43	-0.45	-0.40	-0.37	-0.40
B	0.14	0.15	0.15	0.98	1.00	1.07	0.80	0.74	0.85
F	0.09	0.09	0.10	-0.48	-0.48	-0.50	-0.44	-0.42	-0.44
F	0.05	0.05	0.05	-0.45	-0.46	-0.48	-0.40	-0.39	-0.42
F	0.13	0.13	0.14	-0.48	-0.48	-0.50	-0.44	-0.42	-0.44

Invariance with alkyl chain for chloride and NTf_2 ILs

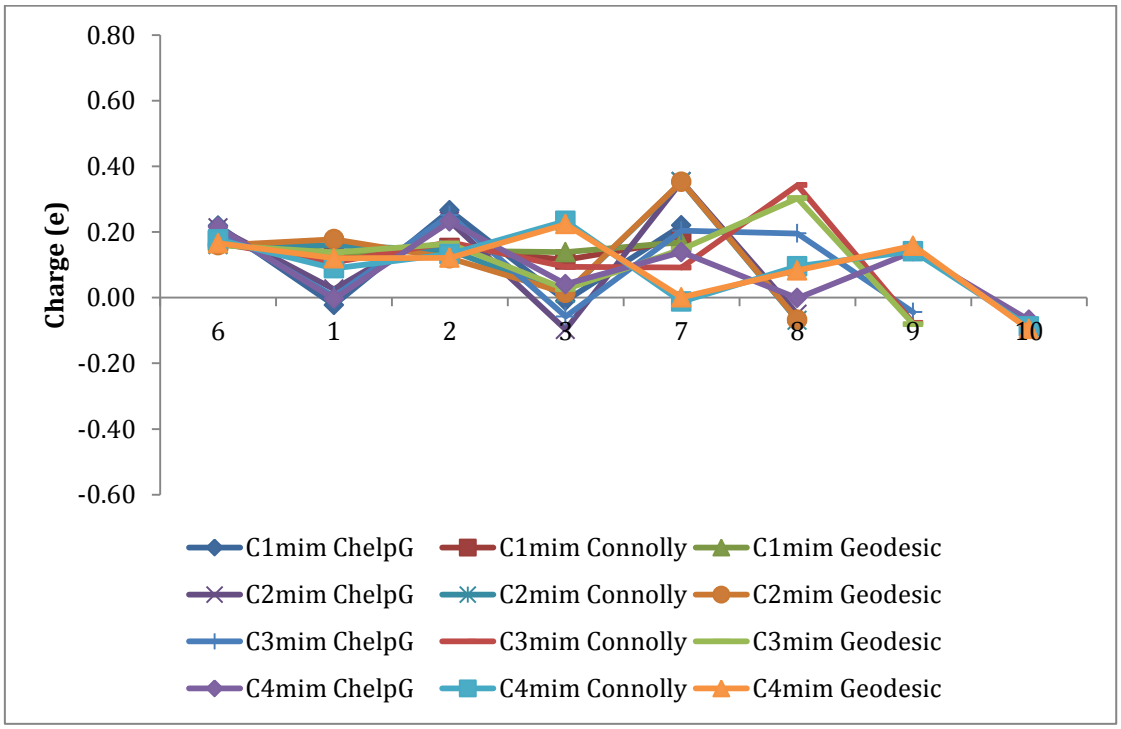

Figure S2. Charge distribution for chloride-based imidazolium ionic liquids using RESP charge schemes.

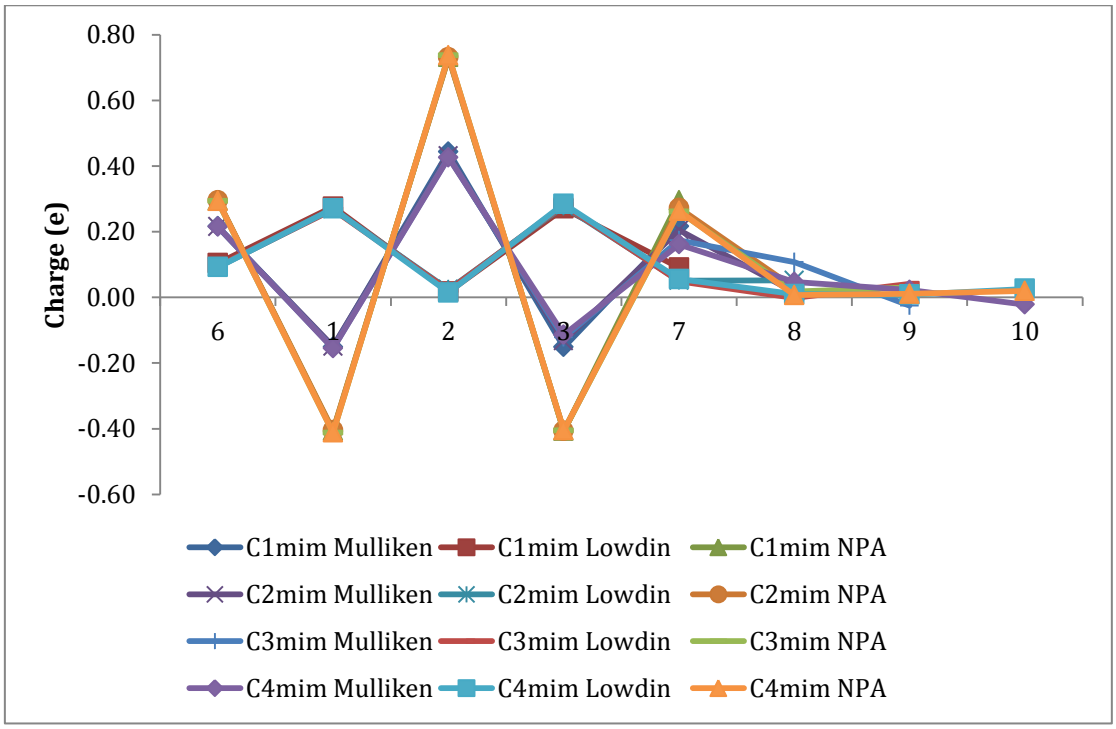

Figure S3. Charge distribution for chloride-based imidazolium ionic liquids using density matrix-based charge schemes.

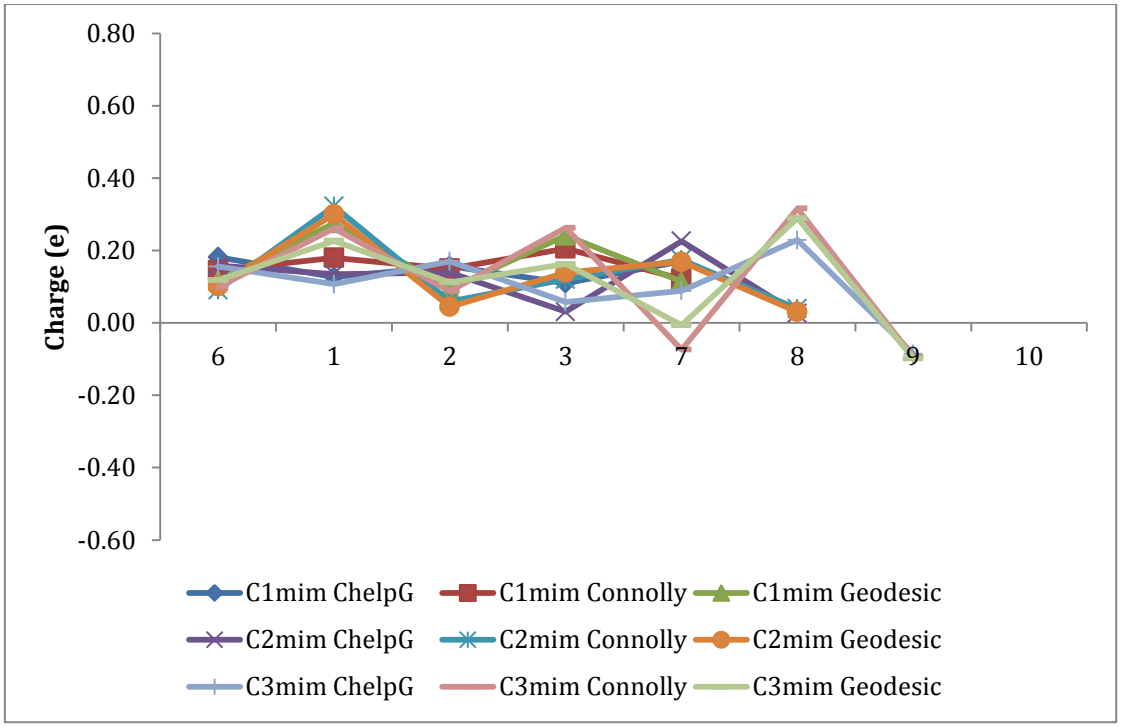

Figure S4. Charge distribution for NTf_2-based imidazolium ionic liquids using RESP charge schemes.

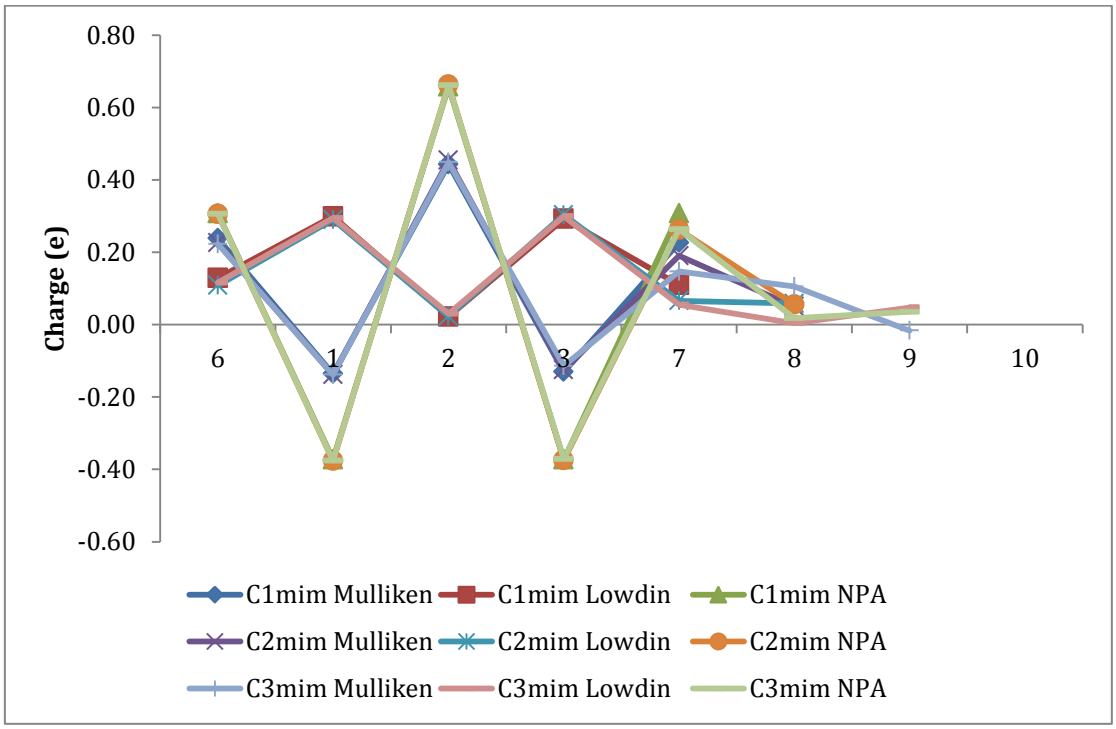

Figure S5. Charge distribution for NTf_2-based imidazolium ionic liquids using density matrix-based charge schemes.

Cluster dipole moments

Table S26. Dipole moments for ionic liquid clusters

		[NMe_4][BF_4]		[C_1mim][BF_4]		[C_1mim]Cl
	Ion	Cation	Anion	Cation	Anion	Cation
ChelpG	1	0.44	0.39	3.06	0.35	3.12
	2	1.05	0.41	2.81	0.29	2.74
	3	0.38	0.34	1.10	0.43	2.18
	4	0.88	0.37	3.63	0.95	2.93
	5	0.46	0.15	3.17	0.95	2.95
	6	0.54	0.58	2.08	0.58	2.18
	7	0.74	0.26	3.32	0.37	2.74
	8	0.91	0.37	3.21	0.63	3.10
	Mean	0.68	0.36	2.80	0.57	2.74
	Std. dev.	0.25	0.12	0.82	0.26	0.37
Connolly	1	1.13	0.67	3.27	0.53	3.27
	2	1.36	0.78	2.95	0.51	2.45
	3	0.58	0.60	2.04	0.54	2.38
	4	3.89	0.60	4.90	0.85	3.59
	5	0.35	0.37	3.63	0.73	3.69
	6	0.78	0.69	2.14	0.62	2.39
	7	0.61	0.56	3.37	0.53	2.45
	8	2.56	0.76	3.80	0.96	3.28
	Mean	1.41	0.63	3.26	0.66	2.94
	Std. dev.	1.22	0.13	0.92	0.17	0.57
Geodesic	1	0.54	0.51	3.85	0.78	3.46
	2	0.80	0.59	3.05	0.62	2.68
	3	0.38	0.22	1.74	0.49	2.58
	4	0.91	0.48	6.36	1.45	3.56
	5	0.42	0.34	3.55	0.78	3.55
	6	0.34	0.64	2.91	0.65	2.64
	7	0.44	0.51	3.23	0.52	2.69
	8	1.05	0.70	3.67	0.86	3.47
	Mean	0.61	0.50	3.55	0.77	3.08
	Std. dev.	0.27	0.16	1.31	0.31	0.46
Mulliken	1	0.37	0.83	3.61	0.61	2.93
	2	0.42	0.64	3.15	0.70	2.59
	3	0.43	0.61	1.99	0.54	2.43
	4	0.68	0.72	2.62	0.30	2.64
	5	0.36	0.48	1.71	0.20	2.64
	6	0.72	0.59	2.06	0.52	2.43
	7	0.71	0.78	3.03	0.75	2.59
	8	0.36	0.61	3.53	0.65	2.93
	Mean	0.51	0.66	2.71	0.53	2.65
	Std. dev.	0.17	0.11	0.73	0.19	0.19

Löwdin	1	0.47	0.13	2.59	0.16	1.88
	2	0.25	0.15	2.48	0.16	1.81
	3	0.47	0.18	2.31	0.18	2.15
	4	0.32	0.26	2.64	0.13	1.95
	5	0.17	0.16	2.42	0.12	1.96
	6	0.21	0.19	2.29	0.14	2.15
	7	0.32	0.27	2.31	0.19	1.81
	8	0.49	0.19	2.86	0.20	1.87
	Mean	0.34	0.19	0.34	0.19	1.95
	Std. dev.	0.13	0.05	0.13	0.05	0.13
NPA	1	0.40	0.74	4.14	0.63	2.29
	2	0.79	0.55	3.51	0.72	1.56
	3	0.72	0.52	2.92	0.50	1.06
	4	0.36	0.63	3.50	0.27	1.95
	5	0.73	0.47	3.34	0.24	1.96
	6	0.21	0.62	2.97	0.49	1.06
	7	0.31	0.71	3.53	0.75	1.56
	8	0.78	0.50	4.07	0.64	2.29
	Mean	0.54	0.59	3.50	0.53	1.72
	Std. dev.	0.24	0.10	0.44	0.19	0.49