

Supplemental Material

Paper: A correlation-based predictor for Pair-Association in Ionic Liquids

Authors: A. Maiti and R. D. Rogers

Atomic coordinates for the structures in Figs. 1(a-d)
(Cartesian coordinates in *Angstroms*)

Structure for Fig. 1(a)

C₄mim⁺Br⁻ (gas phase)

C	2.304503279	1.321892380	0.225295108
N	2.585872021	0.007244650	-0.119046582
C	1.012909777	1.571510110	-0.129184443
N	0.506512962	0.402700885	-0.685487266
C	1.445260964	-0.567997995	-0.576245144
C	-0.895398546	0.151739997	-1.039766250
C	-1.822491443	0.194557529	0.175129278
C	-3.260978071	-0.173878716	-0.197700031
C	-4.206694146	-0.113164100	1.003000262
C	3.735468104	-0.772977525	0.321479793
H	3.048580670	1.962506759	0.681625565
H	0.420335135	2.473440372	-0.044831292
H	1.383065688	-1.543843302	-1.032509509
H	-0.924229069	-0.844297913	-1.500086060
H	-1.193381255	0.885587823	-1.804302703
H	-1.805207878	1.204946271	0.618452465
H	-1.421520167	-0.504676093	0.927971593
H	-3.272595748	-1.190535987	-0.625534401
H	-3.625384215	0.501051232	-0.992682056
H	-5.234402782	-0.380721726	0.718136278
H	-4.229085966	0.897256507	1.439715318
H	-3.880485513	-0.808558147	1.790120553
H	4.491784248	-0.091307095	0.723970979
H	4.162332425	-1.326772180	-0.523995303
H	3.378788257	-1.477203465	1.092891394
Br	0.737096451	-2.257596170	1.481274318

Structure for Fig. 1(b)
C₄mim⁺Br⁻ (water)

C	2.410816285	1.242156120	0.311001118
N	2.547812491	-0.119236134	0.103578880
C	1.138060849	1.575971153	-0.063619890
N	0.526201642	0.413993418	-0.496443027
C	1.394514873	-0.604744472	-0.383781891
C	-0.870494534	0.275330279	-0.946914235
C	-1.826849284	0.007194844	0.213702798
C	-3.268229112	-0.161275675	-0.275625028
C	-4.247530638	-0.435666857	0.867323484
C	3.753758296	-0.906939385	0.366532606
H	3.223201525	1.848300566	0.693036504
H	0.629616925	2.532465628	-0.068046073
H	1.166944584	-1.642769448	-0.651922227
H	-0.889075555	-0.558676365	-1.660563497
H	-1.128789843	1.199995813	-1.478704669
H	-1.770273063	0.833595341	0.941050319
H	-1.504464632	-0.911707920	0.730765286
H	-3.302407142	-0.990130527	-1.002413330
H	-3.576805850	0.746857249	-0.820732583
H	-5.274824856	-0.550366812	0.490557125
H	-4.246783317	0.389460848	1.596319562
H	-3.979423062	-1.358149649	1.405503339
H	4.575908023	-0.534700704	-0.255258151
H	3.548689217	-1.951971577	0.119333186
H	4.017549310	-0.821492609	1.426336736
Br	-0.238470825	-3.604196297	-1.393538079

Structure for Fig. 1(c)
C₄mim⁺BF₄⁻ (water)

C	2.274633421	1.692526215	-0.188007352
N	2.546706338	0.358190205	0.053388181
C	0.975352574	1.764419674	-0.608215777
N	0.480780982	0.472561656	-0.620599978
C	1.447067490	-0.364986446	-0.211563075
C	-0.904131610	0.090444388	-0.950431231
C	-1.850566223	0.291962793	0.231638927
C	-3.291337559	-0.085059850	-0.126706451
C	-4.249806631	0.109161228	1.050269523
C	3.815816726	-0.180575233	0.549314280
H	3.023784484	2.463779937	-0.052825226
H	0.371446097	2.612100656	-0.908140202
H	1.362571659	-1.442707964	-0.101026567
H	-0.882486357	-0.958928460	-1.268706771
H	-1.205182358	0.698991713	-1.813046869
H	-1.814140371	1.345578440	0.553489685
H	-1.501778255	-0.323860805	1.076211065
H	-3.318512950	-1.135934135	-0.459850300
H	-3.626369482	0.524206728	-0.983157831
H	-5.277361539	-0.169945685	0.775367350
H	-4.261586500	1.160058656	1.379093495
H	-3.950023897	-0.509209903	1.910732326
H	4.637266941	0.283103309	-0.005952457
H	3.824803087	-1.262094275	0.389504630
H	3.914183715	0.038484922	1.618816285
B	0.860725877	-3.114763582	2.061763229
F	-0.454955768	-2.670426883	1.760089098
F	1.563865568	-3.353108779	0.836136686
F	1.545723386	-2.118337687	2.805631437
F	0.801250850	-4.319607463	2.809167909

Structure for Fig. 1(d)
C₄mim⁺PF₆⁻ (water)

C	2.082053933	2.113318068	-1.329236756
N	2.551036481	1.134944551	-0.470612447
C	0.787316362	1.794178728	-1.629086523
N	0.490582557	0.623293965	-0.954638601
C	1.571943559	0.242919941	-0.256467353
C	-0.819725284	-0.050514938	-0.931779389
C	-1.811540501	0.648331923	-0.002631882
C	-3.171284903	-0.056696178	-0.002471732
C	-4.177792392	0.613531407	0.933795627
C	3.906597744	1.052262626	0.078425342
H	2.705496148	2.939479379	-1.648736997
H	0.060106330	2.292626084	-2.258369791
H	1.639774939	-0.632790710	0.377716614
H	-0.641803877	-1.084491333	-0.612757333
H	-1.185325037	-0.072184213	-1.966380018
H	-1.936974482	1.696178860	-0.321413365
H	-1.393516235	0.661052673	1.016301852
H	-3.032886716	-1.110482188	0.293163177
H	-3.573251193	-0.071075863	-1.029095201
H	-5.152187720	0.103763075	0.899884871
H	-4.339944586	1.666862439	0.655227353
H	-3.825654761	0.594515303	1.976774446
H	4.598459542	0.717977073	-0.703163683
H	3.906024237	0.336574850	0.905492054
H	4.202846752	2.040039250	0.445154700
P	0.846166124	-0.995507717	3.521557576
F	1.612472173	-0.347686864	4.827941183
F	-0.613359642	-0.701191981	4.223965014
F	0.890727704	-2.481971845	4.228985054
F	2.309299918	-1.292524159	2.811227631
F	0.087696925	-1.645467133	2.206250053
F	0.806571656	0.489608904	2.808196242