SUPPORTING INFORMATION

The Role of the Cation in the Solvation of Cellulose by Imidazolium-Based Ionic Liquids

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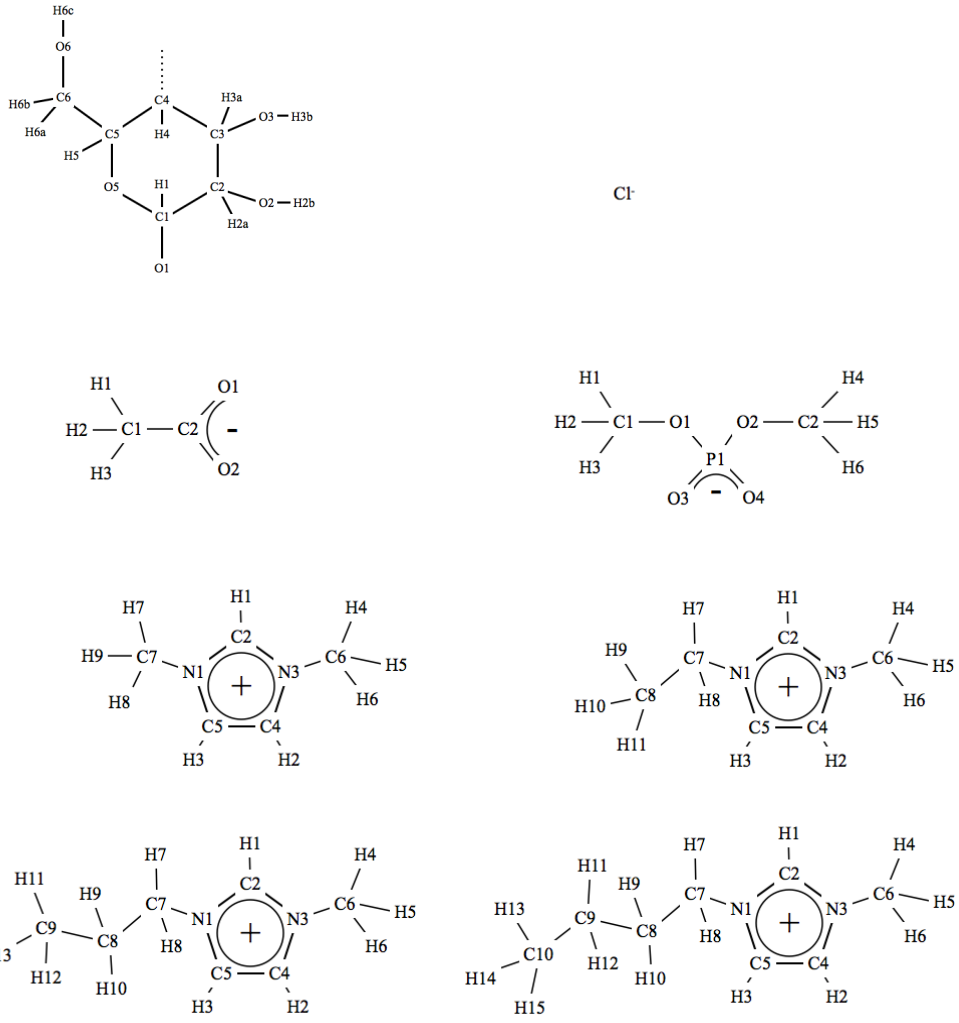


Figure S1: Atom naming within the different molecules.

Table S1: Number of contacts between the ring hydrogens of the cation and cellulose–bound anions and cellulose oxygens.

Simulation	Number of contacts[a]	
	bound anion	cellulose
$[C_2MIM]Ac$ (1x8 glucans)	0.39	0.32
$[C_2MIM]Ac$ (1x16 glucans)	0.94	0.50
$[C_2MIM]Ac$ (4x16 glucans)	0.95	0.49
$[C_2MIM]Ac$ (1x32 glucans)	0.93	0.49

[a]Normalized by the average number of cations present in the primary solvation shell of cellulose.

Table S2: Number of contacting ions for simulations with different cellulose lengths.

Simulation	Contacting Ions per Glucan	
	Anion	Cation
$[C_2MIM]Ac$ (1x8 glucans)	2.626 ± 0.005	4.700 ± 0.007
$[C_2MIM]Ac$ (1x16 glucans)	2.427 ± 0.003	4.325 ± 0.004
$[C_2MIM]Ac$ (4x16 glucans)[a]	2.437 ± 0.003	4.296 ± 0.005
	2.436 ± 0.003	4.335 ± 0.005
	2.447 ± 0.003	4.271 ± 0.005
	2.438 ± 0.004	4.276 ± 0.005
$[C_2MIM]Ac$ (1x32 glucans)	2.418 ± 0.003	4.131 ± 0.004

[a]each entry refers to the statistics for one of the four strands.

Table S3: Number of C–H···O hydrogen bonds for simulations with different cellulose lengths.

Simulation	C–H···O H-Bonds per Glucan
$[C_2MIM]Ac$ (1x8 glucans)	0.279
$[C_2MIM]Ac$ (1x16 glucans)	0.255
$[C_2MIM]Ac$ (4x16 glucans)	0.248
$[C_2MIM]Ac$ (1x32 glucans)	0.244

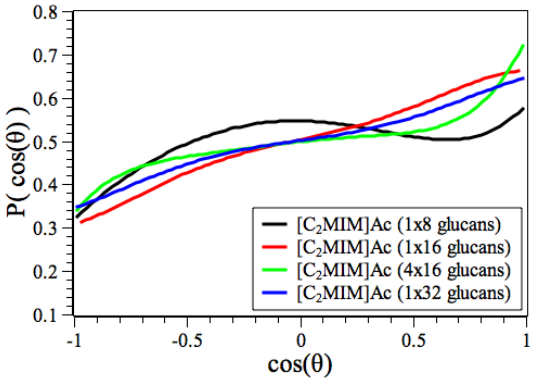


Figure S2: Orientation of the alkyl tail for different cellulose chain lengths.

Table S4: Energy contributions, in kcal/mol per glucan, between the different IL components and the cellulose strand.

Simulation	Anion (elec)	Anion (vdW)	Cation (elec)	Cation (vdW)	Total
[C_2MIM]Ac (1x8 glucans)	−50.0	−8.97	1.97	−14.4	−71.3
[C_2MIM]Ac (1x16 glucans)	−50.8	−7.50	2.10	−14.0	−70.2
[C_2MIM]Ac (4x16 glucans)[a]	−48.5	−7.63	2.04	−14.0	−68.1
	−47.5	−8.15	1.55	−13.8	−67.9
	−48.1	−4.02	2.15	−13.8	−63.8
	−47.2	−5.41	1.86	−14.0	−64.8
[C_2MIM]Ac (1x32 glucans)	−46.2	−8.16	1.44	−13.8	−66.7

[a]each entry refers to individual statistics for each of the four strands.

Table S5: Occurrences of different hydrogen-bonding patterns per glucan.

Simulation	nonbridging			bridging[c]				Total[d]
	H_6	H_3	H_2	H_{2i}–H_{3i}	H_{2i}–H_{6j}	H_{3i}–H_{6j}	H_{2i}–H_{3j}	
[C_2MIM]Ac (1x8 glucans)	0.63	0.28	0.18	0.52	0.34	0.12	0.61	2.91
[C_2MIM]Ac (1x16 glucans)	0.63	0.31	0.22	0.58	0.37	0.14	0.56	2.80
[C_2MIM]Ac (4x16 glucans)	0.56	0.30	0.25	0.50	0.32	0.20	0.39	2.89
[C_2MIM]Ac (1x32 glucans)	0.54	0.27	0.30	0.49	0.23	0.15	0.44	2.84

[c]Indices i and j indicate separate glucans, where $i \neq j$. [d]Includes other, less significant patterns not shown in preceding columns.

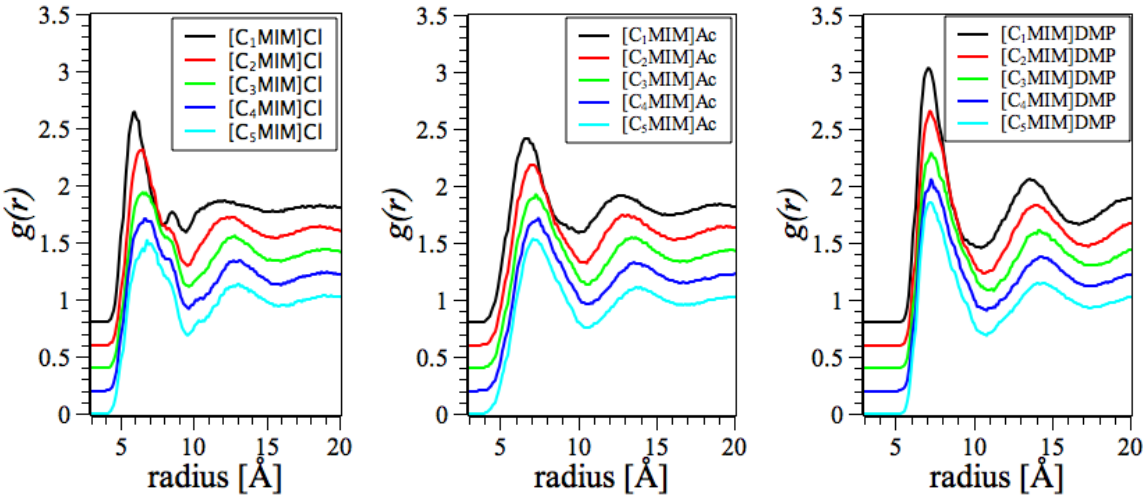
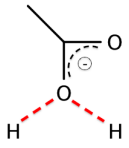


Figure S3: Anion-anion radial distribution functions for (a) the chlorides using the Cl atoms, (b) the acetates using the C2 atoms and (c) the dimethylphosphates using the P1 atoms.

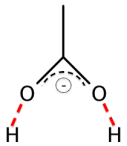
Table S6: Hydrogen bonding for the chlorides

		same glucan ($i = j$)			different glucan ($i \neq j$)		
IL		H_2	H_3	H_6	H_2	H_3	H_6
	H_2	0.44	0.21	0	0.09	0.10	0.08
$[C_1mim]Cl$	H_3	0.21	0.50	0	0.10	0	0.13
	H_6	0	0	0.65	0.08	0.13	0.06
	H_2	0.47	0.22	0	0	0.09	0.11
$[C_2mim]Cl$	H_3	0.22	0.46	0	0.09	0	0.13
	H_6	0	0	0.55	0.11	0.13	0.14
	H_2	0.39	0.36	0	0	0.06	0.12
$[C_3mim]Cl$	H_3	0.36	0.24	0.01	0.06	0	0.10
	H_6	0	0.01	0.56	0.12	0.10	0.11
	H_2	0.24	0.31	0	0.11	0.05	0.20
$[C_4mim]Cl$	H_3	0.31	0.27	0.03	0.05	0	0.15
	H_6	0	0.03	0.35	0.20	0.15	0.07
	H_2	0.23	0.34	0	0.07	0.08	0.11
$[C_5mim]Cl$	H_3	0.34	0.29	0	0.08	0	0.09
	H_6	0	0	0.47	0.11	0.09	0.13

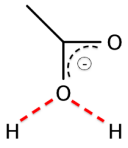
Table S7: Hydrogen bonding for the acetates



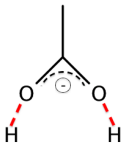
same glucan ($i = j$)



same glucan ($i = j$)



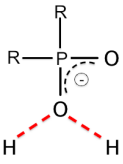
different glucan ($i \neq j$)



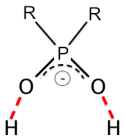
different glucan ($i \neq j$)

IL		H_2	H_3	H_6	H_2	H_3	H_6	H_2	H_3	H_6	H_2	H_3	H_6
	H_2	0.26	0.06	0	0.08	0.17	0	0.05	0.01	0.03	0.07	0.23	0.19
$[C_1mim]Ac$	H_3	0.06	0.44	0	0.17	0.05	0	0.01	0	0.04	0.23	0.01	0.03
	H_6	0	0	0.62	0	0	0.06	0.03	0.04	0	0.19	0.03	0
	H_2	0.19	0.09	0	0.03	0.20	0	0	0	0.03	0	0.28	0.15
$[C_2mim]Ac$	H_3	0.09	0.28	0	0.20	0.03	0	0	0	0.04	0.28	0	0.05
	H_6	0	0	0.60	0	0	0.03	0.03	0.04	0	0.15	0.05	0
	H_2	0.27	0.12	0	0.04	0.18	0	0	0.02	0.06	0.02	0.25	0.17
$[C_3mim]Ac$	H_3	0.12	0.26	0	0.18	0.04	0	0.02	0	0.09	0.25	0.01	0.08
	H_6	0	0	0.48	0	0	0.03	0.06	0.09	0	0.17	0.08	0.02
	H_2	0.16	0.11	0	0.04	0.29	0	0.06	0.03	0.05	0.01	0.17	0.18
$[C_4mim]Ac$	H_3	0.11	0.29	0	0.29	0.04	0	0.03	0	0.05	0.17	0	0.09
	H_6	0	0	0.45	0	0	0.04	0.05	0.05	0.03	0.18	0.09	0.08
	H_2	0.16	0.14	0	0.01	0.21	0	0	0.01	0.04	0	0.14	0.13
$[C_5mim]Ac$	H_3	0.14	0.23	0	0.21	0.01	0.02	0.01	0	0.01	0.14	0.02	0.01
	H_6	0	0	0.58	0	0.02	0.02	0.04	0.01	0.01	0.13	0.01	0.01

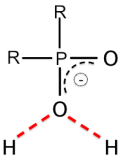
Table S8: Hydrogen bonding for the dimethylphosphates



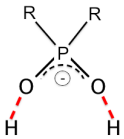
same glucan ($i = j$)



same glucan ($i = j$)



different glucan ($i \neq j$)



different glucan ($i \neq j$)

IL		H_2	H_3	H_6	H_2	H_3	H_6	H_2	H_3	H_6	H_2	H_3	H_6
	H_2	0.25	0.05	0	0	0.08	0	0	0	0.02	0	0.29	0.09
$[C_1mim]DMP$	H_3	0.05	0.33	0	0.08	0	0.02	0	0	0.03	0.29	0	0.06
	H_6	0	0	0.52	0	0.02	0	0.02	0.03	0.01	0.09	0.06	0.01
	H_2	0.26	0.10	0	0	0.12	0	0.01	0	0.03	0	0.24	0.09
$[C_2mim]DMP$	H_3	0.10	0.29	0	0.12	0	0	0	0	0.04	0.24	0	0.08
	H_6	0	0	0.50	0	0	0	0.03	0.04	0	0.09	0.08	0
	H_2	0.27	0.14	0	0	0.12	0	0	0	0.05	0	0.16	0.12
$[C_3mim]DMP$	H_3	0.14	0.25	0	0.12	0	0.02	0	0	0.06	0.16	0	0.05
	H_6	0	0	0.38	0	0.02	0	0.05	0.06	0	0.12	0.05	0.05
	H_2	0.37	0.04	0	0	0.10	0	0	0	0.02	0	0.24	0.07
$[C_4mim]DMP$	H_3	0.04	0.23	0	0.10	0	0.05	0	0	0.05	0.24	0	0.05
	H_6	0	0	0.42	0	0.05	0	0.02	0.05	0	0.07	0.05	0.05
	H_2	0.26	0.11	0	0	0.05	0	0.04	0.01	0.01	0.01	0.15	0.06
$[C_5mim]DMP$	H_3	0.11	0.30	0.01	0.05	0	0.05	0.01	0	0.03	0.15	0.06	0.06
	H_6	0	0.1	0.44	0	0.05	0	0.01	0.03	0.01	0.06	0.06	0.02

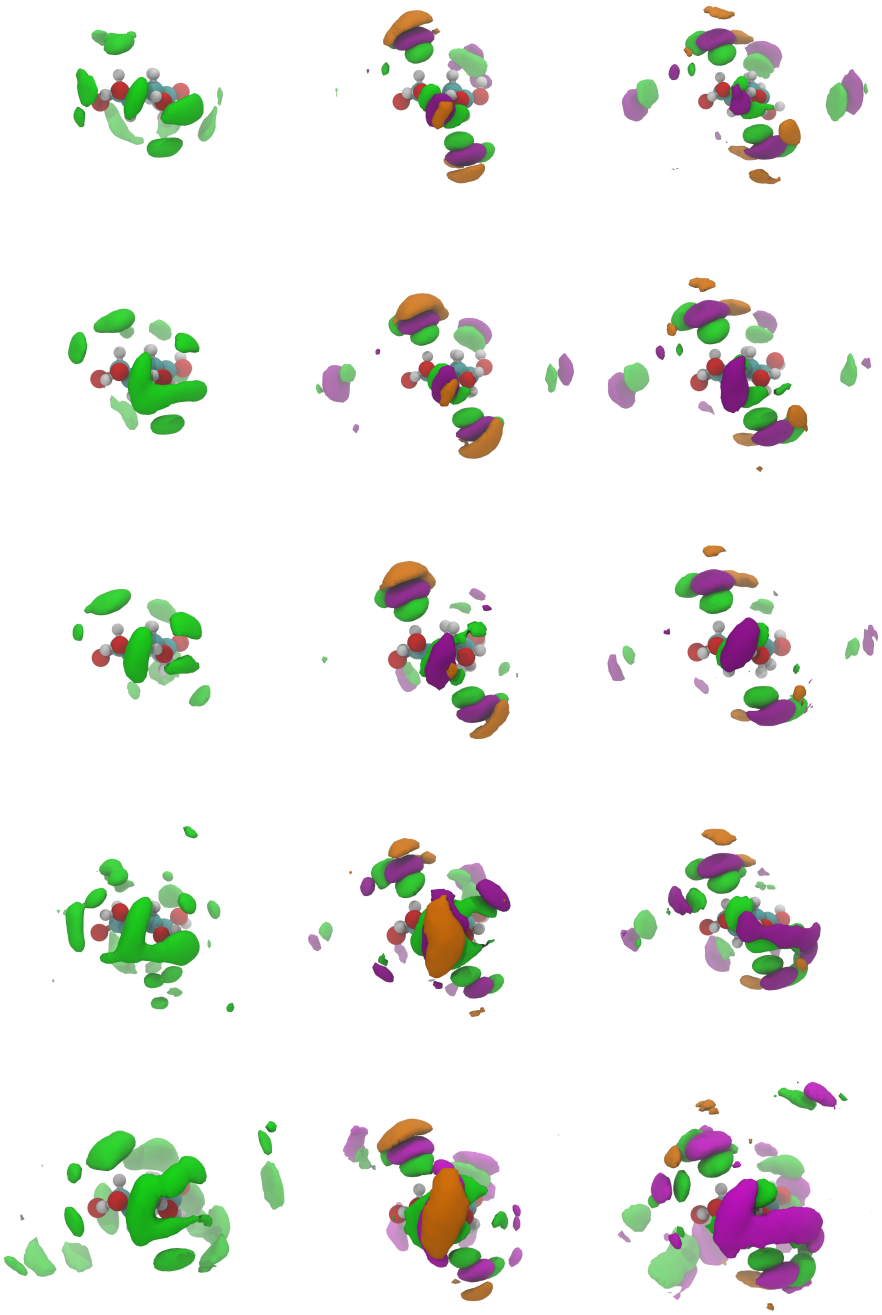


Figure S4: (Top to bottom): [C_1mim], [C_2mim], [C_3mim], [C_4mim] and [C_5mim]. (Left to right) Cl, Ac and DMP. Isosurfaces indicate 5 times the normal density and the colors indicate (green) Chloride and oxygens, (purple) carboxylic carbon and phosphorous and (orange) methyl groups.

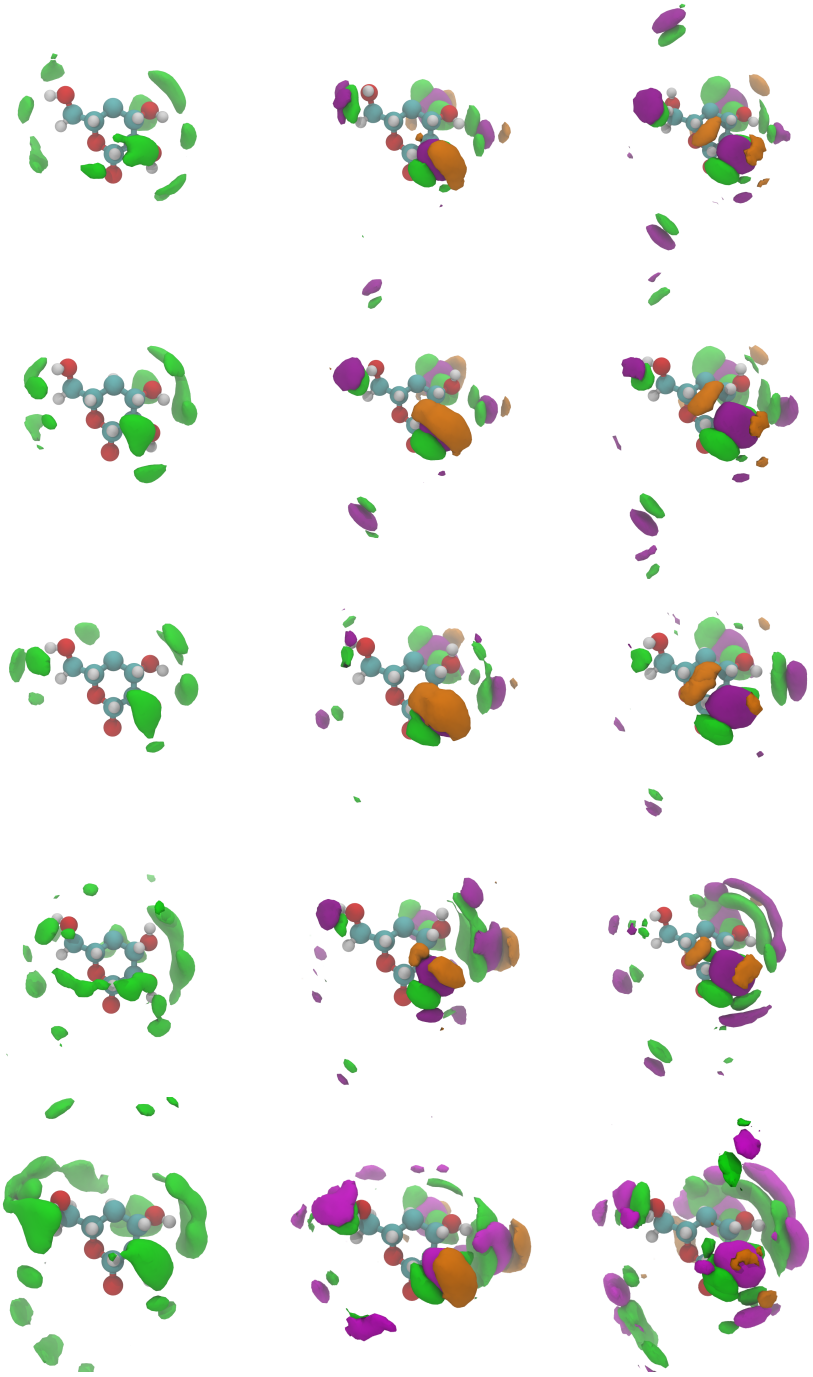


Figure S5: (Top to bottom): [C_1mim], [C_2mim], [C_3mim], [C_4mim] and [C_5mim]. (Left to right) Cl, Ac and DMP. Isosurfaces indicate 5 times the normal density and the colors indicate (green) Chloride and oxygens, (purple) carboxylic carbon and phosphorous and (orange) methyl groups.

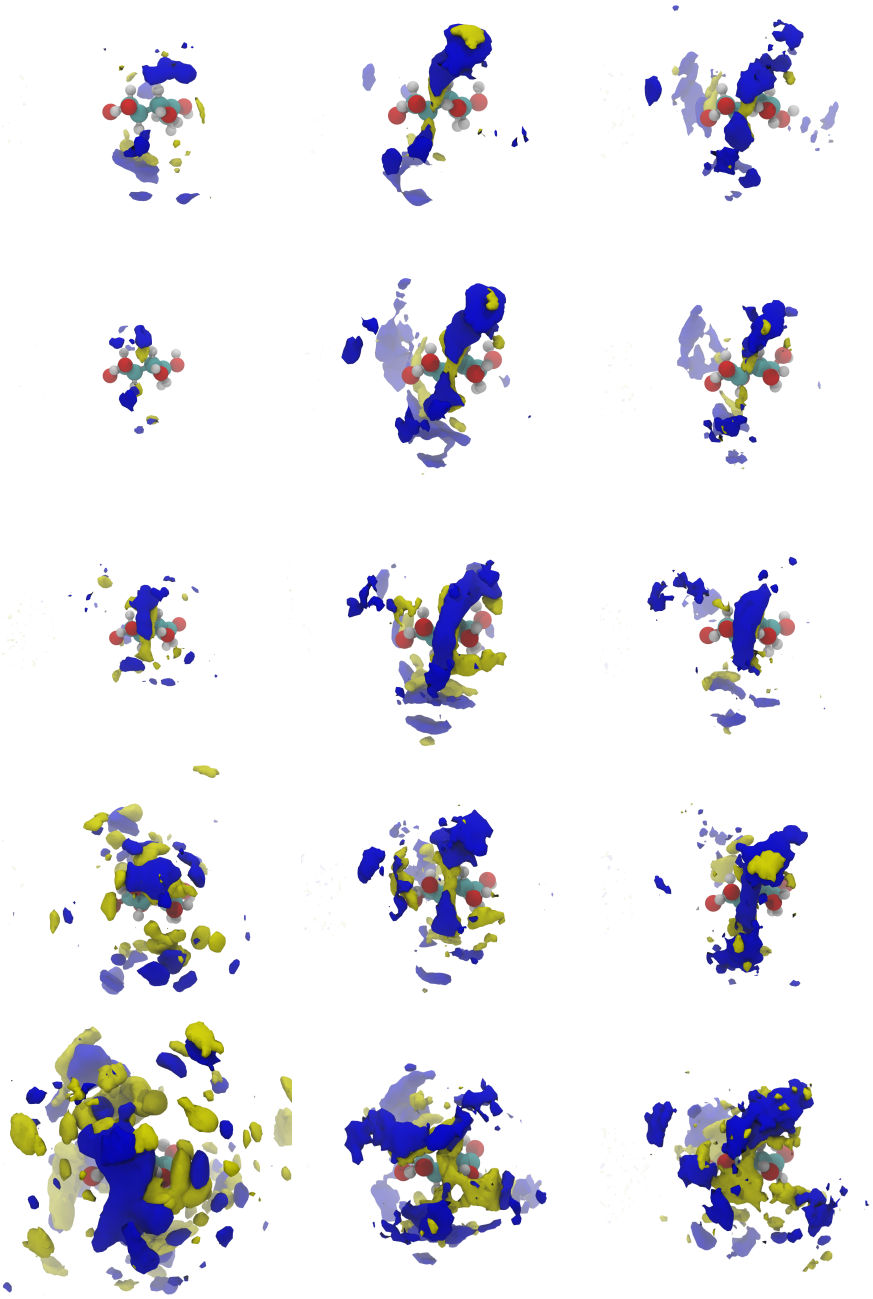


Figure S6: (Top to bottom): [C_1mim], [C_2mim], [C_3mim], [C_4mim] and [C_5mim]. (Left to right) Cl, Ac and DMP. Isosurfaces indicate 3 times the normal density and the colors indicate (blue) the C_2 atom of the cation and (yellow) the H_1, H_2 and H_3 atoms of the cation.

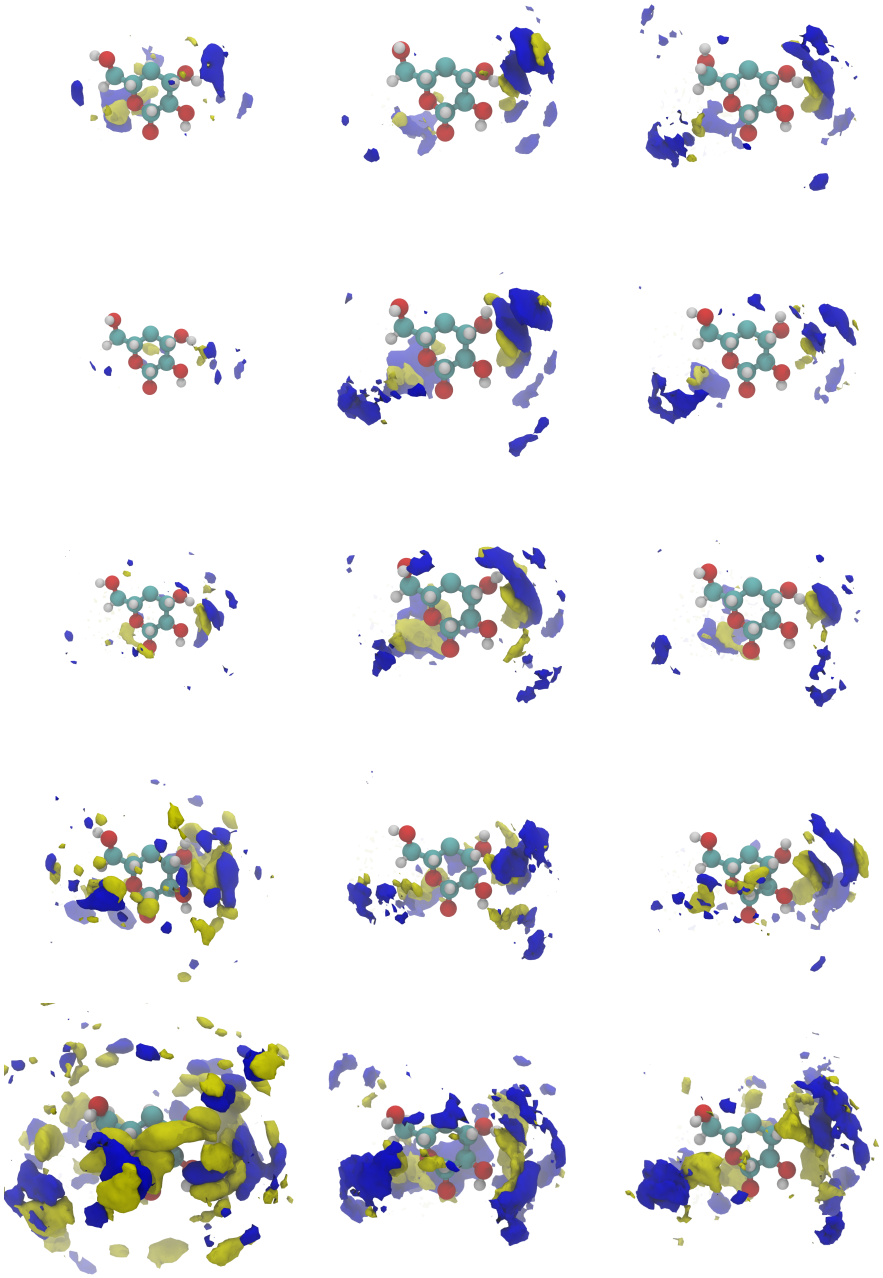


Figure S7: (Top to bottom): [C_1mim], [C_2mim], [C_3mim], [C_4mim] and [C_5mim]. (Left to right) Cl, Ac and DMP. Isosurfaces indicate 3 times the normal density and the colors indicate (blue) the C_2 atom of the cation and (yellow) the H_1, H_2 and H_3 atoms of the cation.

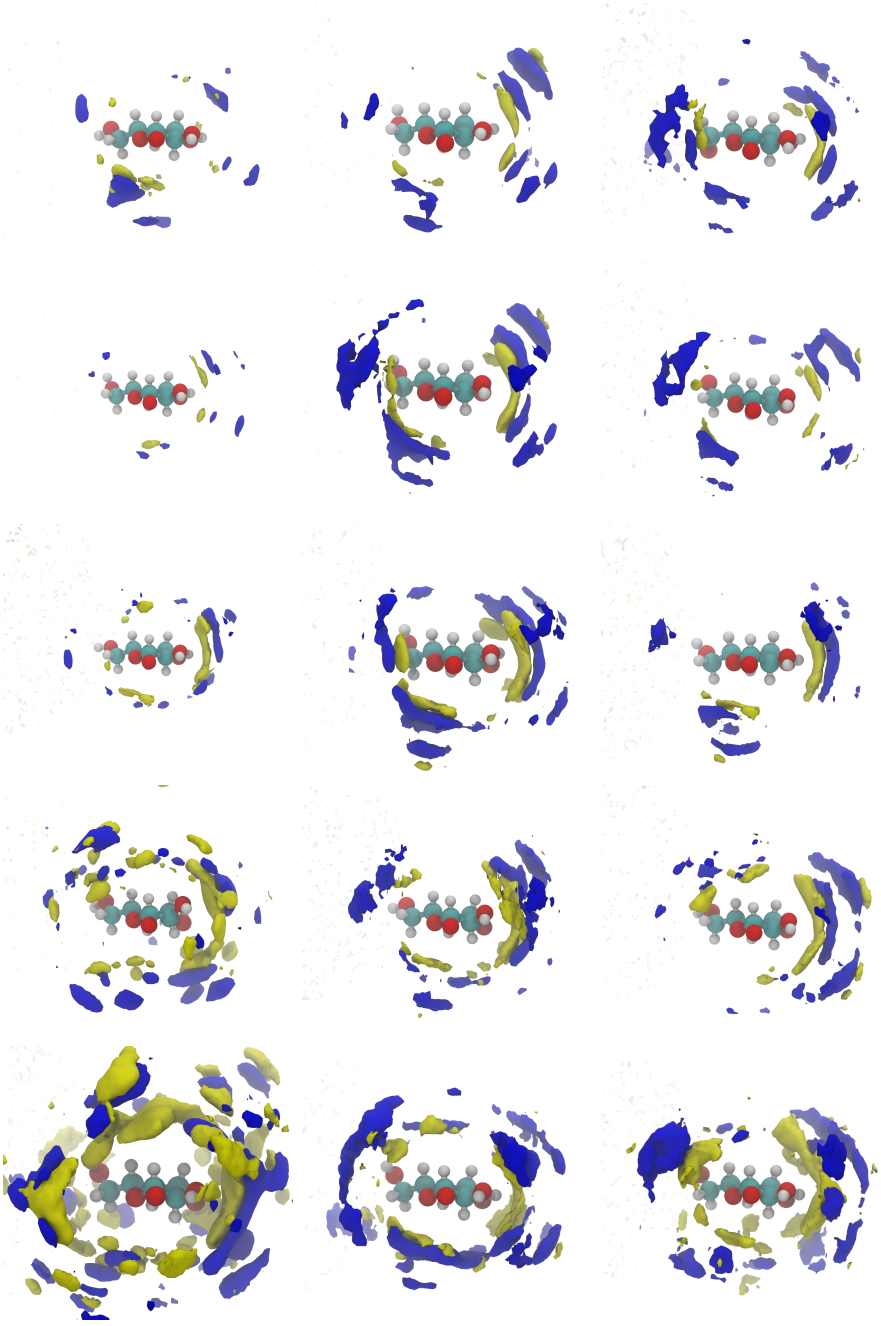


Figure S8: (Top to bottom): [C_1mim], [C_2mim], [C_3mim], [C_4mim] and [C_5mim]. (Left to right) Cl, Ac and DMP. Isosurfaces indicate 3 times the normal density and the colors indicate (blue) the C_2 atom of the cation and (yellow) the H_1, H_2 and H_3 atoms of the cation.

Table S9: Pairwise electrostatic energies for the chlorides.

[DMIM]Cl	Cl	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-14536	14536	1568	-3001	-2132	2420	-1859	-1859	-1860	1861	-3027	1871	-3062	-2151	2467	-1900	-1899	0	-1900	0	0	0	0	0	0	0	0	-14463	72
H2b	-9363	-9363	-983	1881	1340	-1515	1163	1163	1164	-1168	1898	-1172	1914	1347	-1538	1184	1184	0	1185	0	0	0	0	0	0	0	0	9045	-317
C2	-4176	-4176	-453	866	616	-698	536	536	537	-537	874	-540	883	622	-712	548	548	0	548	0	0	0	0	0	0	0	0	4175	-1
H2a	-1234	-1234	-134	256	182	-207	159	159	159	-159	259	-160	262	184	-211	162	162	0	162	0	0	0	0	0	0	0	0	1236	2
O3	-14425	14425	1579	-3009	-2149	2433	-1867	-1867	-1868	1874	-3039	1887	-3070	-2172	2480	-1906	-1905	0	-1906	0	0	0	0	0	0	0	0	-14504	-79
H3b	-9304	-9304	-992	1889	1350	-1522	1168	1168	1168	-1178	1904	-1184	1923	1364	-1551	1192	1192	0	1191	0	0	0	0	0	0	0	0	9083	-221
C3	-4152	-4152	-454	867	616	-698	536	536	537	-538	874	-542	884	625	-714	549	549	0	549	0	0	0	0	0	0	0	0	4176	25
H3a	-1232	-1232	-134	257	182	-206	158	158	158	-159	258	-160	261	184	-211	163	163	0	163	0	0	0	0	0	0	0	0	1234	2
C4	-3469	-3469	-375	722	511	-581	447	447	448	-446	731	-449	738	515	-593	457	457	0	458	0	0	0	0	0	0	0	0	3486	18
O4t	961	961	104	-198	-142	160	-123	-123	-123	122	-200	122	-201	-141	162	-125	-125	0	-125	0	0	0	0	0	0	0	0	-954	7
H4t	-622	-622	-65	124	89	-101	77	77	77	-77	126	-77	126	88	-101	78	78	0	78	0	0	0	0	0	0	0	0	598	-24
H4	-652	-652	-70	135	96	-109	84	84	84	-84	137	-84	138	97	-111	86	86	0	86	0	0	0	0	0	0	0	0	653	0
C5	-3442	-3442	-372	714	506	-574	442	442	442	-443	725	-445	731	509	-583	450	450	0	450	0	0	0	0	0	0	0	0	3444	2
H5	-613	-613	-66	126	90	-102	79	79	79	-79	129	-79	130	91	-103	80	80	0	80	0	0	0	0	0	0	0	0	611	-1
H6b	-1235	-1235	-135	258	184	-209	161	161	161	-161	262	-162	264	185	-211	162	162	0	163	0	0	0	0	0	0	0	0	1245	10
C6	-2956	-2956	-324	619	443	-502	385	385	385	-387	628	-388	632	445	-507	390	390	0	390	0	0	0	0	0	0	0	0	2984	28
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H6c	-8927	-8927	-963	1830	1312	-1475	1131	1132	1132	-1147	1855	-1148	1862	1316	-1488	1143	1144	0	1144	0	0	0	0	0	0	0	0	8780	-146
H6a	-1235	-1235	-135	258	185	-210	161	161	161	-161	262	-162	263	186	-212	163	163	0	163	0	0	0	0	0	0	0	0	1245	9
O5	8201	8201	875	-1689	-1187	1350	-1040	-1040	-1040	1040	-1707	1046	-1723	-1195	1372	-1060	-1060	0	-1060	0	0	0	0	0	0	0	0	-8117	83
C1	-6202	-6202	-662	1276	902	-1028	791	790	791	-788	1293	-792	1305	905	-1045	806	806	0	806	0	0	0	0	0	0	0	0	6157	-46
H1	-2050	-2050	-219	420	299	-340	266	266	261	-261	427	-262	431	300	-345	266	266	0	266	0	0	0	0	0	0	0	0	2032	-18
O1	8548	8548	916	-1770	-1247	1427	-1098	-1098	-1099	1094	-1796	1096	-1808	-1254	1449	-1118	-1117	0	-1118	0	0	0	0	0	0	0	0	-8543	6
H1t	-619	-619	-67	127	91	-103	79	79	79	-79	129	-79	127	90	-100	77	77	0	77	0	0	0	0	0	0	0	0	605	-14
TOT	-699	-699	-6	-12	13	10	-7	-8	-7	-6	-8	-1	-12	9	10	-10	-9	0	-10	0	0	0	0	0	0	0	0	-54	-753

[EMIM]Cl	Cl	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-12606	12606	1369	-2630	-1866	2131	-1641	-1641	-1640	1617	-2630	1613	-2618	-1857	2102	-1620	-1620	618	-745	-745	0	-745	0	0	0	0	0	-12547	59
H2b	-8114	-8114	-859	1646	1173	-1335	1027	1027	1026	-1015	1645	-1012	1637	1165	-1317	1014	1014	-387	467	467	0	467	0	0	0	0	0	7850	-264
C2	-3636	-3636	-393	757	537	-615	474	474	474	-464	756	-463	752	535	-606	467	467	-178	215	215	0	215	0	0	0	0	0	3618	-18
H2a	-1075	-1075	-117	224	159	-183	141	141	141	-138	224	-137	223	158	-180	138	138	-53	64	64	0	64	0	0	0	0	0	1071	-4
O3	-12615	12615	1368	-2632	-1877	2157	-1660	-1660	-1659	1617	-2633	1605	-2603	-1851	2103	-1618	-1618	619	-746	-746	0	-746	0	0	0	0	0	-12578	37
H3b	-8126	-8126	-861	1655	1181	-1354	1042	1042	1042	-1017	1652	-1009	1630	1163	-1314	1012	1011	-387	466	466	0	466	0	0	0	0	0	7886	-240
C3	-3631	-3631	-393	756	536	-616	475	475	475	-463	755	-462	750	532	-605	467	467	-178	215	215	0	215	0	0	0	0	0	3616	-16
H3a	-1076	-1076	-115	223	158	-182	140	140	140	-137	223	-136	222	157	-179	138	138	-53	63	63	0	63	0	0	0	0	0	1067	-10
C4	-3055	-3055	-326	633	443	-512	396	396	396	-385	632	-384	629	441	-504	391	391	-149	180	180	0	180	0	0	0	0	0	3027	-28
O4t	852	852	91	-178	-125	145	-112	-112	-112	107	-176	106	-172	-122	138	-106	-106	40	-49	-49	0	-49	0	0	0	0	0	-841	11
H4t	-549	-549	-57	111	78	-90	70	70	70	-67	110	-66	107	76	-86	66	66	-25	30	31	0	30	0	0	0	0	0	524	-24
H4	-571	-571	-61	119	84	-96	74	74	74	-72	119	-72	118	83	-95	73	73	-28	34	34	0	34	0	0	0	0	0	568	-3
C5	-2996	-2996	-322	623	438	-503	389	389	389	-381	623	-380	621	438	-500	387	387	-148	178	178	0	178	0	0	0	0	0	2983	-13
H5	-533	-533	-57	111	78	-90	69	69	69	-68	111	-68	110	78	-89	69	69	-26	32	32	0	32	0	0	0	0	0	530	-3
H6b	-1073	-1073	-116	224	159	-182	140	140	140	-138	225	-138	223	158	-180	139	139	-53	64	64	0	64	0	0	0	0	0	1073	0
C6	-2568	-2568	-280	539	383	-437	337	337	337	-332	540	-331	537	382	-434	334	334	-128	154	155	0	155	0	0	0	0	0	2580	12
O6	-12221	12221	1354	-2586	-1848	2103	-1616	-1616	-1616	1599	-2589	1594	-2571	-1841	2084	-1601	-1601	614	-740	-740	0	-740	0	0	0	0	0	-12358	-138
H6c	-7740	-7740	-837	1595	1144	-1298	997	997	997	-987	1595	-985	1583	1138	-1282	985	985	-377	455	455	0	455	0	0	0	0	0	7611	-129
H6a	-1072	-1072	-117	224	160	-183	140	140	140	-139	225	-138	224	159	-181	139	140	-54	65	65	0	65	0	0	0	0	0	1076	3
O5	7099	7099	759	-1467	-1032	1184	-915	-914	-914	897	-1468	896	-1464	-1032	1178	-911	-911	348	-420	-420	0	-420	0	0	0	0	0	-7027	73
C1	-5420	-5420	-575	1113	783	-902	696	696	695	-680	1114	-679	1112	781	-893	691	690	-263	318	318	0	318	0	0	0	0	0	5333	-86
H1	-1795	-1795	-191	369	261	-299	230	230	230	-226	369	-225	368	259	-296	228	228	-87	105	105	0	105	0	0	0	0	0	1765	-31
O1	7505	7505	793	-1545	-1081	1246	-962	-962	-962	941	-1546	941	-1546	-1079	1236	-957	-957	365	-441	-441	0	-441	0	0	0	0	0	-7398	107
H1t	-527	-527	-56	106	76	-86	66	66	66	-66	107	-67	109	77	-87	67	67	-26	31	31	0	31	0	0	0	0	0	512	-15
TOT	-660	-660	0	-10	3	4	-3	-2	-3	4	-18	4	-19	-3	12	-11	-10	4	-4	-4	0	-4	0	0	0	0	0	-60	-720

[PMIM]Cl	Cl	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-11184	11184	1215	-2337	-1668	1918	-1475	-1475	-1476	1435	-2334	1419	-2287	-1637	1846	-1421	-1424	-107	-648	-648	1923	-644	-643	0	-644	0	0	-11114	70
H2b	-7238	-7238	-764	1467	1048	-1202	924	924	924	-901	1463	-889	1429	1028	-1155	889	890	67	405	405	-1200	402	402	0	402	0	0	6957	-281
C2	-3214	-3214	-348	670	477	-549	423	423	423	-411	671	-408	660	470	-531	409	410	31	187	187	-558	187	187	0	187	0	0	3198	-17
H2a	-946	-946	-103	198	141	-162	125	125	125	-122	198	-121	196	139	-157	121	121	9	56	56	-166	56	56	0	56	0	0	945	-2
O3	-11137	11137	1207	-2330	-1654	1910	-1472	-1471	-1472	1426	-2334	1412	-2284	-1627	1840	-1418	-1421	-107	-648	-648	1927	-646	-645	0	-645	0	0	-11101	36
H3b	-7177	-7177	-761	1464	1041	-1198	922	922	923	-896	1461	-887	1430	1025	-1152	888	889	67	405	406	-1203	404	403	0	403	0	0	6957	-220
C3	-3211	-3211	-347	669	475	-549	423	423	423	-410	670	-406	659	468	-530	409	410	31	187	187	-556	186	186	0	186	0	0	3196	-15
H3a	-951	-951	-102	198	140	-162	125	125	125	-121	198	-120	194	138	-156	121	121	9	55	55	-164	55	55	0	55	0	0	943	-8
C4	-2680	-2680	-287	556	393	-454	351	351	351	-341	560	-338	552	388	-443	343	344	26	157	157	-467	157	156	0	157	0	0	2669	-11
O4t	742	742	78	-153	-105	121	-93	-93	-93	91	-148	92	-151	-107	125	-98	-98	-7	-45	-45	135	-45	-45	0	-45	0	0	-727	15
H4t	-480	-480	-50	96	67	-76	58	58	58	-58	93	-58	95	68	-79	61	61	5	28	28	-84	28	28	0	28	0	0	456	-24
H4	-501	-501	-54	104	74	-85	65	65	66	-64	105	-63	103	73	-83	64	64	5	30	30	-88	30	30	0	30	0	0	499	-2
C5	-2646	-2646	-285	549	389	-448	346	346	346	-337	553	-335	546	386	-438	339	339	26	155	155	-461	155	154	0	155	0	0	2635	-11
H5	-471	-471	-51	98	69	-80	62	62	62	-60	98	-60	97	69	-78	60	60	5	28	28	-82	27	27	0	27	0	0	468	-3
H6b	-944	-944	-103	198	141	-161	124	124	124	-122	198	-121	197	140	-158	122	122	9	56	56	-168	56	56	0	56	0	0	947	3
C6	-2270	-2270	-248	477	338	-388	299	299	299	-293	478	-292	472	337	-380	293	293	22	134	134	-401	134	134	0	134	0	0	2276	6
O6	-10863	10863	1196	-2288	-1634	1866	-1435	-1434	-1435	1412	-2293	1402	-2257	-1618	1821	-1402	-1403	-106	-642	-641	1909	-639	-639	0	-639	0	0	-10901	-37
H6c	-6898	-6898	-739	1413	1012	-1151	885	885	885	-873	1415	-864	1392	999	-1122	864	865	65	395	394	-1171	392	392	0	392	0	0	6724	-174
H6a	-947	-947	-103	198	141	-162	125	125	125	-122	199	-122	197	140	-158	122	122	9	56	56	-168	56	56	0	56	0	0	949	1
O5	6283	6283	669	-1296	-915	1059	-818	-818	-818	793	-1304	788	-1288	-905	1029	-796	-797	-60	-365	-365	1085	-364	-364	0	-364	0	0	-6212	71
C1	-4782	-4782	-509	986	698	-807	623	623	624	-604	994	-599	977	687	-779	603	604	46	276	276	-821	275	275	0	275	0	0	4722	-60
H1	-1588	-1588	-169	326	232	-268	206	206	206	-201	327	-199	323	224	-257	199	199	15	91	91	-271	91	91	0	91	0	0	1569	-27
O1	6592	6592	704	-1371	-965	1119	-865	-865	-865	839	-1384	832	-1359	-951	1081	-837	-838	-63	-383	-382	1137	-381	-381	0	-381	0	0	-6560	32
H1t	-484	-484	-52	99	73	-85	65	65	65	-63	104	-61	98	69	-76	58	59	4	26	26	-78	26	26	0	26	0	0	476	-8
TOT	-628	-628	-5	-7	8	6	-6	-5	-5	-2	-10	-0	-9	4	6	-4	-6	-0	-2	-2	10	-3	-2	0	-2	0	0	-37	-664

[BMIM]Cl	Cl	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-9896	9896	1074	-2071	-1467	1683	-1296	-1296	-1296	1264	-2053	1253	-2023	-1446	1638	-1261	-1266	-96	-582	-581	1145	-574	-575	1721	-577	-577	-577	-9837	59
H2b	-6465	-6465	-680	1307	931	-1066	820	820	820	-801	1296	-792	1275	915	-1028	789	791	60	362	362	-712	357	358	-1066	356	357	357	6189	-276
C2	-2830	-2830	-307	595	418	-478	369	369	369	-360	585	-359	580	416	-471	365	365	28	168	168	-331	166	167	-500	168	168	168	2823	-7
H2a	-841	-841	-91	177	124	-143	110	110	110	-107	174	-107	172	124	-140	108	108	8	50	50	-98	49	49	-147	49	49	49	837	-3
O3	9890	9890	1074	-2072	-1462	1668	-1281	-1281	-1281	1260	-2040	1255	-2025	-1454	1645	-1269	-1266	-96	-582	-580	1145	-574	-576	1726	-579	-579	-579	-9802	88
H3b	-6452	-6452	-679	1307	925	-1050	806	807	806	-795	1284	-791	1268	918	-1033	794	794	60	364	364	-719	360	361	-1081	362	362	363	6158	-294
C3	-2837	-2837	-307	594	416	-475	366	366	366	-358	583	-357	579	414	-472	365	365	28	168	168	-332	166	167	-501	168	168	168	2814	-22
H3a	-843	-843	-90	176	123	-141	108	108	108	-106	172	-105	171	122	-139	107	108	8	49	49	-98	49	49	-148	50	50	50	832	-11
C4	-2376	-2376	-252	492	340	-389	300	300	300	-294	482	-295	483	343	-395	306	306	23	142	141	-280	141	141	-424	143	142	143	2336	-41
O4t	677	677	70	-133	-97	107	-82	-82	-82	87	-142	88	-148	-99	113	-87	-88	-6	-38	-38	75	-38	-38	112	-38	-38	-38	-659	18
H4t	-438	-438	-44	83	60	-66	51	51	51	-54	88	-55	92	62	-71	55	55	4	24	24	-47	24	24	-70	24	24	24	410	-28
H4	-444	-444	-47	92	64	-73	56	56	56	-55	90	-56	91	65	-74	58	57	4	27	26	-53	26	26	-80	27	27	27	438	-6
C5	-2300	-2300	-249	483	335	-381	294	294	294	-290	470	-290	472	338	-390	301	301	23	141	140	-279	140	140	-423	142	142	142	2290	-10
H5	-408	-408	-44	86	60	-68	52	52	52	-52	83	-52	84	60	-69	54	53	4	25	25	-50	25	25	-76	25	25	25	406	-2
H6b	-816	-816	-89	173	120	-137	106	105	105	-104	167	-105	170	122	-141	109	108	8	50	51	-101	51	51	-154	52	52	52	825	6
C6	-1946	-1946	-215	416	290	-329	253	253	253	-250	402	-251	407	294	-338	261	260	20	122	122	-243	122	122	-369	124	124	124	1973	27
O6	9248	9248	1035	-1992	-1390	1569	-1202	-1202	-1202	1195	-1907	1207	-1948	-1411	1622	-1250	-1249	-97	-584	-582	1164	-583	-584	1767	-594	-593	-593	-9408	-160
H6c	-5920	-5920	-638	1230	856	-966	741	740	741	-734	1171	-742	1197	869	-997	768	767	59	358	356	-711	356	357	-1077	362	361	362	5786	-134
H6a	-814	-814	-90	173	121	-137	106	106	106	-104	168	-105	170	122	-141	109	108	8	51	51	-101	51	51	-154	52	52	52	823	9
O5	5471	5471	584	-1139	-790	902	-696	-696	-696	684	-1111	685	-1115	-795	916	-710	-707	-54	-329	-328	655	-328	-329	996	-334	-334	-334	5403	68
C1	-4212	-4212	-445	869	605	-694	535	535	535	-523	853	-523	854	604	-693	538	537	41	249	248	-492	247	247	-746	250	250	250	4134	-78
H1	-1393	-1393	-148	288	200	-229	176	176	176	-173	281	-173	283	200	-230	178	178	14	82	82	-163	82	82	-247	83	83	83	1365	-28
O1	5881	5881	617	-1204	-838	967	-748	-748	-747	725	-1190	724	-1183	-836	962	-744	-744	-57	-344	-343	679	-340	-341	1029	-345	-345	-345	-5741	140
H1t	-446	-446	-46	87	64	-75	59	59	59	-56	93	-54	88	61	-67	51	51	4	23	23	-45	22	22	-65	22	22	22	423	-23
TOT	-718	-718	-9	15	8	-1	3	2	3	-2	1	-1	-4	9	5	-8	-5	-0	-4	-3	10	-4	-4	22	-8	-8	-8	9	-709

Table S10: Pairwise dispersion energies for the chlorides.

[DMIM]Cl	Cl	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	39.4	39	-1.8	0.1	-3.6	-2.1	-0.3	-0.2	-0.2	-2.2	-0.2	-2.2	0.1	-3.7	-2.2	-0.2	-0.2	0	-0.2	0	0	0	0	0	0	0	0	-19	20
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-1.5	-1	-1.9	-0.6	-2.4	-2.0	-0.7	-0.7	-0.7	-2.0	-0.6	-2.0	-0.7	-2.4	-2.2	-0.7	-0.7	0	-0.7	0	0	0	0	0	0	0	0	-21	-23
H2a	-0.4	-0	-0.5	-0.1	-0.9	-0.6	-0.0	-0.0	-0.1	-0.5	-0.1	-0.4	-0.1	-0.8	-0.6	-0.0	-0.0	0	-0.1	0	0	0	0	0	0	0	0	-5	-5
O3	39.9	40	-2.1	0.1	-3.6	-2.3	-0.2	-0.2	-0.3	-2.2	0.3	-2.3	0.5	-3.8	-2.4	-0.3	-0.2	0	-0.3	0	0	0	0	0	0	0	0	-19	21
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-1.4	-1	-1.9	-0.6	-2.3	-2.0	-0.7	-0.7	-0.7	-2.0	-0.6	-2.0	-0.7	-2.4	-2.2	-0.8	-0.8	0	-0.7	0	0	0	0	0	0	0	0	-21	-22
H3a	0.6	1	-0.4	-0.0	-0.8	-0.6	-0.1	-0.1	-0.0	-0.5	-0.1	-0.5	-0.1	-0.8	-0.7	0	-0.0	0	-0.0	0	0	0	0	0	0	0	0	-5	-4
C4	-3.3	-3	-1.7	-0.5	-2.0	-1.8	-0.6	-0.6	-0.6	-1.8	-0.6	-1.8	-0.6	-2.1	-1.9	-0.7	-0.6	0	-0.7	0	0	0	0	0	0	0	0	-19	-22
O4t	2.9	3	-0.1	0	-0.2	-0.2	-0.0	-0.0	-0.0	-0.1	0	-0.2	0	-0.2	-0.1	-0.0	-0.0	0	-0.0	0	0	0	0	0	0	0	0	-1	2
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	0.1	0	-0.5	-0.1	-0.7	-0.5	-0.1	-0.1	-0.1	-0.5	-0.0	-0.5	-0.1	-0.7	-0.6	-0.1	-0.0	0	-0.1	0	0	0	0	0	0	0	0	-5	-5
C5	-3.7	-4	-1.8	-0.6	-2.2	-1.8	-0.6	-0.6	-0.6	-1.9	-0.6	-1.9	-0.6	-2.3	-2.0	-0.7	-0.7	0	-0.7	0	0	0	0	0	0	0	0	-20	-23
H5	-0.8	-1	-0.5	-0.0	-0.8	-0.5	-0.0	-0.0	-0.0	-0.4	-0.1	-0.4	-0.1	-0.8	-0.6	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-4	-5
H6b	-0.7	-1	-0.6	-0.1	-0.9	-0.7	-0.1	-0.1	-0.1	-0.6	-0.1	-0.6	-0.0	-0.9	-0.7	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-6	-7
C6	-1.2	-1	-2.1	-0.7	-2.9	-2.3	-0.7	-0.7	-0.7	-2.2	-0.7	-2.2	-0.7	-2.9	-2.3	-0.8	-0.8	0	-0.8	0	0	0	0	0	0	0	0	-24	-25
O6	35.0	35	-2.0	0.2	-4.3	-2.5	-0.3	-0.3	-0.2	-2.6	0.1	-2.7	0	-4.3	-2.5	-0.3	-0.3	0	-0.3	0	0	0	0	0	0	0	0	-22	13
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.6	-1	-0.6	-0.1	-0.9	-0.7	-0.1	-0.1	-0.1	-0.6	-0.1	-0.6	-0.2	-0.9	-0.7	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-6	-6
O5	-3.5	-4	-1.6	-0.1	-2.3	-1.7	-0.4	-0.4	-0.4	-1.8	-0.3	-1.8	-0.3	-2.5	-1.9	-0.3	-0.4	0	-0.4	0	0	0	0	0	0	0	0	-16	-20
C1	-2.8	-3	-1.7	-0.5	-2.1	-1.8	-0.6	-0.6	-0.6	-1.8	-0.6	-1.8	-0.6	-2.2	-2.0	-0.7	-0.7	0	-0.7	0	0	0	0	0	0	0	0	-19	-22
H1	1.8	2	-0.5	-0.1	-0.6	-0.5	-0.1	-0.1	-0.1	-0.5	-0.1	-0.5	-0.1	-0.7	-0.6	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-5	-3
O1	-0.4	-0	-1.7	-0.4	-2.3	-1.8	-0.4	-0.4	-0.4	-1.8	-0.5	-1.8	-0.4	-2.4	-1.9	-0.4	-0.4	0	-0.3	0	0	0	0	0	0	0	0	-17	-18
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	99	99	-24	-4	-36	-26	-6	-6	-6	-26	-5	-26	-5	-37	-28	-6	-6	0	-6	0	0	0	0	0	0	0	0	-254	-155

[EMIM]Cl	Cl	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	38.8	39	-1.5	0.5	-3.3	-1.9	-0.1	-0.1	-0.1	-1.9	0.2	-1.9	0.2	-3.1	-2.1	-0.1	-0.1	-2.1	-0.4	-0.4	0	-0.4	0	0	0	0	0	-19	20
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.8	-1	-1.7	-0.6	-2.1	-1.9	-0.7	-0.7	-0.7	-1.7	-0.6	-1.7	-0.5	-1.9	-1.6	-0.6	-0.6	-1.7	-0.5	-0.6	0	-0.6	0	0	0	0	0	-21	-22
H2a	-0.0	-0	-0.4	-0.1	-0.7	-0.5	-0.0	-0.0	-0.0	-0.4	-0.1	-0.4	-0.1	-0.7	-0.5	-0.0	-0.0	-0.5	-0.0	-0.0	0	-0.0	0	0	0	0	0	-5	-5
O3	38.3	38	-1.7	0.4	-3.3	-2.1	-0.1	-0.1	-0.2	-2.0	0.1	-1.9	0	-2.9	-2.0	-0.2	-0.2	-2.0	-0.4	-0.4	0	-0.4	0	0	0	0	0	-20	19
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-1.1	-1	-1.6	-0.6	-2.0	-1.9	-0.7	-0.7	-0.6	-1.7	-0.6	-1.6	-0.5	-1.8	-1.6	-0.6	-0.6	-1.6	-0.5	-0.5	0	-0.5	0	0	0	0	0	-20	-21
H3a	0.8	1	-0.5	-0.0	-0.7	-0.6	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.0	-0.1	-0.5	-0.1	-0.1	0	-0.0	0	0	0	0	0	-5	-4
C4	-2.9	-3	-1.5	-0.5	-1.8	-1.6	-0.6	-0.6	-0.6	-1.5	-0.5	-1.5	-0.4	-1.7	-1.4	-0.5	-0.5	-1.5	-0.5	-0.5	0	-0.5	0	0	0	0	0	-18	-21
O4t	2.7	3	-0.1	0	-0.2	-0.2	-0.0	-0.0	-0.0	-0.1	0	-0.1	0	-0.2	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	0	-0.0	0	0	0	0	0	-1	1
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	0.1	0	-0.4	-0.1	-0.7	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.0	-0.0	-0.5	-0.1	-0.1	0	-0.1	0	0	0	0	0	-5	-5
C5	-3.2	-3	-1.5	-0.5	-1.9	-1.6	-0.6	-0.6	-0.6	-1.5	-0.5	-1.5	-0.5	-1.8	-1.5	-0.5	-0.5	-1.6	-0.5	-0.5	0	-0.5	0	0	0	0	0	-19	-22
H5	-0.6	-1	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.5	-0.0	-0.1	0	-0.0	0	0	0	0	0	-5	-5
H6b	-0.8	-1	-0.5	-0.1	-0.8	-0.6	-0.1	-0.1	-0.1	-0.4	-0.1	-0.5	-0.1	-0.7	-0.6	-0.1	-0.1	-0.6	-0.1	-0.1	0	-0.1	0	0	0	0	0	-5	-6
C6	-1.4	-1	-1.8	-0.6	-2.4	-1.9	-0.6	-0.7	-0.6	-1.8	-0.6	-1.8	-0.6	-2.3	-1.9	-0.6	-0.6	-1.9	-0.6	-0.6	0	-0.6	0	0	0	0	0	-23	-24
O6	32.9	33	-1.8	0.2	-3.6	-2.1	-0.2	-0.2	-0.2	-2.2	0	-2.2	0.1	-3.5	-2.5	-0.2	-0.2	-2.5	-0.5	-0.5	0	-0.5	0	0	0	0	0	-22	11
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.8	-1	-0.5	-0.1	-0.8	-0.6	-0.1	-0.1	-0.1	-0.5	-0.1	-0.4	-0.1	-0.8	-0.6	-0.1	-0.0	-0.6	-0.0	-0.0	0	-0.0	0	0	0	0	0	-6	-6
O5	-3.2	-3	-1.3	-0.2	-2.0	-1.5	-0.3	-0.4	-0.3	-1.4	-0.3	-1.4	-0.3	-2.0	-1.5	-0.3	-0.3	-1.6	-0.4	-0.4	0	-0.4	0	0	0	0	0	-16	-20
C1	-2.1	-2	-1.5	-0.5	-1.9	-1.7	-0.6	-0.6	-0.6	-1.5	-0.5	-1.5	-0.5	-1.8	-1.5	-0.5	-0.5	-1.6	-0.5	-0.5	0	-0.5	0	0	0	0	0	-19	-21
H1	2.7	3	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.5	-0.1	-0.1	0	-0.1	0	0	0	0	0	-5	-3
O1	-0.1	-0	-1.5	-0.3	-2.0	-1.7	-0.4	-0.4	-0.4	-1.5	-0.3	-1.5	-0.3	-2.0	-1.6	-0.3	-0.3	-1.6	-0.4	-0.4	0	-0.4	0	0	0	0	0	-17	-18
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	99	99	-21	-3	-32	-24	-5	-5	-5	-22	-4	-21	-4	-30	-23	-5	-5	-23	-6	-6	0	-6	0	0	0	0	0	-250	-151

[PMIM]Cl	Cl	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	43.1	43	-1.6	0.3	-3.0	-1.8	-0.1	-0.1	-0.1	-1.8	0.1	-1.8	0.1	-2.7	-1.8	-0.1	-0.2	-1.8	-0.3	-0.3	-1.7	-0.4	-0.4	0	-0.5	0	0	-20	23
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	0	0	-1.5	-0.5	-1.9	-1.7	-0.6	-0.6	-0.6	-1.6	-0.5	-1.5	-0.5	-1.8	-1.4	-0.5	-0.5	-1.3	-0.5	-0.5	-1.4	-0.5	-0.5	0	-0.5	0	0	-21	-21
H2a	-0.3	-0	-0.3	-0.1	-0.7	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.0	-0.0	-0.5	-0.0	-0.0	-0.5	-0.0	-0.0	0	-0.0	0	0	-5	-5
O3	32.8	33	-1.8	0.2	-3.0	-1.8	-0.1	-0.1	-0.1	-1.7	0	-1.6	-0.0	-2.6	-1.7	-0.1	-0.1	-1.7	-0.3	-0.3	-1.7	-0.5	-0.5	0	-0.4	0	0	-20	13
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-1.0	-1	-1.5	-0.5	-1.9	-1.7	-0.6	-0.6	-0.6	-1.5	-0.5	-1.4	-0.4	-1.7	-1.3	-0.5	-0.5	-1.3	-0.4	-0.4	-1.3	-0.4	-0.4	0	-0.4	0	0	-20	-21
H3a	0.5	0	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.0	-0.4	-0.1	-0.4	-0.1	-0.5	-0.4	-0.1	-0.0	-0.4	-0.1	-0.1	-0.4	-0.1	-0.0	0	-0.0	0	0	-5	-4
C4	-2.7	-3	-1.3	-0.4	-1.6	-1.4	-0.5	-0.5	-0.5	-1.3	-0.4	-1.3	-0.4	-1.5	-1.2	-0.5	-0.5	-1.2	-0.4	-0.4	-1.4	-0.5	-0.5	0	-0.5	0	0	-18	-21
O4t	2.7	3	-0.1	0	-0.2	-0.1	-0.0	-0.0	-0.0	-0.1	-0.0	-0.1	-0.0	-0.2	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.2	-0.0	-0.0	0	-0.0	0	0	-1	1
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	-0.3	-0	-0.4	-0.1	-0.6	-0.4	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.5	-0.4	-0.1	-0.0	-0.4	-0.0	-0.1	-0.4	-0.0	-0.0	0	-0.0	0	0	-5	-5
C5	-2.8	-3	-1.4	-0.4	-1.7	-1.5	-0.5	-0.5	-0.5	-1.4	-0.5	-1.4	-0.4	-1.6	-1.3	-0.5	-0.5	-1.3	-0.4	-0.4	-1.4	-0.5	-0.5	0	-0.5	0	0	-19	-22
H5	-0.4	-0	-0.4	-0.1	-0.6	-0.4	-0.0	-0.0	-0.0	-0.4	-0.1	-0.3	-0.1	-0.6	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	0	-0.0	0	0	-4	-5
H6b	-0.7	-1	-0.5	-0.1	-0.7	-0.6	-0.1	-0.1	-0.1	-0.5	-0.1	-0.5	-0.1	-0.7	-0.5	-0.1	-0.1	-0.5	-0.1	-0.1	-0.5	-0.1	-0.1	0	-0.1	0	0	-6	-7
C6	-0.7	-1	-1.6	-0.5	-2.2	-1.8	-0.6	-0.6	-0.6	-1.6	-0.5	-1.6	-0.5	-2.0	-1.6	-0.5	-0.6	-1.6	-0.5	-0.5	-1.7	-0.5	-0.5	0	-0.5	0	0	-23	-24
O6	35.0	35	-1.6	0.2	-3.4	-2.0	-0.2	-0.2	-0.2	-2.0	0.1	-2.1	-0.0	-3.1	-2.1	-0.1	-0.1	-2.1	-0.4	-0.3	-2.1	-0.5	-0.5	0	-0.5	0	0	-23	12
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.7	-1	-0.5	-0.1	-0.7	-0.5	-0.0	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.7	-0.5	-0.1	-0.1	-0.6	-0.1	-0.1	-0.5	-0.1	-0.1	0	-0.1	0	0	-6	-7
O5	-2.8	-3	-1.2	-0.2	-1.8	-1.4	-0.3	-0.3	-0.3	-1.3	-0.2	-1.3	-0.3	-1.7	-1.3	-0.2	-0.2	-1.3	-0.3	-0.3	-1.4	-0.4	-0.4	0	-0.4	0	0	-17	-19
C1	-1.7	-2	-1.3	-0.4	-1.7	-1.5	-0.5	-0.5	-0.5	-1.4	-0.4	-1.3	-0.4	-1.5	-1.3	-0.4	-0.5	-1.2	-0.4	-0.4	-1.3	-0.4	-0.4	0	-0.4	0	0	-18	-20
H1	2.5	2	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.5	-0.4	-0.1	-0.1	-0.4	-0.1	-0.1	-0.4	-0.1	-0.1	0	-0.1	0	0	-5	-3
O1	-0.1	-0	-1.2	-0.1	-1.8	-1.5	-0.4	-0.4	-0.4	-1.3	-0.2	-1.3	-0.3	-1.7	-1.4	-0.3	-0.3	-1.4	-0.3	-0.3	-1.4	-0.4	-0.4	0	-0.4	0	0	-17	-17
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	102	102	-19	-3	-29	-22	-5	-5	-5	-20	-4	-19	-4	-26	-20	-4	-4	-20	-5	-5	-20	-5	-5	0	-5	0	0	-254	-151

[BMIM]	Cl	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	40.5	40	-1.5	0.2	-2.8	-1.7	-0.2	-0.2	-0.2	-1.5	0.1	-1.5	-0.1	-2.4	-1.6	-0.1	-0.1	-1.6	-0.3	-0.3	-1.5	-0.3	-0.3	-1.5	-0.4	-0.4	-0.4	-21	20
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.3	-0	-1.4	-0.5	-1.7	-1.6	-0.5	-0.5	-0.5	-1.4	-0.5	-1.3	-0.4	-1.5	-1.3	-0.5	-0.5	-1.2	-0.4	-0.4	-1.1	-0.4	-0.4	-1.2	-0.4	-0.4	-0.4	-20	-21
H2a	-0.2	-0	-0.4	-0.1	-0.6	-0.5	-0.0	-0.0	-0.0	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	0	0	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	-0.0	-5	-5
O3	40.5	40	-1.5	0.2	-2.8	-1.7	-0.1	-0.1	-0.2	-1.7	-0.0	-1.5	0.3	-2.4	-1.6	-0.0	-0.1	-1.5	-0.3	-0.3	-1.4	-0.4	-0.4	-1.4	-0.4	-0.4	-0.4	-20	20
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-0.4	-0	-1.4	-0.5	-1.7	-1.5	-0.5	-0.5	-0.5	-1.4	-0.5	-1.3	-0.4	-1.5	-1.2	-0.4	-0.4	-1.1	-0.4	-0.4	-1.0	-0.4	-0.4	-1.1	-0.4	-0.4	-0.4	-20	-20
H3a	0.1	0	-0.3	0	-0.6	-0.5	-0.0	-0.0	-0.0	-0.4	-0.1	-0.4	-0.1	-0.5	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	-0.3	-0.0	-0.0	-0.4	-0.0	-0.1	-0.0	-5	-5
C4	-2.3	-2	-1.1	-0.4	-1.3	-1.3	-0.4	-0.4	-0.4	-1.1	-0.4	-1.1	-0.3	-1.2	-1.1	-0.4	-0.4	-1.0	-0.4	-0.4	-1.1	-0.4	-0.4	-1.2	-0.4	-0.4	-0.4	-17	-20
O4t	2.7	3	-0.1	-0.0	-0.2	-0.1	-0.0	0	-0.0	-0.1	-0.0	-0.1	0	-0.2	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.0	-1	1
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	0	0	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.0	-0.4	-0.4	0	-0.0	-0.4	-0.0	-0.1	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	-0.1	-4	-4
C5	-2.3	-2	-1.1	-0.4	-1.4	-1.3	-0.4	-0.4	-0.4	-1.2	-0.4	-1.2	-0.4	-1.3	-1.1	-0.4	-0.4	-1.1	-0.4	-0.4	-1.1	-0.4	-0.4	-1.3	-0.4	-0.4	-0.4	-18	-20
H5	-0.1	-0	-0.4	-0.1	-0.5	-0.4	-0.0	-0.0	-0.1	-0.3	-0.1	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	-0.4	-0.1	-0.0	-0.1	-5	-5
H6b	-0.6	-1	-0.4	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.4	-0.1	-0.3	-0.1	-0.6	-0.5	-0.1	-0.1	-0.5	-0.1	-0.1	-0.5	-0.1	-0.1	-0.5	-0.1	-0.1	-0.1	-6	-6
C6	-0.7	-1	-1.4	-0.5	-1.8	-1.5	-0.5	-0.5	-0.5	-1.3	-0.4	-1.3	-0.4	-1.7	-1.4	-0.5	-0.5	-1.4	-0.5	-0.5	-1.5	-0.5	-0.5	-1.6	-0.5	-0.5	-0.5	-22	-23
O6	27.5	27	-1.3	0.3	-2.8	-1.5	-0.2	-0.1	-0.1	-1.7	0.1	-1.7	0.1	-2.7	-1.9	-0.1	-0.1	-1.9	-0.3	-0.3	-2.0	-0.4	-0.5	-2.0	-0.5	-0.6	-0.5	-23	5
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.7	-1	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.5	-0.5	-0.1	-0.1	-0.5	-0.1	-0.1	-0.5	-0.0	-0.0	-0.6	-0.0	-0.1	-0.1	-6	-6
O5	-2.6	-3	-1.1	-0.2	-1.5	-1.2	-0.2	-0.3	-0.2	-1.0	-0.2	-1.1	-0.2	-1.4	-1.1	-0.3	-0.3	-1.1	-0.3	-0.3	-1.1	-0.3	-0.3	-1.2	-0.3	-0.4	-0.4	-16	-19
C1	-2.1	-2	-1.2	-0.4	-1.5	-1.4	-0.5	-0.5	-0.5	-1.2	-0.4	-1.1	-0.3	-1.3	-1.1	-0.4	-0.4	-1.0	-0.4	-0.4	-1.0	-0.3	-0.4	-1.1	-0.4	-0.4	-0.4	-18	-20
H1	0.7	1	-0.4	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.5	-0.3	-0.1	-0.1	-0.3	-0.1	-0.1	-0.3	-0.1	-0.0	-0.4	-0.0	-0.1	-0.1	-5	-4
O1	0.9	1	-1.1	-0.2	-1.6	-1.4	-0.3	-0.3	-0.3	-1.2	-0.2	-1.1	-0.3	-1.4	-1.2	-0.2	-0.3	-1.1	-0.3	-0.3	-1.1	-0.3	-0.3	-1.2	-0.4	-0.3	-0.3	-17	-16
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	101	101	-17	-3	-25	-19	-4	-4	-4	-17	-3	-17	-3	-23	-18	-4	-4	-17	-4	-4	-17	-4	-4	-18	-5	-5	-5	-248	-148

Table S11: Pairwise electrostatic energies for the acetates.

[DMIM]Ac	H2	H3	H1	C2	C1	O2	O1	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-663	-664	-664	3097	-7932	9262	9282	11718	1261	-2436	-1714	1965	-1514	-1513	-1514	1487	-2425	1487	-2425	-1715	1963	-1512	-1512	0	-1513	0	0	0	0	0	0	0	0	-11630	88
H2b	418	418	418	-1954	5054	-5962	-5978	-7585	-790	1519	1075	-1229	946	945	946	-931	1513	-931	1514	1076	-1229	945	946	0	946	0	0	0	0	0	0	0	0	7261	-324
C2	193	193	192	-897	2291	-2674	-2681	-3384	-363	702	494	-567	437	436	437	-429	699	-428	699	494	-566	436	436	0	437	0	0	0	0	0	0	0	0	3355	-29
H2a	57	57	57	-267	682	-794	-795	-1003	-108	208	147	-168	130	130	130	-127	208	-127	207	147	-168	130	130	0	130	0	0	0	0	0	0	0	0	995	-7
O3	-663	-663	-663	3094	-7913	9252	9262	11706	1269	-2443	-1728	1977	-1520	-1520	-1521	1496	-2434	1495	-2429	-1726	1971	-1516	-1516	0	-1516	0	0	0	0	0	0	0	0	-11661	45
H3b	418	418	418	-1954	5036	-5951	-5962	-7577	-796	1528	1086	-1240	953	952	953	-938	1522	-937	1519	1085	-1237	950	949	0	950	0	0	0	0	0	0	0	0	7297	-280
C3	192	192	192	-895	2280	-2667	-2669	-3374	-364	701	494	-566	437	436	437	-428	698	-429	698	494	-565	436	435	0	436	0	0	0	0	0	0	0	0	3351	-23
H3a	57	57	57	-265	677	-790	-791	-998	-107	207	146	-167	129	129	129	-127	206	-127	206	146	-167	129	129	0	129	0	0	0	0	0	0	0	0	990	-9
C4	161	161	161	-753	1928	-2240	-2242	-2822	-302	583	411	-471	364	364	365	-356	582	-356	581	411	-470	363	363	0	363	0	0	0	0	0	0	0	0	2795	-27
O4t	-42	-42	-42	197	-498	579	581	733	79	-153	-107	123	-94	-94	-94	92	-151	92	-151	-107	124	-95	-95	0	-95	0	0	0	0	0	0	0	0	-728	4
H4t	27	27	27	-124	318	-373	-376	-476	-49	96	67	-77	59	59	59	-58	95	-58	95	67	-78	60	60	0	60	0	0	0	0	0	0	0	0	456	-20
H4	30	30	30	-142	362	-419	-420	-528	-57	109	77	-89	68	68	68	-67	109	-67	109	77	-88	68	68	0	68	0	0	0	0	0	0	0	0	523	-4
C5	160	160	160	-744	1902	-2211	-2214	-2789	-299	578	407	-466	360	360	360	-353	577	-353	577	407	-465	359	359	0	359	0	0	0	0	0	0	0	0	2765	-24
H5	28	28	28	-132	338	-393	-393	-495	-53	102	72	-83	64	64	64	-63	102	-63	102	72	-83	64	64	0	64	0	0	0	0	0	0	0	0	490	-4
H6b	58	58	58	-270	687	-796	-797	-1003	-109	210	148	-170	131	130	131	-129	210	-129	210	148	-169	130	130	0	130	0	0	0	0	0	0	0	0	1003	-0
C6	139	139	139	-646	1641	-1905	-1907	-2402	-261	503	356	-406	313	313	313	-309	503	-309	502	356	-405	312	312	0	312	0	0	0	0	0	0	0	0	2403	1
O6	-660	-660	-660	3072	-7788	9078	9082	11465	1260	-2420	-1716	1955	-1503	-1502	-1503	1488	-2416	1486	-2410	-1713	1948	-1497	-1497	0	-1497	0	0	0	0	0	0	0	0	-11537	-72
H6c	409	409	409	-1905	4865	-5727	-5735	-7274	-779	1489	1062	-1207	927	926	927	-919	1485	-918	1483	1060	-1203	923	923	0	923	0	0	0	0	0	0	0	0	7103	-171
H6a	58	58	58	-270	685	-794	-795	-1001	-109	210	149	-170	131	131	131	-129	210	-129	209	148	-169	130	130	0	130	0	0	0	0	0	0	0	0	1002	1
O5	-375	-376	-376	1757	-4508	5218	5230	6571	706	-1364	-961	1103	-851	-851	-852	834	-1366	833	-1364	-960	1100	-849	-849	0	-849	0	0	0	0	0	0	0	0	-6540	30
C1	285	285	285	-1337	3429	-3968	-3979	-5000	-532	1031	725	-836	645	644	645	-629	1032	-628	1030	724	-835	644	644	0	644	0	0	0	0	0	0	0	0	4948	-52
H1	94	94	94	-442	1132	-1312	-1315	-1654	-175	339	239	-276	212	212	212	-207	340	-207	339	239	-275	212	212	0	212	0	0	0	0	0	0	0	0	1630	-24
O1	-395	-395	-395	1854	-4770	5516	5521	6936	739	-1434	-1007	1160	-896	-895	-895	875	-1436	874	-1434	-1007	1159	-895	-894	0	-894	0	0	0	0	0	0	0	0	-6878	58
H1t	28	28	28	-129	334	-396	-394	-501	-53	101	72	-81	63	62	62	-62	101	-63	102	72	-83	63	63	0	63	0	0	0	0	0	0	0	0	483	-18
TOT	13	13	13	-55	231	-467	-484	-737	9	-34	-7	15	-11	-13	-12	12	-36	10	-32	-5	11	-10	-11	0	-10	0	0	0	0	0	0	0	0	-124	-861

[EMIM]Ac	H2	H3	H1	C2	C1	O2	O1	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-597	-598	-597	2793	-7210	8440	8451	10681	1139	-2202	-1552	1781	-1373	-1373	-1374	1344	-2193	1341	-2183	-1545	1760	-1361	-1361	517	-624	-623	0	-623	0	0	0	0	0	-10504	176
H2b	377	377	377	-1764	4599	-5441	-5471	-6947	-713	1373	974	-1117	859	860	860	-842	1370	-838	1360	967	-1101	850	849	-323	389	389	0	389	0	0	0	0	0	6556	-391
C2	173	173	173	-809	2080	-2438	-2438	-3085	-328	635	446	-512	395	395	395	-386	631	-386	629	444	-507	393	392	-149	180	180	0	180	0	0	0	0	0	3028	-57
H2a	51	51	51	-239	616	-720	-719	-909	-97	188	132	-152	117	117	117	-114	187	-114	186	132	-150	116	116	-44	53	53	0	53	0	0	0	0	0	895	-14
O3	-596	-596	-596	2785	-7167	8418	8390	10637	1145	-2211	-1561	1784	-1374	-1374	-1374	1349	-2191	1345	-2184	-1552	1764	-1363	-1363	517	-624	-624	0	-623	0	0	0	0	0	-10511	126
H3b	376	376	376	-1758	4562	-5442	-5395	-6905	-718	1381	980	-1119	860	860	860	-846	1371	-842	1363	973	-1105	851	852	-324	390	390	0	390	0	0	0	0	0	6567	-338
C3	173	173	173	-807	2074	-2433	-2429	-3076	-328	635	446	-512	394	395	395	-387	630	-386	628	444	-506	393	393	-149	180	180	0	180	0	0	0	0	0	3027	-50
H3a	51	51	51	-240	616	-720	-720	-910	-97	187	132	-151	117	117	117	-114	186	-114	186	132	-150	116	116	-44	53	53	0	53	0	0	0	0	0	895	-15
C4	145	145	145	-680	1754	-2044	-2040	-2574	-273	528	371	-427	330	330	330	-321	526	-320	524	370	-424	329	328	-125	151	151	0	151	0	0	0	0	0	2528	-47
O4t	-41	-41	-41	191	-485	562	560	705	75	-146	-102	117	-90	-90	-90	88	-144	88	-144	-102	117	-90	-90	35	-42	-42	0	-42	0	0	0	0	0	-692	13
H4t	26	26	26	-119	307	-361	-359	-456	-47	91	64	-73	56	56	56	-55	90	-55	90	64	-74	57	57	-22	26	26	0	26	0	0	0	0	0	433	-23
H4	27	27	27	-128	329	-382	-382	-482	-51	99	70	-80	62	62	62	-60	98	-60	98	69	-79	61	61	-23	28	28	0	28	0	0	0	0	0	473	-9
C5	144	144	144	-672	1726	-2008	-2008	-2531	-270	522	368	-423	327	327	327	-319	522	-318	519	367	-420	325	325	-124	150	149	0	149	0	0	0	0	0	2505	-26
H5	26	26	26	-120	308	-357	-357	-450	-48	93	66	-76	58	58	58	-57	93	-57	92	65	-75	58	58	-22	27	27	0	27	0	0	0	0	0	445	-4
H6b	52	52	52	-241	616	-718	-718	-906	-98	189	133	-153	118	118	118	-116	189	-115	188	133	-152	117	117	-45	54	54	0	54	0	0	0	0	0	903	-3
C6	124	124	124	-578	1477	-1720	-1720	-2169	-235	454	321	-368	283	283	283	-278	453	-278	452	320	-364	281	281	-107	130	130	0	130	0	0	0	0	0	2169	0
O6	-590	-591	-590	2745	-6978	8163	8172	10330	1136	-2183	-1549	1771	-1362	-1362	-1363	1343	-2181	1338	-2168	-1542	1749	-1348	-1348	515	-621	-620	0	-621	0	0	0	0	0	-10416	-85
H6c	367	367	367	-1708	4369	-5166	-5176	-6580	-700	1340	958	-1095	842	841	842	-828	1343	-823	1330	950	-1076	828	828	-316	381	381	0	381	0	0	0	0	0	6405	-175
H6a	52	52	52	-241	616	-717	-717	-904	-98	189	134	-153	118	118	118	-116	189	-116	188	133	-152	117	117	-45	54	54	0	54	0	0	0	0	0	904	0
O5	-338	-338	-337	1583	-4077	4729	4733	5955	637	-1235	-868	998	-771	-771	-771	753	-1235	752	-1231	-867	992	-768	-768	293	-353	-353	0	-353	0	0	0	0	0	-5916	39
C1	257	257	257	-1206	3115	-3615	-3619	-4555	-480	934	655	-756	584	584	584	-568	933	-567	929	653	-749	580	580	-221	267	267	0	267	0	0	0	0	0	4475	-80
H1	85	85	85	-400	1032	-1199	-1201	-1513	-159	308	217	-251	194	194	194	-188	308	-187	307	216	-247	191	191	-73	88	88	0	88	0	0	0	0	0	1478	-34
O1	-355	-355	-355	1670	-4325	5003	5004	6287	666	-1295	-907	1047	-808	-808	-809	788	-1294	786	-1289	-905	1040	-805	-805	307	-370	-370	0	-370	0	0	0	0	0	-6202	85
H1t	25	25	25	-118	303	-357	-360	-457	-48	92	65	-74	57	57	57	-56	92	-56	91	65	-74	56	56	-22	26	26	0	26	0	0	0	0	0	437	-20
TOT	13	13	13	-61	254	-525	-518	-812	11	-35	-6	8	-8	-7	-8	13	-26	17	-38	-15	16	-15	-16	5	-6	-6	0	-6	0	0	0	0	0	-120	-932

[PMIM]Ac	H2	H3	H1	C2	C1	O2	O1	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-538	-538	-538	2517	-6517	7658	7647	9691	1029	-1986	-1410	1628	-1257	-1257	-1258	1219	-2000	1207	-1961	-1387	1564	-1211	-1209	-90	-547	-547	1611	-539	-539	0	-539	0	0	-9479	212
H2b	340	340	340	-1595	4174	-4966	-4957	-6323	-643	1237	885	-1020	786	786	786	-764	1249	-756	1225	867	-976	753	753	56	340	340	-1004	335	335	0	335	0	0	5909	-414
C2	156	156	156	-729	1884	-2209	-2205	-2791	-296	572	405	-468	362	362	362	-351	577	-348	565	399	-450	348	348	26	158	158	-465	156	156	0	156	0	0	2731	-60
H2a	46	46	46	-215	554	-649	-647	-819	-88	169	120	-139	107	107	107	-104	171	-103	168	119	-134	103	103	8	47	47	-139	46	46	0	46	0	0	808	-11
O3	-539	-539	-539	2518	-6498	7632	7612	9648	1032	-1990	-1416	1631	-1259	-1259	-1259	1226	-2009	1215	-1972	-1391	1562	-1208	-1206	-90	-546	-546	1607	-538	-538	0	-538	0	0	-9492	156
H3b	339	340	340	-1590	4151	-4938	-4924	-6283	-645	1241	887	-1019	785	786	786	-766	1252	-759	1230	871	-976	753	752	56	341	340	-1004	336	336	0	336	0	0	5919	-364
C3	156	156	156	-730	1883	-2209	-2203	-2790	-296	571	405	-468	362	362	362	-351	577	-348	566	398	-448	347	347	26	157	157	-463	155	155	0	155	0	0	2729	-60
H3a	46	46	46	-216	559	-654	-652	-825	-87	169	120	-138	107	107	107	-104	170	-103	167	117	-132	102	102	8	46	46	-137	46	46	0	46	0	0	805	-20
C4	131	131	131	-615	1591	-1853	-1849	-2332	-245	475	337	-390	301	301	302	-291	481	-288	470	330	-374	290	290	22	132	132	-390	131	131	0	130	0	0	2276	-56
O4t	-36	-37	-37	171	-438	511	508	642	67	-130	-92	106	-82	-82	-82	79	-130	79	-129	-91	103	-79	-80	-6	-36	-36	108	-36	-36	0	-36	0	0	-621	21
H4t	23	23	23	-108	279	-330	-327	-417	-42	81	57	-66	51	51	51	-50	81	-50	80	57	-65	50	50	4	23	23	-68	23	23	0	23	0	0	387	-30
H4	25	25	25	-115	298	-346	-346	-435	-46	88	63	-73	56	56	56	-55	90	-54	88	62	-70	54	54	4	25	25	-73	24	24	0	24	0	0	425	-10
C5	130	130	129	-607	1561	-1816	-1814	-2287	-243	469	334	-385	298	298	298	-289	476	-285	465	328	-371	287	287	22	131	131	-387	130	130	0	129	0	0	2251	-36
H5	23	23	23	-108	278	-322	-323	-406	-43	83	59	-69	53	53	53	-52	85	-51	83	58	-66	51	51	4	23	23	-69	23	23	0	23	0	0	400	-6
H6b	47	47	47	-217	556	-647	-648	-817	-88	169	121	-139	107	107	107	-105	172	-104	168	119	-134	104	104	8	47	47	-141	47	47	0	47	0	0	812	-5
C6	111	111	111	-519	1330	-1549	-1551	-1954	-211	407	290	-334	258	258	258	-251	412	-249	404	286	-322	249	249	19	113	113	-337	113	113	0	113	0	0	1950	-5
O6	-529	-529	-529	2458	-6268	7333	7356	9293	1018	-1957	-1394	1603	-1236	-1236	-1236	1207	-1974	1196	-1933	-1374	1543	-1192	-1191	-90	-542	-542	1609	-539	-539	0	-539	0	0	-9334	-42
H6c	329	329	329	-1531	3940	-4656	-4676	-5937	-626	1202	860	-988	761	761	761	-742	1211	-735	1186	845	-949	732	732	55	333	332	-987	330	330	0	330	0	0	5733	-204
H6a	47	47	47	-217	557	-647	-647	-815	-88	170	121	-140	108	108	108	-105	172	-104	168	119	-135	104	104	8	47	47	-141	47	47	0	47	0	0	813	-2
O5	-304	-304	-304	1425	-3687	4289	4282	5398	571	-1106	-787	911	-704	-705	-705	683	-1125	675	-1100	-772	874	-677	-677	-51	-307	-307	911	-305	-305	0	-304	0	0	-5312	86
C1	231	231	231	-1088	2826	-3282	-3280	-4131	-432	839	595	-692	535	535	535	-516	852	-510	834	582	-661	513	512	38	232	232	-689	230	230	0	230	0	0	4027	-104
H1	77	77	77	-362	940	-1092	-1092	-1375	-143	277	197	-229	177	177	177	-170	281	-168	275	192	-218	169	169	13	77	77	-227	76	76	0	76	0	0	1329	-46
O1	-319	-319	-319	1501	-3901	4528	4528	5698	600	-1167	-825	960	-743	-743	-743	716	-1183	708	-1159	-808	918	-712	-711	-53	-323	-323	956	-320	-320	0	-320	0	0	-5595	103
H1t	23	23	23	-106	274	-322	-326	-412	-43	83	59	-69	53	53	53	-51	83	-50	81	57	-65	50	50	4	22	23	-67	22	22	0	22	0	0	394	-18
TOT	15	14	14	-79	328	-537	-534	-780	12	-35	-10	14	-14	-13	-14	15	-30	15	-30	-15	19	-18	-16	-1	-7	-7	17	-6	-6	0	-6	0	0	-134	-914

[BMIM]Ac	H2	H3	H1	C2	C1	O2	O1	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-488	-488	-487	2287	-5959	7026	6995	8887	950	-1828	-1320	1542	-1193	-1193	-1193	1139	-1877	1111	-1790	-1264	1396	-1081	-1082	-79	-477	-476	916	-462	-462	1340	-447	-447	-447	-8727	160
H2b	309	309	309	-1452	3828	-4583	-4541	-5823	-596	1145	828	-964	744	744	745	-713	1173	-694	1117	793	-875	675	677	49	298	298	-574	289	289	-840	280	280	280	5449	-373
C2	141	141	141	-661	1720	-2024	-2020	-2560	-272	525	379	-444	344	344	344	-328	542	-319	516	363	-401	311	311	23	137	137	-264	133	134	-387	129	129	129	2517	-43
H2a	42	42	42	-195	508	-596	-596	-754	-81	155	112	-132	102	102	102	-97	161	-95	153	108	-119	92	92	7	41	41	-79	40	40	-115	38	38	38	745	-9
O3	-489	-489	-489	2296	-5968	7013	7013	8885	950	-1827	-1325	1547	-1197	-1194	-1196	1144	-1888	1114	-1795	-1267	1402	-1085	-1084	-79	-478	-477	921	-464	-465	1348	-450	-450	-449	-8744	141
H3b	311	311	311	-1460	3842	-4559	-4586	-5831	-597	1148	832	-970	749	747	748	-717	1180	-698	1124	796	-879	679	680	50	299	299	-577	290	291	-845	282	282	282	5475	-357
C3	141	141	141	-662	1721	-2024	-2021	-2562	-273	525	380	-444	344	343	344	-328	542	-319	515	364	-402	311	311	23	138	137	-265	134	134	-387	129	129	129	2515	-47
H3a	42	42	42	-197	512	-602	-599	-760	-81	155	112	-131	102	101	101	-97	160	-95	153	108	-119	92	92	7	41	41	-78	39	40	-115	38	38	38	743	-16
C4	118	118	118	-554	1445	-1690	-1690	-2135	-226	435	315	-369	286	286	286	-272	452	-265	429	301	-334	259	259	19	115	115	-222	112	112	-326	109	108	109	2093	-42
O4t	-33	-33	-33	154	-398	460	465	583	60	-119	-82	95	-74	-73	-73	71	-117	71	-116	-82	94	-73	-72	-5	-33	-33	64	-32	-32	96	-32	-32	-32	-561	22
H4t	21	21	21	-97	255	-298	-302	-381	-38	75	52	-60	46	46	46	-45	73	-45	72	51	-58	45	45	3	20	20	-40	20	20	-60	20	20	20	351	-30
H4	22	22	22	-104	271	-316	-316	-398	-42	81	59	-69	54	53	53	-51	84	-50	80	56	-63	49	49	4	22	21	-42	21	21	-61	20	20	20	391	-7
C5	116	116	116	-545	1419	-1660	-1658	-2095	-223	430	312	-364	282	282	282	-270	447	-262	424	298	-331	257	256	19	114	114	-220	111	111	-323	108	108	108	2068	-27
H5	21	21	21	-97	253	-296	-295	-373	-40	76	55	-65	50	50	50	-48	79	-47	75	53	-59	46	46	3	20	20	-39	20	20	-57	19	19	19	367	-6
H6b	42	42	42	-195	503	-588	-587	-742	-81	155	112	-130	101	101	101	-97	160	-95	153	108	-120	93	93	7	41	41	-80	40	40	-118	39	39	39	743	0
C6	100	100	100	-468	1209	-1417	-1414	-1789	-194	373	270	-314	243	243	243	-233	385	-228	368	259	-288	223	222	16	99	99	-192	97	97	-282	94	94	94	1787	-2
O6	-477	-477	-477	2223	-5728	6743	6736	8543	933	-1788	-1294	1501	-1159	-1159	-1159	1120	-1843	1096	-1762	-1248	1380	-1066	-1065	-78	-474	-473	916	-462	-462	1346	-450	-450	-449	-8547	-5
H6c	298	297	298	-1391	3625	-4313	-4307	-5493	-575	1102	798	-923	711	711	711	-689	1129	-673	1084	769	-849	655	655	48	291	291	-564	283	284	-828	276	276	276	5252	-242
H6a	42	42	42	-196	506	-591	-590	-746	-81	155	112	-131	101	101	101	-97	160	-95	153	108	-120	93	93	7	41	41	-80	40	40	-118	39	39	39	744	-2
O5	-274	-273	-274	1287	-3357	3916	3905	4929	526	-1015	-735	861	-668	-667	-668	637	-1059	621	-1006	-703	780	-605	-605	-44	-268	-268	518	-260	-261	759	-253	-253	-253	-4889	41
C1	208	208	208	-982	2565	-2995	-2986	-3774	-399	770	557	-656	508	508	508	-482	802	-469	763	532	-590	458	458	33	202	202	-391	197	197	-573	191	191	191	3708	-65
H1	69	69	69	-326	852	-994	-991	-1252	-132	254	184	-217	168	168	168	-160	265	-155	252	176	-195	151	151	11	67	67	-129	65	65	-189	63	63	63	1224	-28
O1	-288	-288	-287	1355	-3548	4133	4127	5205	553	-1066	-774	911	-705	-705	-705	669	-1112	652	-1060	-739	821	-637	-637	-47	-281	-281	543	-273	-273	796	-265	-265	-265	-5144	61
H1t	20	20	20	-96	255	-304	-301	-385	-40	75	56	-64	50	50	50	-48	80	-47	76	53	-59	45	45	3	20	20	-39	20	20	-57	19	19	19	364	-21
TOT	15	15	16	-77	332	-560	-560	-821	3	-9	-4	11	-11	-10	-10	10	-22	12	-20	-6	12	-13	-8	-1	-5	-3	2	-2	-2	4	-2	-2	-2	-76	-897

Table S12: Pairwise dispersion energies for the acetates.

[DMIM]Ac	H2	H3	H1	C2	C1	O2	O1	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-0.5	-0.5	-0.5	-1.8	-1.8	19.0	20.0	34	-1.5	0.4	-3.2	-1.8	-0.1	-0.1	-0.1	-1.8	0.2	-1.8	0.2	-3.2	-1.7	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-15	19
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.4	-0.4	-0.4	-1.3	-1.8	-1.8	-1.7	-8	-1.7	-0.6	-2.1	-1.8	-0.6	-0.6	-0.6	-1.7	-0.6	-1.7	-0.6	-2.1	-1.8	-0.6	-0.6	0	-0.6	0	0	0	0	0	0	0	0	-18	-26
H2a	-0.1	-0.0	-0.0	-0.4	-0.6	-0.3	-0.3	-2	-0.4	-0.1	-0.7	-0.5	-0.0	-0.0	-0.0	-0.4	-0.1	-0.4	-0.0	-0.8	-0.6	-0.0	-0.0	0	-0.0	0	0	0	0	0	0	0	0	-4	-6
O3	-0.5	-0.5	-0.5	-1.8	-1.9	18.7	19.5	33	-1.5	0.5	-3.3	-1.8	-0.1	-0.1	-0.0	-1.9	0.2	-1.9	0.3	-3.3	-1.8	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-15	18
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-0.4	-0.4	-0.4	-1.3	-1.8	-1.8	-1.8	-8	-1.7	-0.6	-2.1	-1.8	-0.6	-0.6	-0.6	-1.7	-0.5	-1.7	-0.6	-2.1	-1.8	-0.6	-0.6	0	-0.6	0	0	0	0	0	0	0	0	-18	-26
H3a	-0.0	-0.1	-0.1	-0.4	-0.6	-0.1	-0.1	-1	-0.4	-0.0	-0.7	-0.5	-0.0	-0.0	-0.0	-0.4	-0.0	-0.4	-0.0	-0.7	-0.5	-0.0	-0.0	0	-0.0	0	0	0	0	0	0	0	0	-4	-5
C4	-0.3	-0.3	-0.3	-1.2	-1.5	-2.1	-2.2	-8	-1.5	-0.5	-1.8	-1.6	-0.5	-0.5	-0.5	-1.5	-0.5	-1.5	-0.5	-1.8	-1.6	-0.5	-0.5	0	-0.5	0	0	0	0	0	0	0	0	-16	-24
O4t	-0.0	-0.0	-0.0	-0.1	-0.1	1.1	1.3	2	-0.1	0	-0.2	-0.1	-0.0	-0.0	-0.0	-0.1	-0.0	-0.1	0	-0.2	-0.1	-0.0	-0.0	0	-0.0	0	0	0	0	0	0	0	0	-1	1
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	-0.0	-0.0	-0.0	-0.3	-0.2	0.1	0.1	-1	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.0	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-4	-4
C5	-0.4	-0.4	-0.4	-1.2	-1.5	-2.2	-2.2	-8	-1.5	-0.5	-1.9	-1.6	-0.6	-0.5	-0.6	-1.6	-0.5	-1.6	-0.5	-1.9	-1.6	-0.6	-0.6	0	-0.6	0	0	0	0	0	0	0	0	-16	-25
H5	-0.0	-0.0	-0.0	-0.4	-0.4	-0.5	-0.5	-2	-0.4	-0.1	-0.6	-0.5	-0.1	-0.0	-0.1	-0.3	-0.1	-0.4	-0.1	-0.6	-0.4	-0.0	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-4	-6
H6b	-0.1	-0.1	-0.1	-0.5	-0.6	-0.7	-0.7	-3	-0.5	-0.1	-0.8	-0.6	-0.1	-0.1	-0.1	-0.5	-0.1	-0.5	-0.1	-0.8	-0.6	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-5	-8
C6	-0.5	-0.5	-0.5	-1.5	-1.8	-1.8	-1.8	-8	-1.8	-0.6	-2.4	-2.0	-0.7	-0.7	-0.7	-1.8	-0.6	-1.8	-0.6	-2.4	-1.9	-0.7	-0.7	0	-0.6	0	0	0	0	0	0	0	0	-20	-28
O6	-0.6	-0.6	-0.6	-2.1	-1.9	15.3	15.6	25	-1.7	0.2	-3.7	-2.0	-0.1	-0.1	-0.1	-2.1	0.2	-2.1	0.2	-3.7	-1.9	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-17	8
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.0	-0.0	-0.0	-0.5	-0.6	-0.7	-0.7	-3	-0.5	-0.1	-0.8	-0.6	-0.1	-0.1	-0.1	-0.5	-0.1	-0.5	-0.1	-0.8	-0.6	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-5	-8
O5	-0.3	-0.3	-0.3	-1.1	-1.3	-1.9	-2.0	-7	-1.4	-0.1	-2.1	-1.5	-0.3	-0.3	-0.3	-1.4	-0.2	-1.5	-0.2	-2.1	-1.5	-0.3	-0.3	0	-0.3	0	0	0	0	0	0	0	0	-14	-21
C1	-0.3	-0.3	-0.3	-1.1	-1.5	-2.0	-2.0	-8	-1.5	-0.5	-1.8	-1.6	-0.5	-0.5	-0.5	-1.5	-0.5	-1.5	-0.5	-1.8	-1.6	-0.5	-0.5	0	-0.5	0	0	0	0	0	0	0	0	-16	-24
H1	-0.1	-0.1	-0.1	-0.4	-0.3	0.6	0.7	0	-0.4	-0.1	-0.5	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-4	-4
O1	-0.3	-0.3	-0.3	-1.1	-1.3	-0.6	-0.7	-5	-1.4	-0.2	-2.1	-1.6	-0.4	-0.4	-0.4	-1.5	-0.3	-1.5	-0.2	-2.1	-1.6	-0.4	-0.3	0	-0.4	0	0	0	0	0	0	0	0	-15	-19
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	-5	-5	-5	-19	-21	38	40	24	-20	-3	-31	-23	-5	-5	-5	-22	-4	-22	-3	-31	-23	-5	-5	0	-5	0	0	0	0	0	0	0	0	-211	-187

[EMIM]Ac	H2	H3	H1	C2	C1	O2	O1	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-0.4	-0.4	-0.4	-1.6	-1.7	18.6	21.6	36	-1.4	0.4	-3.0	-1.7	-0.0	-0.1	-0.1	-1.8	0.2	-1.7	0.2	-2.7	-1.8	-0.1	-0.1	-1.7	-0.3	-0.3	0	-0.3	0	0	0	0	0	-16	19
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.3	-0.3	-0.3	-1.1	-1.7	-1.7	-1.6	-7	-1.5	-0.5	-1.9	-1.7	-0.6	-0.6	-0.6	-1.6	-0.5	-1.5	-0.5	-1.8	-1.4	-0.5	-0.5	-1.4	-0.5	-0.5	0	-0.5	0	0	0	0	0	-18	-26
H2a	-0.1	-0.1	-0.1	-0.4	-0.5	-0.3	-0.4	-2	-0.4	-0.1	-0.7	-0.5	-0.0	-0.0	-0.0	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.0	-0.0	-0.4	-0.0	-0.0	0	-0.0	0	0	0	0	0	-4	-6
O3	-0.4	-0.4	-0.4	-1.6	-1.6	21.0	17.1	34	-1.4	0.6	-3.0	-1.7	-0.0	-0.0	-0.0	-1.7	0.2	-1.7	0.2	-2.7	-1.8	-0.1	-0.1	-1.7	-0.3	-0.4	0	-0.4	0	0	0	0	0	-16	18
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-0.3	-0.3	-0.3	-1.1	-1.7	-1.7	-1.8	-7	-1.5	-0.5	-2.0	-1.7	-0.6	-0.6	-0.6	-1.6	-0.5	-1.5	-0.5	-1.8	-1.4	-0.5	-0.5	-1.4	-0.5	-0.5	0	-0.5	0	0	0	0	0	-18	-26
H3a	-0.1	-0.1	-0.0	-0.4	-0.5	-0.0	0.1	-1	-0.4	-0.0	-0.7	-0.5	0	0	0	-0.4	-0.0	-0.4	-0.0	-0.6	-0.5	-0.0	-0.0	-0.4	-0.0	-0.0	0	-0.0	0	0	0	0	0	-4	-5
C4	-0.3	-0.3	-0.3	-1.0	-1.4	-2.0	-2.1	-7	-1.4	-0.4	-1.7	-1.5	-0.5	-0.5	-0.5	-1.4	-0.5	-1.4	-0.4	-1.6	-1.3	-0.5	-0.5	-1.3	-0.4	-0.4	0	-0.4	0	0	0	0	0	-17	-24
O4t	-0.0	-0.0	-0.0	-0.1	-0.1	1.1	1.2	2	-0.1	0	-0.2	-0.1	-0.0	-0.0	-0.0	-0.1	0	-0.1	0	-0.2	-0.1	-0.0	0	-0.1	-0.0	-0.0	0	-0.0	0	0	0	0	0	-1	1
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	-0.0	-0.0	-0.0	-0.3	-0.3	0.1	-0.0	-1	-0.4	-0.1	-0.6	-0.4	-0.0	-0.1	-0.0	-0.4	-0.1	-0.4	-0.1	-0.5	-0.4	-0.0	-0.1	-0.4	-0.1	-0.0	0	-0.1	0	0	0	0	0	-4	-5
C5	-0.3	-0.3	-0.3	-1.1	-1.4	-2.1	-2.1	-7	-1.5	-0.5	-1.8	-1.6	-0.6	-0.6	-0.6	-1.5	-0.5	-1.5	-0.5	-1.7	-1.4	-0.5	-0.5	-1.4	-0.5	-0.5	0	-0.5	0	0	0	0	0	-18	-25
H5	-0.0	-0.0	-0.0	-0.3	-0.4	-0.5	-0.5	-2	-0.4	-0.1	-0.6	-0.5	-0.0	-0.0	-0.0	-0.3	-0.1	-0.3	-0.1	-0.5	-0.4	-0.0	-0.1	-0.4	-0.0	-0.0	0	-0.1	0	0	0	0	0	-4	-6
H6b	-0.1	-0.1	-0.1	-0.4	-0.5	-0.6	-0.7	-2	-0.5	-0.1	-0.7	-0.6	-0.1	-0.1	-0.1	-0.5	-0.1	-0.5	-0.1	-0.7	-0.6	-0.1	-0.1	-0.5	-0.1	-0.1	0	-0.1	0	0	0	0	0	-5	-8
C6	-0.4	-0.4	-0.4	-1.3	-1.6	-1.7	-1.7	-7	-1.7	-0.6	-2.3	-1.9	-0.6	-0.6	-0.6	-1.7	-0.6	-1.7	-0.6	-2.2	-1.7	-0.6	-0.6	-1.7	-0.6	-0.6	0	-0.6	0	0	0	0	0	-21	-29
O6	-0.5	-0.5	-0.5	-1.9	-1.8	15.0	15.6	25	-1.5	0.3	-3.4	-1.8	-0.1	-0.1	-0.1	-1.9	0.2	-1.9	0.2	-3.3	-2.2	-0.1	-0.1	-2.1	-0.4	-0.4	0	-0.4	0	0	0	0	0	-19	6
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.1	-0.1	-0.1	-0.4	-0.5	-0.7	-0.7	-2	-0.4	-0.1	-0.8	-0.6	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.7	-0.6	-0.0	-0.0	-0.5	-0.0	-0.0	0	-0.0	0	0	0	0	0	-5	-8
O5	-0.3	-0.3	-0.3	-1.0	-1.2	-1.9	-1.8	-7	-1.3	-0.0	-2.1	-1.5	-0.3	-0.3	-0.3	-1.4	-0.1	-1.3	-0.1	-1.9	-1.4	-0.2	-0.2	-1.4	-0.3	-0.3	0	-0.3	0	0	0	0	0	-15	-21
C1	-0.3	-0.3	-0.3	-1.0	-1.4	-2.0	-1.9	-7	-1.4	-0.5	-1.8	-1.6	-0.5	-0.5	-0.5	-1.4	-0.5	-1.4	-0.4	-1.6	-1.3	-0.5	-0.5	-1.3	-0.4	-0.4	0	-0.4	0	0	0	0	0	-17	-24
H1	-0.1	-0.1	-0.1	-0.4	-0.2	0.7	0.8	1	-0.4	-0.1	-0.5	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.5	-0.4	-0.1	-0.1	-0.4	-0.1	-0.1	0	-0.1	0	0	0	0	0	-5	-4
O1	-0.3	-0.3	-0.3	-1.0	-1.3	-0.7	-0.5	-4	-1.3	-0.2	-1.9	-1.5	-0.4	-0.3	-0.3	-1.4	-0.3	-1.3	-0.2	-1.8	-1.4	-0.3	-0.3	-1.4	-0.3	-0.3	0	-0.3	0	0	0	0	0	-15	-20
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	-4	-4	-4	-16	-20	41	41	33	-19	-2	-30	-22	-5	-5	-5	-20	-3	-20	-3	-27	-21	-4	-4	-20	-5	-5	0	-5	0	0	0	0	0	-224	-191

[PMIM]Ac	H2	H3	H1	C2	C1	O2	O1	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-0.4	-0.4	-0.4	-1.6	-1.6	19.7	19.3	35	-1.4	0.6	-2.8	-1.6	-0.0	-0.1	-0.0	-1.6	0.3	-1.6	0.2	-2.5	-1.6	-0.0	-0.0	-1.5	-0.3	-0.3	-1.4	-0.3	-0.3	0	-0.4	0	0	-17	18
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.3	-0.3	-0.3	-1.1	-1.7	-1.7	-1.7	-7	-1.4	-0.5	-1.8	-1.6	-0.6	-0.6	-0.6	-1.5	-0.5	-1.4	-0.5	-1.6	-1.3	-0.5	-0.5	-1.1	-0.4	-0.4	-1.0	-0.3	-0.3	0	-0.3	0	0	-19	-26
H2a	-0.1	-0.1	-0.0	-0.3	-0.5	-0.3	-0.4	-2	-0.3	-0.1	-0.6	-0.5	-0.0	-0.0	-0.0	-0.3	-0.1	-0.3	-0.0	-0.6	-0.4	-0.0	0	-0.4	0	-0.0	-0.3	-0.0	-0.0	0	-0.0	0	0	-4	-6
O3	-0.4	-0.4	-0.4	-1.5	-1.5	17.5	16.7	30	-1.3	0.7	-3.0	-1.5	0	0.1	0.1	-1.6	0.4	-1.5	0.4	-2.6	-1.6	0	-0.0	-1.5	-0.3	-0.3	-1.3	-0.3	-0.3	0	-0.3	0	0	-16	14
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-0.3	-0.3	-0.3	-1.1	-1.7	-1.8	-1.8	-7	-1.4	-0.5	-1.9	-1.7	-0.6	-0.6	-0.6	-1.5	-0.5	-1.4	-0.5	-1.6	-1.2	-0.4	-0.4	-1.1	-0.4	-0.4	-1.0	-0.3	-0.3	0	-0.3	0	0	-18	-26
H3a	-0.0	-0.0	-0.0	-0.4	-0.5	0.1	0.1	-1	-0.4	0	-0.6	-0.5	-0.0	0	0	-0.3	-0.0	-0.3	-0.0	-0.5	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	-0.3	-0.1	-0.0	0	-0.0	0	0	-4	-5
C4	-0.3	-0.3	-0.3	-1.0	-1.4	-2.0	-2.0	-7	-1.2	-0.4	-1.6	-1.4	-0.5	-0.5	-0.5	-1.4	-0.5	-1.3	-0.4	-1.4	-1.1	-0.4	-0.4	-1.0	-0.3	-0.3	-1.0	-0.3	-0.3	0	-0.3	0	0	-16	-24
O4t	-0.0	-0.0	-0.0	-0.1	-0.1	1.3	1.1	2	-0.1	0	-0.2	-0.1	-0.0	-0.0	-0.0	-0.1	0	-0.1	0	-0.2	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	0	-0.0	0	0	-1	1
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	-0.0	-0.0	-0.0	-0.3	-0.3	-0.0	-0.0	-1	-0.4	-0.1	-0.5	-0.4	-0.0	-0.1	-0.0	-0.3	-0.1	-0.3	-0.1	-0.5	-0.4	-0.0	-0.0	-0.3	-0.0	-0.0	-0.3	-0.1	-0.0	0	-0.0	0	0	-4	-5
C5	-0.3	-0.3	-0.3	-1.0	-1.3	-2.0	-2.0	-7	-1.3	-0.4	-1.7	-1.5	-0.5	-0.5	-0.5	-1.4	-0.5	-1.3	-0.4	-1.5	-1.1	-0.4	-0.4	-1.0	-0.4	-0.4	-1.1	-0.3	-0.3	0	-0.3	0	0	-17	-25
H5	-0.0	-0.0	-0.0	-0.3	-0.4	-0.5	-0.5	-2	-0.3	-0.1	-0.5	-0.4	-0.0	-0.0	-0.0	-0.2	-0.1	-0.2	-0.1	-0.5	-0.4	-0.1	-0.0	-0.4	-0.0	-0.1	-0.3	-0.0	-0.0	0	-0.0	0	0	-4	-6
H6b	-0.0	-0.0	-0.0	-0.4	-0.5	-0.6	-0.6	-2	-0.4	-0.1	-0.7	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.5	-0.1	-0.1	-0.4	-0.0	-0.1	0	-0.1	0	0	-5	-8
C6	-0.4	-0.4	-0.4	-1.2	-1.5	-1.6	-1.7	-7	-1.5	-0.5	-2.1	-1.7	-0.6	-0.6	-0.6	-1.6	-0.5	-1.5	-0.5	-1.9	-1.4	-0.5	-0.5	-1.3	-0.4	-0.4	-1.3	-0.4	-0.4	0	-0.4	0	0	-21	-28
O6	-0.5	-0.5	-0.5	-1.7	-1.6	12.4	13.7	21	-1.3	0.4	-3.2	-1.7	-0.0	-0.1	-0.1	-1.7	0.3	-1.8	0.2	-2.9	-1.8	0	0	-1.8	-0.3	-0.3	-1.8	-0.4	-0.4	0	-0.5	0	0	-19	2
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.0	-0.1	-0.0	-0.4	-0.5	-0.6	-0.5	-2	-0.4	-0.1	-0.7	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.0	-0.1	-0.5	-0.0	-0.0	-0.4	-0.0	-0.0	0	-0.0	0	0	-5	-7
O5	-0.3	-0.3	-0.3	-0.9	-1.2	-1.9	-1.9	-7	-1.2	-0.0	-1.8	-1.4	-0.3	-0.3	-0.3	-1.3	-0.2	-1.3	-0.1	-1.6	-1.1	-0.2	-0.2	-1.1	-0.3	-0.3	-1.0	-0.3	-0.3	0	-0.3	0	0	-15	-21
C1	-0.3	-0.3	-0.3	-1.0	-1.4	-1.9	-1.8	-7	-1.3	-0.4	-1.6	-1.5	-0.5	-0.5	-0.5	-1.4	-0.5	-1.3	-0.4	-1.4	-1.1	-0.4	-0.4	-1.0	-0.3	-0.3	-1.0	-0.3	-0.3	0	-0.3	0	0	-17	-24
H1	-0.0	-0.0	-0.1	-0.4	-0.0	1.1	1.0	1	-0.4	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.4	-0.3	-0.1	-0.1	-0.3	-0.1	-0.1	-0.3	-0.1	-0.1	0	-0.1	0	0	-5	-3
O1	-0.3	-0.3	-0.3	-1.0	-1.3	-0.8	-0.4	-4	-1.2	-0.1	-1.9	-1.4	-0.3	-0.3	-0.3	-1.3	-0.2	-1.3	-0.2	-1.7	-1.2	-0.2	-0.2	-1.1	-0.2	-0.2	-1.0	-0.3	-0.3	0	-0.3	0	0	-15	-20
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	-4	-4	-4	-16	-19	36	37	27	-17	-2	-28	-20	-4	-4	-4	-19	-3	-18	-3	-25	-17	-3	-3	-16	-4	-4	-15	-4	-4	0	-4	0	0	-222	-196

[BMIM]Ac	H2	H3	H1	C2	C1	O2	O1	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-0.3	-0.3	-0.3	-1.4	-1.4	20.2	16.9	33	-1.2	0.4	-2.9	-1.6	0.1	0	-0.0	-1.6	0.2	-1.4	0.2	-2.4	-1.4	0.1	-0.0	-1.2	-0.2	-0.2	-1.1	-0.3	-0.3	-0.9	-0.2	-0.2	-0.2	-16	17
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.3	-0.3	-0.3	-1.0	-1.5	-1.4	-1.5	-6	-1.4	-0.5	-1.9	-1.7	-0.6	-0.6	-0.6	-1.5	-0.5	-1.4	-0.4	-1.6	-1.1	-0.4	-0.4	-0.9	-0.3	-0.3	-0.7	-0.2	-0.3	-0.7	-0.2	-0.2	-0.2	-19	-25
H2a	-0.0	-0.0	-0.0	-0.3	-0.5	-0.4	-0.4	-2	-0.4	-0.0	-0.7	-0.5	0	0	0	-0.4	-0.0	-0.3	-0.0	-0.6	-0.4	-0.0	0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.2	-0.0	-0.0	-0.0	-4	-6
O3	-0.3	-0.4	-0.3	-1.4	-1.5	17.5	20.9	34	-1.3	0.5	-3.0	-1.6	0	0	0	-1.6	0.4	-1.6	0.1	-2.4	-1.5	-0.0	-0.1	-1.3	-0.2	-0.2	-1.1	-0.3	-0.3	-1.0	-0.3	-0.2	-0.2	-17	17
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-0.3	-0.3	-0.3	-1.0	-1.5	-1.5	-1.4	-6	-1.4	-0.5	-1.9	-1.7	-0.6	-0.6	-0.6	-1.5	-0.5	-1.4	-0.4	-1.6	-1.1	-0.4	-0.4	-0.9	-0.3	-0.3	-0.7	-0.2	-0.3	-0.7	-0.2	-0.2	-0.2	-19	-25
H3a	-0.0	-0.0	-0.0	-0.3	-0.5	-0.2	-0.2	-1	-0.3	-0.0	-0.6	-0.5	0	0	-0.0	-0.4	-0.0	-0.3	-0.0	-0.5	-0.4	-0.0	0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.2	-0.0	-0.0	-0.0	-4	-5
C4	-0.2	-0.2	-0.2	-0.8	-1.2	-1.8	-1.7	-6	-1.2	-0.4	-1.5	-1.5	-0.5	-0.5	-0.5	-1.3	-0.4	-1.2	-0.4	-1.3	-1.0	-0.4	-0.4	-0.8	-0.3	-0.3	-0.7	-0.2	-0.2	-0.7	-0.2	-0.2	-0.2	-16	-23
O4t	-0.0	-0.0	-0.0	-0.1	-0.1	1.0	1.3	2	-0.1	0.1	-0.2	-0.1	-0.0	0	0	-0.1	0	-0.1	0	-0.2	-0.1	0	-0.0	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.0	-1	1
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	-0.0	-0.0	-0.0	-0.2	-0.3	-0.3	-0.2	-1	-0.3	-0.1	-0.5	-0.4	-0.0	-0.0	-0.1	-0.3	-0.1	-0.3	-0.1	-0.5	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.2	-0.0	-0.0	-0.0	-4	-5
C5	-0.3	-0.3	-0.3	-0.9	-1.2	-1.7	-1.7	-6	-1.2	-0.4	-1.6	-1.5	-0.5	-0.5	-0.5	-1.3	-0.4	-1.2	-0.4	-1.3	-1.0	-0.4	-0.4	-0.9	-0.3	-0.3	-0.8	-0.3	-0.3	-0.8	-0.3	-0.3	-0.3	-17	-23
H5	-0.0	-0.0	-0.0	-0.3	-0.4	-0.5	-0.4	-2	-0.3	-0.1	-0.5	-0.4	-0.0	-0.1	-0.0	-0.3	-0.1	-0.3	-0.0	-0.4	-0.3	-0.0	-0.1	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.0	-4	-6
H6b	-0.0	-0.0	-0.1	-0.3	-0.4	-0.5	-0.5	-2	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.4	-0.0	-0.1	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	-0.3	-0.0	-0.0	-0.1	-5	-7
C6	-0.3	-0.3	-0.3	-1.1	-1.4	-1.4	-1.4	-6	-1.4	-0.5	-2.0	-1.6	-0.6	-0.6	-0.6	-1.5	-0.5	-1.4	-0.5	-1.7	-1.3	-0.4	-0.5	-1.1	-0.4	-0.4	-1.1	-0.3	-0.3	-1.0	-0.3	-0.3	-0.3	-21	-27
O6	-0.4	-0.4	-0.4	-1.6	-1.5	14.7	14.3	25	-1.2	0.4	-3.0	-1.5	-0.0	-0.0	0	-1.7	0.2	-1.6	0.3	-2.7	-1.6	0	0.1	-1.5	-0.2	-0.2	-1.4	-0.3	-0.3	-1.3	-0.3	-0.3	-0.4	-19	6
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.0	-0.0	-0.0	-0.4	-0.5	-0.5	-0.5	-2	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.4	-0.0	-0.0	-0.4	-0.1	-0.0	-0.4	-0.0	-0.0	-0.4	-0.0	-0.1	-0.0	-5	-7
O5	-0.2	-0.2	-0.2	-0.8	-1.1	-1.6	-1.6	-6	-1.1	-0.1	-1.8	-1.3	-0.3	-0.3	-0.2	-1.2	-0.1	-1.1	-0.2	-1.5	-1.0	-0.2	-0.2	-0.9	-0.2	-0.2	-0.8	-0.2	-0.2	-0.8	-0.2	-0.2	-0.2	-15	-20
C1	-0.2	-0.2	-0.2	-0.8	-1.2	-1.6	-1.7	-6	-1.2	-0.4	-1.6	-1.5	-0.5	-0.5	-0.5	-1.3	-0.5	-1.2	-0.4	-1.4	-1.0	-0.4	-0.4	-0.8	-0.3	-0.3	-0.7	-0.2	-0.2	-0.7	-0.2	-0.2	-0.2	-17	-23
H1	-0.0	-0.0	-0.1	-0.3	-0.2	0.4	0.2	-0	-0.4	-0.1	-0.5	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.3	-0.1	-0.4	-0.3	-0.1	-0.1	-0.3	-0.1	-0.0	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.0	-4	-5
O1	-0.2	-0.2	-0.2	-0.8	-1.1	-0.1	-0.4	-3	-1.2	-0.2	-1.8	-1.5	-0.4	-0.4	-0.3	-1.3	-0.2	-1.2	-0.2	-1.5	-1.1	-0.2	-0.2	-0.9	-0.2	-0.2	-0.8	-0.2	-0.2	-0.7	-0.2	-0.2	-0.2	-16	-19
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	-3	-3	-3	-14	-17	40	40	39	-16	-2	-27	-20	-4	-4	-4	-18	-3	-17	-3	-23	-16	-3	-3	-13	-3	-3	-12	-3	-3	-11	-3	-3	-3	-223	-184

Table S13: Pairwise electrostatic energies for the dimethylphosphates.

[DMIM]DMP	H1	H2	H3	C1	O1	P1	O3	O4	O2	C2	H4	H5	H6	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-531	-531	-531	-176	3775	-7014	6146	6110	3765	-175	-529	-529	-529	9251	998	-1926	-1356	1550	-1195	-1195	-1195	1177	-1920	1177	-1916	-1355	1551	-1194	-1194	0	-1194	0	0	0	0	0	0	0	0	-9189	63
H2b	333	334	333	111	-2372	4431	-3959	-3899	-2369	110	332	332	332	-5953	-622	1200	847	-968	746	746	746	-734	1196	-733	1195	847	-969	746	746	0	746	0	0	0	0	0	0	0	0	5735	-218
C2	154	154	154	51	-1096	2029	-1774	-1769	-1088	51	153	153	153	-2674	-287	556	390	-446	344	344	344	-339	553	-339	553	390	-447	344	344	0	344	0	0	0	0	0	0	0	0	2648	-26
H2a	46	46	46	15	-325	602	-525	-524	-323	15	45	45	45	-792	-85	164	116	-132	102	102	102	-100	164	-100	163	116	-132	102	102	0	102	0	0	0	0	0	0	0	0	784	-8
O3	-534	-534	-534	-177	3795	-7011	6120	6147	3772	-175	-529	-529	-529	9281	999	-1928	-1356	1552	-1195	-1196	-1197	1175	-1915	1175	-1917	-1358	1554	-1196	-1197	0	-1196	0	0	0	0	0	0	0	0	-9196	85
H3b	337	336	336	112	-2395	4452	-3943	-3973	-2380	111	334	333	333	-6007	-623	1202	847	-971	748	748	749	-733	1194	-733	1195	848	-972	748	748	0	748	0	0	0	0	0	0	0	0	5745	-262
C3	154	154	154	51	-1096	2027	-1767	-1770	-1089	51	153	153	153	-2673	-287	555	390	-446	344	343	344	-338	552	-339	552	390	-447	344	344	0	344	0	0	0	0	0	0	0	0	2647	-26
H3a	46	46	46	15	-325	601	-525	-523	-323	15	45	45	45	-792	-85	164	115	-132	102	102	102	-100	163	-100	163	115	-132	102	102	0	102	0	0	0	0	0	0	0	0	782	-10
C4	129	129	129	43	-916	1690	-1470	-1475	-911	42	128	128	128	-2225	-239	461	326	-373	288	288	288	-283	461	-282	460	326	-372	287	288	0	288	0	0	0	0	0	0	0	0	2209	-15
O4t	-36	-36	-36	-12	259	-476	415	408	257	-12	-36	-36	-36	622	66	-127	-89	102	-79	-79	-79	77	-127	77	-127	-89	103	-79	-79	0	-80	0	0	0	0	0	0	0	0	-607	15
H4t	23	23	23	8	-162	300	-265	-260	-161	8	23	23	23	-397	-41	80	56	-64	49	49	49	-48	79	-48	79	56	-65	50	50	0	50	0	0	0	0	0	0	0	0	381	-16
H4	24	24	24	8	-172	317	-276	-277	-171	8	24	24	24	-417	-45	86	61	-70	54	54	54	-53	86	-53	86	61	-70	54	54	0	54	0	0	0	0	0	0	0	0	413	-4
C5	128	128	128	42	-906	1670	-1449	-1449	-903	42	127	127	127	-2187	-238	456	324	-370	285	285	285	-281	457	-281	457	324	-369	284	284	0	284	0	0	0	0	0	0	0	0	2189	2
H5	23	23	23	8	-162	298	-258	-258	-161	8	23	23	23	-390	-42	81	58	-66	51	51	51	-50	81	-50	81	57	-66	51	51	0	51	0	0	0	0	0	0	0	0	389	-1
H6b	46	46	46	15	-327	601	-521	-522	-325	15	46	46	46	-786	-86	165	117	-134	103	103	103	-102	166	-101	165	117	-133	102	102	0	102	0	0	0	0	0	0	0	0	790	3
C6	111	111	111	37	-782	1440	-1248	-1251	-779	37	110	110	110	-1882	-205	396	281	-321	247	247	247	-244	398	-244	397	280	-320	246	246	0	246	0	0	0	0	0	0	0	0	1896	13
O6	-529	-529	-528	-175	3703	-6796	5932	5943	3696	-174	-526	-526	-526	8967	988	-1901	-1347	1543	-1186	-1187	-1187	1171	-1905	1169	-1900	-1343	1534	-1180	-1180	0	-1179	0	0	0	0	0	0	0	0	-9089	-122
H6c	327	327	327	108	-2298	4234	-3746	-3757	-2295	108	325	325	325	-5688	-606	1165	827	-947	729	729	730	-717	1168	-716	1165	824	-944	726	726	0	726	0	0	0	0	0	0	0	0	5584	-104
H6a	47	47	47	15	-328	604	-522	-522	-326	15	46	46	46	-785	-86	165	117	-134	103	103	103	-102	166	-102	165	117	-133	103	103	0	103	0	0	0	0	0	0	0	0	790	5
O5	-301	-301	-301	-100	2130	-3936	3415	3407	2120	-99	-299	-299	-299	5139	561	-1078	-764	874	-673	-674	-674	664	-1082	664	-1082	-765	874	-673	-673	0	-673	0	0	0	0	0	0	0	0	-5173	-34
C1	228	228	228	76	-1616	2991	-2611	-2605	-1607	75	227	226	226	-3934	-422	815	575	-661	509	509	509	-500	817	-500	817	576	-662	509	510	0	510	0	0	0	0	0	0	0	0	3913	-20
H1	76	76	75	25	-536	994	-869	-868	-533	25	75	75	75	-1309	-139	269	190	-218	168	169	168	-165	270	-165	270	190	-219	168	168	0	169	0	0	0	0	0	0	0	0	1293	-17
O1	-315	-316	-315	-105	2232	-4148	3592	3595	2222	-104	-313	-313	-313	5402	585	-1128	-798	917	-706	-707	-707	694	-1133	694	-1132	-799	918	-706	-706	0	-706	0	0	0	0	0	0	0	0	-5420	-19
H1t	23	23	23	7	-160	296	-261	-261	-158	7	22	22	22	-395	-41	80	57	-65	50	50	50	-49	81	-50	81	57	-65	50	50	0	50	0	0	0	0	0	0	0	0	384	-11
TOT	8	7	7	3	-80	197	-368	-353	-68	3	6	7	6	-625	17	-30	-18	21	-13	-14	-13	21	-31	20	-29	-19	19	-11	-12	0	-11	0	0	0	0	0	0	0	0	-103	-727

[EMIM]DMP	H1	H2	H3	C1	O1	P1	O3	O4	O2	C2	H4	H5	H6	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-487	-487	-488	-162	3472	-6468	5663	5647	3459	-161	-484	-484	-484	8537	909	-1759	-1240	1429	-1103	-1103	-1103	1076	-1764	1071	-1744	-1231	1401	-1083	-1082	412	-498	-497	0	-498	0	0	0	0	0	-8410	127
H2b	306	306	306	102	-2189	4105	-3673	-3627	-2184	101	304	304	304	-5535	-566	1094	775	-893	689	689	689	-671	1099	-666	1086	767	-872	674	674	-257	310	309	0	310	0	0	0	0	0	5242	-293
C2	141	141	141	47	-1008	1872	-1633	-1638	-1002	46	140	140	140	-2470	-262	508	357	-411	318	318	317	-310	508	-308	502	354	-403	312	312	-119	144	143	0	144	0	0	0	0	0	2424	-47
H2a	42	42	42	14	-298	553	-480	-484	-297	14	42	42	42	-728	-77	150	106	-122	94	94	94	-92	150	-91	149	105	-120	92	92	-35	43	43	0	43	0	0	0	0	0	717	-11
O3	-490	-490	-491	-163	3496	-6500	5658	5693	3477	-161	-484	-485	-484	8577	912	-1763	-1247	1432	-1105	-1106	-1105	1080	-1767	1073	-1747	-1234	1402	-1083	-1083	412	-497	-497	0	-497	0	0	0	0	0	-8421	156
H3b	309	309	309	103	-2210	4133	-3643	-3693	-2195	102	305	305	305	-5563	-569	1101	780	-897	691	692	691	-674	1104	-669	1089	769	-874	675	675	-257	310	310	0	310	0	0	0	0	0	5256	-307
C3	142	142	142	47	-1010	1873	-1632	-1638	-1004	46	140	140	140	-2473	-262	508	358	-411	318	318	317	-310	508	-308	502	355	-402	312	311	-118	143	143	0	143	0	0	0	0	0	2423	-49
H3a	42	42	42	14	-299	554	-484	-483	-297	14	41	41	41	-732	-78	150	106	-122	94	94	94	-92	150	-91	148	105	-119	92	92	-35	42	42	0	42	0	0	0	0	0	716	-16
C4	118	119	119	39	-843	1560	-1354	-1360	-839	39	117	117	117	-2051	-219	421	299	-344	266	266	265	-259	423	-257	419	296	-338	261	261	-100	121	121	0	121	0	0	0	0	0	2024	-27
O4t	-33	-34	-33	-11	237	-437	377	375	234	-11	-33	-33	-33	567	60	-115	-81	93	-71	-71	-71	70	-115	71	-116	-81	94	-73	-72	28	-33	-33	0	-34	0	0	0	0	0	-553	14
H4t	21	21	21	7	-150	276	-243	-241	-147	7	20	20	21	-366	-37	72	51	-58	45	45	45	-44	72	-44	72	51	-59	45	45	-17	21	21	0	21	0	0	0	0	0	345	-21
H4	22	22	22	7	-158	294	-255	-256	-158	7	22	22	22	-385	-41	79	56	-64	50	50	50	-48	79	-48	78	55	-63	49	49	-19	23	23	0	23	0	0	0	0	0	378	-7
C5	117	117	117	39	-829	1524	-1324	-1328	-823	38	116	116	116	-2004	-217	417	297	-341	264	264	263	-257	420	-256	416	295	-336	259	259	-99	120	120	0	120	0	0	0	0	0	2008	4
H5	21	21	21	7	-148	272	-236	-236	-147	7	21	21	21	-356	-39	74	53	-61	47	47	47	-46	75	-45	74	52	-60	46	46	-18	21	21	0	21	0	0	0	0	0	357	1
H6b	42	42	42	14	-298	547	-476	-477	-296	14	42	42	42	-719	-78	151	107	-123	95	95	95	-93	152	-93	150	107	-121	94	94	-36	43	43	0	43	0	0	0	0	0	725	6
C6	101	101	102	34	-712	1307	-1140	-1142	-707	33	100	100	100	-1722	-188	362	258	-296	228	228	228	-224	365	-223	361	256	-291	224	224	-86	104	104	0	104	0	0	0	0	0	1740	18
O6	-484	-484	-484	-160	3385	-6201	5432	5438	3365	-158	-478	-479	-479	8213	906	-1738	-1239	1423	-1097	-1097	-1096	1074	-1750	1069	-1732	-1229	1395	-1075	-1074	412	-497	-497	0	-497	0	0	0	0	0	-8340	-128
H6c	299	299	300	99	-2109	3890	-3444	-3453	-2099	98	296	296	296	-5231	-554	1066	760	-875	675	675	675	-658	1074	-653	1061	751	-854	658	658	-252	304	304	0	304	0	0	0	0	0	5117	-115
H6a	42	42	42	14	-298	547	-476	-477	-296	14	42	42	42	-718	-79	151	107	-124	95	95	95	-93	152	-93	151	107	-122	94	94	-36	43	43	0	43	0	0	0	0	0	725	7
O5	-275	-275	-275	-91	1944	-3588	3118	3123	1932	-90	-272	-272	-272	4706	513	-986	-701	807	-623	-623	-622	608	-994	605	-982	-697	794	-612	-612	235	-283	-283	0	-283	0	0	0	0	0	-4738	-32
C1	209	209	209	69	-1486	2759	-2398	-2403	-1477	69	207	207	207	-3619	-385	745	527	-610	471	471	471	-458	751	-455	742	523	-597	461	461	-176	213	213	0	213	0	0	0	0	0	3582	-37
H1	69	69	69	23	-494	920	-802	-802	-491	23	69	69	69	-1209	-127	246	174	-202	156	156	156	-151	248	-150	245	172	-196	152	152	-58	70	70	0	70	0	0	0	0	0	1183	-26
O1	-289	-289	-289	-96	2046	-3808	3292	3308	2041	-95	-286	-286	-286	4965	535	-1033	-734	848	-654	-654	-654	636	-1043	632	-1030	-727	831	-641	-640	245	-296	-296	0	-296	0	0	0	0	0	-4969	-4
H1t	21	21	21	7	-146	271	-239	-243	-146	7	21	20	20	-367	-38	73	52	-60	46	46	46	-46	75	-45	74	52	-58	45	45	-17	21	21	0	21	0	0	0	0	0	351	-16
TOT	7	7	7	3	-103	256	-393	-395	-98	3	7	7	7	-685	19	-27	-20	17	-12	-12	-12	19	-26	23	-33	-27	31	-20	-19	8	-9	-8	0	-9	0	0	0	0	0	-118	-803

[PMIM]DMP	H1	H2	H3	C1	O1	P1	O3	O4	O2	C2	H4	H5	H6	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-445	-445	-445	-148	3177	-5941	5224	5183	3175	-147	-443	-443	-443	7860	838	-1618	-1148	1326	-1024	-1025	-1025	994	-1632	986	-1605	-1131	1278	-986	-990	-75	-452	-452	1337	-448	-449	0	-448	0	0	-7747	113
H2b	280	280	280	93	-2018	3797	-3397	-3363	-2017	93	279	279	280	-5132	-523	1010	717	-828	639	639	639	-620	1017	-615	1002	706	-798	616	618	47	281	281	-832	279	279	0	279	0	0	4831	-301
C2	128	128	128	43	-919	1714	-1507	-1493	-918	42	128	128	128	-2270	-240	465	329	-381	294	294	294	-286	470	-283	462	325	-368	284	285	22	130	130	-387	130	130	0	130	0	0	2231	-39
H2a	38	38	38	13	-271	504	-443	-438	-270	13	38	38	38	-667	-71	137	98	-113	87	87	87	-85	139	-84	137	96	-109	84	84	6	39	39	-115	39	39	0	39	0	0	660	-7
O3	-444	-444	-445	-148	3181	-5931	5229	5179	3177	-147	-443	-443	-444	7876	838	-1620	-1148	1324	-1022	-1022	-1022	996	-1636	988	-1611	-1131	1276	-984	-986	-74	-450	-450	1334	-447	-448	0	-448	0	0	-7744	132
H3b	280	280	280	93	-2017	3794	-3389	-3357	-2019	93	279	279	279	-5123	-524	1011	718	-827	638	638	638	-622	1022	-617	1007	706	-796	614	616	46	280	280	-830	278	278	0	278	0	0	4836	-287
C3	129	129	129	43	-920	1715	-1509	-1495	-919	43	128	128	128	-2272	-240	465	329	-381	294	294	294	-286	471	-283	462	324	-367	283	284	21	130	130	-385	129	129	0	129	0	0	2229	-43
H3a	38	38	38	13	-273	508	-446	-442	-273	13	38	38	38	-673	-71	137	97	-113	87	87	87	-84	139	-84	136	96	-108	84	84	6	38	38	-114	38	38	0	38	0	0	658	-15
C4	108	107	108	36	-768	1435	-1254	-1244	-768	36	107	107	107	-1884	-200	385	275	-318	246	246	246	-239	394	-236	386	271	-307	237	237	18	109	109	-325	109	109	0	109	0	0	1859	-24
O4t	-30	-30	-30	-10	215	-400	344	351	214	-10	-30	-30	-30	524	55	-106	-75	87	-67	-67	-67	66	-109	66	-107	-75	85	-65	-65	-5	-30	-30	88	-29	-29	0	-29	0	0	-510	15
H4t	19	19	19	6	-136	256	-221	-230	-135	6	19	19	19	-341	-34	66	47	-54	42	42	42	-41	68	-41	67	47	-53	41	40	3	18	18	-54	18	18	0	18	0	0	319	-22
H4	20	20	20	7	-144	270	-236	-234	-144	7	20	20	20	-354	-37	72	52	-60	46	46	46	-45	74	-44	72	51	-57	44	44	3	20	20	-61	20	20	0	20	0	0	348	-6
C5	106	106	107	35	-757	1406	-1227	-1218	-757	35	106	106	106	-1846	-198	380	273	-315	244	244	244	-237	390	-234	381	268	-304	234	235	18	108	108	-324	108	108	0	108	0	0	1840	-6
H5	19	19	19	6	-136	251	-219	-217	-135	6	19	19	19	-329	-35	68	49	-56	43	43	43	-42	69	-42	68	48	-54	42	42	3	19	19	-57	19	19	0	19	0	0	327	-2
H6b	38	38	38	13	-272	502	-439	-436	-272	13	38	38	38	-662	-72	137	99	-114	88	88	88	-86	141	-85	138	97	-110	84	85	6	39	39	-117	39	39	0	39	0	0	664	2
C6	92	92	92	30	-650	1200	-1052	-1046	-650	30	92	92	92	-1586	-172	331	237	-274	211	211	211	-206	339	-204	331	233	-264	203	203	15	93	94	-280	94	94	0	94	0	0	1595	9
O6	-437	-437	-437	-145	3081	-5681	5007	4975	3081	-145	-437	-438	-438	7549	830	-1591	-1141	1314	-1012	-1014	-1013	991	-1623	979	-1586	-1122	1263	-971	-974	-74	-446	-447	1330	-445	-446	0	-446	0	0	-7643	-94
H6c	270	270	270	90	-1924	3580	-3192	-3164	-1926	90	271	271	271	-4823	-508	976	699	-806	621	622	621	-606	994	-599	972	685	-772	595	596	45	272	273	-808	271	271	0	271	0	0	4684	-139
H6a	38	38	38	13	-272	502	-439	-437	-271	13	38	38	38	-661	-72	138	99	-114	88	88	88	-86	141	-85	138	97	-110	85	85	6	39	39	-117	39	39	0	39	0	0	665	3
O5	-250	-250	-250	-83	1777	-3306	2884	2863	1776	-83	-249	-249	-249	4333	468	-898	-646	745	-575	-575	-575	561	-922	554	-900	-634	718	-553	-555	-42	-255	-255	763	-255	-255	0	-255	0	0	-4342	-9
C1	190	190	190	63	-1362	2544	-2220	-2202	-1358	63	189	189	189	-3334	-353	681	486	-563	435	436	436	-423	697	-418	681	478	-543	419	420	32	193	193	-575	192	192	0	192	0	0	3288	-46
H1	63	63	63	21	-455	851	-742	-737	-454	21	63	63	63	-1116	-117	225	160	-186	144	144	144	-140	230	-138	225	158	-179	138	138	10	63	63	-189	63	63	0	63	0	0	1087	-29
O1	-263	-263	-263	-87	1873	-3500	3059	3024	1868	-87	-261	-261	-261	4578	489	-943	-674	783	-605	-605	-605	587	-967	580	-947	-662	755	-582	-582	-44	-268	-268	801	-268	-267	0	-268	0	0	-4562	16
H1t	19	19	19	6	-136	254	-230	-222	-132	6	18	18	18	-342	-35	68	48	-56	43	43	43	-42	68	-41	67	47	-53	41	41	3	19	19	-55	18	18	0	18	0	0	324	-18
TOT	8	8	8	4	-127	325	-416	-403	-129	4	8	8	8	-693	15	-24	-20	21	-15	-15	-15	20	-25	19	-23	-22	24	-15	-14	-1	-8	-9	29	-9	-8	0	-9	0	0	-105	-798

[BMIM]DMP	H1	H2	H3	C1	O1	P1	O3	O4	O2	C2	H4	H5	H6	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-415	-414	-414	-137	2951	-5521	4912	4852	2918	-135	-406	-405	-405	7381	790	-1516	-1100	1281	-990	-990	-992	953	-1574	930	-1499	-1056	1166	-901	-903	-66	-401	-402	776	-392	-391	1146	-384	-383	-383	-7283	99
H2b	261	261	261	87	-1876	3538	-3212	-3145	-1856	85	256	256	256	-4828	-492	945	684	-796	615	615	616	-592	977	-578	935	658	-729	564	565	41	250	251	-484	244	244	-715	239	239	239	4536	-292
C2	120	119	119	40	-854	1601	-1418	-1407	-847	39	117	117	117	-2136	-226	436	315	-368	285	285	285	-273	453	-266	431	302	-335	259	259	19	115	116	-224	113	113	-330	111	111	111	2095	-41
H2a	35	35	35	12	-252	471	-416	-413	-249	11	35	35	35	-627	-67	129	93	-109	84	84	84	-81	134	-79	128	89	-99	77	77	6	34	34	-66	33	33	-98	33	33	33	619	-8
O3	-412	-412	-412	-137	2955	-5542	4887	4886	2939	-135	-406	-406	-406	7399	785	-1507	-1092	1272	-985	-985	-985	946	-1566	924	-1494	-1051	1165	-901	-904	-66	-401	-402	782	-394	-394	1159	-388	-388	-388	-7257	142
H3b	260	260	260	87	-1875	3540	-3156	-3181	-1862	86	256	256	256	-4813	-489	942	680	-794	615	614	615	-589	975	-576	933	656	-728	563	565	41	251	251	-487	246	245	-723	242	242	242	4531	-282
C3	120	119	119	40	-857	1613	-1420	-1417	-853	39	118	118	118	-2142	-226	435	314	-366	284	284	284	-272	452	-265	429	301	-334	259	259	19	115	116	-224	113	113	-331	111	111	111	2090	-52
H3a	35	35	35	12	-255	478	-422	-420	-253	12	35	35	35	-638	-67	129	93	-109	84	84	84	-80	133	-78	127	89	-99	76	77	6	34	34	-66	33	33	-98	33	33	33	618	-20
C4	100	100	100	33	-719	1355	-1185	-1177	-715	33	99	98	98	-1781	-187	361	261	-306	237	237	237	-227	377	-221	358	251	-279	216	216	16	97	97	-189	95	95	-279	93	93	93	1742	-39
O4t	-27	-27	-27	-9	197	-372	322	324	201	-9	-28	-28	-28	488	51	-98	-69	80	-62	-62	-62	61	-100	61	-98	-70	79	-61	-61	-5	-27	-28	54	-27	-27	80	-27	-27	-27	-471	17
H4t	17	17	17	6	-125	237	-209	-210	-127	6	18	18	18	-318	-32	62	44	-50	39	39	39	-38	62	-38	61	44	-49	38	38	3	17	17	-34	17	17	-50	17	17	17	295	-23
H4	19	19	19	6	-135	255	-223	-221	-135	6	18	18	18	-335	-35	67	49	-57	44	44	44	-42	70	-41	67	47	-52	41	41	3	18	18	-35	18	18	-52	17	17	17	325	-10
C5	99	99	99	33	-706	1318	-1159	-1152	-702	32	97	97	97	-1748	-186	358	260	-302	234	234	234	-226	374	-220	355	249	-277	214	214	16	96	96	-187	94	94	-277	92	92	92	1725	-22
H5	18	18	18	6	-126	234	-206	-205	-125	6	17	17	17	-310	-33	64	46	-54	42	42	42	-40	67	-39	64	45	-50	38	38	3	17	17	-33	17	17	-49	16	16	16	308	-3
H6b	36	35	35	12	-252	470	-412	-410	-251	12	35	35	35	-621	-67	129	93	-109	84	84	84	-81	134	-79	127	90	-100	77	77	6	35	35	-68	34	34	-101	34	34	34	619	-1
C6	85	85	85	28	-605	1126	-992	-986	-602	28	84	84	84	-1495	-161	309	224	-262	202	202	202	-195	322	-190	307	216	-239	185	185	14	83	83	-162	82	82	-241	81	81	81	1490	-5
O6	-406	-406	-406	-134	2881	-5341	4712	4687	2864	-133	-402	-402	-402	7111	777	-1489	-1081	1256	-970	-969	-970	936	-1543	915	-1474	-1040	1151	-887	-889	-66	-399	-398	778	-393	-393	1155	-387	-387	-387	-7150	-39
H6c	252	252	252	84	-1799	3369	-3007	-2982	-1792	83	250	249	249	-4541	-477	914	662	-769	594	594	594	-572	942	-560	903	638	-705	545	546	40	244	244	-475	240	240	-705	236	236	236	4385	-157
H6a	36	36	36	12	-252	469	-412	-409	-250	12	35	35	35	-620	-67	129	93	-109	84	84	84	-81	133	-79	127	90	-100	77	77	6	35	35	-68	34	34	-101	34	34	34	619	-0
O5	-232	-231	-231	-77	1653	-3097	2719	2696	1643	-76	-228	-228	-228	4083	440	-843	-614	717	-555	-555	-555	533	-883	519	-839	-589	654	-505	-505	-37	-226	-226	439	-220	-220	648	-216	-216	-216	-4071	12
C1	177	177	177	59	-1268	2380	-2095	-2074	-1258	58	174	174	174	-3146	-332	639	464	-544	421	421	422	-403	669	-393	637	445	-495	383	384	28	170	171	-331	167	166	-489	163	163	163	3091	-55
H1	59	59	59	20	-422	795	-701	-694	-419	19	58	58	58	-1052	-110	212	153	-179	139	139	139	-133	221	-130	211	147	-164	127	127	9	56	56	-109	55	55	-161	54	54	54	1022	-31
O1	-245	-245	-245	-81	1756	-3304	2891	2866	1744	-80	-241	-241	-241	4333	461	-888	-644	756	-586	-585	-586	559	-929	546	-886	-617	687	-531	-532	-39	-236	-237	461	-231	-231	682	-228	-228	-227	-4290	43
H1t	18	18	18	6	-128	242	-217	-211	-128	6	18	18	18	-323	-33	64	46	-53	41	41	42	-40	66	-39	64	44	-49	38	38	3	17	17	-32	16	16	-47	16	16	16	306	-17
TOT	8	8	8	3	-114	316	-419	-405	-114	4	9	9	9	-678	18	-21	-25	25	-18	-17	-18	23	-33	21	-25	-23	19	-11	-12	-1	-6	-6	15	-7	-7	24	-7	-7	-8	-107	-785

Table S14: Pairwise dispersion energies for the dimethylphosphates.

[DMIM]DMP	H1	H2	H3	C1	O1	P1	O3	O4	O2	C2	H4	H5	H6	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-0.3	-0.3	-0.4	-1.4	-1.5	-3.4	14.1	9.1	-1.4	-1.3	-0.3	-0.3	-0.3	12	-1.2	0.2	-2.5	-1.4	-0.1	-0.1	-0.1	-1.5	0	-1.5	0	-2.5	-1.4	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-12	0
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.4	-0.4	-0.4	-1.1	-1.1	-2.7	-1.6	-1.7	-1.1	-1.1	-0.3	-0.3	-0.3	-13	-1.3	-0.4	-1.6	-1.4	-0.5	-0.5	-0.5	-1.3	-0.4	-1.3	-0.4	-1.6	-1.4	-0.5	-0.5	0	-0.5	0	0	0	0	0	0	0	0	-14	-26
H2a	-0.0	-0.0	-0.0	-0.3	-0.3	-1.0	-0.3	-0.2	-0.3	-0.3	-0.0	-0.0	-0.0	-3	-0.4	-0.1	-0.6	-0.4	-0.0	-0.0	-0.0	-0.3	-0.0	-0.3	-0.1	-0.6	-0.4	-0.0	-0.0	0	-0.1	0	0	0	0	0	0	0	0	-3	-6
O3	-0.3	-0.3	-0.3	-1.4	-1.5	-3.5	11.4	14.8	-1.5	-1.3	-0.3	-0.3	-0.3	15	-1.1	0.4	-2.4	-1.4	-0.1	-0.1	-0.1	-1.4	0.1	-1.4	0.1	-2.4	-1.4	-0.0	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-12	3
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-0.4	-0.4	-0.4	-1.1	-1.1	-2.8	-1.7	-1.6	-1.1	-1.1	-0.3	-0.3	-0.3	-13	-1.3	-0.4	-1.6	-1.4	-0.5	-0.5	-0.5	-1.3	-0.4	-1.3	-0.4	-1.6	-1.4	-0.5	-0.5	0	-0.5	0	0	0	0	0	0	0	0	-14	-26
H3a	-0.0	-0.0	-0.0	-0.3	-0.3	-1.0	0.2	-0.0	-0.3	-0.3	-0.0	-0.0	-0.0	-2	-0.3	-0.0	-0.6	-0.4	-0.0	-0.0	-0.0	-0.3	-0.1	-0.3	-0.0	-0.6	-0.4	-0.0	-0.0	0	-0.0	0	0	0	0	0	0	0	0	-3	-5
C4	-0.3	-0.3	-0.3	-1.1	-1.0	-2.3	-1.9	-1.8	-0.9	-1.0	-0.3	-0.3	-0.3	-12	-1.1	-0.4	-1.4	-1.2	-0.4	-0.4	-0.4	-1.2	-0.4	-1.2	-0.4	-1.4	-1.2	-0.4	-0.4	0	-0.4	0	0	0	0	0	0	0	0	-12	-24
O4t	-0.0	-0.0	-0.0	-0.1	-0.1	-0.2	0.7	0.7	-0.1	-0.1	-0.0	-0.0	-0.0	1	-0.1	0	-0.2	-0.1	-0.0	-0.0	-0.0	-0.1	-0.0	-0.1	0	-0.2	-0.1	-0.0	-0.0	0	-0.0	0	0	0	0	0	0	0	0	-1	-0
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	-0.0	-0.0	-0.0	-0.3	-0.2	-0.6	-0.0	0.1	-0.2	-0.3	-0.0	-0.0	-0.0	-2	-0.3	-0.1	-0.4	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.4	-0.4	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-3	-5
C5	-0.4	-0.4	-0.4	-1.2	-1.0	-2.2	-1.8	-1.8	-1.0	-1.1	-0.4	-0.4	-0.4	-12	-1.2	-0.4	-1.5	-1.3	-0.4	-0.4	-0.4	-1.3	-0.4	-1.3	-0.4	-1.5	-1.3	-0.4	-0.4	0	-0.4	0	0	0	0	0	0	0	0	-13	-26
H5	-0.0	-0.0	-0.0	-0.3	-0.3	-0.8	-0.4	-0.4	-0.3	-0.3	-0.0	-0.0	-0.0	-3	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	0	-0.0	0	0	0	0	0	0	0	0	-3	-6
H6b	-0.0	-0.1	-0.0	-0.4	-0.4	-0.9	-0.5	-0.5	-0.4	-0.4	-0.0	-0.0	-0.0	-4	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-4	-8
C6	-0.4	-0.5	-0.4	-1.3	-1.2	-2.6	-1.5	-1.5	-1.2	-1.3	-0.4	-0.4	-0.4	-13	-1.4	-0.5	-1.9	-1.6	-0.5	-0.5	-0.5	-1.4	-0.5	-1.4	-0.5	-1.9	-1.5	-0.5	-0.5	0	-0.5	0	0	0	0	0	0	0	0	-16	-29
O6	-0.4	-0.4	-0.4	-1.6	-1.6	-3.5	8.4	9.6	-1.6	-1.6	-0.4	-0.4	-0.4	6	-1.4	0.1	-2.9	-1.6	-0.1	-0.1	-0.1	-1.6	0.1	-1.7	0.1	-2.9	-1.6	-0.2	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-14	-9
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.0	-0.0	-0.0	-0.4	-0.4	-0.9	-0.6	-0.6	-0.4	-0.4	-0.0	-0.0	-0.1	-4	-0.4	-0.1	-0.6	-0.5	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.5	-0.0	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-4	-8
O5	-0.3	-0.3	-0.3	-1.1	-1.0	-2.0	-1.6	-1.7	-0.9	-1.0	-0.3	-0.3	-0.3	-11	-1.0	-0.1	-1.7	-1.2	-0.2	-0.2	-0.2	-1.1	-0.1	-1.1	-0.2	-1.7	-1.2	-0.2	-0.2	0	-0.2	0	0	0	0	0	0	0	0	-11	-22
C1	-0.3	-0.4	-0.3	-1.1	-1.0	-2.3	-1.7	-1.7	-0.9	-1.0	-0.3	-0.3	-0.3	-12	-1.2	-0.4	-1.5	-1.3	-0.4	-0.4	-0.4	-1.2	-0.4	-1.2	-0.4	-1.5	-1.2	-0.4	-0.4	0	-0.4	0	0	0	0	0	0	0	0	-13	-25
H1	-0.0	-0.0	-0.0	-0.3	-0.2	-0.7	0.4	0.2	-0.3	-0.3	-0.0	-0.1	-0.1	-1	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	0	-0.1	0	0	0	0	0	0	0	0	-4	-5
O1	-0.3	-0.3	-0.3	-1.0	-0.9	-2.1	-0.8	-0.5	-0.9	-1.0	-0.3	-0.3	-0.3	-9	-1.1	-0.2	-1.6	-1.2	-0.3	-0.3	-0.3	-1.1	-0.2	-1.1	-0.3	-1.6	-1.2	-0.3	-0.3	0	-0.3	0	0	0	0	0	0	0	0	-11	-21
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	-4	-4	-4	-16	-15	-36	21	21	-15	-15	-4	-4	-4	-80	-16	-3	-25	-18	-4	-4	-4	-17	-3	-17	-3	-24	-18	-4	-4	0	-4	0	0	0	0	0	0	0	0	-167	-247

[EMIM]DMP	H1	H2	H3	C1	O1	P1	O3	O4	O2	C2	H4	H5	H6	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-0.3	-0.3	-0.3	-1.3	-1.4	-3.3	14.7	9.9	-1.4	-1.3	-0.3	-0.3	-0.3	14	-1.1	0.2	-2.3	-1.3	-0.1	-0.1	-0.1	-1.3	0.1	-1.3	0.1	-2.1	-1.4	-0.1	-0.1	-1.4	-0.3	-0.3	0	-0.3	0	0	0	0	0	-13	1
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.3	-0.3	-0.3	-1.0	-1.0	-2.6	-1.4	-1.7	-1.0	-1.0	-0.3	-0.3	-0.3	-12	-1.2	-0.4	-1.5	-1.3	-0.5	-0.5	-0.5	-1.2	-0.4	-1.2	-0.4	-1.4	-1.1	-0.4	-0.4	-1.1	-0.4	-0.4	0	-0.4	0	0	0	0	0	-15	-26
H2a	-0.0	-0.0	-0.0	-0.3	-0.3	-0.9	-0.3	-0.1	-0.3	-0.3	-0.0	-0.0	-0.0	-3	-0.3	-0.1	-0.5	-0.4	-0.0	-0.0	-0.0	-0.3	-0.1	-0.3	-0.1	-0.5	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	0	-0.0	0	0	0	0	0	-4	-6
O3	-0.3	-0.3	-0.3	-1.3	-1.4	-3.3	10.0	14.8	-1.4	-1.2	-0.3	-0.3	-0.3	14	-1.1	0.3	-2.4	-1.3	-0.1	-0.0	-0.1	-1.3	0.2	-1.3	0.1	-2.1	-1.4	-0.1	-0.1	-1.4	-0.3	-0.3	0	-0.3	0	0	0	0	0	-13	1
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-0.3	-0.3	-0.3	-1.0	-1.1	-2.7	-1.6	-1.6	-1.0	-1.0	-0.3	-0.3	-0.3	-12	-1.2	-0.4	-1.5	-1.4	-0.5	-0.5	-0.5	-1.2	-0.4	-1.2	-0.4	-1.3	-1.1	-0.4	-0.4	-1.1	-0.4	-0.4	0	-0.4	0	0	0	0	0	-14	-26
H3a	-0.0	-0.0	-0.0	-0.3	-0.3	-1.0	0.4	-0.1	-0.3	-0.3	-0.0	-0.0	-0.0	-2	-0.3	-0.0	-0.5	-0.4	-0.0	0	0	-0.3	-0.0	-0.3	-0.1	-0.5	-0.4	-0.0	-0.0	-0.3	-0.0	-0.0	0	-0.0	0	0	0	0	0	-3	-5
C4	-0.3	-0.3	-0.3	-1.0	-0.9	-2.2	-1.8	-1.7	-0.8	-0.9	-0.3	-0.3	-0.3	-11	-1.0	-0.3	-1.3	-1.2	-0.4	-0.4	-0.4	-1.1	-0.4	-1.1	-0.3	-1.2	-1.0	-0.4	-0.3	-1.0	-0.3	-0.3	0	-0.3	0	0	0	0	0	-13	-24
O4t	-0.0	-0.0	-0.0	-0.1	-0.1	-0.2	0.8	0.8	-0.1	-0.1	-0.0	-0.0	-0.0	1	-0.1	-0.0	-0.1	-0.1	-0.0	0	-0.0	-0.1	0	-0.1	0	-0.1	-0.1	0	-0.0	-0.1	-0.0	-0.0	0	-0.0	0	0	0	0	0	-1	-0
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	-0.0	-0.0	-0.0	-0.3	-0.3	-0.6	-0.2	0	-0.2	-0.3	-0.0	-0.0	-0.0	-2	-0.3	-0.1	-0.4	-0.3	-0.1	-0.0	-0.1	-0.3	-0.1	-0.3	-0.1	-0.4	-0.3	-0.1	-0.0	-0.3	-0.0	-0.0	0	-0.0	0	0	0	0	0	-3	-5
C5	-0.3	-0.3	-0.3	-1.0	-0.9	-2.0	-1.6	-1.7	-0.9	-1.0	-0.3	-0.3	-0.3	-11	-1.1	-0.3	-1.4	-1.3	-0.4	-0.4	-0.4	-1.2	-0.4	-1.1	-0.4	-1.3	-1.1	-0.4	-0.4	-1.1	-0.4	-0.4	0	-0.4	0	0	0	0	0	-14	-25
H5	-0.0	0	0	-0.3	-0.3	-0.7	-0.4	-0.4	-0.3	-0.3	-0.0	-0.0	-0.0	-3	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.2	-0.1	-0.3	-0.1	-0.4	-0.3	-0.1	-0.0	-0.3	-0.0	-0.0	0	-0.0	0	0	0	0	0	-3	-6
H6b	-0.0	-0.0	-0.0	-0.4	-0.3	-0.8	-0.5	-0.5	-0.3	-0.3	-0.1	-0.0	-0.0	-3	-0.4	-0.1	-0.6	-0.4	-0.1	-0.1	-0.1	-0.4	-0.1	-0.4	-0.1	-0.6	-0.4	-0.1	-0.1	-0.4	-0.1	-0.1	0	-0.1	0	0	0	0	0	-4	-8
C6	-0.4	-0.4	-0.4	-1.2	-1.1	-2.4	-1.4	-1.4	-1.1	-1.2	-0.4	-0.4	-0.4	-12	-1.3	-0.4	-1.8	-1.5	-0.5	-0.5	-0.5	-1.3	-0.5	-1.3	-0.4	-1.7	-1.3	-0.4	-0.4	-1.4	-0.5	-0.5	0	-0.5	0	0	0	0	0	-17	-29
O6	-0.4	-0.4	-0.4	-1.5	-1.5	-3.3	7.9	8.7	-1.4	-1.4	-0.4	-0.4	-0.3	5	-1.2	0.2	-2.7	-1.4	-0.1	-0.1	-0.1	-1.6	0.1	-1.5	0.1	-2.5	-1.7	-0.0	-0.1	-1.7	-0.3	-0.3	0	-0.3	0	0	0	0	0	-16	-10
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.0	-0.0	-0.0	-0.4	-0.4	-0.8	-0.5	-0.5	-0.4	-0.4	-0.0	-0.0	-0.0	-4	-0.4	-0.1	-0.6	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.6	-0.4	-0.1	-0.0	-0.4	-0.0	-0.0	0	-0.0	0	0	0	0	0	-4	-8
O5	-0.3	-0.3	-0.3	-0.9	-0.8	-1.8	-1.5	-1.5	-0.8	-0.9	-0.3	-0.3	-0.3	-10	-1.0	-0.1	-1.6	-1.2	-0.2	-0.2	-0.2	-1.0	-0.2	-1.0	-0.1	-1.5	-1.1	-0.2	-0.2	-1.1	-0.3	-0.3	0	-0.3	0	0	0	0	0	-12	-22
C1	-0.3	-0.3	-0.3	-1.0	-0.9	-2.2	-1.6	-1.7	-0.9	-0.9	-0.3	-0.3	-0.3	-11	-1.0	-0.3	-1.4	-1.2	-0.4	-0.4	-0.4	-1.1	-0.4	-1.1	-0.3	-1.2	-1.0	-0.4	-0.4	-1.1	-0.3	-0.3	0	-0.3	0	0	0	0	0	-13	-24
H1	-0.0	-0.0	-0.0	-0.3	-0.2	-0.6	0.5	0.3	-0.2	-0.3	-0.1	-0.0	-0.1	-1	-0.3	-0.1	-0.4	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.4	-0.3	-0.1	-0.1	-0.3	-0.1	-0.1	0	-0.1	0	0	0	0	0	-4	-5
O1	-0.3	-0.3	-0.3	-0.9	-0.8	-2.0	-0.6	-0.4	-0.8	-0.9	-0.2	-0.3	-0.3	-8	-1.0	-0.2	-1.5	-1.2	-0.3	-0.3	-0.3	-1.1	-0.2	-1.1	-0.2	-1.4	-1.1	-0.2	-0.3	-1.1	-0.3	-0.3	0	-0.3	0	0	0	0	0	-12	-20
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	-4	-4	-4	-14	-14	-33	21	21	-14	-14	-4	-4	-4	-69	-14	-2	-23	-17	-4	-4	-4	-16	-3	-15	-3	-21	-16	-3	-3	-16	-4	-4	0	-4	0	0	0	0	0	-178	-247

[PMIM]DMP	H1	H2	H3	C1	O1	P1	O3	O4	O2	C2	H4	H5	H6	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-0.3	-0.3	-0.3	-1.2	-1.3	-3.1	12.3	11.8	-1.3	-1.2	-0.3	-0.3	-0.3	14	-1.1	0.4	-2.3	-1.3	-0.0	-0.1	-0.1	-1.3	0.1	-1.3	0.2	-2.0	-1.3	-0.0	-0.1	-1.2	-0.2	-0.2	-1.2	-0.3	-0.3	0	-0.3	0	0	-14	0
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.3	-0.3	-0.3	-0.9	-0.9	-2.4	-1.5	-1.4	-0.9	-0.9	-0.3	-0.3	-0.3	-11	-1.1	-0.4	-1.4	-1.3	-0.5	-0.5	-0.5	-1.2	-0.4	-1.1	-0.4	-1.3	-1.0	-0.3	-0.3	-0.9	-0.3	-0.3	-0.9	-0.3	-0.3	0	-0.3	0	0	-15	-26
H2a	-0.0	-0.0	-0.0	-0.3	-0.3	-0.8	-0.2	-0.3	-0.3	-0.3	-0.0	-0.0	-0.0	-3	-0.3	-0.0	-0.5	-0.4	-0.0	-0.0	-0.0	-0.3	-0.1	-0.3	-0.1	-0.4	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	0	-0.0	0	0	-4	-6
O3	-0.3	-0.3	-0.3	-1.1	-1.3	-3.0	11.4	10.4	-1.3	-1.2	-0.3	-0.3	-0.3	12	-1.1	0.4	-2.3	-1.3	-0.1	-0.0	-0.1	-1.3	0.2	-1.2	0.2	-2.0	-1.3	-0.1	-0.1	-1.2	-0.2	-0.2	-1.2	-0.3	-0.3	0	-0.3	0	0	-14	-1
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-0.3	-0.3	-0.3	-0.9	-1.0	-2.5	-1.5	-1.5	-1.0	-0.9	-0.3	-0.3	-0.3	-11	-1.1	-0.4	-1.4	-1.3	-0.4	-0.4	-0.4	-1.2	-0.4	-1.1	-0.4	-1.2	-0.9	-0.3	-0.3	-0.9	-0.3	-0.3	-0.9	-0.3	-0.3	0	-0.3	0	0	-14	-26
H3a	-0.0	-0.0	-0.0	-0.3	-0.3	-0.8	-0.0	0	-0.3	-0.3	-0.0	-0.0	-0.0	-2	-0.3	-0.0	-0.5	-0.4	-0.0	-0.0	-0.0	-0.3	-0.1	-0.3	-0.0	-0.4	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	0	-0.0	0	0	-3	-5
C4	-0.3	-0.3	-0.3	-0.9	-0.8	-2.1	-1.6	-1.6	-0.8	-0.9	-0.3	-0.3	-0.3	-10	-0.9	-0.3	-1.2	-1.1	-0.4	-0.4	-0.4	-1.1	-0.4	-1.0	-0.3	-1.0	-0.8	-0.3	-0.3	-0.8	-0.3	-0.3	-0.8	-0.3	-0.3	0	-0.3	0	0	-13	-23
O4t	-0.0	-0.0	-0.0	-0.1	-0.1	-0.2	0.5	1.1	-0.1	-0.1	-0.0	-0.0	-0.0	1	-0.1	0	-0.1	-0.1	-0.0	-0.0	-0.0	-0.1	0	-0.1	0	-0.1	-0.1	0	0	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	0	-0.0	0	0	-1	-0
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	-0.0	-0.0	-0.0	-0.3	-0.2	-0.6	0	0	-0.2	-0.2	-0.0	-0.0	-0.0	-2	-0.3	-0.1	-0.4	-0.4	-0.0	-0.1	-0.0	-0.3	-0.1	-0.3	-0.1	-0.4	-0.3	-0.1	-0.1	-0.3	-0.0	-0.0	-0.2	-0.0	-0.0	0	-0.0	0	0	-3	-5
C5	-0.3	-0.3	-0.3	-0.9	-0.9	-2.0	-1.6	-1.6	-0.9	-0.9	-0.3	-0.3	-0.3	-11	-1.0	-0.3	-1.3	-1.2	-0.4	-0.4	-0.4	-1.1	-0.4	-1.0	-0.3	-1.1	-0.9	-0.3	-0.3	-0.9	-0.3	-0.3	-0.9	-0.3	-0.3	0	-0.3	0	0	-14	-25
H5	-0.0	-0.0	0	-0.3	-0.2	-0.7	-0.4	-0.3	-0.2	-0.3	-0.0	-0.0	-0.0	-2	-0.3	-0.1	-0.4	-0.4	-0.1	-0.0	-0.0	-0.3	-0.0	-0.2	-0.1	-0.4	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	0	-0.0	0	0	-3	-6
H6b	-0.0	-0.0	-0.0	-0.3	-0.3	-0.8	-0.4	-0.4	-0.3	-0.3	-0.0	-0.0	-0.0	-3	-0.4	-0.1	-0.5	-0.4	-0.0	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	-0.4	-0.0	-0.0	-0.4	-0.1	-0.0	0	-0.1	0	0	-4	-7
C6	-0.4	-0.4	-0.4	-1.1	-1.1	-2.3	-1.4	-1.4	-1.0	-1.1	-0.4	-0.4	-0.4	-12	-1.2	-0.4	-1.7	-1.4	-0.5	-0.5	-0.5	-1.3	-0.5	-1.2	-0.4	-1.5	-1.1	-0.4	-0.4	-1.1	-0.4	-0.4	-1.1	-0.4	-0.4	0	-0.4	0	0	-17	-28
O6	-0.3	-0.3	-0.3	-1.3	-1.4	-3.1	8.0	7.4	-1.4	-1.3	-0.3	-0.3	-0.4	5	-1.2	0.2	-2.6	-1.4	-0.1	-0.0	-0.0	-1.4	0.2	-1.4	0.1	-2.3	-1.5	-0.1	0	-1.5	-0.2	-0.2	-1.5	-0.3	-0.3	0	-0.3	0	0	-16	-11
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.0	-0.0	-0.0	-0.3	-0.3	-0.8	-0.5	-0.4	-0.3	-0.3	-0.0	-0.0	-0.0	-3	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.5	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	-0.4	-0.0	-0.0	0	-0.0	0	0	-4	-7
O5	-0.2	-0.3	-0.3	-0.9	-0.8	-1.8	-1.5	-1.4	-0.8	-0.9	-0.3	-0.2	-0.2	-9	-0.9	-0.1	-1.5	-1.1	-0.2	-0.2	-0.2	-1.0	-0.1	-1.0	-0.2	-1.2	-0.9	-0.2	-0.2	-0.9	-0.2	-0.2	-0.9	-0.2	-0.2	0	-0.2	0	0	-12	-22
C1	-0.3	-0.3	-0.3	-0.9	-0.9	-2.1	-1.6	-1.5	-0.8	-0.9	-0.3	-0.3	-0.3	-10	-0.9	-0.3	-1.3	-1.2	-0.4	-0.4	-0.4	-1.1	-0.4	-1.0	-0.3	-1.1	-0.9	-0.3	-0.3	-0.8	-0.3	-0.3	-0.9	-0.3	-0.3	0	-0.3	0	0	-13	-24
H1	-0.0	-0.0	-0.0	-0.3	-0.2	-0.5	0.4	0.5	-0.2	-0.3	-0.1	-0.0	-0.0	-1	-0.3	-0.1	-0.4	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.3	-0.3	-0.1	-0.1	-0.3	-0.1	-0.1	-0.3	-0.1	-0.1	0	-0.1	0	0	-4	-5
O1	-0.3	-0.2	-0.2	-0.9	-0.8	-1.9	-0.2	-0.6	-0.8	-0.9	-0.3	-0.3	-0.3	-8	-0.9	-0.1	-1.4	-1.1	-0.3	-0.3	-0.3	-1.0	-0.2	-1.0	-0.2	-1.2	-0.9	-0.2	-0.2	-0.9	-0.2	-0.2	-0.9	-0.3	-0.3	0	-0.3	0	0	-12	-20
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	-3	-3	-3	-13	-13	-31	20	19	-13	-13	-3	-3	-3	-66	-13	-2	-22	-17	-4	-4	-4	-15	-3	-14	-2	-19	-14	-3	-3	-13	-3	-3	-13	-4	-4	0	-4	0	0	-181	-246

[BMIM]DMP	H1	H2	H3	C1	O1	P1	O3	O4	O2	C2	H4	H5	H6	ani tot	C2	H1	N3	C6	H4	H5	H6	C4	H2	C5	H3	N1	C7	H7	H8	C8	H9	H10	H11	C9	H12	H13	C10	H14	H15	cat tot	tot
O2	-0.2	-0.3	-0.3	-1.1	-1.3	-3.1	15.0	11.0	-1.3	-1.0	-0.2	-0.3	-0.2	17	-1.0	0.3	-2.4	-1.3	-0.0	-0.0	-0.0	-1.3	0.3	-1.3	0.1	-2.0	-1.2	-0.0	-0.1	-1.1	-0.2	-0.2	-0.9	-0.2	-0.2	-0.9	-0.2	-0.2	-0.2	-14	2
H2b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2	-0.3	-0.3	-0.3	-0.9	-0.9	-2.4	-1.3	-1.5	-0.9	-0.8	-0.3	-0.3	-0.3	-10	-1.1	-0.4	-1.5	-1.4	-0.5	-0.5	-0.5	-1.3	-0.4	-1.1	-0.4	-1.2	-0.9	-0.3	-0.3	-0.7	-0.2	-0.3	-0.6	-0.2	-0.2	-0.6	-0.2	-0.2	-0.2	-15	-26
H2a	-0.0	-0.0	-0.0	-0.3	-0.3	-0.8	-0.2	-0.2	-0.3	-0.2	-0.0	-0.0	-0.0	-2	-0.3	-0.0	-0.5	-0.4	-0.0	-0.0	-0.0	-0.3	-0.0	-0.3	-0.0	-0.5	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.0	-4	-6
O3	-0.3	-0.3	-0.2	-1.1	-1.3	-2.9	8.7	13.0	-1.2	-1.0	-0.2	-0.3	-0.2	13	-1.1	0.1	-2.3	-1.3	-0.0	-0.0	-0.0	-1.3	0.3	-1.3	0.1	-1.9	-1.2	-0.0	-0.0	-1.0	-0.2	-0.2	-0.9	-0.2	-0.2	-0.9	-0.2	-0.2	-0.2	-14	-2
H3b	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C3	-0.3	-0.3	-0.3	-0.9	-0.9	-2.5	-1.6	-1.4	-0.9	-0.8	-0.3	-0.3	-0.3	-11	-1.1	-0.3	-1.5	-1.4	-0.5	-0.5	-0.5	-1.2	-0.4	-1.1	-0.3	-1.2	-0.9	-0.3	-0.3	-0.7	-0.2	-0.2	-0.6	-0.2	-0.2	-0.6	-0.2	-0.2	-0.2	-15	-26
H3a	-0.0	-0.0	-0.0	-0.3	-0.3	-0.9	0.2	0.2	-0.3	-0.3	-0.0	-0.0	-0.0	-2	-0.3	-0.0	-0.5	-0.4	-0.0	-0.0	-0.0	-0.3	-0.0	-0.3	-0.1	-0.4	-0.3	-0.0	-0.0	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.0	-4	-5
C4	-0.3	-0.3	-0.3	-0.8	-0.8	-2.1	-1.7	-1.7	-0.8	-0.8	-0.2	-0.2	-0.2	-10	-0.9	-0.3	-1.2	-1.2	-0.4	-0.4	-0.4	-1.1	-0.4	-1.0	-0.3	-1.0	-0.7	-0.3	-0.3	-0.6	-0.2	-0.2	-0.6	-0.2	-0.2	-0.6	-0.2	-0.2	-0.2	-13	-23
O4t	-0.0	-0.0	-0.0	-0.1	-0.1	-0.2	0.9	0.8	-0.1	-0.1	-0.0	-0.0	-0.0	1	-0.1	0	-0.1	-0.1	-0.0	-0.0	-0.0	-0.1	-0.0	-0.1	0	-0.1	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.1	-0.0	-0.0	-0.0	-1	-0
H4t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	-0.0	-0.0	-0.0	-0.2	-0.2	-0.5	-0.0	0.1	-0.2	-0.2	-0.0	-0.0	-0.0	-2	-0.3	-0.1	-0.4	-0.4	-0.1	-0.1	-0.0	-0.3	-0.1	-0.3	-0.1	-0.3	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.0	-3	-5
C5	-0.3	-0.3	-0.3	-0.9	-0.8	-1.9	-1.6	-1.6	-0.8	-0.8	-0.3	-0.3	-0.3	-10	-1.0	-0.3	-1.4	-1.3	-0.4	-0.4	-0.4	-1.1	-0.4	-1.0	-0.3	-1.1	-0.8	-0.3	-0.3	-0.7	-0.2	-0.2	-0.6	-0.2	-0.2	-0.7	-0.2	-0.2	-0.2	-14	-24
H5	-0.0	-0.0	0	-0.2	-0.2	-0.7	-0.4	-0.4	-0.2	-0.2	-0.0	0	-0.0	-2	-0.3	-0.1	-0.5	-0.4	-0.0	-0.0	-0.0	-0.2	-0.1	-0.3	-0.1	-0.4	-0.3	-0.0	-0.0	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.0	-4	-6
H6b	-0.0	-0.0	-0.0	-0.3	-0.3	-0.7	-0.5	-0.4	-0.3	-0.3	-0.0	-0.0	-0.0	-3	-0.3	-0.1	-0.5	-0.4	-0.0	-0.0	-0.0	-0.3	-0.1	-0.3	-0.1	-0.4	-0.3	-0.0	-0.1	-0.3	-0.1	-0.0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.0	-4	-7
C6	-0.3	-0.3	-0.3	-1.0	-1.0	-2.2	-1.3	-1.3	-0.9	-1.0	-0.3	-0.3	-0.3	-11	-1.1	-0.3	-1.7	-1.4	-0.5	-0.5	-0.5	-1.3	-0.4	-1.1	-0.4	-1.4	-1.0	-0.3	-0.3	-0.9	-0.3	-0.3	-0.8	-0.3	-0.3	-0.9	-0.3	-0.3	-0.3	-17	-27
O6	-0.3	-0.3	-0.3	-1.3	-1.3	-3.1	8.7	7.7	-1.3	-1.2	-0.3	-0.3	-0.3	7	-1.1	0.1	-2.6	-1.4	-0.1	-0.1	-0.0	-1.4	0.2	-1.4	0.2	-2.2	-1.3	-0.0	0	-1.3	-0.2	-0.2	-1.2	-0.3	-0.3	-1.1	-0.3	-0.3	-0.3	-17	-10
H6c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H6a	-0.0	-0.0	-0.0	-0.3	-0.3	-0.7	-0.4	-0.4	-0.3	-0.3	-0.0	-0.0	-0.0	-3	-0.3	-0.1	-0.5	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.4	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.3	-0.0	-0.0	-0.0	-4	-7
O5	-0.2	-0.2	-0.2	-0.8	-0.7	-1.7	-1.5	-1.4	-0.7	-0.8	-0.2	-0.2	-0.2	-9	-0.9	-0.2	-1.5	-1.2	-0.2	-0.3	-0.2	-1.1	-0.1	-0.9	-0.2	-1.2	-0.8	-0.2	-0.2	-0.7	-0.2	-0.2	-0.7	-0.2	-0.2	-0.7	-0.2	-0.2	-0.2	-12	-21
C1	-0.3	-0.3	-0.3	-0.8	-0.8	-2.1	-1.6	-1.6	-0.8	-0.8	-0.3	-0.2	-0.2	-10	-1.0	-0.3	-1.3	-1.2	-0.4	-0.4	-0.4	-1.1	-0.4	-1.0	-0.3	-1.1	-0.8	-0.3	-0.3	-0.6	-0.2	-0.2	-0.6	-0.2	-0.2	-0.6	-0.2	-0.2	-0.2	-14	-24
H1	-0.0	-0.0	-0.0	-0.3	-0.2	-0.5	0.5	0.6	-0.2	-0.3	-0.0	-0.0	-0.0	-1	-0.3	-0.1	-0.4	-0.4	-0.1	-0.1	-0.1	-0.3	-0.1	-0.3	-0.1	-0.4	-0.3	-0.1	-0.1	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.2	-0.0	-0.0	-0.0	-4	-4
O1	-0.2	-0.2	-0.2	-0.8	-0.8	-1.9	-0.7	-1.0	-0.7	-0.8	-0.2	-0.2	-0.2	-8	-0.9	-0.1	-1.5	-1.3	-0.3	-0.3	-0.3	-1.1	-0.2	-1.0	-0.2	-1.2	-0.8	-0.2	-0.2	-0.7	-0.2	-0.2	-0.6	-0.2	-0.2	-0.6	-0.2	-0.2	-0.2	-13	-21
H1t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TOT	-3	-3	-3	-12	-12	-31	21	21	-12	-12	-3	-3	-3	-56	-13	-2	-23	-17	-4	-4	-4	-15	-3	-14	-2	-18	-12	-3	-3	-11	-3	-3	-10	-3	-3	-10	-3	-3	-3	-186	-242