Syntheses and Quadratic Nonlinear Optical Properties of Salts Containing Benzothiazolium Electron Acceptor Groups

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Supporting Information

Cartesian coordinates of optimized geometries used in theoretical calculations (B3P86/6-31G*)

Cation 1: gas phase (vacuum)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.669487	-1.144369	0.000000
2	7	0	5.503151	-0.068472	-0.000003
3	6	0	3.312022	-1.003945	0.000000
4	6	0	2.705807	0.284551	0.000000
5	6	0	3.615779	1.376216	-0.000002
6	6	0	4.968596	1.179860	-0.000011
7	6	0	1.306310	0.526751	0.000000
8	6	0	6.951746	-0.277561	0.000011
9	6	0	0.333575	-0.441464	-0.000002
10	6	0	-1.077353	-0.259718	-0.000001
11	6	0	-1.919182	-1.396919	-0.000003
12	6	0	-3.288847	-1.295886	-0.000002
13	6	0	-3.920040	-0.022866	0.000000
14	6	0	-1.713489	1.005663	0.000001
15	6	0	-3.079596	1.127388	0.000001
16	7	0	-5.269104	0.094872	0.000001
17	6	0	-5.894412	1.406482	0.000004
18	6	0	-6.107390	-1.091895	0.000000
19	1	0	5.152120	-2.115064	0.000002
20	1	0	2.712885	-1.906352	0.000000
21	1	0	3.242171	2.394427	0.000000
22	1	0	5.674241	2.002041	-0.000011
23	1	0	7.247665	-0.832597	-0.893357
24	1	0	7.453623	0.689502	-0.000025
25	1	0	7.247657	-0.832526	0.893426
26	1	0	1.012571	1.573202	0.000001
27	1	0	0.650949	-1.483875	-0.000004
28	1	0	-1.466874	-2.385729	-0.000005
29	1	0	-3.884005	-2.200442	-0.000003
30	1	0	-1.116500	1.912443	0.000002
31	1	0	-3.516946	2.118092	0.000003
32	1	0	-6.976970	1.285465	0.000004
33	1	0	-5.617359	1.982087	0.891051
34	1	0	-5.617360	1.982090	-0.891043
35	1	0	-7.154000	-0.790205	0.000001
36	1	0	-5.930133	-1.705540	-0.891025
37	1	0	-5.930132	-1.705543	0.891023

Cation 1: in acetonitrile (PCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.676788	-1.145044	0.001465
2	7	0	-5.500455	-0.065333	0.001439
3	6	0	-3.315602	-1.006130	0.000112
4	6	0	-2.717820	0.279636	-0.001146
5	6	0	-3.614212	1.374288	-0.001111
6	6	0	-4.971955	1.181354	0.000128
7	6	0	-1.305450	0.522725	-0.002518
8	6	0	-6.950830	-0.271067	0.003265
9	6	0	-0.344818	-0.445530	-0.002000
10	6	0	1.078279	-0.260158	-0.002599
11	6	0	1.917168	-1.394899	-0.001781
12	6	0	3.292329	-1.292976	-0.001042
13	6	0	3.922806	-0.022487	-0.000753
14	6	0	1.711799	1.002672	-0.003094
15	6	0	3.083175	1.124953	-0.002155
16	7	0	5.278368	0.096238	0.001146
17	6	0	5.899136	1.406827	0.005381
18	6	0	6.113013	-1.089461	0.001203
19	1	0	-5.161218	-2.119571	0.002463
20	1	0	-2.717302	-1.913807	-0.000078
21	1	0	-3.235565	2.394648	-0.002166
22	1	0	-5.677503	2.009558	0.000126
23	1	0	-7.240252	-0.825032	0.899464
24	1	0	-7.447373	0.699148	-0.000927
25	1	0	-7.241221	-0.833102	-0.887550
26	1	0	-1.016370	1.573638	-0.003970
27	1	0	-0.659704	-1.491315	-0.000512
28	1	0	1.463201	-2.386107	-0.001454
29	1	0	3.883839	-2.202076	-0.000064
30	1	0	1.114390	1.912835	-0.004036
31	1	0	3.515237	2.119918	-0.002530
32	1	0	6.982845	1.288116	0.010815
33	1	0	5.624298	1.986752	-0.884956
34	1	0	5.615365	1.984950	0.894032
35	1	0	7.160897	-0.788940	-0.003172
36	1	0	5.937847	-1.705239	0.892652
37	1	0	5.931828	-1.708929	-0.886362

Cation 2: gas phase (vacuum)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.149567	-3.466243	0.000000
2	6	0	4.317270	-2.657692	0.000000
3	6	0	4.138402	-1.245519	0.000000
4	6	0	2.883056	-0.690852	0.000000
5	6	0	1.714456	-1.490301	0.000000
6	6	0	1.901129	-2.892460	0.000000
7	7	0	5.556367	-3.208437	0.000000
8	6	0	5.714965	-4.651793	0.000000
9	6	0	6.737485	-2.363522	0.000000
10	6	0	0.393148	-0.964137	0.000000
11	6	0	0.000000	0.354734	0.000000
12	6	0	-1.356512	0.723572	0.000000
13	6	0	-1.814983	2.023544	0.000000
14	6	0	-3.172368	2.425032	0.000000
15	6	0	-3.507714	3.809645	0.000000
16	6	0	-4.805790	4.229266	0.000000
17	7	0	-5.840086	3.343613	0.000000
18	6	0	-5.566956	2.011289	0.000000
19	6	0	-4.286291	1.537781	0.000000
20	6	0	-7.216138	3.838931	0.000000
21	1	0	3.232746	-4.545918	0.000000
22	1	0	5.000664	-0.590268	0.000000
23	1	0	2.797197	0.391511	0.000000
24	1	0	1.026323	-3.538182	0.000000
25	1	0	6.776956	-4.894833	0.000000
26	1	0	5.262837	-5.104285	0.890700
27	1	0	5.262837	-5.104285	-0.890700
28	1	0	7.626526	-2.993227	0.000000
29	1	0	6.773669	-1.725078	-0.890853
30	1	0	6.773669	-1.725078	0.890853
31	1	0	-0.403614	-1.709484	0.000000
32	1	0	0.742009	1.150192	0.000000
33	1	0	-2.077048	-0.094450	0.000000
34	1	0	-1.076540	2.822705	0.000000
35	1	0	-2.721574	4.556927	0.000000
36	1	0	-5.080148	5.278012	0.000000
37	1	0	-6.426012	1.350905	0.000000
38	1	0	-4.147023	0.463610	0.000000
39	1	0	-7.395738	4.442397	-0.893125
40	1	0	-7.902318	2.992550	0.000000
41	1	0	-7.395738	4.442397	0.893125

Cation 2: in acetonitrile (PCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.082737	-3.535314	0.000000
2	6	0	4.264372	-2.751735	0.000000
3	6	0	4.111568	-1.339098	0.000000
4	6	0	2.862138	-0.758259	0.000000
5	6	0	1.681230	-1.533328	0.000000
6	6	0	1.840359	-2.935246	0.000000
7	7	0	5.498505	-3.328530	0.000000
8	6	0	5.626623	-4.772276	0.000000
9	6	0	6.691666	-2.505166	0.000000
10	6	0	0.357921	-0.977304	0.000000
11	6	0	0.000000	0.342516	0.000000
12	6	0	-1.360877	0.744270	0.000000
13	6	0	-1.775138	2.048736	0.000000
14	6	0	-3.134632	2.490985	0.000000
15	6	0	-3.419241	3.880043	0.000000
16	6	0	-4.708665	4.339130	0.000000
17	7	0	-5.759211	3.480130	0.000000
18	6	0	-5.532885	2.142974	0.000000
19	6	0	-4.261620	1.632151	0.000000
20	6	0	-7.123021	4.013698	0.000000
21	1	0	3.139569	-4.618550	0.000000
22	1	0	4.983789	-0.694193	0.000000
23	1	0	2.799875	0.328655	0.000000
24	1	0	0.951160	-3.566048	0.000000
25	1	0	6.684173	-5.037398	0.000000
26	1	0	5.163134	-5.218821	0.889256
27	1	0	5.163134	-5.218821	-0.889256
28	1	0	7.570437	-3.150517	0.000000
29	1	0	6.740109	-1.863667	-0.889406
30	1	0	6.740109	-1.863667	0.889406
31	1	0	-0.454159	-1.710002	0.000000
32	1	0	0.757975	1.127348	0.000000
33	1	0	-2.100220	-0.060435	0.000000
34	1	0	-1.017308	2.833833	0.000000
35	1	0	-2.608332	4.605935	0.000000
36	1	0	-4.951557	5.399975	0.000000
37	1	0	-6.412873	1.503252	0.000000
38	1	0	-4.154835	0.550489	0.000000
39	1	0	-7.277470	4.623475	-0.893438
40	1	0	-7.829514	3.183821	0.000000
41	1	0	-7.277470	4.623475	0.893438

Cation 3: gas phase (vacuum)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.698579	-1.330085	0.000000
2	6	0	6.241315	-0.018361	0.000000
3	6	0	5.325730	1.070633	0.000000
4	6	0	3.969592	0.855558	0.000000
5	6	0	3.421010	-0.449088	0.000000
6	6	0	4.337909	-1.525367	0.000000
7	7	0	7.582614	0.190887	0.000000
8	6	0	8.497748	-0.935681	0.000000
9	6	0	8.115429	1.541030	0.000000
10	6	0	2.023881	-0.723465	0.000000
11	6	0	0.979764	0.172121	0.000000
12	1	0	6.353670	-2.192316	0.000000
13	1	0	5.694626	2.088974	0.000000
14	1	0	3.310031	1.718057	0.000000
15	1	0	3.953197	-2.542350	0.000000
16	1	0	9.522063	-0.564335	0.000000
17	1	0	8.362868	-1.561398	0.890571
18	1	0	8.362862	-1.561402	-0.890567
19	1	0	9.204013	1.495152	0.000000
20	1	0	7.799457	2.097594	-0.890633
21	1	0	7.799451	2.097595	0.890631
22	1	0	1.757361	-1.781334	0.000000
23	1	0	1.174282	1.242552	0.000000
24	6	0	-0.361209	-0.249142	0.000000
25	6	0	-1.458783	0.590148	0.000000
26	6	0	-2.776829	0.113017	0.000000
27	6	0	-3.899854	0.917238	0.000000
28	6	0	-5.240936	0.473054	0.000000
29	6	0	-6.307781	1.419075	0.000000
30	6	0	-7.612624	1.024113	0.000000
31	7	0	-7.958082	-0.294198	0.000000
32	6	0	-6.972773	-1.233007	0.000000
33	6	0	-5.651371	-0.892073	0.000000
34	6	0	-9.370010	-0.671937	0.000000
35	1	0	-2.898890	-0.970205	0.000000
36	1	0	-3.749631	1.994994	0.000000
37	1	0	-6.088054	2.481244	0.000000
38	1	0	-8.436084	1.729067	0.000000
39	1	0	-7.302412	-2.265237	0.000000
40	1	0	-4.924377	-1.695107	0.000000
41	1	0	-9.862960	-0.279360	-0.892944
42	1	0	-9.450712	-1.758618	0.000000
43	1	0	-9.862958	-0.279372	0.892950
44	1	0	-0.544021	-1.324990	0.000000
45	1	0	-1.298213	1.667278	0.000000

Cation 3: in acetonitrile (PCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.707234	-1.324799	0.000104
2	6	0	-6.248906	-0.015119	0.000611
3	6	0	-5.331898	1.069646	-0.001656
4	6	0	-3.970674	0.851797	-0.003617
5	6	0	-3.424709	-0.450566	-0.003723
6	6	0	-4.341257	-1.522693	-0.002088
7	7	0	-7.595905	0.196684	0.003471
8	6	0	-8.508633	-0.928713	0.007643
9	6	0	-8.123894	1.546294	0.002938
10	6	0	-2.015311	-0.730891	-0.004720
11	6	0	-0.979907	0.161643	-0.004655
12	1	0	-6.359881	-2.191165	0.001587
13	1	0	-5.693819	2.092345	-0.001460
14	1	0	-3.310869	1.717741	-0.004913
15	1	0	-3.957914	-2.543328	-0.002228
16	1	0	-9.533881	-0.557613	0.010126
17	1	0	-8.376334	-1.559515	-0.881091
18	1	0	-8.371086	-1.557031	0.897329
19	1	0	-9.213385	1.503223	0.005296
20	1	0	-7.803590	2.106852	0.890815
21	1	0	-7.807372	2.104573	-0.887715
22	1	0	-1.752915	-1.792637	-0.004962
23	1	0	-1.171318	1.236079	-0.004104
24	6	0	0.374802	-0.260980	-0.004514
25	6	0	1.458285	0.580621	-0.003425
26	6	0	2.790756	0.101367	-0.002655
27	6	0	3.896894	0.910170	-0.001150
28	6	0	5.254334	0.465710	0.000034
29	6	0	6.304160	1.419477	0.002031
30	6	0	7.615972	1.029972	0.003269
31	7	0	7.957833	-0.283907	0.002643
32	6	0	6.985839	-1.230210	0.000805
33	6	0	5.658246	-0.893061	-0.000519
34	6	0	9.373422	-0.658564	0.003891
35	1	0	2.912774	-0.984532	-0.003111
36	1	0	3.747710	1.991136	-0.000600
37	1	0	6.077513	2.483940	0.002616
38	1	0	8.437983	1.742971	0.004801
39	1	0	7.319347	-2.265727	0.000403
40	1	0	4.934054	-1.703519	-0.001992
41	1	0	9.857794	-0.258496	0.897971
42	1	0	9.453198	-1.745507	0.003308
43	1	0	9.859643	-0.257444	-0.888707
44	1	0	0.559592	-1.339352	-0.004901
45	1	0	1.297538	1.660968	-0.002887

Cation 4: gas phase (vacuum)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.913727	-1.332257	0.000126
2	6	0	-7.424590	-0.008588	0.000034
3	6	0	-6.483164	1.057251	-0.000090
4	6	0	-5.132068	0.809276	-0.000119
5	6	0	-4.615006	-0.507452	-0.000028
6	6	0	-5.557416	-1.560597	0.000095
7	7	0	-8.761629	0.233446	0.000063
8	6	0	-9.703363	-0.870192	0.000191
9	6	0	-9.260481	1.595942	-0.000033
10	6	0	-3.222810	-0.814127	-0.000053
11	6	0	-2.161717	0.059434	-0.000166
12	1	0	-7.589560	-2.178440	0.000221
13	1	0	-6.826950	2.084390	-0.000163
14	1	0	-4.452201	1.655900	-0.000215
15	1	0	-5.197426	-2.586651	0.000167
16	1	0	-10.718516	-0.474141	0.000196
17	1	0	-9.584093	-1.499671	-0.890183
18	1	0	-9.584026	-1.499522	0.890660
19	1	0	-10.349949	1.577197	0.000007
20	1	0	-8.930746	2.145155	0.890368
21	1	0	-8.930810	2.145005	-0.890551
22	1	0	-2.979707	-1.877555	0.000026
23	1	0	-2.336258	1.133454	-0.000249
24	6	0	1.594729	-0.044401	-0.000098
25	6	0	2.732205	0.744841	0.000001
26	6	0	4.027188	0.214707	-0.000024
27	6	0	5.182512	0.975662	0.000073
28	6	0	6.504209	0.482878	0.000053
29	6	0	7.606696	1.388864	0.000163
30	6	0	8.895401	0.946061	0.000147
31	7	0	9.192768	-0.384833	0.000026
32	6	0	8.172517	-1.286575	-0.000082
33	6	0	6.865160	-0.897480	-0.000071
34	6	0	10.589296	-0.813477	0.000013
35	1	0	4.107168	-0.872440	-0.000126
36	1	0	5.072329	2.058329	0.000174
37	1	0	7.426342	2.458466	0.000261
38	1	0	9.744392	1.620081	0.000229
39	1	0	8.463749	-2.330281	-0.000176
40	1	0	6.108889	-1.673049	-0.000161
41	1	0	11.096961	-0.439475	0.892844
42	1	0	10.630928	-1.902448	-0.000086
43	1	0	11.096995	-0.439312	-0.892732
44	1	0	1.726870	-1.127597	-0.000199
45	1	0	2.617306	1.827933	0.000102
46	6	0	-0.826485	-0.383252	-0.000180
47	6	0	0.280652	0.442539	-0.000079
48	1	0	-0.658256	-1.461308	-0.000280
49	1	0	0.130179	1.521340	0.000021

Cation 4: in acetonitrile (PCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.924800	-1.326476	-0.000082
2	6	0	-7.432536	-0.003855	0.000981
3	6	0	-6.487797	1.056097	-0.002147
4	6	0	-5.132199	0.802906	-0.004533
5	6	0	-4.619618	-0.512470	-0.004504
6	6	0	-5.563686	-1.559880	-0.002591
7	7	0	-8.774535	0.243670	0.004910
8	6	0	-9.716545	-0.856671	0.012608
9	6	0	-9.265497	1.606746	0.006627
10	6	0	-3.215828	-0.827311	-0.005874
11	6	0	-2.162309	0.042362	-0.006371
12	1	0	-7.599732	-2.175637	0.000993
13	1	0	-6.822889	2.087932	-0.002342
14	1	0	-4.450684	1.651868	-0.006605
15	1	0	-5.207222	-2.590232	-0.003259
16	1	0	-10.731670	-0.458461	0.019306
17	1	0	-9.605305	-1.491089	-0.876630
18	1	0	-9.592649	-1.489061	0.901599
19	1	0	-10.355821	1.593464	0.008731
20	1	0	-8.930234	2.157509	0.895297
21	1	0	-8.933941	2.158084	-0.883006
22	1	0	-2.978510	-1.894855	-0.006440
23	1	0	-2.333955	1.120266	-0.006060
24	6	0	1.610287	-0.054039	-0.006543
25	6	0	2.730426	0.741002	-0.005081
26	6	0	4.041407	0.209329	-0.003741
27	6	0	5.178897	0.975103	-0.001475
28	6	0	6.517571	0.479245	0.000462
29	6	0	7.603880	1.391839	0.003269
30	6	0	8.899486	0.951915	0.005388
31	7	0	9.190658	-0.374450	0.004806
32	6	0	8.182624	-1.282588	0.002010
33	6	0	6.869334	-0.894445	-0.000214
34	6	0	10.590724	-0.802958	0.007172
35	1	0	4.121425	-0.880410	-0.004537
36	1	0	5.071108	2.060994	-0.000826
37	1	0	7.418605	2.464277	0.003789
38	1	0	9.748549	1.632543	0.007607
39	1	0	8.475765	-2.330142	0.001540
40	1	0	6.114260	-1.676221	-0.002504
41	1	0	11.089529	-0.421345	0.901401
42	1	0	10.629406	-1.892190	0.007073
43	1	0	11.092667	-0.421114	-0.885198
44	1	0	1.747763	-1.139396	-0.007233
45	1	0	2.613845	1.827060	-0.004529
46	6	0	-0.812757	-0.400164	-0.007164
47	6	0	0.279448	0.429513	-0.006845
48	1	0	-0.641785	-1.480687	-0.007972
49	1	0	0.125538	1.511101	-0.006320

Cation 5: gas phase (vacuum)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.673846	3.115744	0.000000
2	6	0	3.602581	2.066628	0.000000
3	6	0	4.972184	2.306390	0.000000
4	6	0	5.402208	3.627455	0.000000
5	6	0	4.479662	4.678638	0.000000
6	6	0	3.111489	4.440130	0.000000
7	6	0	1.232510	1.299182	0.000000
8	1	0	5.682565	1.486465	0.000000
9	1	0	6.465442	3.842928	0.000000
10	1	0	4.834921	5.703759	0.000000
11	1	0	2.417902	5.273311	0.000000
12	6	0	0.000000	0.620397	0.000000
13	6	0	-0.107276	-0.752584	0.000000
14	1	0	-0.895888	1.231152	0.000000
15	1	0	0.819249	-1.328415	0.000000
16	6	0	-1.288692	-1.534638	0.000000
17	6	0	-1.178654	-2.947136	0.000000
18	6	0	-2.599449	-0.994126	0.000000
19	6	0	-2.279054	-3.766307	0.000000
20	1	0	-0.188916	-3.396959	0.000000
21	6	0	-3.710451	-1.796077	0.000000
22	1	0	-2.742673	0.082311	0.000000
23	6	0	-3.591022	-3.217186	0.000000
24	1	0	-2.136436	-4.839513	0.000000
25	1	0	-4.690340	-1.335223	0.000000
26	7	0	1.356974	2.646152	0.000000
27	16	0	2.787509	0.519900	0.000000
28	7	0	-4.685201	-4.010930	0.000000
29	6	0	0.191020	3.519705	0.000000
30	1	0	-0.411171	3.343974	0.895086
31	1	0	0.518849	4.556119	0.000000
32	1	0	-0.411171	3.343974	-0.895086
33	6	0	-6.018834	-3.431482	0.000000
34	1	0	-6.186575	-2.816050	0.891406
35	1	0	-6.186575	-2.816050	-0.891406
36	1	0	-6.755976	-4.233227	0.000000
37	6	0	-4.541299	-5.457909	0.000000
38	1	0	-5.529658	-5.915469	0.000000
39	1	0	-4.005357	-5.804491	-0.891125
40	1	0	-4.005357	-5.804491	0.891125

Cation 5: in acetonitrile (PCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.673580	3.112562	0.000000
2	6	0	3.602834	2.063093	0.000000
3	6	0	4.973124	2.302090	0.000000
4	6	0	5.402545	3.624287	0.000000
5	6	0	4.478659	4.675949	0.000000
6	6	0	3.109364	4.438271	0.000000
7	6	0	1.236123	1.298843	0.000000
8	1	0	5.682975	1.477020	0.000000
9	1	0	6.469083	3.840184	0.000000
10	1	0	4.833476	5.704661	0.000000
11	1	0	2.416539	5.275774	0.000000
12	6	0	0.000000	0.619656	0.000000
13	6	0	-0.101808	-0.750241	0.000000
14	1	0	-0.895432	1.231799	0.000000
15	1	0	0.823146	-1.334302	0.000000
16	6	0	-1.290062	-1.531531	0.000000
17	6	0	-1.178582	-2.942532	0.000000
18	6	0	-2.598954	-0.989957	0.000000
19	6	0	-2.281373	-3.763490	0.000000
20	1	0	-0.185382	-3.392035	0.000000
21	6	0	-3.711870	-1.794194	0.000000
22	1	0	-2.748609	0.087467	0.000000
23	6	0	-3.592233	-3.214073	0.000000
24	1	0	-2.132756	-4.837676	0.000000
25	1	0	-4.690280	-1.326257	0.000000
26	7	0	1.358546	2.642837	0.000000
27	16	0	2.788998	0.517200	0.000000
28	7	0	-4.688927	-4.009305	0.000000
29	6	0	0.192049	3.517675	0.000000
30	1	0	-0.409239	3.338943	0.895362
31	1	0	0.520941	4.554375	0.000000
32	1	0	-0.409239	3.338943	-0.895362
33	6	0	-6.020468	-3.428939	0.000000
34	1	0	-6.187628	-2.810487	0.890241
35	1	0	-6.187628	-2.810487	-0.890241
36	1	0	-6.758421	-4.230966	0.000000
37	6	0	-4.544288	-5.454303	0.000000
38	1	0	-5.533358	-5.912145	0.000000
39	1	0	-4.005661	-5.801869	-0.890045
40	1	0	-4.005661	-5.801869	0.890045

Cation 6: gas phase (vacuum)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.692204	-5.015558	0.000000
2	6	0	2.510944	-3.654883	0.000000
3	6	0	1.223596	-3.064221	0.000000
4	6	0	0.114950	-3.947335	0.000000
5	6	0	0.276066	-5.308735	0.000000
6	6	0	1.575037	-5.894701	0.000000
7	1	0	3.699437	-5.412925	0.000000
8	1	0	3.384774	-3.008037	0.000000
9	1	0	-0.894376	-3.547541	0.000000
10	1	0	-0.603431	-5.940529	0.000000
11	7	0	1.736151	-7.238765	0.000000
12	6	0	0.580219	-8.119311	0.000000
13	1	0	0.920040	-9.154210	0.000000
14	1	0	-0.039461	-7.965332	0.891158
15	1	0	-0.039461	-7.965332	-0.891158
16	6	0	3.069207	-7.817514	0.000000
17	1	0	3.633968	-7.518904	-0.890943
18	1	0	3.633968	-7.518904	0.890943
19	1	0	2.987101	-8.903685	0.000000
20	6	0	1.106974	-1.650885	0.000000
21	6	0	-0.044571	-0.890066	0.000000
22	1	0	2.050735	-1.103838	0.000000
23	1	0	-1.020600	-1.370357	0.000000
24	6	0	0.000000	0.509090	0.000000
25	6	0	-1.109732	1.335803	0.000000
26	1	0	0.990966	0.965803	0.000000
27	1	0	-2.094853	0.880022	0.000000
28	6	0	-1.044335	2.735761	0.000000
29	6	0	-1.835440	4.917427	0.000000
30	6	0	-0.454923	5.158743	0.000000
31	6	0	-2.732976	5.985133	0.000000
32	6	0	0.058581	6.450390	0.000000
33	6	0	-2.218734	7.275571	0.000000
34	1	0	-3.806166	5.831198	0.000000
35	6	0	-0.840381	7.510198	0.000000
36	1	0	1.129318	6.625071	0.000000
37	1	0	-2.905727	8.115361	0.000000
38	1	0	-0.466119	8.528449	0.000000
39	6	0	-3.480188	3.014272	0.000000
40	1	0	-3.645294	2.407780	-0.894494
41	1	0	-3.645294	2.407780	0.894494
42	1	0	-4.193024	3.835070	0.000000
43	7	0	-2.127078	3.551047	0.000000
44	16	0	0.436312	3.653251	0.000000

Cation 6: in acetonitrile (PCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.842647	-4.933391	0.000000
2	6	0	2.622202	-3.574781	0.000000
3	6	0	1.319884	-3.022586	0.000000
4	6	0	0.236961	-3.934731	0.000000
5	6	0	0.437887	-5.294435	0.000000
6	6	0	1.751646	-5.843141	0.000000
7	1	0	3.864389	-5.297145	0.000000
8	1	0	3.478848	-2.900451	0.000000
9	1	0	-0.786930	-3.565338	0.000000
10	1	0	-0.428614	-5.946723	0.000000
11	7	0	1.951161	-7.185654	0.000000
12	6	0	0.820961	-8.096727	0.000000
13	1	0	1.189796	-9.122354	0.000000
14	1	0	0.193769	-7.957301	0.889212
15	1	0	0.193769	-7.957301	-0.889212
16	6	0	3.298803	-7.724705	0.000000
17	1	0	3.857487	-7.406683	-0.889060
18	1	0	3.857487	-7.406683	0.889060
19	1	0	3.248028	-8.813442	0.000000
20	6	0	1.164316	-1.605756	0.000000
21	6	0	-0.008933	-0.886807	0.000000
22	1	0	2.094689	-1.030480	0.000000
23	1	0	-0.975986	-1.391596	0.000000
24	6	0	0.000000	0.519246	0.000000
25	6	0	-1.137992	1.299978	0.000000
26	1	0	0.982713	1.000033	0.000000
27	1	0	-2.104888	0.802214	0.000000
28	6	0	-1.120777	2.704893	0.000000
29	6	0	-1.986940	4.852906	0.000000
30	6	0	-0.614992	5.142417	0.000000
31	6	0	-2.923331	5.887879	0.000000
32	6	0	-0.145420	6.451455	0.000000
33	6	0	-2.452830	7.195830	0.000000
34	1	0	-3.994092	5.700297	0.000000
35	6	0	-1.082208	7.479170	0.000000
36	1	0	0.922892	6.659838	0.000000
37	1	0	-3.171676	8.012839	0.000000
38	1	0	-0.742770	8.513049	0.000000
39	6	0	-3.564638	2.894865	0.000000
40	1	0	-3.704323	2.281207	-0.894029
41	1	0	-3.704323	2.281207	0.894029
42	1	0	-4.305315	3.691318	0.000000
43	7	0	-2.229593	3.478632	0.000000
44	16	0	0.327537	3.670823	0.000000

Cation 7: gas phase (vacuum)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.371262	-4.452042	0.000000
2	6	0	-4.081464	-3.979856	0.000000
3	6	0	-3.783925	-2.595931	0.000000
4	6	0	-4.886098	-1.705852	0.000000
5	6	0	-6.180957	-2.158547	0.000000
6	6	0	-6.471141	-3.552745	0.000000
7	1	0	-5.540994	-5.521505	0.000000
8	1	0	-3.260486	-4.692646	0.000000
9	1	0	-4.714329	-0.633896	0.000000
10	1	0	-6.988659	-1.437040	0.000000
11	7	0	-7.749774	-4.002439	0.000000
12	6	0	-8.858947	-3.064695	0.000000
13	1	0	-9.795855	-3.620440	0.000000
14	1	0	-8.843141	-2.425781	0.890954
15	1	0	-8.843141	-2.425781	-0.890954
16	6	0	-8.024880	-5.428581	0.000000
17	1	0	-7.610723	-5.915551	-0.890837
18	1	0	-7.610723	-5.915551	0.890837
19	1	0	-9.103042	-5.584420	0.000000
20	6	0	-2.427600	-2.174221	0.000000
21	6	0	-1.937706	-0.885264	0.000000
22	1	0	-1.687894	-2.975861	0.000000
23	1	0	-2.621586	-0.039229	0.000000
24	6	0	1.379987	0.858843	0.000000
25	6	0	1.993410	2.103343	0.000000
26	1	0	2.009671	-0.032238	0.000000
27	1	0	1.364275	2.987856	0.000000
28	6	0	3.378239	2.294692	0.000000
29	6	0	5.380680	3.470805	0.000000
30	6	0	5.869794	2.157326	0.000000
31	6	0	6.267759	4.547167	0.000000
32	6	0	7.233171	1.888127	0.000000
33	6	0	7.630711	4.276841	0.000000
34	1	0	5.920408	5.574282	0.000000
35	6	0	8.112431	2.964728	0.000000
36	1	0	7.599584	0.866942	0.000000
37	1	0	8.331130	5.105519	0.000000
38	1	0	9.181772	2.781856	0.000000
39	6	0	3.209899	4.740598	0.000000
40	1	0	2.582615	4.792285	-0.894137
41	1	0	2.582615	4.792285	0.894137
42	1	0	3.886275	5.591853	0.000000
43	7	0	3.984768	3.509312	0.000000
44	16	0	4.552764	1.005219	0.000000
45	6	0	-0.562673	-0.615232	0.000000
46	6	0	0.000000	0.651639	0.000000
47	1	0	0.114675	-1.470605	0.000000
48	1	0	-0.658191	1.519189	0.000000

Cation 7: in acetonitrile (PCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.284016	-4.566450	0.000000
2	6	0	-3.998031	-4.073019	0.000000
3	6	0	-3.722757	-2.686460	0.000000
4	6	0	-4.836820	-1.813917	0.000000
5	6	0	-6.127865	-2.288238	0.000000
6	6	0	-6.397082	-3.685313	0.000000
7	1	0	-5.431962	-5.640919	0.000000
8	1	0	-3.163874	-4.774887	0.000000
9	1	0	-4.684192	-0.736205	0.000000
10	1	0	-6.943982	-1.573796	0.000000
11	7	0	-7.672129	-4.155642	0.000000
12	6	0	-8.793372	-3.234541	0.000000
13	1	0	-9.722483	-3.804613	0.000000
14	1	0	-8.786837	-2.592805	0.889956
15	1	0	-8.786837	-2.592805	-0.889956
16	6	0	-7.923430	-5.584436	0.000000
17	1	0	-7.500011	-6.066920	-0.889908
18	1	0	-7.500011	-6.066920	0.889908
19	1	0	-8.999701	-5.757401	0.000000
20	6	0	-2.365143	-2.242592	0.000000
21	6	0	-1.904139	-0.948061	0.000000
22	1	0	-1.611421	-3.035085	0.000000
23	1	0	-2.602431	-0.109646	0.000000
24	6	0	1.381728	0.861131	0.000000
25	6	0	1.951379	2.121382	0.000000
26	1	0	2.029689	-0.020277	0.000000
27	1	0	1.290418	2.984818	0.000000
28	6	0	3.333886	2.355564	0.000000
29	6	0	5.292992	3.593386	0.000000
30	6	0	5.824088	2.295511	0.000000
31	6	0	6.143857	4.699797	0.000000
32	6	0	7.195902	2.068404	0.000000
33	6	0	7.515215	4.471452	0.000000
34	1	0	5.766281	5.719221	0.000000
35	6	0	8.039668	3.174062	0.000000
36	1	0	7.592728	1.054960	0.000000
37	1	0	8.190196	5.324999	0.000000
38	1	0	9.117568	3.025421	0.000000
39	6	0	3.084100	4.794298	0.000000
40	1	0	2.455654	4.822939	-0.894386
41	1	0	2.455654	4.822939	0.894386
42	1	0	3.734947	5.665844	0.000000
43	7	0	3.897939	3.586342	0.000000
44	16	0	4.545426	1.103054	0.000000
45	6	0	-0.526730	-0.652697	0.000000
46	6	0	0.000000	0.624520	0.000000
47	1	0	0.169899	-1.496393	0.000000
48	1	0	-0.677362	1.481084	0.000000

Cation 8: gas phase (vacuum)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.249281	7.561568	0.000000
2	6	0	1.120784	7.265252	0.000000
3	6	0	2.082741	8.267601	0.000000
4	6	0	1.651583	9.589403	0.000000
5	6	0	0.287277	9.891546	0.000000
6	6	0	-0.675789	8.889449	0.000000
7	6	0	-0.339714	5.239737	0.000000
8	1	0	3.140248	8.025019	0.000000
9	1	0	2.383279	10.390384	0.000000
10	1	0	-0.033309	10.928179	0.000000
11	1	0	-1.727725	9.152142	0.000000
12	6	0	-0.923680	3.972274	0.000000
13	6	0	-0.203137	2.783721	0.000000
14	1	0	-2.007867	3.917999	0.000000
15	1	0	0.886733	2.836985	0.000000
16	6	0	-0.767539	1.510472	0.000000
17	6	0	0.000000	0.352580	0.000000
18	1	0	-1.852835	1.420079	0.000000
19	1	0	1.085284	0.465023	0.000000
20	6	0	-0.509836	-0.948108	0.000000
21	6	0	0.302147	-2.069719	0.000000
22	1	0	-1.590683	-1.082153	0.000000
23	6	0	-0.156764	-3.395902	0.000000
24	6	0	0.708032	-4.467654	0.000000
25	1	0	-1.232475	-3.558812	0.000000
26	1	0	1.773585	-4.234328	0.000000
27	6	0	0.388573	-5.853881	0.000000
28	6	0	1.433938	-6.806861	0.000000
29	6	0	-0.934345	-6.358156	0.000000
30	6	0	1.192699	-8.159924	0.000000
31	1	0	2.463230	-6.456474	0.000000
32	6	0	-1.194853	-7.705849	0.000000
33	1	0	-1.774226	-5.670105	0.000000
34	1	0	2.032534	-8.843478	0.000000
35	1	0	-2.225222	-8.039563	0.000000
36	6	0	-0.136991	-8.657762	0.000000
37	7	0	-0.392061	-9.990515	0.000000
38	6	0	-1.759493	-10.476901	0.000000
39	1	0	-1.751606	-11.566373	0.000000
40	1	0	-2.305691	-10.141795	0.890085
41	1	0	-2.305691	-10.141795	-0.890085
42	6	0	0.701928	-10.944738	0.000000
43	1	0	1.333306	-10.828754	-0.889248
44	1	0	1.333306	-10.828754	0.889248
45	1	0	0.296254	-11.955842	0.000000
46	6	0	-2.489228	6.419260	0.000000
47	1	0	-2.871347	5.918761	-0.894061
48	1	0	-2.871347	5.918761	0.894061
49	1	0	-2.840883	7.448074	0.000000
50	16	0	1.381051	5.533587	0.000000
51	7	0	-1.035106	6.407677	0.000000
52	1	0	1.382185	-1.915133	0.000000

Cation 8: in acetonitrile (PCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.189135	7.559373	0.000000
2	6	0	1.179137	7.251872	0.000000
3	6	0	2.150977	8.246094	0.000000
4	6	0	1.728747	9.571454	0.000000
5	6	0	0.365072	9.884479	0.000000
6	6	0	-0.607642	8.890809	0.000000
7	6	0	-0.296434	5.243323	0.000000
8	1	0	3.208949	7.990439	0.000000
9	1	0	2.468332	10.369545	0.000000
10	1	0	0.051555	10.926566	0.000000
11	1	0	-1.659292	9.165817	0.000000
12	6	0	-0.892236	3.975941	0.000000
13	6	0	-0.177372	2.789475	0.000000
14	1	0	-1.978468	3.923164	0.000000
15	1	0	0.916029	2.824956	0.000000
16	6	0	-0.761290	1.517519	0.000000
17	6	0	0.000000	0.361238	0.000000
18	1	0	-1.850544	1.439468	0.000000
19	1	0	1.089097	0.466085	0.000000
20	6	0	-0.523746	-0.942035	0.000000
21	6	0	0.283396	-2.061216	0.000000
22	1	0	-1.608609	-1.068628	0.000000
23	6	0	-0.188424	-3.391285	0.000000
24	6	0	0.670279	-4.461901	0.000000
25	1	0	-1.268670	-3.544717	0.000000
26	1	0	1.740357	-4.235982	0.000000
27	6	0	0.338699	-5.853614	0.000000
28	6	0	1.377219	-6.811463	0.000000
29	6	0	-0.985920	-6.349107	0.000000
30	6	0	1.127197	-8.166787	0.000000
31	1	0	2.411296	-6.466107	0.000000
32	6	0	-1.255032	-7.699013	0.000000
33	1	0	-1.825794	-5.656523	0.000000
34	1	0	1.967170	-8.852962	0.000000
35	1	0	-2.290546	-8.022154	0.000000
36	6	0	-0.204178	-8.657234	0.000000
37	7	0	-0.467288	-9.991953	0.000000
38	6	0	-1.837149	-10.468781	0.000000
39	1	0	-1.835017	-11.558926	0.000000
40	1	0	-2.382330	-10.128557	0.889552
41	1	0	-2.382330	-10.128557	-0.889552
42	6	0	0.621265	-10.950208	0.000000
43	1	0	1.254488	-10.839902	-0.889547
44	1	0	1.254488	-10.839902	0.889547
45	1	0	0.208608	-11.959303	0.000000
46	6	0	-2.438505	6.436365	0.000000
47	1	0	-2.821889	5.936989	-0.894104
48	1	0	-2.821889	5.936989	0.894104
49	1	0	-2.781020	7.468798	0.000000
50	16	0	1.425463	5.520897	0.000000
51	7	0	-0.982472	6.411993	0.000000
52	1	0	1.367371	-1.913019	0.000000

Complete Reference 18:

(18) Gaussian 03, Revision B.05, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, V. G.; Montgomery, J. A., Vreven, Jr. T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian, Inc., Pittsburgh PA, 2003.