Supporting Information for Mark Mascal, *The Energetics of Shooting Ions into the Dodecahedrane Cage*

Contents

S2 H^+@**1** MP2/6-311G(d,p)

S3 He@**1** MP2/6-311G(d,p)

S4 Li^+@**1** MP2/6-311G(d,p)

S5 Be^+@**1** MP2/6-311G(d,p)

S6 Be^{2+}@**1** MP2/6-311G(d,p)

S7 Mg^{2+}@**1** MP2/6-311G(d,p)

S8 **1** + H^+ exohedral complex MP2/6-311G(d,p)

S9 **1** + He exohedral complex HF/6-31G(d)

S10 **1** + Li^+ exohedral complex HF/6-31G(d)

S11 **1** + Be^+ exohedral complex HF/6-31G(d)

S12 **1** + Be^{2+} exohedral complex HF/6-31G(d)

S13 **1** + Mg^{2+} exohedral complex HF/6-31G(d)

S14 Li^+@**1** Cl^- ion pair HF/6-31+G(d)

S15 **1** + H^+ facial complex HF/6-31G(d)

S16 **1** + He facial complex HF/6-31G(d)

S17 **1** + Li^+ facial complex HF/6-31G(d)

S18 **1** + Be^+ facial complex HF/6-31G(d)

S19 **1** + Be^{2+} facial complex HF/6-31G(d)

S20 **1** + Mg^{2+} facial complex HF/6-31G(d)

H^+@**1** MP2/6-311G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.040708	-0.779481
2	6	0	0.000000	2.040708	0.779481
3	6	0	1.261227	1.261227	-1.261227
4	6	0	-1.261227	1.261227	-1.261227
5	6	0	1.261227	1.261227	1.261227
6	6	0	2.040708	0.779481	0.000000
7	6	0	0.779481	0.000000	-2.040708
8	6	0	-1.261227	1.261227	1.261227
9	6	0	-2.040708	0.779481	0.000000
10	6	0	-0.779481	0.000000	-2.040708
11	6	0	0.779481	0.000000	2.040708
12	6	0	2.040708	-0.779481	0.000000
13	6	0	1.261227	-1.261227	-1.261227
14	6	0	-0.779481	0.000000	2.040708
15	6	0	-2.040708	-0.779481	0.000000
16	6	0	-1.261227	-1.261227	-1.261227
17	6	0	1.261227	-1.261227	1.261227
18	6	0	0.000000	-2.040708	-0.779481
19	6	0	-1.261227	-1.261227	1.261227
20	6	0	0.000000	-2.040708	0.779481
21	1	0	-3.061635	1.169441	0.000000
22	1	0	-1.892195	-1.892195	-1.892195
23	1	0	1.169441	0.000000	-3.061635
24	1	0	3.061635	-1.169441	0.000000
25	1	0	1.892195	1.892195	1.892195
26	1	0	-1.169441	0.000000	3.061635
27	1	0	0.000000	3.061635	1.169441
28	1	0	1.892195	1.892195	-1.892195
29	1	0	-1.892195	1.892195	-1.892195
30	1	0	3.061635	1.169441	0.000000
31	1	0	-1.892195	1.892195	1.892195
32	1	0	-1.169441	0.000000	-3.061635
33	1	0	1.169441	0.000000	3.061635
34	1	0	1.892195	-1.892195	-1.892195
35	1	0	-3.061635	-1.169441	0.000000
36	1	0	1.892195	-1.892195	1.892195
37	1	0	0.000000	-3.061635	-1.169441
38	1	0	-1.892195	-1.892195	1.892195
39	1	0	0.000000	-3.061635	1.169441
40	1	0	0.000000	3.061635	-1.169441
41	1	0	0.000000	0.000000	0.000000

He@**1** MP2/6-311G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.072496	1.735335	-0.779214
2	6	0	-1.072496	1.735335	0.779214
3	6	0	0.409657	1.735335	-1.260795
4	6	0	-1.735335	0.409657	-1.260794
5	6	0	0.409657	1.735335	1.260794
6	6	0	1.325678	1.735335	0.000000
7	6	0	0.662839	0.409657	-2.040008
8	6	0	-1.735335	0.409657	1.260795
9	6	0	-2.144992	-0.409657	0.000000
10	6	0	-0.662839	-0.409657	-2.040008
11	6	0	0.662839	0.409657	2.040008
12	6	0	2.144992	0.409657	0.000000
13	6	0	1.735335	-0.409657	-1.260795
14	6	0	-0.662839	-0.409657	2.040008
15	6	0	-1.325678	-1.735335	0.000000
16	6	0	-0.409657	-1.735335	-1.260794
17	6	0	1.735335	-0.409657	1.260794
18	6	0	1.072496	-1.735335	-0.779214
19	6	0	-0.409657	-1.735335	1.260795
20	6	0	1.072496	-1.735335	0.779214
21	1	0	-3.220214	-0.615006	0.000000
22	1	0	-0.615006	-2.605208	-1.892794
23	1	0	0.995101	0.615006	-3.062606
24	1	0	3.220214	0.615006	0.000000
25	1	0	0.615006	2.605208	1.892794
26	1	0	-0.995101	-0.615006	3.062606
27	1	0	-1.610107	2.605208	1.169811
28	1	0	0.615006	2.605208	-1.892794
29	1	0	-2.605208	0.615006	-1.892794
30	1	0	1.990202	2.605208	0.000000
31	1	0	-2.605208	0.615006	1.892794
32	1	0	-0.995101	-0.615006	-3.062606
33	1	0	0.995101	0.615006	3.062606
34	1	0	2.605208	-0.615006	-1.892794
35	1	0	-1.990202	-2.605208	0.000000
36	1	0	2.605208	-0.615006	1.892794
37	1	0	1.610107	-2.605208	-1.169811
38	1	0	-0.615006	-2.605208	1.892794
39	1	0	1.610107	-2.605208	1.169811
40	1	0	-1.610107	2.605208	-1.169811
41	2	0	0.000000	0.000000	0.000000

Li^{+}@**1** MP2/6-311G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.049662	-0.782901
2	6	0	0.000000	2.049662	0.782901
3	6	0	1.266761	1.266761	-1.266761
4	6	0	-1.266761	1.266761	-1.266761
5	6	0	1.266761	1.266761	1.266761
6	6	0	2.049662	0.782901	0.000000
7	6	0	0.782901	0.000000	-2.049662
8	6	0	-1.266761	1.266761	1.266761
9	6	0	-2.049662	0.782901	0.000000
10	6	0	-0.782901	0.000000	-2.049662
11	6	0	0.782901	0.000000	2.049662
12	6	0	2.049662	-0.782901	0.000000
13	6	0	1.266761	-1.266761	-1.266761
14	6	0	-0.782901	0.000000	2.049662
15	6	0	-2.049662	-0.782901	0.000000
16	6	0	-1.266761	-1.266761	-1.266761
17	6	0	1.266761	-1.266761	1.266761
18	6	0	0.000000	-2.049662	-0.782901
19	6	0	-1.266761	-1.266761	1.266761
20	6	0	0.000000	-2.049662	0.782901
21	1	0	-3.068804	1.172179	0.000000
22	1	0	-1.896625	-1.896625	-1.896625
23	1	0	1.172179	0.000000	-3.068804
24	1	0	3.068804	-1.172179	0.000000
25	1	0	1.896625	1.896625	1.896625
26	1	0	-1.172179	0.000000	3.068804
27	1	0	0.000000	3.068804	1.172179
28	1	0	1.896625	1.896625	-1.896625
29	1	0	-1.896625	1.896625	-1.896625
30	1	0	3.068804	1.172179	0.000000
31	1	0	-1.896625	1.896625	1.896625
32	1	0	-1.172179	0.000000	-3.068804
33	1	0	1.172179	0.000000	3.068804
34	1	0	1.896625	-1.896625	-1.896625
35	1	0	-3.068804	-1.172179	0.000000
36	1	0	1.896625	-1.896625	1.896625
37	1	0	0.000000	-3.068804	-1.172179
38	1	0	-1.896625	-1.896625	1.896625
39	1	0	0.000000	-3.068804	1.172179
40	1	0	0.000000	3.068804	-1.172179
41	3	0	0.000000	0.000000	0.000000

Be^{+}@**1** MP2/6-311G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.112736	0.808450	-1.734386
2	6	0	1.112736	-0.808450	-1.734386
3	6	0	-0.425027	1.308100	-1.734386
4	6	0	1.757170	1.276659	-0.380209
5	6	0	-0.425027	-1.308100	-1.734386
6	6	0	-1.375418	0.000000	-1.734386
7	6	0	-0.671179	2.065677	-0.380209
8	6	0	1.757170	-1.276659	-0.380209
9	6	0	2.156775	0.000000	0.435586
10	6	0	0.666480	2.051215	0.435586
11	6	0	-0.671179	-2.065677	-0.380209
12	6	0	-2.171982	0.000000	-0.380209
13	6	0	-1.744868	1.267721	0.435586
14	6	0	0.666480	-2.051215	0.435586
15	6	0	1.323412	0.000000	1.749985
16	6	0	0.408957	1.258640	1.749985
17	6	0	-1.744868	-1.267721	0.435586
18	6	0	-1.070663	0.777882	1.749985
19	6	0	0.408957	-1.258640	1.749985
20	6	0	-1.070663	-0.777882	1.749985
21	1	0	3.235645	0.000000	0.638046
22	1	0	0.614689	1.891819	2.621789
23	1	0	-1.003925	3.089764	-0.590655
24	1	0	-3.248771	0.000000	-0.590655
25	1	0	-0.616882	-1.898567	-2.628427
26	1	0	0.999869	-3.077282	0.638046
27	1	0	1.615018	-1.173379	-2.628427
28	1	0	-0.616882	1.898567	-2.628427
29	1	0	2.628311	1.909579	-0.590655
30	1	0	-1.996272	0.000000	-2.628427
31	1	0	2.628311	-1.909579	-0.590655
32	1	0	0.999869	3.077282	0.638046
33	1	0	-1.003925	-3.089764	-0.590655
34	1	0	-2.617692	1.901865	0.638046
35	1	0	1.989176	0.000000	2.621789
36	1	0	-2.617692	-1.901865	0.638046
37	1	0	-1.609277	1.169208	2.621789
38	1	0	0.614689	-1.891819	2.621789
39	1	0	-1.609277	-1.169208	2.621789
40	1	0	1.615018	1.173379	-2.628427
41	4	0	0.000000	0.000000	-0.583262

Be^{2+}@**1** MP2/6-311G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.109983	1.741068	-0.806456
2	6	0	-1.109982	1.741068	0.806456
3	6	0	0.423987	1.741059	-1.304874
4	6	0	-1.751722	0.384523	-1.272701
5	6	0	0.423989	1.741060	1.304872
6	6	0	1.372034	1.741055	-0.000001
7	6	0	0.669100	0.384510	-2.059275
8	6	0	-1.751721	0.384524	1.272702
9	6	0	-2.152203	-0.436911	0.000001
10	6	0	-0.665070	-0.436919	-2.046864
11	6	0	0.669102	0.384511	2.059274
12	6	0	2.165251	0.384503	-0.000001
13	6	0	1.741164	-0.436932	-1.265032
14	6	0	-0.665068	-0.436918	2.046865
15	6	0	-1.326411	-1.759478	0.000001
16	6	0	-0.409890	-1.759483	-1.261482
17	6	0	1.741165	-0.436931	1.265031
18	6	0	1.073072	-1.759491	-0.779639
19	6	0	-0.409889	-1.759482	1.261484
20	6	0	1.073072	-1.759490	0.779639
21	1	0	-3.226538	-0.630691	0.000002
22	1	0	-0.615340	-2.625447	-1.893774
23	1	0	1.000475	0.588490	-3.079143
24	1	0	3.237604	0.588479	-0.000002
25	1	0	0.618644	2.627843	1.903944
26	1	0	-0.997056	-0.630702	3.068618
27	1	0	-1.619578	2.627854	1.176703
28	1	0	0.618642	2.627841	-1.903947
29	1	0	-2.619272	0.588509	-1.903013
30	1	0	2.001940	2.627835	-0.000002
31	1	0	-2.619270	0.588511	1.903015
32	1	0	-0.997059	-0.630704	-3.068616
33	1	0	1.000479	0.588492	3.079141
34	1	0	2.610317	-0.630723	-1.896511
35	1	0	-1.991247	-2.625439	0.000002
36	1	0	2.610319	-0.630721	1.896509
37	1	0	1.610927	-2.625459	-1.170417
38	1	0	-0.615338	-2.625446	1.893777
39	1	0	1.610929	-2.625458	1.170418
40	1	0	-1.619579	2.627854	-1.176703
41	4	0	0.000003	0.581001	0.000000

Mg^{2+}@**1** MP2/6-311G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.090970	1.765226	-0.792636
2	6	0	-1.090970	1.765226	0.792636
3	6	0	0.416713	1.765226	-1.282512
4	6	0	-1.765226	0.416713	-1.282512
5	6	0	0.416713	1.765226	1.282512
6	6	0	1.348513	1.765226	0.000000
7	6	0	0.674257	0.416713	-2.075148
8	6	0	-1.765226	0.416713	1.282512
9	6	0	-2.181940	-0.416713	0.000000
10	6	0	-0.674256	-0.416713	-2.075148
11	6	0	0.674256	0.416713	2.075148
12	6	0	2.181940	0.416713	0.000000
13	6	0	1.765226	-0.416713	-1.282512
14	6	0	-0.674257	-0.416713	2.075148
15	6	0	-1.348513	-1.765226	0.000000
16	6	0	-0.416713	-1.765226	-1.282512
17	6	0	1.765226	-0.416713	1.282512
18	6	0	1.090970	-1.765226	-0.792636
19	6	0	-0.416713	-1.765226	1.282512
20	6	0	1.090970	-1.765226	0.792636
21	1	0	-3.251663	-0.621012	0.000000
22	1	0	-0.621012	-2.630651	-1.911280
23	1	0	1.004819	0.621012	-3.092515
24	1	0	3.251663	0.621012	0.000000
25	1	0	0.621012	2.630651	1.911280
26	1	0	-1.004819	-0.621012	3.092515
27	1	0	-1.625832	2.630651	1.181236
28	1	0	0.621012	2.630651	-1.911279
29	1	0	-2.630650	0.621012	-1.911280
30	1	0	2.009638	2.630651	0.000000
31	1	0	-2.630651	0.621012	1.911279
32	1	0	-1.004819	-0.621012	-3.092515
33	1	0	1.004819	0.621012	3.092515
34	1	0	2.630651	-0.621012	-1.911279
35	1	0	-2.009638	-2.630651	0.000000
36	1	0	2.630650	-0.621012	1.911280
37	1	0	1.625832	-2.630651	-1.181236
38	1	0	-0.621012	-2.630651	1.911279
39	1	0	1.625831	-2.630651	1.181236
40	1	0	-1.625831	2.630651	-1.181236
41	12	0	0.000000	0.000000	0.000000

1 + H^+ exohedral complex MP2/6-311G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.254581	1.319215	1.234305
2	6	0	1.960069	0.000000	0.781898
3	6	0	0.777647	2.060111	-0.047960
4	6	0	0.000000	1.141722	2.058408
5	6	0	2.010468	0.000000	-0.769905
6	6	0	1.257051	1.254254	-1.279245
7	6	0	-0.777647	2.060111	-0.047960
8	6	0	1.254581	-1.319215	1.234305
9	6	0	0.000000	-1.141722	2.058408
10	6	0	-1.254581	1.319215	1.234305
11	6	0	1.257051	-1.254254	-1.279245
12	6	0	0.000000	0.774870	-2.053618
13	6	0	-1.257051	1.254254	-1.279245
14	6	0	0.777647	-2.060111	-0.047960
15	6	0	-1.254581	-1.319215	1.234305
16	6	0	-1.960069	0.000000	0.781898
17	6	0	0.000000	-0.774870	-2.053618
18	6	0	-2.010468	0.000000	-0.769905
19	6	0	-0.777647	-2.060111	-0.047960
20	6	0	-1.257051	-1.254254	-1.279245
21	1	0	0.000000	-1.591503	3.061339
22	1	0	-2.971219	0.000000	1.196139
23	1	0	-1.166979	3.081440	-0.056478
24	1	0	0.000000	1.168338	-3.073451
25	1	0	3.049002	0.000000	-1.111306
26	1	0	1.166979	-3.081440	-0.056478
27	1	0	2.971219	0.000000	1.196139
28	1	0	1.166979	3.081440	-0.056478
29	1	0	0.000000	1.591503	3.061339
30	1	0	1.901670	1.865815	-1.915893
31	1	0	1.971334	-1.917283	1.804452
32	1	0	-1.971334	1.917283	1.804452
33	1	0	1.901670	-1.865815	-1.915893
34	1	0	-1.901670	1.865815	-1.915893
35	1	0	-1.971334	-1.917283	1.804452
36	1	0	0.000000	-1.168338	-3.073451
37	1	0	-3.049002	0.000000	-1.111306
38	1	0	-1.166979	-3.081440	-0.056478
39	1	0	-1.901670	-1.865815	-1.915893
40	1	0	1.971334	1.917283	1.804452
41	1	0	0.000000	0.000000	2.554414

1 + He exohedral complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.998332	1.690144	-0.773860
2	6	0	-0.998335	1.690139	0.773868
3	6	0	0.473638	1.690003	-1.252100
4	6	0	-1.656706	0.373613	-1.252139
5	6	0	0.473634	1.689995	1.252112
6	6	0	1.383352	1.689942	0.000008
7	6	0	0.724997	0.373446	-2.025953
8	6	0	-1.656710	0.373605	1.252136
9	6	0	-2.063605	-0.440053	-0.000005
10	6	0	-0.591605	-0.440134	-2.025952
11	6	0	0.724990	0.373433	2.025958
12	6	0	2.196969	0.373341	0.000005
13	6	0	1.790079	-0.440306	-1.252120
14	6	0	-0.591612	-0.440147	2.025948
15	6	0	-1.249966	-1.756640	-0.000008
16	6	0	-0.340252	-1.756702	-1.252116
17	6	0	1.790075	-0.440314	1.252123
18	6	0	1.131713	-1.756823	-0.773858
19	6	0	-0.340256	-1.756710	1.252103
20	6	0	1.131710	-1.756828	0.773850
21	1	0	-3.128668	-0.643397	-0.000007
22	1	0	-0.543731	-2.618335	-1.878148
23	1	0	1.054120	0.576845	-3.038888
24	1	0	3.262042	0.576683	0.000007
25	1	0	0.677120	2.551628	1.878147
26	1	0	-0.920730	-0.643550	3.038887
27	1	0	-1.530798	2.551819	1.160775
28	1	0	0.677127	2.551640	-1.878128
29	1	0	-2.518332	0.577074	-1.878167
30	1	0	2.041640	2.551562	0.000012
31	1	0	-2.518338	0.577062	1.878162
32	1	0	-0.920720	-0.643530	-3.038894
33	1	0	1.054110	0.576825	3.038895
34	1	0	2.651717	-0.643767	-1.878149
35	1	0	-1.908249	-2.618266	-0.000012
36	1	0	2.651711	-0.643779	1.878153
37	1	0	1.664184	-2.618510	-1.160767
38	1	0	-0.543738	-2.618347	1.878129
39	1	0	1.664180	-2.618517	1.160755
40	1	0	-1.530794	2.551826	-1.160764
41	2	0	-4.668261	2.334512	0.000000

1 + Li^+ exohedral complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.073655	0.780056	1.649063
2	6	0	1.073655	-0.780056	1.649063
3	6	0	1.727380	1.255015	0.327462
4	6	0	-0.410100	1.262157	1.649063
5	6	0	1.727380	-1.255015	0.327462
6	6	0	2.131582	0.000000	-0.480925
7	6	0	0.658695	2.027255	-0.480925
8	6	0	-0.410100	-1.262157	1.649063
9	6	0	-1.327110	0.000000	1.649063
10	6	0	-0.659800	2.030656	0.327462
11	6	0	0.658695	-2.027255	-0.480925
12	6	0	1.316456	0.000000	-1.796488
13	6	0	0.406807	1.252024	-1.796488
14	6	0	-0.659800	-2.030656	0.327462
15	6	0	-2.135159	0.000000	0.327462
16	6	0	-1.724486	1.252913	-0.480925
17	6	0	0.406807	-1.252024	-1.796488
18	6	0	-1.065035	0.773793	-1.796488
19	6	0	-1.724486	-1.252913	-0.480925
20	6	0	-1.065035	-0.773793	-1.796488
21	1	0	-2.018730	0.000000	2.495613
22	1	0	-2.585245	1.878290	-0.679605
23	1	0	0.987476	3.039138	-0.679605
24	1	0	1.975403	0.000000	-2.655126
25	1	0	2.586153	-1.878950	0.537142
26	1	0	-0.987822	-3.040205	0.537142
27	1	0	1.633187	-1.186580	2.495613
28	1	0	2.586153	1.878950	0.537142
29	1	0	-0.623822	1.919927	2.495613
30	1	0	3.195539	0.000000	-0.679605
31	1	0	-0.623822	-1.919927	2.495613
32	1	0	-0.987822	3.040205	0.537142
33	1	0	0.987476	-3.039138	-0.679605
34	1	0	0.610433	1.878720	-2.655126
35	1	0	-3.196661	0.000000	0.537142
36	1	0	0.610433	-1.878720	-2.655126
37	1	0	-1.598135	1.161113	-2.655126
38	1	0	-2.585245	-1.878290	-0.679605
39	1	0	-1.598135	-1.161113	-2.655126
40	1	0	1.633187	1.186580	2.495613
41	3	0	0.000000	0.000000	3.512168

1 + Be^{+} exohedral complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.089153	0.791316	1.648188
2	6	0	1.089153	-0.791316	1.648188
3	6	0	1.726249	1.254194	0.307133
4	6	0	-0.416019	1.280376	1.648188
5	6	0	1.726249	-1.254193	0.307133
6	6	0	2.129649	0.000000	-0.497055
7	6	0	0.658098	2.025417	-0.497055
8	6	0	-0.416019	-1.280376	1.648188
9	6	0	-1.346267	0.000000	1.648188
10	6	0	-0.659369	2.029328	0.307133
11	6	0	0.658098	-2.025417	-0.497055
12	6	0	1.316349	0.000000	-1.813803
13	6	0	0.406774	1.251922	-1.813803
14	6	0	-0.659368	-2.029328	0.307133
15	6	0	-2.133761	0.000000	0.307133
16	6	0	-1.722923	1.251776	-0.497055
17	6	0	0.406774	-1.251922	-1.813803
18	6	0	-1.064949	0.773730	-1.813803
19	6	0	-1.722922	-1.251777	-0.497055
20	6	0	-1.064949	-0.773731	-1.813803
21	1	0	-2.049163	0.000000	2.478811
22	1	0	-2.583956	1.877354	-0.691430
23	1	0	0.986983	3.037622	-0.691430
24	1	0	1.976655	0.000000	-2.670819
25	1	0	2.583398	-1.876948	0.521688
26	1	0	-0.986770	-3.036966	0.521688
27	1	0	1.657808	-1.204468	2.478811
28	1	0	2.583397	1.876948	0.521688
29	1	0	-0.633226	1.948870	2.478811
30	1	0	3.193945	0.000000	-0.691430
31	1	0	-0.633226	-1.948870	2.478811
32	1	0	-0.986770	3.036966	0.521688
33	1	0	0.986984	-3.037622	-0.691430
34	1	0	0.610820	1.879911	-2.670819
35	1	0	-3.193255	0.000000	0.521688
36	1	0	0.610820	-1.879911	-2.670819
37	1	0	-1.599148	1.161849	-2.670819
38	1	0	-2.583956	-1.877354	-0.691430
39	1	0	-1.599148	-1.161849	-2.670819
40	1	0	1.657808	1.204468	2.478811
41	4	0	0.000000	0.000000	3.118717

1 + Be^{2+} exohedral complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.129011	0.820274	1.675465
2	6	0	1.129011	-0.820274	1.675465
3	6	0	1.735494	1.260911	0.309670
4	6	0	-0.431244	1.327232	1.675465
5	6	0	1.735494	-1.260910	0.309670
6	6	0	2.132105	0.000000	-0.487725
7	6	0	0.658857	2.027753	-0.487725
8	6	0	-0.431244	-1.327232	1.675465
9	6	0	-1.395534	0.000000	1.675465
10	6	0	-0.662900	2.040196	0.309670
11	6	0	0.658857	-2.027753	-0.487725
12	6	0	1.316578	0.000000	-1.803746
13	6	0	0.406845	1.252141	-1.803746
14	6	0	-0.662900	-2.040196	0.309670
15	6	0	-2.145189	0.000000	0.309670
16	6	0	-1.724910	1.253220	-0.487725
17	6	0	0.406845	-1.252141	-1.803746
18	6	0	-1.065134	0.773865	-1.803746
19	6	0	-1.724909	-1.253220	-0.487725
20	6	0	-1.065134	-0.773866	-1.803746
21	1	0	-2.101953	0.000000	2.505780
22	1	0	-2.585487	1.878466	-0.679095
23	1	0	0.987568	3.039422	-0.679095
24	1	0	1.977508	0.000000	-2.658638
25	1	0	2.592567	-1.883610	0.519302
26	1	0	-0.990272	-3.047745	0.519302
27	1	0	1.700516	-1.235497	2.505780
28	1	0	2.592567	1.883610	0.519302
29	1	0	-0.649539	1.999076	2.505780
30	1	0	3.195837	0.000000	-0.679095
31	1	0	-0.649539	-1.999076	2.505780
32	1	0	-0.990273	3.047745	0.519302
33	1	0	0.987568	-3.039422	-0.679095
34	1	0	0.611084	1.880722	-2.658638
35	1	0	-3.204589	0.000000	0.519302
36	1	0	0.611084	-1.880722	-2.658638
37	1	0	-1.599838	1.162350	-2.658638
38	1	0	-2.585486	-1.878466	-0.679095
39	1	0	-1.599838	-1.162350	-2.658638
40	1	0	1.700516	1.235497	2.505780
41	4	0	0.000000	0.000000	2.688332

1 + Mg^{2+} exohedral complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.065203	-0.472192	0.326660
2	6	0	0.065203	-0.472191	1.903032
3	6	0	1.500077	-0.101489	-0.145739
4	6	0	-0.234655	-1.941117	-0.160465
5	6	0	1.500077	-0.101488	2.375430
6	6	0	2.365389	0.130082	1.114846
7	6	0	2.070324	-1.315363	-0.915667
8	6	0	-0.234655	-1.941117	2.390158
9	6	0	-0.419977	-2.848962	1.114846
10	6	0	1.020500	-2.450813	-0.924823
11	6	0	2.070324	-1.315363	3.145358
12	6	0	3.489448	-0.934565	1.114846
13	6	0	3.307477	-1.825996	-0.137405
14	6	0	1.020500	-2.450813	3.154515
15	6	0	0.724104	-3.902776	1.114845
16	6	0	1.592899	-3.654141	-0.140080
17	6	0	3.307476	-1.825996	2.367098
18	6	0	3.013041	-3.268360	0.340912
19	6	0	1.592899	-3.654142	2.369772
20	6	0	3.013040	-3.268360	1.888780
21	1	0	-1.382855	-3.387544	1.114846
22	1	0	1.612171	-4.536050	-0.765077
23	1	0	2.327370	-1.032479	-1.926932
24	1	0	4.460421	-0.459550	1.114846
25	1	0	1.461410	0.780768	2.997856
26	1	0	0.745037	-2.728559	4.161621
27	1	0	-0.637061	0.265904	2.326404
28	1	0	1.461410	0.780767	-0.768164
29	1	0	-1.097987	-1.992051	-0.845496
30	1	0	2.769387	1.132848	1.114845
31	1	0	-1.097988	-1.992051	3.075190
32	1	0	0.745037	-2.728558	-1.931928
33	1	0	2.327370	-1.032478	4.156624
34	1	0	4.187288	-1.797558	-0.764742
35	1	0	0.302293	-4.897442	1.114845
36	1	0	4.187288	-1.797557	2.994434
37	1	0	3.745349	-3.962499	-0.046803
38	1	0	1.612171	-4.536050	2.994768
39	1	0	3.745349	-3.962499	2.276496
40	1	0	-0.637061	0.265903	-0.096712
41	12	0	-1.914904	-1.175201	1.114846

Li^{+}@**1** Cl^{-} ion pair HF/6-31+G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.740581	1.264606	0.112536
2	6	0	-1.074897	0.780958	-1.216668
3	6	0	-2.150438	0.000000	0.936102
4	6	0	-0.664522	2.045188	0.936102
5	6	0	-1.074897	-0.780958	-1.216668
6	6	0	-1.740581	-1.264606	0.112536
7	6	0	-1.327358	0.000000	2.262887
8	6	0	0.410574	1.263617	-1.216668
9	6	0	0.664843	2.046175	0.112536
10	6	0	-0.410176	1.262392	2.262887
11	6	0	0.410574	-1.263617	-1.216668
12	6	0	-0.664522	-2.045188	0.936102
13	6	0	-0.410176	-1.262392	2.262887
14	6	0	1.328646	0.000000	-1.216668
15	6	0	1.739741	1.263996	0.936102
16	6	0	1.073855	0.780201	2.262887
17	6	0	0.664843	-2.046175	0.112536
18	6	0	1.073855	-0.780201	2.262887
19	6	0	2.151476	0.000000	0.112536
20	6	0	1.739741	-1.263996	0.936102
21	1	0	0.992791	3.055495	-0.088255
22	1	0	1.603666	1.165132	3.122805
23	1	0	-1.982240	0.000000	3.122805
24	1	0	-0.992320	-3.054048	1.141375
25	1	0	-1.581757	-1.149214	-2.091767
26	1	0	1.955159	0.000000	-2.091767
27	1	0	-1.581757	1.149214	-2.091767
28	1	0	-3.211216	0.000000	1.141375
29	1	0	-0.992320	3.054048	1.141375
30	1	0	-2.599160	-1.888400	-0.088255
31	1	0	0.604177	1.859467	-2.091767
32	1	0	-0.612546	1.885222	3.122805
33	1	0	0.604177	-1.859467	-2.091767
34	1	0	-0.612546	-1.885222	3.122805
35	1	0	2.597928	1.887505	1.141375
36	1	0	0.992791	-3.055495	-0.088255
37	1	0	1.603666	-1.165132	3.122805
38	1	0	3.212738	0.000000	-0.088255
39	1	0	2.597928	-1.887505	1.141375
40	1	0	-2.599160	1.888400	-0.088255
41	3	0	0.000000	0.000000	0.423753
42	17	0	0.000000	0.000000	-4.384575

1 + H^+ facial complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.253395	1.623984	-0.812891
2	6	0	-1.253394	1.623985	0.812892
3	6	0	0.209671	1.764613	-1.260429
4	6	0	-1.764104	0.164551	-1.315285
5	6	0	0.209672	1.764613	1.260428
6	6	0	1.103298	1.874367	-0.000001
7	6	0	0.616349	0.482834	-2.029163
8	6	0	-1.764103	0.164552	1.315287
9	6	0	-2.079739	-0.737428	0.000001
10	6	0	-0.582210	-0.498312	-2.039416
11	6	0	0.616351	0.482835	2.029162
12	6	0	2.073873	0.669370	-0.000001
13	6	0	1.773340	-0.189449	-1.252350
14	6	0	-0.582208	-0.498311	2.039417
15	6	0	-1.071618	-1.896875	0.000001
16	6	0	-0.171549	-1.768712	-1.254091
17	6	0	1.773341	-0.189449	1.252348
18	6	0	1.287069	-1.579048	-0.773995
19	6	0	-0.171548	-1.768712	1.254092
20	6	0	1.287069	-1.579048	0.773994
21	1	0	-3.121500	-1.008208	0.000001
22	1	0	-0.267829	-2.646310	-1.879023
23	1	0	0.912691	0.727214	-3.040324
24	1	0	3.101663	1.007212	-0.000001
25	1	0	0.305484	2.642330	1.885330
26	1	0	-0.878998	-0.742518	3.050529
27	1	0	-1.936842	2.377141	1.165371
28	1	0	0.305482	2.642329	-1.885331
29	1	0	-2.669002	0.284880	-1.885608
30	1	0	1.642294	2.812167	-0.000001
31	1	0	-2.669000	0.284881	1.885610
32	1	0	-0.879001	-0.742518	-3.050528
33	1	0	0.912693	0.727215	3.040323
34	1	0	2.650873	-0.280990	-1.878485
35	1	0	-1.611050	-2.834469	0.000001
36	1	0	2.650874	-0.280990	1.878483
37	1	0	1.921481	-2.365344	-1.160967
38	1	0	-0.267827	-2.646309	1.879023
39	1	0	1.921482	-2.365344	1.160966
40	1	0	-1.936842	2.377141	-1.165370
41	1	0	-1.624111	0.568336	0.000001

1 + He facial complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.156282	2.167599	-0.924537
2	6	0	0.156282	2.167599	0.924537
3	6	0	1.312560	1.231409	-1.281563
4	6	0	-1.339650	1.243062	-1.495932
5	6	0	1.312560	1.231409	1.281563
6	6	0	2.043163	0.748125	0.000000
7	6	0	0.790398	-0.026127	-2.027016
8	6	0	-1.339650	1.243062	1.495932
9	6	0	-2.264187	0.671666	0.000000
10	6	0	-0.761053	-0.050154	-2.073613
11	6	0	0.790398	-0.026127	2.027016
12	6	0	2.040909	-0.798647	0.000000
13	6	0	1.267250	-1.276795	-1.251806
14	6	0	-0.761053	-0.050154	2.073613
15	6	0	-2.042616	-0.842204	0.000000
16	6	0	-1.236617	-1.278892	-1.252765
17	6	0	1.267251	-1.276795	1.251806
18	6	0	0.015444	-2.050454	-0.773659
19	6	0	-1.236617	-1.278892	1.252765
20	6	0	0.015444	-2.050454	0.773659
21	1	0	-3.309443	0.961764	0.000000
22	1	0	-1.857028	-1.911068	-1.877670
23	1	0	1.181105	-0.033398	-3.038134
24	1	0	3.052906	-1.187708	0.000000
25	1	0	2.020975	1.751145	1.917909
26	1	0	-1.082266	-0.166765	3.103242
27	1	0	0.244589	3.158278	1.357520
28	1	0	2.020975	1.751145	-1.917909
29	1	0	-1.951924	1.800758	-2.196513
30	1	0	3.058774	1.127067	0.000000
31	1	0	-1.951924	1.800758	2.196513
32	1	0	-1.082267	-0.166765	-3.103242
33	1	0	1.181105	-0.033398	3.038134
34	1	0	1.893475	-1.904276	-1.875998
35	1	0	-3.000175	-1.352099	0.000000
36	1	0	1.893475	-1.904275	1.875998
37	1	0	0.017478	-3.063706	-1.159430
38	1	0	-1.857028	-1.911068	1.877670
39	1	0	0.017478	-3.063706	1.159430
40	1	0	0.244589	3.158278	-1.357520
41	2	0	-0.926934	1.499809	0.000000

1 + Li^+ facial complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.218700	1.784358	-0.931189
2	6	0	-1.218692	1.784356	0.931202
3	6	0	0.263155	1.788329	-1.289526
4	6	0	-1.803738	0.112528	-1.506698
5	6	0	0.263165	1.788326	1.289528
6	6	0	1.131941	1.870615	-0.000002
7	6	0	0.643632	0.475225	-2.034795
8	6	0	-1.803727	0.112525	1.506712
9	6	0	-2.165305	-0.920722	0.000007
10	6	0	-0.547012	-0.526836	-2.086498
11	6	0	0.643648	0.475220	2.034791
12	6	0	2.096958	0.661219	-0.000007
13	6	0	1.796436	-0.197555	-1.252292
14	6	0	-0.546996	-0.526840	2.086501
15	6	0	-1.047713	-1.957689	0.000002
16	6	0	-0.146452	-1.782570	-1.257573
17	6	0	1.796445	-0.197558	1.252278
18	6	0	1.310189	-1.587083	-0.773961
19	6	0	-0.146443	-1.782572	1.257570
20	6	0	1.310195	-1.587084	0.773948
21	1	0	-3.183863	-1.267594	0.000011
22	1	0	-0.230970	-2.662055	-1.880977
23	1	0	0.950776	0.714974	-3.043485
24	1	0	3.126037	0.994495	-0.000011
25	1	0	0.469485	2.640517	1.923444
26	1	0	-0.738941	-0.812757	3.112198
27	1	0	-1.840599	2.570970	1.321396
28	1	0	0.469470	2.640521	-1.923442
29	1	0	-2.670792	0.198610	-2.138037
30	1	0	1.681149	2.802089	-0.000003
31	1	0	-2.670775	0.198605	2.138058
32	1	0	-0.738965	-0.812750	-3.112194
33	1	0	0.950799	0.714967	3.043479
34	1	0	2.676141	-0.291128	-1.874738
35	1	0	-1.485804	-2.946993	0.000002
36	1	0	2.676156	-0.291132	1.874717
37	1	0	1.948209	-2.371314	-1.158655
38	1	0	-0.230956	-2.662060	1.880973
39	1	0	1.948217	-2.371317	1.158635
40	1	0	-1.840609	2.570973	-1.321376
41	3	0	-1.643360	0.575074	0.000007

1 + Be^{+} facial complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.200191	1.756398	-0.916458
2	6	0	-1.200186	1.756397	0.916466
3	6	0	0.273603	1.786657	-1.290887
4	6	0	-1.775973	0.111019	-1.482863
5	6	0	0.273610	1.786655	1.290888
6	6	0	1.139982	1.869509	-0.000001
7	6	0	0.651308	0.473067	-2.036327
8	6	0	-1.775966	0.111017	1.482871
9	6	0	-2.131822	-0.905882	0.000004
10	6	0	-0.537418	-0.530950	-2.088699
11	6	0	0.651318	0.473063	2.036325
12	6	0	2.102741	0.658375	-0.000004
13	6	0	1.802396	-0.199894	-1.251554
14	6	0	-0.537408	-0.530954	2.088701
15	6	0	-1.038650	-1.963312	0.000001
16	6	0	-0.139373	-1.786428	-1.258520
17	6	0	1.802402	-0.199896	1.251545
18	6	0	1.316434	-1.588606	-0.773504
19	6	0	-0.139368	-1.786430	1.258518
20	6	0	1.316438	-1.588607	0.773496
21	1	0	-3.164972	-1.223873	0.000006
22	1	0	-0.222053	-2.667042	-1.882257
23	1	0	0.960499	0.712284	-3.045555
24	1	0	3.132885	0.990576	-0.000007
25	1	0	0.467480	2.644376	1.925609
26	1	0	-0.742309	-0.812785	3.115700
27	1	0	-1.850094	2.533575	1.293469
28	1	0	0.467471	2.644379	-1.925607
29	1	0	-2.662739	0.211347	-2.092860
30	1	0	1.691366	2.800820	-0.000002
31	1	0	-2.662729	0.211343	2.092873
32	1	0	-0.742324	-0.812780	-3.115698
33	1	0	0.960513	0.712280	3.045551
34	1	0	2.683320	-0.294111	-1.873368
35	1	0	-1.490009	-2.949424	0.000001
36	1	0	2.683328	-0.294114	1.873355
37	1	0	1.955915	-2.372781	-1.157807
38	1	0	-0.222044	-2.667045	1.882254
39	1	0	1.955921	-2.372783	1.157794
40	1	0	-1.850100	2.533577	-1.293456
41	4	0	-1.618144	0.566250	0.000004

1 + Be^{2+} facial complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.204181	1.771894	-0.926127
2	6	0	-1.204176	1.771892	0.926135
3	6	0	0.278385	1.786400	-1.291858
4	6	0	-1.786038	0.109156	-1.498507
5	6	0	0.278391	1.786398	1.291859
6	6	0	1.147259	1.871782	-0.000001
7	6	0	0.657547	0.472373	-2.040654
8	6	0	-1.786031	0.109153	1.498516
9	6	0	-2.145641	-0.918474	0.000004
10	6	0	-0.533247	-0.532951	-2.090270
11	6	0	0.657556	0.472369	2.040651
12	6	0	2.108473	0.657925	-0.000004
13	6	0	1.807793	-0.201302	-1.252950
14	6	0	-0.533237	-0.532954	2.090272
15	6	0	-1.034856	-1.966390	0.000001
16	6	0	-0.134815	-1.791923	-1.261194
17	6	0	1.807799	-0.201304	1.252941
18	6	0	1.321289	-1.591563	-0.774367
19	6	0	-0.134809	-1.791925	1.261192
20	6	0	1.321293	-1.591564	0.774359
21	1	0	-3.183639	-1.200515	0.000007
22	1	0	-0.223584	-2.669590	-1.884371
23	1	0	0.960297	0.713533	-3.048976
24	1	0	3.135803	0.992564	-0.000007
25	1	0	0.453844	2.645986	1.923441
26	1	0	-0.754583	-0.807282	3.112193
27	1	0	-1.878251	2.529816	1.284134
28	1	0	0.453835	2.645989	-1.923439
29	1	0	-2.685031	0.224347	-2.077756
30	1	0	1.691984	2.804415	-0.000002
31	1	0	-2.685021	0.224343	2.077769
32	1	0	-0.754597	-0.807277	-3.112190
33	1	0	0.960311	0.713528	3.048972
34	1	0	2.685589	-0.293975	-1.876069
35	1	0	-1.501441	-2.941516	0.000001
36	1	0	2.685598	-0.293978	1.876056
37	1	0	1.957136	-2.375642	-1.159477
38	1	0	-0.223575	-2.669593	1.884368
39	1	0	1.957142	-2.375644	1.159464
40	1	0	-1.878257	2.529818	-1.284121
41	4	0	-1.626523	0.569182	0.000004

1 + Mg^{2+} facial complex HF/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.071555	2.000670	-1.114844
2	6	0	-1.071553	2.000669	1.114848
3	6	0	0.401909	1.800158	-1.330937
4	6	0	-1.771973	-0.000881	-1.803857
5	6	0	0.401912	1.800157	1.330936
6	6	0	1.235974	1.849903	-0.000001
7	6	0	0.744291	0.444850	-2.048880
8	6	0	-1.771969	-0.000881	1.803861
9	6	0	-2.204852	-1.237907	0.000002
10	6	0	-0.434270	-0.589353	-2.153500
11	6	0	0.744296	0.444849	2.048879
12	6	0	2.188839	0.630347	-0.000002
13	6	0	1.888045	-0.229216	-1.253436
14	6	0	-0.434266	-0.589354	2.153501
15	6	0	-0.951055	-2.066152	0.000001
16	6	0	-0.051264	-1.828574	-1.266278
17	6	0	1.888048	-0.229217	1.253431
18	6	0	1.401352	-1.620018	-0.774666
19	6	0	-0.051261	-1.828575	1.266277
20	6	0	1.401354	-1.620018	0.774663
21	1	0	-3.199505	-1.645509	0.000003
22	1	0	-0.129131	-2.707762	-1.887881
23	1	0	1.056954	0.681665	-3.054656
24	1	0	3.218313	0.958525	-0.000003
25	1	0	0.747435	2.606989	1.967151
26	1	0	-0.488453	-0.924758	3.182919
27	1	0	-1.640024	2.810947	1.534091
28	1	0	0.747431	2.606990	-1.967152
29	1	0	-2.603840	0.056706	-2.482204
30	1	0	1.789999	2.776445	-0.000001
31	1	0	-2.603834	0.056705	2.482210
32	1	0	-0.488460	-0.924756	-3.182918
33	1	0	1.056961	0.681664	3.054654
34	1	0	2.769216	-0.324834	-1.871426
35	1	0	-1.252278	-3.107496	0.000001
36	1	0	2.769220	-0.324835	1.871420
37	1	0	2.042565	-2.401354	-1.156606
38	1	0	-0.129126	-2.707763	1.887880
39	1	0	2.042568	-2.401354	1.156600
40	1	0	-1.640027	2.810947	-1.534086
41	12	0	-1.579834	0.552842	0.000002