Meta-hybrid Density Function Theory Study of Adsorption of Imidazolium and Ammonium-Based Ionic Liquids on Graphene Sheet

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Table S1. Bond critical point data (in au) obtained from QTAIM analysis for the H-bonds and other interactions in ionic liquids at the M06-2X/cc-pVDZ level of theory

Structure	BCP	ρ(r)	∑ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	H(r)	$^{a}E_{X\ldots Y}$	$\sum E_{X\ldots Y}$
[Bmim][BF_4]	F20…H14-C6	0.0171	0.1134	0.0572	0.0144	-0.0145	-0.0001	-4.56	-30.50
	F20…H13-C2	0.0210		0.0772	0.0190	-0.0188	0.0002	-5.93	
	F22…H13-C2	0.0168		0.0677	0.0160	-0.0150	0.0009	-4.73	
	F22…H18-C7	0.0127		0.0538	0.0122	-0.0109	0.0012	-3.44	
	F22…H26-C24	0.0068		0.0320	0.0066	-0.0053	0.0013	-1.66	
	F22…H16-C8	0.0115		0.0503	0.0111	-0.0097	0.0014	-3.06	
	F21…H16-C9	0.0113		0.0394	0.0095	-0.0092	0.0003	-2.89	
	F21…C2	0.0161		0.0634	0.0146	-0.0134	0.0012	-4.23	
[Bmim][PF_6]	F13…H18-C6	0.0149	0.1145	0.0519	0.0129	-0.0128	0.0001	-4.02	-31.01
	F13…H20-C2	0.0158		0.0594	0.0144	-0.0140	0.0004	-4.38	
	F14…H20-C2	0.0183		0.0710	0.0171	-0.0166	0.0005	-5.22	
	F14…H24-C7	0.0135		0.0585	0.0133	-0.0120	0.0013	-3.77	
	F14…H28-C9	0.0076		0.0348	0.0074	-0.0061	0.0013	-1.92	
	F15…C2	0.0175		0.0689	0.0163	-0.0155	0.0008	-4.85	

	F15…H25-C8	0.0135		0.0456	0.0114	-0.0115	-0.0001	-3.59	
	F16…H25-C8	0.0066		0.0316	0.0065	-0.0052	0.00134	-1.64	
	F16…H29-C10	0.0065		0.0285	0.0061	-0.0051	0.0010	-1.61	
[Bmim][DCA]	N28…H12-C9	0.0136	0.0678	0.0426	0.0098	-0.0090	0.0008	-2.83	-13.58
	N28…N3	0.0112		0.0387	0.0085	-0.0074	0.0011	-2.33	
	N26…H18-C16	0.0101		0.0330	0.0073	-0.0064	0.0009	-2.01	
	N30…H21-C19	0.0050		0.0167	0.0034	-0.0028	0.0006	-0.88	
	N30…H15-C13	0.0141		0.0426	0.0099	-0.0091	0.0007	-2.87	
	N30…H6-C2	0.0137		0.0443	0.0097	-0.0084	0.0013	-2.65	
[Bmim][Tf_2N]	O31…H11-C9	0.0143	0.1163	0.0428	0.0107	-0.0108	-0.0001	-3.39	-25.70
	O31…C4	0.0075		0.0261	0.0055	-0.0045	0.0009	-1.42	
	N26…C2	0.0175		0.0614	0.0140	-0.0127	0.0013	-3.99	
	N26…H17-C16	0.0105		0.0299	0.0070	-0.0066	0.0004	-2.09	
	O29…H6-C2	0.0143		0.0510	0.0118	-0.0108	0.0009	-3.39	
	O29…H14-C13	0.0125		0.0430	0.0101	-0.0095	0.0006	-2.98	
	O29…H20-C19	0.0065		0.0242	0.0052	-0.0044	0.0008	-1.38	
	O30…H20-C19	0.0054		0.0226	0.0045	-0.0034	0.0011	-1.1	
	O30…H23-C22	0.0074		0.0277	0.0061	-0.0053	0.0008	-1.68	
	F40…H23-C22	0.0026		0.0144	0.0026	-0.0016	0.0009	-0.52	
	F40…H17-C16	0.0046		0.0206	0.0042	-0.0031	0.0009	-0.99	
	F38…H17-C16	0.0050		0.0228	0.0046	-0.0035	0.0010	-1.11	
	F38…C5	0.0078		0.0312	0.0065	-0.0051	0.0013	-1.62	
[Btma][BF_4]	F30…H4…C2	0.0205	0.1123	0.0714	0.0178	-0.0179	-0.0001	-5.62	-30.38
	F30…H14-C15	0.0121		0.0486	0.0112	-0.0104	0.0008	-3.27	
	F31…H14-C15	0.0184		0.0619	0.0155	-0.0156	-0.0001	-4.90	
	F31…H22-C20	0.0117		0.0406	0.0099	-0.0096	0.0002	-3.03	
	F30…H13-C10	0.0181		0.0622	0.0157	-0.0159	-0.0001	-5.00	
	F28…H13-C10	0.0160		0.0563	0.0139	-0.0139	0.0001	-4.36	
	F28…H19-C17	0.0150		0.0587	0.0140	-0.0133	0.0006	-4.18	
[Btma][PF_6]	F29…H3-C2	0.0147	0.1172	0.0501	0.0124	-0.0125	0.0001	-3.91	-31.89
	F29…H7-C6	0.0171		0.0587	0.0148	-0.0149	-0.0001	-4.69	
	F31…H7-C6	0.0158		0.0549	0.0137	-0.0137	-0.0001	-4.31	
	F31…H18-C17	0.0126		0.0557	0.0126	-0.0113	0.0013	-3.56	
	F31…H21-C20	0.0069		0.0330	0.0068	-0.0054	0.0014	-1.70	
	F31…H16-C15	0.0156		0.0611	0.0147	-0.0141	0.0005	-4.43	
	F28…H16-C15	0.0220		0.0763	0.0191	-0.0193	-0.0001	-6.04	
	F28…H3-C2	0.0122		0.0452	0.0108	-0.0104	0.0004	-3.25	
[Btma][DCA]	N31…H5-C2	0.0134	0.0683	0.0378	0.0090	-0.0086	0.0004	-2.71	-13.36
	N31…H12-C10	0.0141		0.0425	0.0096	-0.0086	0.0010	-2.71	
	N29…H11-C10	0.0131		0.0393	0.0090	-0.0082	0.0007	-2.59	
	N29…H9-C6	0.0133		0.0402	0.0092	-0.0084	0.0008	-2.64	
	N31…H8-C6	0.0142		0.0428	0.0096	-0.0086	0.0010	-2.72	

[Btma][Tf_2N]	O32…H3-C2	0.0157	0.1307	0.0520	0.0126	-0.0122	0.0003	-3.83	-30.23
	O32…H16-C15	0.0121		0.0362	0.0090	-0.0090	-0.0001	-2.85	
	F39…H16-C15	0.0080		0.0316	0.0071	-0.0064	0.0007	-2.02	
	F39…H21-C20	0.0057		0.0253	0.0052	-0.0042	0.0010	-1.33	
	O32…H7-C6	0.0142		0.0418	0.0106	-0.0108	-0.0001	-3.39	
	N27…H7-C6	0.0127		0.0403	0.0094	-0.0087	0.0006	-2.76	
	N27…H16-C15	0.0144		0.0457	0.0108	-0.0102	0.0006	-3.20	
	N27…H18-C17	0.0098		0.0354	0.0077	-0.0066	0.0011	-2.08	
	N27…H21-C20	0.0078		0.0249	0.0056	-0.0050	0.0006	-1.57	
	O30…H25-C23	0.0112		0.0384	0.0091	-0.0086	0.0004	-2.71	
	O30…H18-C17	0.0116		0.0356	0.0088	-0.0087	0.0001	-2.74	
	F37…H9-C6	0.0069		0.0318	0.0067	-0.0056	0.0011	-1.75	

[a] X in $E_{X...Y}$ is N, O, and F electronegative atoms and Y is H, C, and N atoms.

Table S2. Bond Critical Point Data (in au) obtained from QTAIM analysis for the H-bonds and other interactions in ILs adsorbed on the graphene surface at the M06-2X/cc-pVDZ level of theory.

Structure	BCP	ρ(r)	∑ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	H(r)	$^{a}E_{X\ldots Y}$	$\sum E_{X\ldots Y}$
G[Bmim][BF_4]	F20…H14-C6	0.0049	0.0967	0.0231	0.0046	-0.0034	0.0011	-1.09	-25.54
	F20…H13-C2	0.0275		0.1042	0.0250	-0.0240	0.0010	-7.53	
	F22…H13-C2	0.0167		0.0628	0.0152	-0.0148	0.0004	-4.64	
	F22…H18-C7	0.0135		0.0558	0.0129	-0.0120	0.0009	-3.76	
	F22…H26-C24	0.0084		0.0372	0.0080	-0.0067	0.0012	-2.13	
	F22…H16-C8	0.0122		0.0533	0.0119	-0.0106	0.0013	-3.32	
	F21…H16-C9	0.0102		0.0359	0.0085	-0.0081	0.0004	-2.56	
	F21…H30-C27	0.0027		0.0143	0.0026	-0.0016	0.0009	-0.51	
G[Bmim][PF_6]	F13…H18-C6	0.0061	0.0990	0.0268	0.0056	-0.0045	0.0010	-1.43	-26.34
	F13…H20-C2	0.0191		0.0677	0.0167	-0.0165	0.0001	-5.19	
	F14…H20-C2	0.0191		0.0687	0.0171	-0.0171	0.0001	-5.35	
	F14…H24-C7	0.0116		0.0491	0.0112	-0.0101	0.0010	-3.18	
	F14…H28-C9	0.0074		0.0335	0.0071	-0.0059	0.0012	-1.87	
	F15…C2	0.0147		0.0648	0.0144	-0.0126	0.0017	-3.97	
	F15…H25-C8	0.0145		0.0477	0.0121	-0.0123	-0.0001	-3.85	
	F16…H29-C10	0.0061		0.0270	0.0057	-0.0047	0.0010	-1.49	
G[Bmim][DCA]	N28…H12-C9	0.0130	0.0648	0.0411	0.0094	-0.0085	0.0008	-2.68	-12.34
	N28…C2	0.0101		0.0310	0.006	-0.0052	0.0012	-1.66	
	N30…H6-C2	0.0139		0.0426	0.0094	-0.0082	0.001	-2.59	
	N30…H15-C13	0.0119		0.0348	0.0081	-0.0075	0.0005	-2.38	
	N30…H21-C19	0.0062		0.0193	0.0042	0.0035	0.0006	-1.12	
	N26…H18-C16	0.0095		0.0320	0.0070	-0.0068	0.0009	-1.91	
G[Bmim][Tf_2N]	O31…H11-C9	0.0116	0.1154	0.0356	0.0087	-0.0086	0.0001	-2.71	-25.31
	O31…C4	0.0081		0.0278	0.0059	-0.0048	0.0010	-1.53	
	N26…C2	0.0171		0.0593	0.0135	-0.0122	0.0013	-3.84	
	N26…H17-C16	0.0098		0.0275	0.0065	-0.0062	0.0003	-1.95	
	O29…H20-C19	0.0085		0.0300	0.0068	-0.0061	0.0006	-1.93	
	O29…H14-C13	0.0109		0.0411	0.0092	-0.0082	0.0009	-2.60	
	O29…H17-C16	0.0084		0.0338	0.0071	-0.0057	0.0013	-1.81	
	O29…H6-C2	0.0127		0.0455	0.0104	-0.0094	0.0009	-2.96	
	O30…H23-C22	0.0027		0.0118	0.0022	-0.0014	0.0007	-0.46	
	F40…H23-C22	0.0024		0.0134	0.0024	-0.0015	0.0009	-0.48	
	F40…H17-C16	0.0067		0.0272	0.0059	-0.0051	0.0008	-1.61	
	F38…H17-C16	0.0048		0.0228	0.0045	-0.0033	0.0011	-1.06	
	F38…C5	0.0077		0.0307	0.0063	-0.0051	0.0012	-1.60	
	F36…H10-C9	0.0035		0.0186	0.0035	-0.0024	0.0011	-0.76	
G[Btma][BF_4]	F31…H4-C2	0.0159	0.1047	0.0560	0.0139	-0.0138	0.0001	-4.33	-28.08
	F31…H14-C15	0.0198		0.0665	0.0168	-0.0170	-0.0002	-5.35	
	F30…H4-C2	0.0135		0.0475	0.0116	-0.0113	0.0002	-3.56	

	F30…H13-C10	0.0168		0.0569	0.0143	-0.0144	-0.0001	-4.53	
	F28…H13-C10	0.0128		0.0456	0.0110	-0.0106	0.0003	-3.35	
	F28…H14-C15	0.0140		0.0549	0.0130	-0.0123	0.0006	-3.88	
	F28…H19-C17	0.0115		0.0469	0.0107	-0.0098	0.0009	-3.08	
G[Btma][PF_6]	F100…H75-C74	0.0056	0.1106	0.0272	0.0055	-0.0043	0.0012	-1.35	-29.79
	F100…H79-C78	0.0187		0.0642	0.0163	-0.0166	-0.0003	-5.23	
	F100…H88-C87	0.0207		0.0697	0.0178	-0.0182	-0.0003	-5.71	
	F101…H79-C78	0.0115		0.0444	0.0104	-0.0098	0.0006	-3.08	
	F103…H81-C78	0.0126		0.0538	0.0121	-0.0107	0.0013	-3.38	
	F103…H88-C87	0.0107		0.0488	0.0107	-0.0092	0.0015	-2.89	
	F103…H90-C89	0.0152		0.0646	0.0150	-0.0139	0.0010	-4.39	
	F103…H93-C92	0.0083		0.0394	0.0083	-0.0067	0.0015	-2.12	
	F104…H93-C92	0.0069		0.0274	0.0060	-0.0052	0.0008	-1.63	
G[Btma][DCA]	N101…H83-C82	0.0125	0.0619	0.0377	0.0086	-0.0079	0.0007	-2.48	-12.03
	N101…H81-C78	0.0110		0.0335	0.0075	-0.0067	0.0008	-2.12	
	N103…H77-C74	0.0116		0.0322	0.0077	-0.0073	0.0003	-2.30	
	N103…H84-C82	0.0120		0.0349	0.0079	-0.0072	0.0007	-2.27	
	N103…H80-C78	0.0146		0.0454	0.0102	-0.0090	0.0011	-2.85	
G[Btma][Tf_2N]	O32…H7-C6	0.0082	0.1268	0.0289	0.0066	-0.0060	0.0005	-1.91	-29.03
	O32…H3-C2	0.0160		0.0517	0.0126	-0.0122	0.0003	-3.85	
	O32…H16-C15	0.0110		0.0333	0.0082	-0.0080	0.0001	-2.54	
	O30…H18-C17	0.0130		0.0385	0.0097	-0.0098	-0.0001	-3.10	
	O30…H25-C23	0.0088		0.0296	0.0069	-0.0064	0.0004	-2.02	
	N27…H7-C6	0.0155		0.0449	0.0110	-0.010	0.0002	-3.39	
	N27…H16-C15	0.0148		0.0465	0.0110	-0.0104	0.0005	-3.29	
	N27…H18-C17	0.0087		0.0330	0.0070	-0.0057	0.0012	-1.82	
	N27…H21-C20	0.0086		0.0263	0.0060	-0.0055	0.0005	-1.74	
	F37…H7-C6	0.0059		0.0313	0.0061	-0.0043	0.0017	-1.38	
	F39…H16-C15	0.0087		0.0336	0.0077	-0.0070	0.0006	-2.22	
	F39…H21-C20	0.0072		0.0301	0.0065	-0.0056	0.0009	-1.76	

[a] X in $E_{X...Y}$ is N, O, and F electronegative atoms and Y is H and C atoms.

Table S3. Bond Critical Point Data (in au) obtained from QTAIM analysis for the interactions between $[Bmim]^+$ and $[Btma]^+$ cations of ILs and graphene surface at the M06-2X/cc-pVDZ level of theory.

Structure	BCP	ρ(r)	∑ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	H(r)	[a]$E_{X...Y}$	$\sum E_{X...Y}$
G[bmim][BF_4]	C2…C33	0.0073	0.0309	0.0227	0.0047	-0.0038	0.0009	-1.19	-5.19
	C46…H18	0.0081		0.0263	0.0056	-0.0047	0.0009	-1.49	
	C47…H12	0.0087		0.0300	0.0061	-0.0048	0.0014	-1.51	
	C5…C37	0.0069		0.0178	0.0038	-0.0032	0.0006	-1.01	
G[bmim][PF_6]	C2…C40	0.0089	0.0399	0.0286	0.0059	-0.0046	0.0013	-1.45	-6.83
	C37…H24	0.0086		0.0282	0.0060	-0.0051	0.0009	-1.61	
	C35…H24	0.0087		0.0327	0.0065	-0.0049	0.0016	-1.56	
	C45…H19	0.0082		0.0287	0.0057	-0.0044	0.0014	-1.38	
	C5…C41	0.0055		0.0139	0.0030	-0.0026	0.0004	-0.83	
G[bmim][DCA]	C2…C39	0.0091	0.0431	0.0289	0.0059	-0.0046	0.0013	-1.46	-6.81
	C33…H11	0.0062		0.0217	0.0042	-0.0031	0.0011	-0.98	
	C37…H10	0.0068		0.0238	0.0046	-0.0034	0.0013	-1.05	
	C4…C38	0.0062		0.0172	0.0037	-0.0031	0.0006	-0.97	
	C5…C44	0.0063		0.0172	0.0036	-0.0030	0.0006	-0.94	
	C42…H14	0.0084		0.0301	0.0059	-0.0044	0.0015	-1.38	
G[bmim][Tf_2N]	C43…H14	0.0087	0.0344	0.0281	0.0060	-0.0051	0.0009	-1.61	-5.85
	C46…H21	0.0045		0.0137	0.0028	-0.0022	0.0006	-0.68	
	C44…H20	0.0061		0.0185	0.0038	-0.0031	0.0007	-0.96	
	C60…H6	0.0108		0.0335	0.0072	-0.0062	0.0010	-1.95	
	C87…H10	0.0042		0.0123	0.0025	-0.0020	0.0005	-0.63	
G[Btma][BF_4]	C39…H19	0.0042	0.0227	0.0132	0.0027	-0.0022	0.0005	-0.69	-4.00
	C35…H11	0.0105		0.0362	0.0075	-0.0060	0.0015	-1.89	
	C43…H26	0.0080		0.0251	0.0054	-0.0045	0.0009	-1.41	
G[Btma][PF_6]	C9…H80	0.0091	0.0393	0.0337	0.0067	-0.0050	0.0017	-1.57	-6.87
	C10…H81	0.0093		0.0341	0.0070	-0.0055	0.0015	-1.72	
	C3…H90	0.0060		0.0180	0.0038	-0.0032	0.0006	-1.01	
	C21…H83	0.0069		0.0227	0.0047	-0.0038	0.0009	-1.21	
	C51…H97	0.0078		0.0274	0.0055	-0.0043	0.0013	-1.34	
G[Btma][DCA]	C10…H79	0.0108	0.0295	0.0382	0.0080	-0.0065	0.0015	-2.04	-5.23
	C7…H90	0.0047		0.0145	0.0030	-0.0024	0.0006	-0.75	
	C4…H93	0.0064		0.0202	0.0043	-0.0036	0.0007	-1.12	
	C17…H97	0.0075		0.0241	0.0051	-0.0042	0.0009	-1.31	
G[Btma][Tf_2N]	C44…H18	0.0034	0.0366	0.0105	0.0021	-0.0016	0.0005	-0.50	-6.06
	C43…H9	0.0051		0.0164	0.0034	-0.0028	0.0006	-0.87	
	C66…H11	0.0091		0.0336	0.0068	-0.0053	0.0015	-1.67	
	C58…H19	0.0056		0.0168	0.0035	-0.0028	0.0007	-0.87	
	C61…H25	0.0065		0.0225	0.0044	-0.0032	0.0012	-0.99	
	C87…H26	0.0068		0.0222	0.0046	-0.0037	0.0009	-1.16	

[a] X in $E_{X...Y}$ is C atom and Y is H and C atoms.

Table S4. Bond Critical Point Data (in au) obtained from QTAIM analysis for the interactions between $[BF_4]^-$, $[PF_6]^-$, $[DCA]^-$, and $[Tf_2N]^-$ anions of ILs and graphene surface at the M06-2X/cc-pVDZ level of theory.

Structure	BCP	ρ(r)	∑ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	H(r)	[a]$E_{X\cdots Y}$	$\sum E_{X\cdots Y}$
G[bmim][BF_4]	F20…C36	0.0073	0.0407	0.0314	0.0064	-0.0050	0.0014	-1.57	-8.74
	F22…C56	0.0092		0.0397	0.0082	-0.0065	0.0016	-2.06	
	F23…C56	0.0087		0.0367	0.0075	-0.0058	0.0016	-1.84	
	F20…C56	0.0074		0.0327	0.0066	-0.0051	0.0015	-1.60	
	F20…C57	0.0079		0.0325	0.0067	-0.0053	0.0014	-1.66	
G[bmim][PF_6]	F14…C48	0.0070	0.0313	0.0293	0.0060	-0.0047	0.0012	-1.49	-6.64
	F13…C63	0.0080		0.0329	0.0068	-0.0054	0.0014	-1.70	
	F17…C62	0.0092		0.0378	0.0078	-0.0061	0.0016	-1.93	
	F14…C62	0.0070		0.0297	0.0061	-0.0048	0.0013	-1.50	
G[bmim][DCA]	N30…C53	0.0066	0.0199	0.0213	0.0045	-0.0037	0.0008	-1.16	-3.47
	N30…C54	0.0065		0.0210	0.0044	-0.0036	0.0008	-1.14	
	N30…C73	0.0067		0.0210	0.0044	-0.0037	0.0007	-1.15	
G[bmim][Tf_2N]	O29…C50	0.0091	0.0256	0.0335	0.0072	-0.0060	0.0011	-1.89	-5.56
	F36…C61	0.0075		0.0322	0.0067	-0.0054	0.0013	-1.69	
	F37…C64	0.0089		0.0363	0.0077	-0.0063	0.0013	-1.97	
G[Btma][BF_4]	F30…C53	0.0083	0.0254	0.0356	0.0073	-0.0057	0.0015	-1.80	-5.50
	F28…C41	0.0082		0.0348	0.0071	-0.0056	0.0015	-1.78	
	F29…C53	0.0088		0.0378	0.0077	-0.0061	0.0016	-1.91	
G[Btma][PF_6]	F103…C4	0.0057	0.0313	0.0236	0.0047	-0.0035	0.0011	-1.12	-6.83
	F102…C6	0.0084		0.0365	0.0075	-0.0060	0.0015	-1.89	
	F101…C16	0.0087		0.0367	0.0076	-0.0060	0.0015	-1.90	
	F102…C26	0.0084		0.0370	0.0076	-0.0061	0.0015	-1.91	
G[Btma][DCA]	N99…C44	0.0061	0.0138	0.0189	0.0040	-0.0033	0.0007	-1.04	-2.33
	N101…C46	0.0076		0.0238	0.0050	-0.0041	0.0009	-1.29	
G[Btma][Tf_2N]	F37…C49	0.0084	0.0275	0.0345	0.0056	-0.0043	0.0013	-1.35	-5.57
	F38…C54	0.0100		0.0426	0.0090	-0.0075	0.0015	-2.35	
	O30…C51	0.0090		0.0337	0.0072	-0.0059	0.0012	-1.87	

[a] X in $E_{X\cdots Y}$ is N, O, and F electronegative atoms and Y is C atom.

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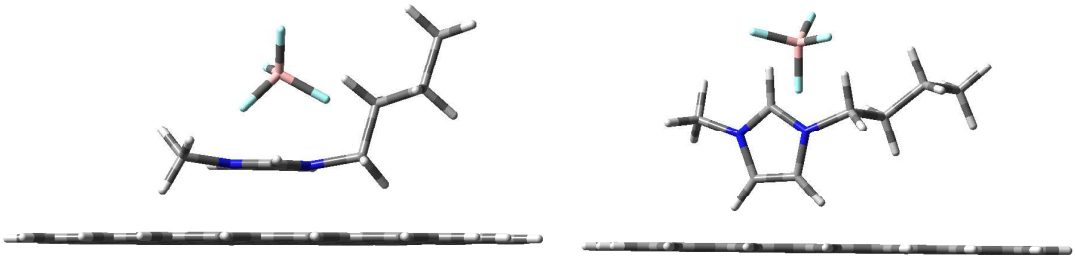
Table S5. Changes in the binding energy (ΔE_b in kcal/mol), enthalpy (ΔH_{ads} in kcal/mol), free energy (ΔG_{ads} in kcal/mol), entropy (ΔS_{ads} in cal/mol.K), translational entropy (ΔS_t in cal/mol.K), rotational entropy (ΔS_r in cal/mol.K), and vibrational entropy (ΔS_v in cal/mol.K) of ILs upon adsorption on the graphene surface

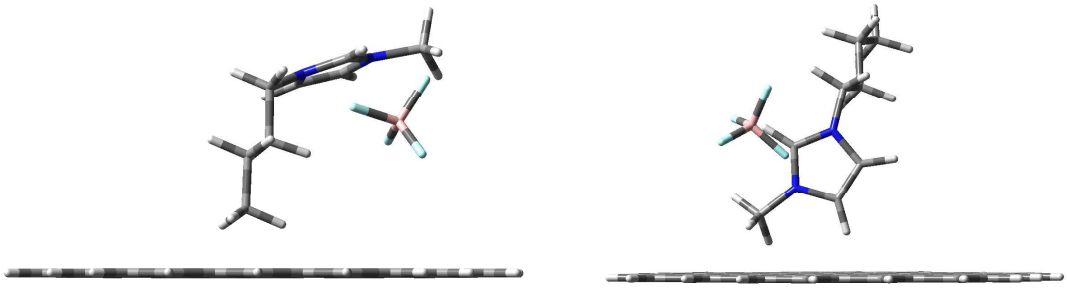
Structure	ΔE_b	ΔH_{ads}	ΔG_{ads}	ΔS_{ads}	ΔS_t	ΔS_r	ΔS_v
[Bmim][BF_4]	-20.54	-20.18	-6.35	-46.41	-41.27	-28.66	23.523
[Bmim][PF_6]	-22.35	-21.69	-9.29	-41.61	-41.77	-29.15	29.307
[Bmim][DCA]	-18.25	-17.78	-5.64	-40.72	-41.06	-28.36	28.697
[Bmim][Tf_2N]	-16.64	-15.73	-5.40	-34.65	-42.53	-30.40	38.283
[Btma][BF_4]	-16.51	-16.05	-2.56	-45.23	-41.04	-28.30	24.105
[Btma][PF_6]	-19.82	-19.24	-6.14	-43.94	-41.59	-29.11	26.757
[Btma][DCA]	-17.30	-16.80	-4.15	-42.45	-40.79	-28.38	26.717
[Btma][Tf_2N]	-17.98	-17.54	-3.22	-48.00	-42.43	-30.45	24.872

G[Bmim][BF_4]1 G[Bmim][BF_4]2



G[Bmim][BF_4]3 G[Bmim][BF_4]4

G[Bmim][BF_4]5 G[Bmim][BF_4]6



G[Bmim][BF_4]7 G[Bmim][BF_4]8

G[Bmim][BF_4]9 G[Bmim][BF_4]10

Figure S1. The initial structures for adsorption of [Bmim][BF_4] ionic liquid on the graphene surface.

XYZ Coordinates

$[BF_4]^-$ SCF energy: -424.410955602

B	-0.000296000	0.000362000	-0.000317000
F	0.323811000	-1.042956000	-0.894920000
F	-1.361190000	0.346262000	-0.152613000
F	0.806787000	1.125512000	-0.277273000
F	0.230757000	-0.429019000	1.324982000

$[PF_6]^-$ SCF energy: -940.489376193

P	0.000000000	0.000000000	0.000000000
F	0.000000000	0.000000000	1.643000000
F	0.000000000	1.643000000	0.000000000
F	0.000000000	0.000000000	-1.643000000
F	-1.643000000	0.000000000	0.000000000
F	0.000000000	-1.643000000	0.000000000
F	1.643000000	0.000000000	0.000000000

$[DCA]^-$ SCF energy: -240.428635030

N	0.000000000	0.000000000	0.733816000
C	0.000000000	1.137562000	0.064829000
N	0.000000000	2.205209000	-0.422476000
C	0.000000000	-1.137562000	0.064829000
N	0.000000000	-2.205209000	-0.422476000

$[Tf_2N]^-$ SCF energy: -1826.90221757

N	0.000000000	0.000000000	1.239493000
S	-0.840595000	1.089169000	0.390218000
S	0.840595000	-1.089169000	0.390218000
O	-1.597183000	1.923070000	1.331572000

O	-1.507516000	0.550429000	-0.808271000
O	1.597183000	-1.923070000	1.331572000
O	1.507516000	-0.550429000	-0.808271000
C	-0.450305000	-2.275746000	-0.309867000
C	0.450305000	2.275746000	-0.309867000
F	0.660320000	2.062908000	-1.602122000
F	1.607945000	2.185588000	0.339450000
F	0.000000000	3.530012000	-0.171652000
F	-1.607945000	-2.185588000	0.339450000
F	0.000000000	-3.530012000	-0.171652000
F	-0.660320000	-2.062908000	-1.602122000

$[Bmim]^+$ SCF energy: -423.006209240

N	-0.485141000	0.185563000	0.489885000
C	-1.411679000	-0.760697000	0.341398000
N	-2.519663000	-0.207275000	-0.155489000
C	-2.293241000	1.139568000	-0.334590000
C	-1.013755000	1.384866000	0.068075000
H	-1.286913000	-1.810831000	0.589841000
H	-3.056598000	1.804137000	-0.725216000
H	-0.442340000	2.306781000	0.095589000
C	-3.770387000	-0.908292000	-0.451739000
H	-3.645291000	-1.968161000	-0.208573000
H	-4.001728000	-0.799368000	-1.517315000
H	-4.576409000	-0.483095000	0.156935000
C	0.897303000	-0.026380000	0.955898000
H	0.911064000	-0.989683000	1.482979000
H	1.110331000	0.760173000	1.692491000
C	1.897717000	-0.005299000	-0.192599000
H	1.629027000	-0.787308000	-0.921876000
H	1.831446000	0.961394000	-0.719199000
C	3.323942000	-0.223764000	0.309864000
H	3.377610000	-1.187320000	0.842854000
H	3.572291000	0.555996000	1.048483000
C	4.338386000	-0.203021000	-0.828177000
H	4.124127000	-0.993226000	-1.562600000

H	5.355972000	-0.361987000	-0.449419000
H	4.321322000	0.762587000	-1.354528000

$[Btma]^{+}$ SCF energy: -331.942534310

N	-1.425337000	-0.006439000	0.000002000
C	-2.477760000	1.056043000	-0.000247000
H	-2.355792000	1.671401000	-0.899131000
H	-2.355734000	1.671890000	0.898296000
H	-3.463754000	0.576889000	-0.000086000
C	-1.594861000	-0.853111000	-1.219676000
H	-1.421598000	-0.230894000	-2.106071000
H	-2.617982000	-1.246811000	-1.228632000
H	-0.877574000	-1.679118000	-1.188246000
C	-1.594971000	-0.852638000	1.219992000
H	-0.877583000	-1.678574000	1.189034000
H	-2.618047000	-1.246464000	1.228926000
H	-1.421947000	-0.230038000	2.106165000
H	-0.066129000	1.323076000	0.889234000
C	-0.069580000	0.676221000	-0.000066000
H	-0.066156000	1.322950000	-0.889457000
C	1.140465000	-0.242136000	-0.000024000
H	1.141309000	-0.891777000	-0.889158000
H	1.141275000	-0.891762000	0.889122000
C	2.424641000	0.595174000	-0.000004000
H	2.427981000	1.253730000	-0.883650000
H	2.427956000	1.253730000	0.883642000
C	3.671801000	-0.281627000	0.000015000
H	4.580393000	0.333479000	0.000030000
H	3.701177000	-0.927096000	-0.889929000
H	3.701152000	-0.927093000	0.889960000

[Bmim][BF_4] SCF energy: -847.578083391

N	-2.334975000	-0.897421000	-0.039838000
C	-1.264417000	-0.641967000	0.708207000
N	-0.369047000	-1.607395000	0.523501000
C	-0.874078000	-2.506663000	-0.392090000
C	-2.112905000	-2.061686000	-0.743097000
C	-3.453642000	0.027420000	-0.203301000
C	1.025324000	-1.520613000	0.979307000
C	1.934341000	-1.093762000	-0.169361000
H	-0.310791000	-3.374667000	-0.715184000
H	-2.846247000	-2.466192000	-1.430923000
H	-3.698920000	0.082416000	-1.269717000
H	-4.322310000	-0.319441000	0.369678000
H	-1.123063000	0.248726000	1.315476000
H	-3.112657000	1.012513000	0.136944000
H	2.085664000	-1.940046000	-0.862424000
H	1.420643000	-0.288419000	-0.714794000
H	1.305193000	-2.493679000	1.407353000
H	1.041299000	-0.757959000	1.766422000
B	-0.180685000	2.004563000	-0.034301000
F	-1.417353000	2.181209000	0.663424000
F	-0.421900000	1.088013000	-1.093542000
F	0.720657000	1.370411000	0.876436000
F	0.317233000	3.198616000	-0.489569000
C	3.274375000	-0.582908000	0.349666000
H	3.752489000	-1.348447000	0.985866000
H	3.072199000	0.294158000	0.984320000
C	4.210078000	-0.190144000	-0.787416000
H	5.159699000	0.207704000	-0.403925000
H	4.440168000	-1.053539000	-1.431001000
H	3.746035000	0.585463000	-1.414469000

[Bmim][PF_6] SCF energy: -1363.64779912

N	1.477187000	-1.662746000	0.468464000
C	1.793873000	-0.403801000	0.758551000
N	2.818042000	-0.028725000	-0.004270000
C	3.163296000	-1.080596000	-0.825083000
C	2.317832000	-2.106977000	-0.529731000
C	3.342447000	1.333158000	-0.060227000
C	0.250405000	-2.335098000	0.925975000
C	-0.804174000	-2.346129000	-0.179087000
C	-2.208577000	-2.545678000	0.382873000
C	-3.262587000	-2.446862000	-0.714065000
P	-0.887926000	1.539086000	-0.026497000
F	-0.835090000	2.736068000	-1.111803000
F	0.439280000	2.167575000	0.762973000
F	-0.869620000	0.291849000	1.087436000
F	0.171278000	0.653406000	-0.957934000
F	-2.134525000	0.813523000	-0.782938000
F	-1.877228000	2.376328000	0.937856000
H	2.564826000	2.004479000	0.321655000
H	4.264117000	1.411580000	0.529218000
H	1.249141000	0.245308000	1.438015000
H	3.969755000	-1.006141000	-1.545289000
H	2.236290000	-3.104394000	-0.946264000
H	0.526482000	-3.344079000	1.263214000
H	-0.109935000	-1.757459000	1.784697000
H	-0.766606000	-1.378734000	-0.699108000
H	-0.568687000	-3.134374000	-0.915270000
H	-2.278913000	-3.516291000	0.904236000
H	-2.387349000	-1.755179000	1.128640000
H	-3.214601000	-1.453091000	-1.182203000
H	-4.273592000	-2.586998000	-0.307413000
H	-3.101857000	-3.208445000	-1.493008000
H	3.541268000	1.580977000	-1.108577000

[Bmim][DCA] SCF energy: -663.582940686

N	-0.444623000	1.286705000	-0.405041000
C	-1.329759000	0.434665000	-0.920724000
N	-2.482562000	0.565840000	-0.265343000
C	-2.321019000	1.504691000	0.724960000
C	-1.042415000	1.965486000	0.632788000
H	-1.104254000	-0.282033000	-1.708991000
H	-3.116472000	1.744026000	1.420485000
H	-0.509588000	2.707806000	1.215482000
C	-3.624109000	-0.332658000	-0.392463000
H	-3.564691000	-0.836177000	-1.363427000
H	-4.549065000	0.252509000	-0.337257000
H	-3.555220000	-1.067564000	0.420830000
C	0.966916000	1.384846000	-0.807305000
H	1.166229000	2.433049000	-1.072990000
H	1.077051000	0.750198000	-1.695421000
C	1.889738000	0.885635000	0.298326000
H	1.906790000	1.605313000	1.135273000
H	1.489649000	-0.062021000	0.691593000
C	3.302961000	0.653717000	-0.228892000
H	3.708824000	1.593263000	-0.642317000
H	3.242339000	-0.067556000	-1.059905000
C	4.226468000	0.114813000	0.857481000
H	4.305201000	0.820439000	1.699021000
H	5.238692000	-0.062644000	0.468977000
H	3.840262000	-0.837607000	1.250173000
N	0.445794000	-2.401575000	0.461605000
C	-0.618528000	-1.889437000	1.051770000
N	-1.547831000	-1.452938000	1.620000000
C	0.646704000	-1.978154000	-0.767179000
N	0.863866000	-1.591264000	-1.856093000

[Bmim][Tf_2N] SCF energy: -2250.05821800

N	-2.319198000	0.185008000	-1.643914000
C	-1.314627000	0.689497000	-2.355356000
N	-1.185944000	1.982845000	-2.070140000
C	-2.109535000	2.310908000	-1.104341000
C	-2.829929000	1.185029000	-0.845352000
H	-0.642768000	0.102497000	-2.973672000
H	-2.147120000	3.299279000	-0.661868000
H	-3.634346000	1.006115000	-0.142042000
C	-0.060430000	2.818645000	-2.470656000
H	0.513825000	2.285066000	-3.235477000
H	0.557559000	2.994385000	-1.580073000
H	-0.433996000	3.764129000	-2.881165000
C	-2.610591000	-1.251315000	-1.522266000
H	-1.879208000	-1.758926000	-2.162739000
H	-3.622144000	-1.437393000	-1.909662000
C	-2.447536000	-1.719958000	-0.075934000
H	-1.634602000	-1.145525000	0.392176000
H	-3.362480000	-1.500649000	0.500472000
C	-2.112186000	-3.205990000	0.010774000
H	-1.180458000	-3.377136000	-0.552535000
H	-2.905616000	-3.800943000	-0.474036000
C	-1.918878000	-3.643782000	1.457513000
H	-1.095222000	-3.072610000	1.910339000
H	-1.668546000	-4.711769000	1.519466000
H	-2.831514000	-3.473539000	2.050217000
N	0.348966000	0.412438000	-0.215180000
S	0.995761000	-1.062485000	-0.419282000
S	0.769483000	1.346543000	1.037848000
O	0.461885000	-1.541258000	-1.716364000
O	0.939453000	-1.960669000	0.739031000
O	0.396722000	2.730136000	0.689291000
O	2.083798000	1.039469000	1.610521000
C	-0.463114000	0.893263000	2.353414000
C	2.825401000	-0.769766000	-0.754862000
F	3.545326000	-1.007987000	0.320828000
F	3.019052000	0.481465000	-1.161428000

F	3.203478000	-1.594517000	-1.725778000
F	-1.706377000	1.109518000	1.908034000
F	-0.262781000	1.644946000	3.427057000
F	-0.353183000	-0.384597000	2.683592000

[Btma][BF_4] SCF energy: -756.511751209

N	1.925429000	-0.633502000	0.001936000
C	1.889648000	-1.855914000	-0.856718000
H	2.198826000	-1.572148000	-1.870043000
H	0.858324000	-2.229024000	-0.850701000
H	2.585818000	-2.594283000	-0.440361000
C	3.319444000	-0.133528000	0.100320000
H	3.697008000	0.066579000	-0.909760000
H	3.935533000	-0.898920000	0.587960000
H	3.326762000	0.786431000	0.694317000
C	1.426262000	-0.997379000	1.366463000
H	1.592733000	-0.148808000	2.037700000
H	2.003947000	-1.865884000	1.706391000
H	0.358090000	-1.228631000	1.287161000
H	0.096351000	-0.106848000	-0.898639000
C	1.033302000	0.407597000	-0.652810000
H	1.545622000	0.673875000	-1.590526000
C	0.743034000	1.639063000	0.183533000
H	1.658049000	2.219301000	0.395451000
H	0.276848000	1.337674000	1.130563000
C	-0.267203000	2.511742000	-0.566059000
H	0.174780000	2.857605000	-1.516459000
H	-1.132708000	1.880385000	-0.817154000
C	-0.709388000	3.704730000	0.271412000
H	-1.423231000	4.331816000	-0.279960000
H	0.146353000	4.336767000	0.557328000
H	-1.204360000	3.361591000	1.192154000
B	-1.970804000	-0.940431000	0.013485000
F	-1.458759000	-0.070072000	1.018978000
F	-3.209574000	-1.426506000	0.348660000

F	-1.015971000	-2.012503000	-0.109015000
F	-1.974510000	-0.238549000	-1.211206000

[Btma][PF_6] SCF energy: -1272.57833666

N	-1.975546000	-1.456778000	-0.001854000
C	-1.156087000	-2.419056000	-0.802661000
H	-0.102439000	-2.129395000	-0.704372000
H	-1.477318000	-2.354111000	-1.849266000
H	-1.327845000	-3.429096000	-0.410610000
C	-1.459660000	-1.454452000	1.403356000
H	-0.450887000	-1.027524000	1.402219000
H	-1.437168000	-2.496035000	1.746465000
H	-2.141323000	-0.866287000	2.026504000
C	-3.397632000	-1.883843000	-0.001317000
H	-3.994949000	-1.124467000	0.516213000
H	-3.480438000	-2.845623000	0.519409000
H	-3.736415000	-1.986944000	-1.038962000
H	-2.464790000	-0.146131000	-1.564324000
C	-1.842890000	-0.091230000	-0.657662000
H	-0.792196000	-0.006536000	-0.953214000
C	-2.226067000	1.095295000	0.204812000
H	-1.625187000	1.091644000	1.123826000
H	-3.296240000	1.084469000	0.476397000
C	-1.889471000	2.380412000	-0.555508000
H	-0.813251000	2.358475000	-0.788811000
H	-2.433771000	2.400513000	-1.514894000
C	-2.220016000	3.625623000	0.258046000
H	-1.964001000	4.538650000	-0.295965000
H	-1.651182000	3.633912000	1.199509000
H	-3.291778000	3.669090000	0.506922000
P	2.004211000	0.046601000	0.008149000
F	1.136205000	-0.314265000	-1.368834000
F	1.494624000	-1.417377000	0.621715000
F	2.771441000	0.367905000	1.395800000

F	0.603088000	0.713180000	0.639898000
F	2.393068000	1.489727000	-0.617863000
F	3.312439000	-0.659466000	-0.626349000

[Btma][DCA] SCF energy: -572.514778607

N	0.092542000	-1.109013000	0.000237000
C	-0.446378000	-2.502182000	-0.007430000
H	-0.077368000	-3.022446000	0.885217000
H	-0.091522000	-3.007390000	-0.914123000
H	-1.543766000	-2.432594000	0.000577000
C	-0.410189000	-0.424398000	1.237493000
H	0.085092000	-0.891881000	2.098272000
H	-1.494177000	-0.582785000	1.280829000
H	-0.202086000	0.649284000	1.173132000
C	-0.398918000	-0.407752000	-1.231111000
H	-0.192092000	0.664879000	-1.142777000
H	-1.481497000	-0.570651000	-1.290969000
H	0.110789000	-0.857082000	-2.093713000
H	1.886787000	-1.793618000	-0.841249000
C	1.595063000	-1.154465000	0.005657000
H	1.880251000	-1.672116000	0.934006000
C	2.276882000	0.200913000	-0.088576000
H	1.877762000	0.892554000	0.669055000
H	2.077546000	0.659649000	-1.069074000
C	3.786863000	0.053643000	0.101564000
H	3.987722000	-0.379477000	1.095746000
H	4.181946000	-0.664871000	-0.636214000
C	4.510671000	1.388156000	-0.036491000
H	5.592003000	1.271427000	0.115943000
H	4.138663000	2.113603000	0.701849000
H	4.353361000	1.820022000	-1.035887000
N	-3.473015000	1.437639000	-0.000923000
C	-2.270890000	1.980179000	0.017088000
N	-1.205377000	2.473772000	0.033107000

C	-3.459648000	0.124241000	-0.007632000
N	-3.441315000	-1.051900000	-0.014421000

[Btma][Tf_2N] SCF energy: -2158.99006130

N	-3.051727000	-0.525146000	-1.022665000
C	-3.401978000	0.541119000	-2.008085000
H	-2.518053000	1.180169000	-2.130098000
H	-4.251979000	1.112414000	-1.615731000
H	-3.671594000	0.062883000	-2.957728000
C	-1.927923000	-1.332146000	-1.594764000
H	-1.119518000	-0.642107000	-1.853855000
H	-2.312844000	-1.852655000	-2.480794000
H	-1.576891000	-2.048126000	-0.846103000
C	-4.226234000	-1.404682000	-0.793289000
H	-3.927094000	-2.239778000	-0.151441000
H	-4.575729000	-1.783686000	-1.761130000
H	-5.017610000	-0.820426000	-0.307525000
H	-3.512946000	0.784578000	0.542050000
C	-2.644744000	0.164982000	0.268884000
H	-1.811770000	0.820616000	-0.005479000
C	-2.253958000	-0.751092000	1.412487000
H	-1.418824000	-1.407242000	1.127171000
H	-3.107482000	-1.372402000	1.732971000
C	-1.779774000	0.099490000	2.594309000
H	-0.888317000	0.660152000	2.273508000
H	-2.555329000	0.842783000	2.850494000
C	-1.444590000	-0.758292000	3.808208000
H	-1.120424000	-0.133928000	4.652129000
H	-0.628333000	-1.450162000	3.559550000
H	-2.319633000	-1.341682000	4.135897000
N	0.437415000	0.018070000	-0.049362000
S	1.581590000	-0.870643000	0.691938000
S	0.806703000	1.301956000	-0.960740000

O	0.901267000	-1.644263000	1.742161000
O	2.852160000	-0.198120000	0.955614000
O	-0.387379000	1.542936000	-1.808611000
O	2.139741000	1.362940000	-1.554524000
C	0.724707000	2.678208000	0.284126000
C	1.929209000	-2.134051000	-0.625174000
F	2.296707000	-1.547170000	-1.755384000
F	0.817411000	-2.845481000	-0.865949000
F	2.883108000	-2.963228000	-0.227938000
F	-0.529863000	2.782793000	0.742626000
F	1.065451000	3.827811000	-0.279992000
F	1.525772000	2.428382000	1.307060000

Graphene SCF energy: -2068.41647517

C	0.000000000	1.226629000	3.553263000
C	0.000000000	0.000000000	2.846060000
C	0.000000000	0.000000000	1.415091000
C	0.000000000	1.225548000	0.707573000
C	0.000000000	2.464694000	1.423045000
C	0.000000000	2.463774000	2.839033000
C	0.000000000	-1.225548000	0.707573000
C	0.000000000	1.225548000	-0.707573000
C	0.000000000	0.000000000	-1.415091000
C	0.000000000	-1.225548000	-0.707573000
C	0.000000000	0.000000000	-2.846060000
C	0.000000000	1.226629000	-3.553263000
C	0.000000000	2.463774000	-2.839033000
C	0.000000000	2.464694000	-1.423045000
C	0.000000000	3.690509000	-0.714345000
C	0.000000000	3.690509000	0.714345000
C	0.000000000	-1.226629000	3.553263000
C	0.000000000	-2.463774000	2.839033000
C	0.000000000	-2.464694000	1.423045000
C	0.000000000	-3.690509000	0.714345000
C	0.000000000	-3.690509000	-0.714345000

C	0.000000000	-2.464694000	-1.423045000
C	0.000000000	-1.226629000	-3.553263000
C	0.000000000	-2.463774000	-2.839033000
C	0.000000000	1.221663000	4.977395000
C	0.000000000	3.699443000	3.546894000
C	0.000000000	3.663349000	4.987713000
C	0.000000000	2.487167000	5.666610000
C	0.000000000	4.900396000	2.829486000
C	0.000000000	4.921339000	1.430746000
C	0.000000000	6.151026000	0.679046000
C	0.000000000	6.151026000	-0.679046000
C	0.000000000	4.921339000	-1.430746000
C	0.000000000	3.699443000	-3.546894000
C	0.000000000	4.900396000	-2.829486000
C	0.000000000	1.221663000	-4.977395000
C	0.000000000	3.663349000	-4.987713000
C	0.000000000	2.487167000	-5.666610000
C	0.000000000	-1.221663000	-4.977395000
C	0.000000000	0.000000000	-5.658617000
C	0.000000000	-3.699443000	-3.546894000
C	0.000000000	-3.663349000	-4.987713000
C	0.000000000	-2.487167000	-5.666610000
C	0.000000000	-4.921339000	-1.430746000
C	0.000000000	-4.900396000	-2.829486000
C	0.000000000	-4.921339000	1.430746000
C	0.000000000	-6.151026000	0.679046000
C	0.000000000	-6.151026000	-0.679046000
C	0.000000000	-3.699443000	3.546894000
C	0.000000000	-4.900396000	2.829486000
C	0.000000000	-1.221663000	4.977395000
C	0.000000000	-2.487167000	5.666610000
C	0.000000000	-3.663349000	4.987713000
C	0.000000000	0.000000000	5.658617000
H	0.000000000	4.611773000	5.527652000
H	0.000000000	5.846031000	3.376387000
H	0.000000000	7.092074000	1.231635000
H	0.000000000	7.092074000	-1.231635000

H	0.000000000	5.846031000	-3.376387000
H	0.000000000	4.611773000	-5.527652000
H	0.000000000	2.479612000	-6.757834000
H	0.000000000	0.000000000	-6.750942000
H	0.000000000	-2.479612000	-6.757834000
H	0.000000000	-4.611773000	-5.527652000
H	0.000000000	-5.846031000	-3.376387000
H	0.000000000	-7.092074000	-1.231635000
H	0.000000000	-7.092074000	1.231635000
H	0.000000000	-5.846031000	3.376387000
H	0.000000000	-4.611773000	5.527652000
H	0.000000000	-2.479612000	6.757834000
H	0.000000000	0.000000000	6.750942000
H	0.000000000	2.479612000	6.757834000

G[Bmim][BF_4] SCF energy: -2916.02807560

N	0.363162000	-2.158556000	2.168893000
C	1.195048000	-1.145588000	1.921120000
N	0.540511000	-0.001738000	2.113767000
C	-0.753258000	-0.288922000	2.486913000
C	-0.867698000	-1.649521000	2.523048000
C	0.770190000	-3.561248000	2.132346000
C	1.184366000	1.319369000	2.008246000
C	2.185418000	1.546492000	3.132972000
H	-1.485195000	0.491169000	2.667327000
H	-1.715690000	-2.288398000	2.744664000
H	0.926915000	-3.921062000	3.157343000
H	-0.006698000	-4.153761000	1.634013000
H	2.231016000	-1.254207000	1.592615000
H	1.711702000	-3.621389000	1.569879000
H	1.661074000	1.678745000	4.094721000
H	2.829571000	0.656497000	3.207675000
H	0.377818000	2.066247000	1.985056000
H	1.717748000	1.335557000	1.051091000
B	4.547311000	-0.866346000	1.458388000
F	3.846282000	-2.073470000	1.125122000
F	4.680731000	-0.786939000	2.846809000
F	3.701096000	0.214278000	1.040516000
F	5.760141000	-0.815806000	0.791714000
C	3.079705000	2.745032000	2.827134000
H	2.477884000	3.669440000	2.781944000
H	3.521346000	2.590305000	1.829103000
C	4.194514000	2.878418000	3.858496000
H	4.848874000	3.732088000	3.633312000
H	3.785648000	3.022022000	4.870932000
H	4.807830000	1.965182000	3.863621000
C	2.054698000	-2.220832000	-1.401258000
C	0.658362000	-2.293821000	-1.174390000
C	-0.110262000	-1.091126000	-1.048098000
C	0.526005000	0.168664000	-1.171204000
C	1.934544000	0.237931000	-1.409704000
C	2.693855000	-0.951161000	-1.522179000

C	-1.492255000	-1.160789000	-0.749755000
C	-0.223353000	1.358579000	-0.998004000
C	-1.605545000	1.287799000	-0.696736000
C	-2.239914000	0.028571000	-0.571508000
C	-2.355913000	2.490524000	-0.492815000
C	-1.716241000	3.749980000	-0.598921000
C	-0.319258000	3.820230000	-0.891245000
C	0.425270000	2.631284000	-1.087268000
C	1.819351000	2.697750000	-1.332051000
C	2.576900000	1.496902000	-1.487469000
C	0.029415000	-3.552693000	-1.016105000
C	-1.365363000	-3.623440000	-0.712172000
C	-2.123473000	-2.433706000	-0.575470000
C	-3.497813000	-2.503489000	-0.237414000
C	-4.254729000	-1.302742000	-0.069723000
C	-3.628368000	-0.042298000	-0.231193000
C	-3.734960000	2.419354000	-0.176378000
C	-4.373191000	1.148231000	-0.042404000
C	2.825174000	-3.417068000	-1.481239000
C	4.100285000	-0.877547000	-1.711828000
C	4.853145000	-2.101551000	-1.783103000
C	4.246134000	-3.310420000	-1.682963000
C	4.716958000	0.373985000	-1.786292000
C	3.985303000	1.559082000	-1.680496000
C	4.611648000	2.854740000	-1.736730000
C	3.891171000	3.998894000	-1.604229000
C	2.466749000	3.966116000	-1.388425000
C	0.332936000	5.083620000	-0.969722000
C	1.709163000	5.129899000	-1.217771000
C	-2.467791000	4.943874000	-0.398799000
C	-0.455590000	6.274235000	-0.775695000
C	-1.785576000	6.208568000	-0.506990000
C	-4.478526000	3.618569000	0.019181000
C	-3.831784000	4.853126000	-0.100008000
C	-5.756821000	1.072338000	0.289016000
C	-6.486138000	2.302595000	0.469128000
C	-5.879257000	3.510714000	0.340683000

C	-5.637265000	-1.368340000	0.268011000
C	-6.359586000	-0.181764000	0.434663000
C	-4.118436000	-3.772538000	-0.051984000
C	-5.520032000	-3.807579000	0.282618000
C	-6.241447000	-2.666359000	0.432284000
C	-1.991664000	-4.887839000	-0.506848000
C	-3.353809000	-4.936059000	-0.189792000
C	0.805695000	-4.744279000	-1.104036000
C	0.142618000	-6.007861000	-0.903410000
C	-1.184836000	-6.077409000	-0.619951000
C	2.182191000	-4.651824000	-1.337823000
H	5.935579000	-2.030984000	-1.892964000
H	5.801969000	0.422452000	-1.892817000
H	5.692198000	2.896032000	-1.883771000
H	4.384592000	4.971479000	-1.648757000
H	2.208427000	6.100505000	-1.269529000
H	0.045836000	7.241188000	-0.848323000
H	-2.365178000	7.121997000	-0.361263000
H	-4.404867000	5.771217000	0.050612000
H	-6.447036000	4.432151000	0.482840000
H	-7.547690000	2.241922000	0.715826000
H	-7.420568000	-0.234886000	0.690276000
H	-7.302141000	-2.712021000	0.686119000
H	-5.993950000	-4.781826000	0.415708000
H	-3.830986000	-5.907630000	-0.040571000
H	-1.667262000	-7.044623000	-0.467207000
H	0.738527000	-6.919729000	-0.976046000
H	2.774608000	-5.568292000	-1.392732000
H	4.831638000	-4.230077000	-1.724274000

G[Bmim][PF_6] SCF energy: -3432.10069635

N	-0.721979000	0.220106000	1.668214000
C	0.460148000	-0.385197000	1.749246000
N	1.397748000	0.528852000	1.988563000
C	0.799834000	1.771801000	2.044960000
C	-0.535339000	1.574753000	1.844164000
C	2.791204000	0.194892000	2.270882000
C	-1.990840000	-0.513173000	1.532974000
C	-2.513236000	-1.035076000	2.865177000
C	-3.564060000	-2.117581000	2.626070000
C	-4.017734000	-2.760578000	3.931672000
P	0.454149000	-3.710885000	3.048284000
F	1.482588000	-4.238703000	4.179123000
F	1.721169000	-3.112738000	2.146829000
F	-0.573364000	-3.118926000	1.867299000
F	0.371149000	-2.233570000	3.795821000
F	-0.840499000	-4.213546000	3.894903000
F	0.540979000	-5.126234000	2.246751000
H	2.951632000	-0.849913000	1.973806000
H	3.453161000	0.859742000	1.702567000
H	0.638973000	-1.450065000	1.628488000
H	1.370917000	2.678836000	2.207641000
H	-1.359366000	2.277977000	1.794102000
H	-2.700168000	0.153727000	1.022216000
H	-1.777857000	-1.368302000	0.881688000
H	-1.672295000	-1.474033000	3.421090000
H	-2.927915000	-0.209926000	3.468677000
H	-4.424328000	-1.695438000	2.076928000
H	-3.113322000	-2.889566000	1.979858000
H	-3.161749000	-3.246381000	4.421893000
H	-4.787333000	-3.524419000	3.752978000
H	-4.437319000	-2.011935000	4.621706000
H	2.971989000	0.296606000	3.348340000
C	-2.767122000	-2.393779000	-1.440517000
C	-2.810829000	-0.996078000	-1.669099000
C	-1.602340000	-0.228726000	-1.634726000
C	-0.361615000	-0.871840000	-1.401492000

C	-0.320042000	-2.283459000	-1.168129000
C	-1.518794000	-3.037426000	-1.179220000
C	-1.655770000	1.180740000	-1.765545000
C	0.827693000	-0.105906000	-1.317729000
C	0.772125000	1.303420000	-1.441840000
C	-0.469629000	1.947272000	-1.664086000
C	1.965363000	2.082203000	-1.300669000
C	3.202997000	1.440186000	-1.047355000
C	3.258763000	0.017605000	-0.920165000
C	2.075606000	-0.752239000	-1.038293000
C	2.114528000	-2.151246000	-0.816820000
C	0.911232000	-2.917783000	-0.873715000
C	-4.054637000	-0.348960000	-1.871215000
C	-4.105872000	1.070231000	-2.030722000
C	-2.914566000	1.834287000	-1.964831000
C	-2.969718000	3.245248000	-2.079861000
C	-1.772942000	4.018551000	-1.974787000
C	-0.529553000	3.374398000	-1.758681000
C	1.904679000	3.494924000	-1.391763000
C	0.653014000	4.143306000	-1.626719000
C	-3.977038000	-3.146991000	-1.429142000
C	-1.478645000	-4.430143000	-0.887719000
C	-2.717587000	-5.165491000	-0.884837000
C	-3.903609000	-4.558708000	-1.148744000
C	-0.253716000	-5.036234000	-0.598926000
C	0.940238000	-4.310195000	-0.589744000
C	2.202247000	-4.924371000	-0.271804000
C	3.350297000	-4.202747000	-0.238662000
C	3.349506000	-2.786191000	-0.496419000
C	4.492001000	-0.626877000	-0.613720000
C	4.512897000	-2.012000000	-0.415739000
C	4.384224000	2.221732000	-0.883365000
C	5.672623000	0.187658000	-0.472232000
C	5.622218000	1.539650000	-0.599193000
C	3.093176000	4.266203000	-1.240723000
C	4.305755000	3.614902000	-0.989250000
C	0.588629000	5.563295000	-1.723355000

C	1.809239000	6.315779000	-1.578702000
C	2.997709000	5.700411000	-1.347461000
C	-1.826504000	5.438832000	-2.075726000
C	-0.646577000	6.180133000	-1.950419000
C	-4.223284000	3.889868000	-2.286448000
C	-4.244187000	5.326546000	-2.399336000
C	-3.106888000	6.061966000	-2.298916000
C	-5.355789000	1.724501000	-2.230943000
C	-5.387027000	3.117243000	-2.362998000
C	-5.255882000	-1.114246000	-1.885847000
C	-6.502994000	-0.427021000	-2.107839000
C	-6.550564000	0.919906000	-2.276065000
C	-5.191718000	-2.494859000	-1.667135000
H	-2.680918000	-6.231880000	-0.656842000
H	-0.229908000	-6.096128000	-0.340414000
H	2.208228000	-5.987981000	-0.032213000
H	4.297571000	-4.679811000	0.016492000
H	5.458729000	-2.499860000	-0.169136000
H	6.617859000	-0.310186000	-0.248570000
H	6.526512000	2.139544000	-0.482458000
H	5.214372000	4.209500000	-0.868903000
H	3.911394000	6.287341000	-1.238253000
H	1.756823000	7.403041000	-1.657930000
H	-0.691406000	7.268918000	-2.027759000
H	-3.143058000	7.149451000	-2.383531000
H	-5.205353000	5.816258000	-2.565207000
H	-6.346848000	3.615082000	-2.519157000
H	-7.505204000	1.422881000	-2.439434000
H	-7.419567000	-1.018977000	-2.132799000
H	-6.116332000	-3.076639000	-1.665281000
H	-4.832371000	-5.131492000	-1.138831000

G[Bmim][DCA] SCF energy: -2732.03003542

N	1.908100000	0.985093000	1.644594000
C	1.325705000	-0.213449000	1.659366000
N	0.078577000	-0.081629000	2.106784000
C	-0.145395000	1.245903000	2.397915000
C	1.005103000	1.917582000	2.106449000
H	1.813774000	-1.136630000	1.343644000
H	-1.100432000	1.597544000	2.771883000
H	1.251231000	2.972215000	2.166532000
C	-0.808016000	-1.196900000	2.427164000
H	-0.515695000	-2.057031000	1.812674000
H	-1.841252000	-0.912647000	2.189658000
H	-0.667948000	-1.445102000	3.487353000
C	3.327725000	1.206649000	1.334187000
H	3.404079000	2.177802000	0.823267000
H	3.623602000	0.408515000	0.638782000
C	4.195046000	1.141239000	2.584326000
H	4.013834000	2.023006000	3.222724000
H	3.909265000	0.254362000	3.171244000
C	5.670924000	1.036692000	2.209776000
H	5.980222000	1.938088000	1.651638000
H	5.787726000	0.177455000	1.528543000
C	6.551139000	0.840563000	3.438302000
H	6.447804000	1.681070000	4.142168000
H	7.611956000	0.758704000	3.162956000
H	6.262901000	-0.080655000	3.966934000
N	3.726876000	-2.318048000	3.484204000
C	2.565036000	-1.896851000	3.954496000
N	1.551461000	-1.516714000	4.405493000
C	3.871200000	-2.142645000	2.188143000
N	4.025495000	-1.971666000	1.034466000
C	-4.377947000	0.977817000	0.106858000
C	-3.616684000	-0.186315000	-0.160125000
C	-2.244858000	-0.069414000	-0.554974000
C	-1.648447000	1.208968000	-0.671614000
C	-2.413069000	2.383577000	-0.380941000
C	-3.772805000	2.267506000	0.000201000

C	-1.475484000	-1.234122000	-0.792973000
C	-0.287183000	1.323881000	-1.044668000
C	0.480556000	0.160012000	-1.290123000
C	-0.109459000	-1.119779000	-1.147356000
C	1.871075000	0.273679000	-1.613113000
C	2.469368000	1.553321000	-1.716639000
C	1.696002000	2.727763000	-1.463454000
C	0.324642000	2.615234000	-1.125716000
C	-0.431078000	3.776636000	-0.831866000
C	-1.806557000	3.660757000	-0.462240000
C	-4.206875000	-1.466754000	-0.021911000
C	-3.427660000	-2.641814000	-0.253403000
C	-2.066152000	-2.527626000	-0.626238000
C	-1.279911000	-3.692125000	-0.805496000
C	0.104928000	-3.575997000	-1.136193000
C	0.689309000	-2.297024000	-1.308455000
C	2.659043000	-0.892446000	-1.769011000
C	2.067294000	-2.181686000	-1.611213000
C	-5.743870000	0.856709000	0.492521000
C	-4.530043000	3.439404000	0.286564000
C	-5.911955000	3.286699000	0.666290000
C	-6.488606000	2.060816000	0.761769000
C	-3.914325000	4.692341000	0.196628000
C	-2.570061000	4.826658000	-0.166562000
C	-1.921047000	6.110637000	-0.251429000
C	-0.611505000	6.220574000	-0.594649000
C	0.187096000	5.058580000	-0.893600000
C	2.308840000	4.013752000	-1.510060000
C	1.541736000	5.150502000	-1.231015000
C	3.860163000	1.660200000	-2.003010000
C	3.711932000	4.092620000	-1.830820000
C	4.447870000	2.974379000	-2.064671000
C	4.049985000	-0.776561000	-2.050910000
C	4.618398000	0.496077000	-2.169631000
C	2.864092000	-3.353302000	-1.742456000
C	4.264605000	-3.204045000	-2.038791000
C	4.828413000	-1.979827000	-2.186163000

C	0.906892000	-4.743154000	-1.281967000
C	2.267223000	-4.607174000	-1.579655000
C	-1.869471000	-4.977403000	-0.632130000
C	-1.037688000	-6.141586000	-0.803684000
C	0.281441000	-6.029469000	-1.107814000
C	-4.011280000	-3.931044000	-0.092724000
C	-3.223046000	-5.069584000	-0.290236000
C	-5.574117000	-1.578044000	0.362970000
C	-6.142931000	-2.895254000	0.498103000
C	-5.400401000	-4.012032000	0.282919000
C	-6.313990000	-0.415841000	0.606103000
H	-6.490354000	4.187243000	0.880383000
H	-4.497355000	5.588783000	0.420569000
H	-2.510041000	7.001798000	-0.027361000
H	-0.135682000	7.201340000	-0.652092000
H	2.014567000	6.134680000	-1.274367000
H	4.176537000	5.079353000	-1.876664000
H	5.511926000	3.051954000	-2.295748000
H	5.687369000	0.582568000	-2.377879000
H	5.894846000	-1.882880000	-2.394689000
H	4.870768000	-4.106968000	-2.126731000
H	2.881874000	-5.505004000	-1.677078000
H	0.898914000	-6.922246000	-1.222210000
H	-1.493176000	-7.124634000	-0.672383000
H	-3.672923000	-6.056719000	-0.160706000
H	-5.846399000	-5.001500000	0.398323000
H	-7.192373000	-2.975884000	0.787055000
H	-7.362049000	-0.503884000	0.902023000
H	-7.536278000	1.965279000	1.052678000

G[Bmim][Tf_2N] SCF energy: -4318.50207088

N	-2.278403000	-2.564332000	0.577106000
C	-2.843109000	-1.667744000	-0.225652000
N	-4.163955000	-1.726764000	-0.082588000
C	-4.458153000	-2.664013000	0.881318000
C	-3.273250000	-3.198930000	1.288021000
H	-2.301089000	-0.936702000	-0.818707000
H	-5.472558000	-2.837748000	1.219435000
H	-3.055914000	-3.952668000	2.035395000
C	-5.091948000	-0.749363000	-0.634447000
H	-4.543551000	-0.116212000	-1.342625000
H	-5.479254000	-0.148620000	0.199571000
H	-5.907252000	-1.266635000	-1.154600000
C	-0.832632000	-2.642022000	0.818432000
H	-0.384974000	-1.925132000	0.120866000
H	-0.485062000	-3.653653000	0.560203000
C	-0.469467000	-2.236261000	2.243420000
H	-1.146597000	-1.428910000	2.555563000
H	-0.624717000	-3.075456000	2.942776000
C	0.971201000	-1.735612000	2.311107000
H	1.073893000	-0.918290000	1.577906000
H	1.667077000	-2.537957000	2.004427000
C	1.325049000	-1.213285000	3.697998000
H	0.664483000	-0.373568000	3.962879000
H	2.363656000	-0.855318000	3.732544000
H	1.208756000	-1.995954000	4.463774000
N	-3.082779000	0.165850000	1.797150000
S	-1.794685000	1.123577000	1.588967000
S	-4.152136000	0.400925000	2.996226000
O	-0.916385000	0.427245000	0.619194000
O	-1.212188000	1.732425000	2.785374000
O	-5.389915000	-0.292940000	2.594782000
O	-4.204266000	1.748174000	3.564880000
C	-3.446820000	-0.660143000	4.349970000
C	-2.507332000	2.513030000	0.576825000
F	-3.555079000	3.056145000	1.174136000
F	-2.901009000	2.024835000	-0.606699000

F	-1.586795000	3.446124000	0.369510000
F	-3.449538000	-1.945474000	3.983677000
F	-4.179857000	-0.531658000	5.447627000
F	-2.195884000	-0.303044000	4.614361000
C	2.734290000	-3.475279000	-0.833966000
C	1.695250000	-2.733825000	-1.448597000
C	1.704962000	-1.303643000	-1.389477000
C	2.750342000	-0.631485000	-0.711985000
C	3.801219000	-1.380958000	-0.094988000
C	3.794784000	-2.795462000	-0.159724000
C	0.649138000	-0.562257000	-1.972438000
C	2.739178000	0.780502000	-0.620310000
C	1.683998000	1.520011000	-1.205376000
C	0.639390000	0.849204000	-1.882097000
C	1.663196000	2.945737000	-1.093392000
C	2.704930000	3.617105000	-0.408087000
C	3.772646000	2.871306000	0.177421000
C	3.787959000	1.458994000	0.077805000
C	4.835121000	0.717710000	0.676605000
C	4.840058000	-0.708122000	0.593421000
C	0.623700000	-3.408845000	-2.084146000
C	-0.452398000	-2.662069000	-2.655605000
C	-0.434317000	-1.245154000	-2.611515000
C	-1.514301000	-0.505124000	-3.157886000
C	-1.515870000	0.920717000	-3.076942000
C	-0.445605000	1.594631000	-2.439392000
C	0.596240000	3.683700000	-1.658209000
C	-0.464652000	3.005283000	-2.331419000
C	2.707244000	-4.899237000	-0.873745000
C	4.837127000	-3.537411000	0.465705000
C	4.792275000	-4.976004000	0.393570000
C	3.780554000	-5.623155000	-0.240261000
C	5.860473000	-2.854739000	1.132192000
C	5.882873000	-1.458089000	1.209253000
C	6.926874000	-0.742828000	1.898719000
C	6.924721000	0.613308000	1.972970000
C	5.877469000	1.397645000	1.369261000

C	4.819501000	3.543090000	0.871425000
C	5.850265000	2.793904000	1.448600000
C	2.677562000	5.036185000	-0.294305000
C	4.771425000	4.980531000	0.960020000
C	3.753194000	5.689398000	0.407832000
C	0.569931000	5.101017000	-1.527886000
C	1.611977000	5.747879000	-0.855177000
C	-1.555417000	3.743132000	-2.873758000
C	-1.552990000	5.176808000	-2.731001000
C	-0.543529000	5.821255000	-2.091595000
C	-2.604979000	1.666403000	-3.612185000
C	-2.598235000	3.061066000	-3.508675000
C	-2.615146000	-1.191613000	-3.749660000
C	-3.699827000	-0.410664000	-4.289276000
C	-3.691477000	0.947292000	-4.227594000
C	-1.559110000	-3.338424000	-3.247223000
C	-2.615588000	-2.591055000	-3.778923000
C	0.598509000	-4.832846000	-2.107639000
C	-0.522632000	-5.488424000	-2.732817000
C	-1.548952000	-4.779356000	-3.270234000
C	1.642765000	-5.547482000	-1.510392000
H	5.595585000	-5.540155000	0.871100000
H	6.659497000	-3.426448000	1.610239000
H	7.726041000	-1.320194000	2.367134000
H	7.722807000	1.138389000	2.500787000
H	6.650971000	3.312516000	1.981002000
H	5.576384000	5.492026000	1.490630000
H	3.729122000	6.777482000	0.490083000
H	1.588677000	6.835847000	-0.758461000
H	-0.560418000	6.907584000	-1.987570000
H	-2.391143000	5.738041000	-3.148227000
H	-3.435505000	3.630349000	-3.919548000
H	-4.520151000	1.523186000	-4.644535000
H	-4.533415000	-0.938125000	-4.757193000
H	-3.460763000	-3.113542000	-4.233696000
H	-2.392094000	-5.293517000	-3.735143000
H	-0.532574000	-6.579630000	-2.758778000

H	1.622189000	-6.639633000	-1.533684000
H	3.760524000	-6.713740000	-0.279022000

G[Btma][BF_4] SCF energy: -2824.95618659

N	0.196623000	0.786885000	3.554506000
C	-1.005840000	0.267982000	4.275196000
H	-0.711694000	0.023782000	5.303475000
H	-1.356434000	-0.631207000	3.755057000
H	-1.771495000	1.053676000	4.270020000
C	0.586098000	2.103259000	4.119671000
H	0.725388000	1.996610000	5.202168000
H	-0.210432000	2.827302000	3.909952000
H	1.518497000	2.432537000	3.646776000
C	-0.144400000	0.956162000	2.109083000
H	0.679032000	1.492506000	1.627334000
H	-1.068765000	1.545512000	2.043934000
H	-0.289368000	-0.037835000	1.667605000
H	0.873044000	-1.204402000	3.655836000
C	1.329298000	-0.209233000	3.729923000
H	1.690422000	-0.054525000	4.758843000
C	2.461308000	-0.085370000	2.725065000
H	2.847225000	0.947490000	2.658049000
H	2.097576000	-0.387323000	1.730123000
C	3.594973000	-1.023839000	3.139312000
H	3.954923000	-0.744041000	4.144584000
H	3.187082000	-2.044549000	3.216370000
C	4.748703000	-1.001731000	2.145172000
H	5.573985000	-1.646830000	2.477999000
H	5.143741000	0.018402000	2.013120000
H	4.415563000	-1.361762000	1.161728000
B	-0.690444000	-2.631383000	2.138595000
F	0.548856000	-2.154169000	1.615151000
F	-1.000763000	-3.878865000	1.636463000
F	-1.685188000	-1.671067000	1.800486000

F	-0.578403000	-2.656287000	3.552832000
C	-1.846962000	3.637375000	-0.613717000
C	-2.215417000	2.271316000	-0.688046000
C	-1.208519000	1.264715000	-0.840299000
C	0.156215000	1.635133000	-0.911968000
C	0.528957000	3.014401000	-0.820885000
C	-0.469071000	4.010883000	-0.678599000
C	-1.573592000	-0.103172000	-0.878018000
C	1.154891000	0.636377000	-1.017334000
C	0.787774000	-0.729774000	-1.063623000
C	-0.576249000	-1.100055000	-0.997037000
C	1.797479000	-1.737192000	-1.168713000
C	3.161944000	-1.367151000	-1.231137000
C	3.535328000	0.009943000	-1.159432000
C	2.537223000	1.008903000	-1.047805000
C	2.905692000	2.374132000	-0.962188000
C	1.898014000	3.381534000	-0.847914000
C	-3.579062000	1.898187000	-0.595245000
C	-3.946485000	0.518366000	-0.643522000
C	-2.949749000	-0.478180000	-0.777532000
C	-3.311965000	-1.845546000	-0.810432000
C	-2.305629000	-2.848844000	-0.937621000
C	-0.944010000	-2.479300000	-1.027632000
C	1.429206000	-3.102879000	-1.212084000
C	0.054238000	-3.474416000	-1.138916000
C	-2.853292000	4.634874000	-0.463737000
C	-0.092921000	5.382362000	-0.590994000
C	-1.133851000	6.369877000	-0.452271000
C	-2.443592000	6.014621000	-0.391773000
C	1.262662000	5.725946000	-0.637266000
C	2.263833000	4.755613000	-0.757459000
C	3.664412000	5.093814000	-0.791926000
C	4.621914000	4.136335000	-0.901184000
C	4.282771000	2.738236000	-0.989659000
C	4.909717000	0.384453000	-1.196672000
C	5.254218000	1.738052000	-1.107512000
C	4.163391000	-2.373876000	-1.350306000

C	5.899679000	-0.654928000	-1.324757000
C	5.543750000	-1.964125000	-1.402361000
C	2.436774000	-4.102997000	-1.326795000
C	3.780204000	-3.718318000	-1.397722000
C	-0.316879000	-4.846869000	-1.170135000
C	0.722469000	-5.837123000	-1.285153000
C	2.031857000	-5.484914000	-1.361940000
C	-2.667464000	-4.223699000	-0.965687000
C	-1.667781000	-5.193567000	-1.084026000
C	-4.683878000	-2.214523000	-0.714620000
C	-5.021787000	-3.614726000	-0.748995000
C	-4.062459000	-4.568656000	-0.867278000
C	-5.316121000	0.140404000	-0.547678000
C	-5.656031000	-1.215814000	-0.587625000
C	-4.578361000	2.903415000	-0.447584000
C	-5.956367000	2.491020000	-0.360288000
C	-6.305303000	1.179068000	-0.408821000
C	-4.195522000	4.248117000	-0.387815000
H	-0.843843000	7.420872000	-0.396371000
H	1.546816000	6.779327000	-0.574752000
H	3.941642000	6.147962000	-0.729687000
H	5.677872000	4.412825000	-0.927045000
H	6.309379000	2.021362000	-1.134721000
H	6.951687000	-0.365117000	-1.357478000
H	6.307418000	-2.737962000	-1.500642000
H	4.550518000	-4.488017000	-1.488441000
H	2.807316000	-6.248141000	-1.448900000
H	0.432298000	-6.889239000	-1.304990000
H	-1.948860000	-6.249174000	-1.099065000
H	-4.334266000	-5.625705000	-0.885346000
H	-6.074365000	-3.893675000	-0.672645000
H	-6.707811000	-1.503126000	-0.513730000
H	-7.354517000	0.884979000	-0.340378000
H	-6.720341000	3.262855000	-0.251076000
H	-4.964910000	5.015583000	-0.274291000
H	-3.217578000	6.776922000	-0.284426000

G[Btma][PF_6] SCF energy: -3341.02579055

C	2.390974000	-2.107779000	-1.578385000
C	0.987096000	-2.180578000	-1.408023000
C	0.225774000	-0.979808000	-1.246415000
C	0.877076000	0.276854000	-1.253920000
C	2.296159000	0.345736000	-1.403525000
C	3.046682000	-0.840835000	-1.569636000
C	-1.178070000	-1.050625000	-1.069667000
C	0.121207000	1.464878000	-1.101752000
C	-1.284795000	1.396354000	-0.948020000
C	-1.934274000	0.138079000	-0.920780000
C	-2.041940000	2.594830000	-0.748816000
C	-1.386976000	3.851186000	-0.740936000
C	0.029553000	3.919364000	-0.912597000
C	0.782313000	2.732972000	-1.083964000
C	2.188021000	2.797936000	-1.232080000
C	2.946035000	1.600839000	-1.396714000
C	0.336550000	-3.438093000	-1.398723000
C	-1.072261000	-3.512901000	-1.176400000
C	-1.827880000	-2.325147000	-1.010912000
C	-3.224972000	-2.397829000	-0.784299000
C	-3.986265000	-1.198790000	-0.618882000
C	-3.344747000	0.063531000	-0.688231000
C	-3.440128000	2.521866000	-0.529058000
C	-4.093615000	1.251220000	-0.492610000
C	3.142233000	-3.304469000	-1.764268000
C	4.457839000	-0.766950000	-1.732782000
C	5.193691000	-1.992686000	-1.907542000
C	4.569943000	-3.199183000	-1.925977000
C	5.084362000	0.481937000	-1.717100000
C	4.358490000	1.664660000	-1.548378000
C	4.994305000	2.956565000	-1.520037000
C	4.274285000	4.096724000	-1.359761000
C	2.841514000	4.062176000	-1.212290000
C	0.691425000	5.179989000	-0.895370000
C	2.080924000	5.225033000	-1.047424000
C	-2.144987000	5.042035000	-0.545330000

C	-0.103148000	6.368473000	-0.713630000
C	-1.449719000	6.304335000	-0.546923000
C	-4.187878000	3.717565000	-0.327305000
C	-3.527384000	4.950550000	-0.348471000
C	-5.495021000	1.171231000	-0.245482000
C	-6.227105000	2.398762000	-0.057624000
C	-5.606535000	3.606627000	-0.098821000
C	-5.387106000	-1.268234000	-0.367209000
C	-6.111390000	-0.083973000	-0.190123000
C	-3.863908000	-3.669476000	-0.711529000
C	-5.283671000	-3.707091000	-0.465261000
C	-6.006276000	-2.568427000	-0.300532000
C	-1.723656000	-4.778740000	-1.119353000
C	-3.102244000	-4.830329000	-0.882291000
C	1.094639000	-4.627944000	-1.591389000
C	0.406380000	-5.892458000	-1.547967000
C	-0.930478000	-5.966220000	-1.314940000
C	2.477954000	-4.536203000	-1.777028000
H	6.277241000	-1.930633000	-2.023356000
H	6.169578000	0.534500000	-1.829787000
H	6.079829000	2.998724000	-1.624789000
H	4.773135000	5.067191000	-1.334331000
H	2.587547000	6.193046000	-1.029952000
H	0.408413000	7.332862000	-0.707437000
H	-2.033358000	7.215887000	-0.405520000
H	-4.104162000	5.866370000	-0.197695000
H	-6.177541000	4.525771000	0.045895000
H	-7.302313000	2.336321000	0.119859000
H	-7.186344000	-0.140300000	-0.002394000
H	-7.080739000	-2.618079000	-0.114422000
H	-5.772038000	-4.682047000	-0.412057000
H	-3.597727000	-5.803053000	-0.832644000
H	-1.432980000	-6.934451000	-1.274895000
H	0.990601000	-6.802750000	-1.696287000
H	3.057304000	-5.451960000	-1.917671000
H	5.143113000	-4.118418000	-2.058872000
N	-1.217516000	-0.288995000	3.098219000

C	-1.410037000	0.527560000	4.327486000
H	-0.417636000	0.847576000	4.668971000
H	-1.905958000	-0.084396000	5.090454000
H	-2.026033000	1.399427000	4.076623000
C	-0.628136000	0.606471000	2.050270000
H	0.233636000	1.128513000	2.474730000
H	-1.414949000	1.305047000	1.737636000
H	-0.291667000	-0.005814000	1.210562000
C	-2.521483000	-0.817343000	2.616618000
H	-2.359867000	-1.331940000	1.661812000
H	-3.213104000	0.022508000	2.469534000
H	-2.918590000	-1.518272000	3.362077000
H	-0.699937000	-1.877481000	4.361193000
C	-0.279962000	-1.428282000	3.447555000
H	0.675382000	-0.947535000	3.686484000
C	-0.074465000	-2.485954000	2.378287000
H	0.190470000	-2.021446000	1.417000000
H	-0.979976000	-3.098430000	2.228149000
C	1.093535000	-3.372465000	2.822540000
H	1.935447000	-2.721452000	3.105374000
H	0.798218000	-3.943354000	3.719773000
C	1.545594000	-4.311410000	1.714096000
H	2.311595000	-5.012610000	2.074407000
H	1.984779000	-3.725898000	0.892615000
H	0.705452000	-4.898557000	1.306789000
P	3.035004000	0.396576000	2.321769000
F	1.955252000	0.640512000	3.580649000
F	2.292393000	1.620072000	1.508631000
F	4.049687000	0.143178000	1.077055000
F	1.937376000	-0.652875000	1.632916000
F	3.663454000	-0.861768000	3.150374000
F	4.064778000	1.434520000	3.014362000

G[Btma][DCA] SCF energy: -2640.95958144

C	3.144633000	-2.540218000	-0.526634000
C	1.758776000	-2.395631000	-0.780301000
C	1.176876000	-1.089498000	-0.848590000
C	1.986148000	0.056393000	-0.654103000
C	3.385642000	-0.090837000	-0.392158000
C	3.960799000	-1.384251000	-0.329254000
C	-0.211566000	-0.945228000	-1.088728000
C	1.406522000	1.347467000	-0.697114000
C	0.018434000	1.491794000	-0.938352000
C	-0.789164000	0.346265000	-1.144384000
C	-0.577039000	2.794590000	-0.926333000
C	0.229628000	3.939325000	-0.711078000
C	1.634190000	3.794670000	-0.493569000
C	2.219696000	2.504827000	-0.475679000
C	3.606334000	2.358176000	-0.227154000
C	4.191185000	1.055217000	-0.183041000
C	0.943094000	-3.542453000	-0.946332000
C	-0.459979000	-3.396868000	-1.168243000
C	-1.037181000	-2.105430000	-1.239573000
C	-2.431575000	-1.962684000	-1.429781000
C	-3.019252000	-0.661682000	-1.453758000
C	-2.203314000	0.488373000	-1.317754000
C	-1.976527000	2.933382000	-1.098182000
C	-2.793157000	1.775575000	-1.283180000
C	3.716976000	-3.842471000	-0.451750000
C	5.351921000	-1.526398000	-0.057821000
C	5.903732000	-2.856339000	0.008632000
C	5.127401000	-3.955485000	-0.179130000
C	6.132977000	-0.382112000	0.136615000
C	5.582673000	0.902994000	0.080134000
C	6.374392000	2.089914000	0.285118000
C	5.818545000	3.328636000	0.241186000
C	4.411661000	3.512973000	-0.010931000
C	2.447341000	4.943394000	-0.273550000
C	3.817525000	4.779139000	-0.042621000
C	-0.368510000	5.231749000	-0.696164000

C	1.818356000	6.240113000	-0.286864000
C	0.481354000	6.376415000	-0.484819000
C	-2.568882000	4.229081000	-1.058034000
C	-1.751888000	5.349085000	-0.870751000
C	-4.207044000	1.907450000	-1.390916000
C	-4.777791000	3.230112000	-1.342160000
C	-3.999906000	4.333358000	-1.194066000
C	-4.430287000	-0.518892000	-1.566369000
C	-4.994544000	0.760083000	-1.525451000
C	-3.252114000	-3.118417000	-1.554987000
C	-4.673790000	-2.941210000	-1.697351000
C	-5.236197000	-1.706038000	-1.692569000
C	-1.286804000	-4.547124000	-1.306338000
C	-2.662514000	-4.383822000	-1.499160000
C	1.524718000	-4.841146000	-0.866857000
C	0.665508000	-5.987524000	-1.022179000
C	-0.669776000	-5.846707000	-1.228478000
C	2.897907000	-4.962773000	-0.625631000
H	6.970418000	-2.962564000	0.214425000
H	7.200427000	-0.495424000	0.340366000
H	7.441729000	1.970048000	0.479608000
H	6.434206000	4.215918000	0.400958000
H	4.438573000	5.662527000	0.125073000
H	2.445537000	7.118915000	-0.125260000
H	0.021585000	7.366552000	-0.483898000
H	-2.208091000	6.341731000	-0.846341000
H	-4.449978000	5.326987000	-1.157275000
H	-5.861945000	3.325014000	-1.422271000
H	-6.080336000	0.861547000	-1.580001000
H	-6.318367000	-1.587297000	-1.760425000
H	-5.298231000	-3.832562000	-1.775426000
H	-3.296229000	-5.269309000	-1.585719000
H	-1.307709000	-6.726137000	-1.334494000
H	1.114285000	-6.980628000	-0.961333000
H	3.339900000	-5.960037000	-0.561602000
H	5.562976000	-4.954922000	-0.123355000
N	-1.630904000	0.242676000	3.176735000

C	-1.824161000	1.582980000	3.804238000
H	-1.204702000	2.310251000	3.264612000
H	-1.515570000	1.524871000	4.855212000
H	-2.890709000	1.836975000	3.720245000
C	-2.092461000	0.338111000	1.756476000
H	-1.424113000	1.044795000	1.251189000
H	-3.119892000	0.720922000	1.760858000
H	-2.065111000	-0.657083000	1.296498000
C	-2.454199000	-0.756666000	3.927252000
H	-2.491988000	-1.691971000	3.357623000
H	-3.466312000	-0.342826000	4.018664000
H	-1.997194000	-0.895954000	4.916045000
H	0.162600000	0.051225000	4.247297000
C	-0.170135000	-0.123356000	3.212561000
H	0.340347000	0.603687000	2.561212000
C	0.159632000	-1.546711000	2.789123000
H	-0.263851000	-1.775658000	1.796582000
H	-0.280472000	-2.262444000	3.500608000
C	1.678107000	-1.738821000	2.753799000
H	2.098296000	-1.150510000	1.920465000
H	2.121755000	-1.328746000	3.677903000
C	2.070564000	-3.204609000	2.609160000
H	3.159143000	-3.312276000	2.494874000
H	1.593042000	-3.656708000	1.726378000
H	1.758732000	-3.783563000	3.492208000
N	-5.613382000	-0.779876000	1.570276000
C	-4.640770000	-1.673549000	1.548547000
N	-3.781674000	-2.472603000	1.498249000
C	-5.358160000	0.249091000	2.351569000
N	-5.118342000	1.176944000	3.032078000

G[Btma][Tf_2N] SCF energy: -4227.43613805

N	3.855481000	-1.272340000	1.116355000
C	4.616195000	-2.183907000	2.019446000
H	4.039908000	-2.296372000	2.947057000
H	5.595688000	-1.733235000	2.220425000
H	4.741309000	-3.148893000	1.513346000
C	2.534098000	-1.912317000	0.819091000
H	2.027315000	-2.089644000	1.772393000
H	2.730281000	-2.847423000	0.277436000
H	1.931061000	-1.239467000	0.198296000
C	4.605988000	-1.069548000	-0.147951000
H	4.039544000	-0.382552000	-0.783505000
H	4.717326000	-2.037036000	-0.654275000
H	5.588460000	-0.641624000	0.089481000
H	4.715817000	0.410254000	2.012306000
C	3.688933000	0.053527000	1.835945000
H	3.233097000	-0.196494000	2.798791000
C	2.867410000	1.101188000	1.106574000
H	1.875897000	0.707841000	0.833131000
H	3.377305000	1.442396000	0.188423000
C	2.635556000	2.300727000	2.027927000
H	2.093933000	1.953421000	2.920524000
H	3.604371000	2.701732000	2.374454000
C	1.829812000	3.383359000	1.322870000
H	1.665746000	4.250897000	1.977793000
H	0.847871000	2.981758000	1.029153000
H	2.350431000	3.732054000	0.415967000
N	0.885695000	-0.463380000	3.045629000
S	-0.590325000	0.032929000	2.588050000
S	1.167956000	-1.126472000	4.493633000
O	-0.407985000	0.815230000	1.350948000
O	-1.473782000	0.509210000	3.651201000
O	2.400026000	-1.931605000	4.332325000
O	0.026580000	-1.671010000	5.226638000
C	1.743010000	0.343785000	5.475358000
C	-1.329968000	-1.556576000	1.976123000
F	-1.450566000	-2.443258000	2.949821000

F	-0.545956000	-2.081174000	1.023212000
F	-2.526766000	-1.310219000	1.454801000
F	2.930321000	0.756022000	5.014713000
F	1.877008000	0.015766000	6.752863000
F	0.879412000	1.342798000	5.363524000
C	2.507496000	-1.295092000	-2.814096000
C	1.967340000	-0.017332000	-2.519682000
C	0.612591000	0.102505000	-2.071781000
C	-0.190072000	-1.054287000	-1.930949000
C	0.366361000	-2.346449000	-2.191926000
C	1.710742000	-2.466189000	-2.624450000
C	0.065667000	1.379957000	-1.803180000
C	-1.545957000	-0.932204000	-1.544249000
C	-2.092568000	0.344633000	-1.281919000
C	-1.284672000	1.499716000	-1.402927000
C	-3.465613000	0.468282000	-0.902878000
C	-4.280920000	-0.685339000	-0.809646000
C	-3.728591000	-1.974765000	-1.075941000
C	-2.365013000	-2.099610000	-1.433706000
C	-1.807279000	-3.379547000	-1.665351000
C	-0.434417000	-3.505064000	-2.039611000
C	2.766592000	1.143568000	-2.675672000
C	2.220962000	2.430699000	-2.377270000
C	0.875423000	2.549523000	-1.951904000
C	0.328092000	3.827291000	-1.682468000
C	-1.030378000	3.946008000	-1.260322000
C	-1.835350000	2.789044000	-1.127289000
C	-4.008997000	1.745176000	-0.625158000
C	-3.189485000	2.909854000	-0.732783000
C	3.847775000	-1.405844000	-3.287483000
C	2.261804000	-3.756248000	-2.874725000
C	3.626120000	-3.838893000	-3.333644000
C	4.375108000	-2.723332000	-3.542670000
C	1.465355000	-4.890931000	-2.685133000
C	0.128566000	-4.791188000	-2.282585000
C	-0.713731000	-5.949450000	-2.121384000
C	-2.020073000	-5.828966000	-1.769073000

C	-2.621553000	-4.540519000	-1.534885000
C	-4.538144000	-3.139815000	-0.955970000
C	-3.968867000	-4.397005000	-1.187146000
C	-5.646895000	-0.556672000	-0.430573000
C	-5.921447000	-2.978325000	-0.584863000
C	-6.447607000	-1.751478000	-0.335561000
C	-5.376018000	1.864697000	-0.244848000
C	-6.165582000	0.713218000	-0.155792000
C	-3.734850000	4.196246000	-0.458449000
C	-5.118597000	4.285901000	-0.066142000
C	-5.898164000	3.178451000	0.034873000
C	-1.582462000	5.227950000	-0.978841000
C	-2.920057000	5.326806000	-0.582206000
C	1.139466000	4.989443000	-1.822834000
C	0.557500000	6.272635000	-1.520960000
C	-0.735251000	6.384941000	-1.119449000
C	3.023794000	3.598484000	-2.519545000
C	2.469321000	4.851477000	-2.235843000
C	4.110008000	1.021237000	-3.137195000
C	4.900594000	2.220305000	-3.263654000
C	4.385774000	3.441583000	-2.964262000
C	4.618154000	-0.247730000	-3.444281000
H	4.045270000	-4.828173000	-3.528306000
H	1.891702000	-5.879047000	-2.874830000
H	-0.276986000	-6.934161000	-2.297482000
H	-2.645328000	-6.717103000	-1.659209000
H	-4.591537000	-5.289646000	-1.090108000
H	-6.541148000	-3.873087000	-0.502464000
H	-7.495797000	-1.648433000	-0.049015000
H	-7.213322000	0.807281000	0.139441000
H	-6.944712000	3.264129000	0.332822000
H	-5.530968000	5.273535000	0.148452000
H	-3.340880000	6.312378000	-0.368814000
H	-1.160469000	7.365265000	-0.895988000
H	1.184188000	7.160695000	-1.621464000
H	3.089296000	5.745050000	-2.342021000
H	5.000138000	4.338348000	-3.066316000

H	5.930779000	2.125565000	-3.612050000
H	5.645354000	-0.335643000	-3.807097000
H	5.400788000	-2.807400000	-3.907495000