

**Cartesian coordinates of theoretically optimized geometries:**Cation in salt **1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.598513	1.560953	2.138306
2	6	0	0.449923	2.893088	0.585969
3	6	0	2.102176	2.684072	2.797739
4	1	0	1.850627	0.566171	2.481684
5	6	0	0.941476	4.056105	1.205632
6	6	0	1.782150	3.979290	2.335827
7	1	0	2.761914	2.537192	3.646031
8	1	0	0.650750	5.028544	0.824487
9	6	0	-1.598513	1.560953	-2.138306
10	6	0	-0.449923	2.893088	-0.585969
11	6	0	-2.102176	2.684072	-2.797739
12	1	0	-1.850627	0.566171	-2.481684
13	6	0	-0.941476	4.056105	-1.205632
14	6	0	-1.782150	3.979290	-2.335827
15	1	0	-2.761914	2.537192	-3.646031
16	1	0	-0.650750	5.028544	-0.824487
17	6	0	2.151081	0.603876	-2.138306
18	6	0	2.730449	-1.056899	-0.585969
19	6	0	3.375563	0.478502	-2.797739
20	1	0	1.415632	1.319604	-2.481684
21	6	0	3.983429	-1.212710	-1.205632
22	6	0	4.337241	-0.446258	-2.335827
23	1	0	3.578230	1.123292	-3.646031
24	1	0	4.680221	-1.950706	-0.824487
25	6	0	2.280526	-1.836189	0.585969
26	6	0	0.552568	-2.164829	2.138306
27	6	0	3.041952	-2.843395	1.205632
28	6	0	1.273387	-3.162574	2.797739
29	1	0	-0.434995	-1.885776	2.481684
30	6	0	2.555091	-3.533032	2.335827
31	1	0	4.029472	-3.077838	0.824487
32	1	0	0.816316	-3.660484	3.646031
33	6	0	-0.552568	-2.164829	-2.138306
34	6	0	-2.280526	-1.836189	-0.585969
35	6	0	-1.273387	-3.162574	-2.797739
36	1	0	0.434995	-1.885776	-2.481684
37	6	0	-3.041952	-2.843395	-1.205632
38	6	0	-2.555091	-3.533032	-2.335827
39	1	0	-0.816316	-3.660484	-3.646031
40	1	0	-4.029472	-3.077838	-0.824487
41	6	0	-2.730449	-1.056899	0.585969
42	6	0	-2.151081	0.603876	2.138306
43	6	0	-3.983429	-1.212710	1.205632
44	6	0	-3.375563	0.478502	2.797739
45	1	0	-1.415632	1.319604	2.481684
46	6	0	-4.337241	-0.446258	2.335827
47	1	0	-4.680221	-1.950706	0.824487
48	1	0	-3.578230	1.123292	3.646031
49	7	0	0.784036	1.640185	1.052309
50	7	0	-1.812460	-0.141098	1.052309
51	7	0	-1.028424	-1.499087	-1.052309

52	7	0	1.028424	-1.499087	1.052309
53	7	0	1.812460	-0.141098	-1.052309
54	7	0	-0.784036	1.640185	-1.052309
55	6	0	2.316836	5.192276	3.022693
56	6	0	2.465145	5.226105	4.427345
57	6	0	2.712957	6.341253	2.307203
58	6	0	2.982069	6.356501	5.056295
59	1	0	2.163271	4.397121	5.056789
60	6	0	3.230235	7.449992	2.979655
61	1	0	2.665782	6.389003	1.225483
62	1	0	3.101638	6.415214	6.132092
63	1	0	3.555641	8.340175	2.455215
64	6	0	-2.316836	5.192276	-3.022693
65	6	0	-2.465145	5.226105	-4.427345
66	6	0	-2.712957	6.341253	-2.307203
67	6	0	-2.982069	6.356501	-5.056295
68	1	0	-2.163271	4.397121	-5.056789
69	6	0	-3.230235	7.449992	-2.979655
70	1	0	-2.665782	6.389003	-1.225483
71	1	0	-3.101638	6.415214	-6.132092
72	1	0	-3.555641	8.340175	-2.455215
73	6	0	-3.338225	-4.602576	-3.022693
74	6	0	-4.135208	-5.520116	-2.307203
75	6	0	-3.293367	-4.747930	-4.427345
76	6	0	-4.836765	-6.522462	-2.979655
77	1	0	-4.200148	-5.503136	-1.225483
78	6	0	-4.013857	-5.760798	-5.056295
79	1	0	-2.726383	-4.072008	-5.056789
80	1	0	-5.444983	-7.249363	-2.455215
81	1	0	-4.004919	-5.893704	-6.132092
82	6	0	3.338225	-4.602576	3.022693
83	6	0	3.293367	-4.747930	4.427345
84	6	0	4.135208	-5.520116	2.307203
85	6	0	4.013857	-5.760798	5.056295
86	1	0	2.726383	-4.072008	5.056789
87	6	0	4.836765	-6.522462	2.979655
88	1	0	4.200148	-5.503136	1.225483
89	1	0	4.004919	-5.893704	6.132092
90	1	0	5.444983	-7.249363	2.455215
91	6	0	5.655060	-0.589699	-3.022693
92	6	0	5.758512	-0.478174	-4.427345
93	6	0	6.848165	-0.821137	-2.307203
94	6	0	6.995926	-0.595703	-5.056295
95	1	0	4.889654	-0.325113	-5.056789
96	6	0	8.067000	-0.927531	-2.979655
97	1	0	6.865930	-0.885866	-1.225483
98	1	0	9.000624	-1.090812	-2.455215
99	6	0	-5.655060	-0.589699	3.022693
100	6	0	-6.848165	-0.821137	2.307203
101	6	0	-5.758512	-0.478174	4.427345
102	6	0	-8.067000	-0.927531	2.979655
103	1	0	-6.865930	-0.885866	1.225483
104	6	0	-6.995926	-0.595703	5.056295
105	1	0	-4.889654	-0.325113	5.056789
106	1	0	-9.000624	-1.090812	2.455215
107	1	0	-7.106557	-0.521510	6.132092
108	6	0	-9.445423	-0.921237	5.051620
109	1	0	-9.677724	0.037955	5.520750
110	1	0	-10.230688	-1.175427	4.340129
111	1	0	-9.380567	-1.703474	5.811143
112	6	0	5.520526	-7.719357	5.051620

113	1	0	4.805992	-8.400133	5.520750
114	1	0	6.133293	-8.272323	4.340129
115	1	0	6.165535	-7.272073	5.811143
116	6	0	-5.520526	-7.719357	-5.051620
117	1	0	-6.165535	-7.272073	-5.811143
118	1	0	-4.805992	-8.400133	-5.520750
119	1	0	-6.133293	-8.272323	-4.340129
120	6	0	-3.924897	8.640595	-5.051620
121	1	0	-4.871732	8.362177	-5.520750
122	1	0	-4.097395	9.447749	-4.340129
123	1	0	-3.215032	8.975546	-5.811143
124	6	0	3.924897	8.640595	5.051620
125	1	0	4.871732	8.362177	5.520750
126	1	0	4.097395	9.447749	4.340129
127	1	0	3.215032	8.975546	5.811143
128	1	0	7.106557	-0.521510	-6.132092
129	6	0	9.445423	-0.921237	-5.051620
130	1	0	9.677724	0.037955	-5.520750
131	1	0	10.230688	-1.175427	-4.340129
132	1	0	9.380567	-1.703474	-5.811143
133	7	0	4.771788	-6.633659	4.334188
134	7	0	8.130811	-0.815660	-4.334188
135	7	0	-3.359023	7.449319	-4.334188
136	7	0	-4.771788	-6.633659	-4.334188
137	7	0	-8.130811	-0.815660	4.334188
138	7	0	3.359023	7.449319	4.334188
139	44	0	0.000000	0.000000	0.000000

-----

Cation in salt **5**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.576749	1.448233	2.129305
2	6	0	0.450058	2.794239	0.585731
3	6	0	2.097722	2.564742	2.790887
4	1	0	1.816041	0.452292	2.476947
5	6	0	0.954128	3.953411	1.201488
6	6	0	1.794622	3.864335	2.331877
7	1	0	2.755316	2.407851	3.639044
8	1	0	0.675559	4.928909	0.818892
9	6	0	-1.576749	1.448233	-2.129305
10	6	0	-0.450058	2.794239	-0.585731
11	6	0	-2.097722	2.564742	-2.790887
12	1	0	-1.816041	0.452292	-2.476947
13	6	0	-0.954128	3.953411	-1.201488
14	6	0	-1.794622	3.864335	-2.331877
15	1	0	-2.755316	2.407851	-3.639044
16	1	0	-0.675559	4.928909	-0.818892
17	6	0	2.042581	0.641388	-2.129305
18	6	0	2.644911	-1.007358	-0.585731
19	6	0	3.269992	0.534310	-2.790887
20	1	0	1.299717	1.346592	-2.476947
21	6	0	3.900819	-1.150406	-1.201488
22	6	0	4.243923	-0.377980	-2.331877
23	1	0	3.462918	1.182248	-3.639044
24	1	0	4.606340	-1.879403	-0.818892

25	6	0	2.194853	-1.786881	0.585731
26	6	0	0.465832	-2.089621	2.129305
27	6	0	2.946690	-2.803005	1.201488
28	6	0	1.172270	-3.099051	2.790887
29	1	0	-0.516325	-1.798884	2.476947
30	6	0	2.449301	-3.486355	2.331877
31	1	0	3.930781	-3.049506	0.818892
32	1	0	0.707602	-3.590099	3.639044
33	6	0	-0.465832	-2.089621	-2.129305
34	6	0	-2.194853	-1.786881	-0.585731
35	6	0	-1.172270	-3.099051	-2.790887
36	1	0	0.516325	-1.798884	-2.476947
37	6	0	-2.946690	-2.803005	-1.201488
38	6	0	-2.449301	-3.486355	-2.331877
39	1	0	-0.707602	-3.590099	-3.639044
40	1	0	-3.930781	-3.049506	-0.818892
41	6	0	-2.644911	-1.007358	0.585731
42	6	0	-2.042581	0.641388	2.129305
43	6	0	-3.900819	-1.150406	1.201488
44	6	0	-3.269992	0.534310	2.790887
45	1	0	-1.299717	1.346592	2.476947
46	6	0	-4.243923	-0.377980	2.331877
47	1	0	-4.606340	-1.879403	0.818892
48	1	0	-3.462918	1.182248	3.639044
49	7	0	0.763676	1.538384	1.046106
50	7	0	-1.714118	-0.107829	1.046106
51	7	0	-0.950441	-1.430555	-1.046106
52	7	0	0.950441	-1.430555	1.046106
53	7	0	1.714118	-0.107829	-1.046106
54	7	0	-0.763676	1.538384	-1.046106
55	6	0	2.343998	5.070320	3.020668
56	6	0	2.494519	5.099910	4.425083
57	6	0	2.750176	6.216648	2.306724
58	6	0	3.023164	6.224274	5.055508
59	1	0	2.185779	4.272750	5.053600
60	6	0	3.278980	7.319248	2.980584
61	1	0	2.701229	6.267491	1.225217
62	1	0	3.144866	6.279738	6.131262
63	1	0	3.611629	8.207505	2.457381
64	6	0	-2.343998	5.070320	-3.020668
65	6	0	-2.494519	5.099910	-4.425083
66	6	0	-2.750176	6.216648	-2.306724
67	6	0	-3.023164	6.224274	-5.055508
68	1	0	-2.185779	4.272750	-5.053600
69	6	0	-3.278980	7.319248	-2.980584
70	1	0	-2.701229	6.267491	-1.225217
71	1	0	-3.144866	6.279738	-6.131262
72	1	0	-3.611629	8.207505	-2.457381
73	6	0	-3.219027	-4.565122	-3.020668
74	6	0	-4.008687	-5.490046	-2.306724
75	6	0	-3.169392	-4.710272	-4.425083
76	6	0	-4.699164	-6.499304	-2.980584
77	1	0	-4.077192	-5.473079	-1.225217
78	6	0	-3.878798	-5.730274	-5.055508
79	1	0	-2.607421	-4.029316	-5.053600
80	1	0	-5.302093	-7.231515	-2.457381
81	1	0	-3.865980	-5.863403	-6.131262
82	6	0	3.219027	-4.565122	3.020668
83	6	0	3.169392	-4.710272	4.425083
84	6	0	4.008687	-5.490046	2.306724
85	6	0	3.878798	-5.730274	5.055508

86	1	0	2.607421	-4.029316	5.053600
87	6	0	4.699164	-6.499304	2.980584
88	1	0	4.077192	-5.473079	1.225217
89	1	0	3.865980	-5.863403	6.131262
90	1	0	5.302093	-7.231515	2.457381
91	6	0	5.563025	-0.505198	-3.020668
92	6	0	5.663911	-0.389638	-4.425083
93	6	0	6.758863	-0.726602	-2.306724
94	6	0	6.901962	-0.494000	-5.055508
95	1	0	4.793200	-0.243435	-5.053600
96	6	0	7.978145	-0.819944	-2.980584
97	1	0	6.778421	-0.794412	-1.225217
98	1	0	8.913723	-0.975990	-2.457381
99	6	0	-5.563025	-0.505198	3.020668
100	6	0	-6.758863	-0.726602	2.306724
101	6	0	-5.663911	-0.389638	4.425083
102	6	0	-7.978145	-0.819944	2.980584
103	1	0	-6.778421	-0.794412	1.225217
104	6	0	-6.901962	-0.494000	5.055508
105	1	0	-4.793200	-0.243435	5.053600
106	1	0	-8.913723	-0.975990	2.457381
107	1	0	-7.010846	-0.416335	6.131262
108	6	0	-9.354481	-0.797047	5.053989
109	1	0	-9.577602	0.165206	5.521379
110	1	0	-10.142720	-1.045667	4.343812
111	1	0	-9.295734	-1.578271	5.815072
112	6	0	5.367503	-7.702695	5.053989
113	1	0	4.645728	-8.377049	5.521379
114	1	0	5.976934	-8.261020	4.343812
115	1	0	6.014689	-7.261206	5.815072
116	6	0	-5.367503	-7.702695	-5.053989
117	1	0	-6.014689	-7.261206	-5.815072
118	1	0	-4.645728	-8.377049	-5.521379
119	1	0	-5.976934	-8.261020	-4.343812
120	6	0	-3.986978	8.499742	-5.053989
121	1	0	-4.931873	8.211844	-5.521379
122	1	0	-4.165786	9.306686	-4.343812
123	1	0	-3.281044	8.839477	-5.815072
124	6	0	3.986978	8.499742	5.053989
125	1	0	4.931873	8.211844	5.521379
126	1	0	4.165786	9.306686	4.343812
127	1	0	3.281044	8.839477	5.815072
128	1	0	7.010846	-0.416335	-6.131262
129	6	0	9.354481	-0.797047	-5.053989
130	1	0	9.577602	0.165206	-5.521379
131	1	0	10.142720	-1.045667	-4.343812
132	1	0	9.295734	-1.578271	-5.815072
133	7	0	4.630080	-6.610037	4.334932
134	7	0	8.039500	-0.704749	-4.334932
135	7	0	-3.409420	7.314785	-4.334932
136	7	0	-4.630080	-6.610037	-4.334932
137	7	0	-8.039500	-0.704749	4.334932
138	7	0	3.409420	7.314785	4.334932
139	26	0	0.000000	0.000000	0.000000

---

**Complete References 4e, 4k, 21, 29c, 29d and 30:**

- (4) (e) Malaun, M.; Kowallick, R.; McDonagh, A. M.; Marcaccio, M.; Paul, R. L.; Asselberghs, I.; Clays, K.; Persoons, A.; Bildstein, B.; Fiorini, C.; Nunzi, J.-M.; Ward, M. D.; McCleverty, J. A. *J. Chem. Soc., Dalton Trans.* **2001**, 3025–3038.
- (k) Sporer, C.; Ratera, I.; Ruiz-Molina, D.; Zhao, Y.-X.; Vidal-Gancedo, J.; Wurst, K.; Jaitner, P.; Clays, K.; Persoons, A.; Rovira, C.; Veciana, J. *Angew. Chem. Int. Ed.* **2004**, *43*, 5266–5268.
- (21) 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.
- (29) (c) Garcia, M. H.; Robalo, M. P.; Dias, A. R.; Duarte, M. T.; Wenseleers, W.; Aerts, G.; Goovaerts, E.; Cifuentes, M. P.; Hurst, S.; Humphrey, M. G.; Samoc, M.; Luther-Davies B. *Organometallics* **2002**, *21*, 2107–2118. (d) Garcia, M. H.; Royer, S.; Robalo, M. P.; Dias, A. R.; Tranchier, J.-P.; Chavignon, R.; Prim, D.; Auffrant, A.; Rose-Munch, F.; Rose, E.; Vaissermann, J.; Persoons, A.; Asselberghs, I. *Eur. J. Inorg. Chem.* **2003**, 3895–3904.

- (30) Powell, C. E.; Cifuentes, M. P.; McDonagh, A. M.; Hurst, S. K.; Lucas, N. T.; Delfs, C. D.; Stranger, R.; Humphrey, M. G.; Houbrechts, S.; Asselberghs, I.; Persoons, A.; Hockless, D. C. R. *Inorg. Chim. Acta* **2003**, *352*, 9–18.