Supplementary Material (ESI) for Dalton Transactions

SUPPORTING INFORMATION

Calcium Carbene Complexes with Boranophosphorano Side-Arms: $CaC[P(Ph)_2BH_3]_2$

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Calculational details:

Energies are given in Hartree and (XYZ) coordinates of the atoms in Angstrom.

7-H2 C2-symmetry E(B3LYP/TZVPP) = -777.5934965015

coordinates:

H	-0.3434293	-0.8177943	-1.7661663
C	0.0000000	0.0000000	-1.1325090
H	0.3434293	0.8177943	-1.7661663
P	-1.4477515	0.5438111	-0.1232607
H	-2.2426185	1.1753928	-1.1014670
P	1.4477515	-0.5438111	-0.1232607
H	2.2426185	-1.1753928	-1.1014670
H	-0.9512326	1.6696506	0.5605924
H	0.9512326	-1.6696506	0.5605924
B	2.3027236	0.8498614	0.9023207
H	3.2436259	0.3195858	1.4331443
H	1.4536976	1.2272596	1.6706820
H	2.6008741	1.6632146	0.0606123
B	-2.3027236	-0.8498614	0.9023207
H	-1.4536976	-1.2272596	1.6706820
H	-2.6008741	-1.6632146	0.0606123
H	-3.2436259	-0.3195858	1.4331443

vibrational modes:

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	45.85	11.82798	YES	YES
8	b	84.02	16.85638	YES	YES
9	a	133.69	4.32733	YES	YES
10	a	167.09	1.20415	YES	YES
11	b	177.38	9.54930	YES	YES
12	b	201.49	3.40596	YES	YES
13	a	247.71	0.23083	YES	YES
14	b	374.98	0.01404	YES	YES
15	a	396.54	0.25998	YES	YES
16	a	518.51	0.59458	YES	YES
17	b	534.01	3.86346	YES	YES
18	b	601.17	2.73026	YES	YES
19	a	607.96	2.59968	YES	YES
20	a	680.91	2.21064	YES	YES
21	b	686.40	15.07980	YES	YES
22	b	783.55	58.63714	YES	YES
23	a	797.90	9.20494	YES	YES
24	b	829.47	8.01545	YES	YES
25	b	906.82	24.90841	YES	YES
26	a	916.18	8.98931	YES	YES
27	b	958.49	189.71792	YES	YES
28	a	964.10	42.24703	YES	YES
29	a	1072.57	40.75923	YES	YES
30	b	1084.17	99.52587	YES	YES
31	a	1117.94	3.59197	YES	YES

32	b	1118.19	6.46309	YES	YES
33	a	1143.54	4.50675	YES	YES
34	b	1151.88	10.10991	YES	YES
35	a	1153.48	0.19464	YES	YES
36	b	1155.38	8.92278	YES	YES
37	a	1160.69	0.28343	YES	YES
38	b	1200.64	3.16922	YES	YES
39	a	1427.18	9.07541	YES	YES
40	a	2445.48	16.80035	YES	YES
41	b	2446.59	80.14990	YES	YES
42	b	2449.79	12.66685	YES	YES
43	a	2449.91	3.95312	YES	YES
44	a	2468.04	1.38769	YES	YES
45	b	2470.53	19.72414	YES	YES
46	b	2510.75	77.31200	YES	YES
47	a	2514.96	157.94856	YES	YES
48	b	2531.58	216.40904	YES	YES
49	a	2531.68	8.39871	YES	YES
50	a	3060.39	0.07618	YES	YES
51	b	3118.80	0.61423	YES	YES

atomic populations:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 h	0.26063	0.73762	0.00154	0.00021	0.00000	0.00000
2 c	-0.98586	3.22504	3.74601	0.01361	0.00121	0.00000
3 h	0.26063	0.73762	0.00154	0.00021	0.00000	0.00000
4 p	0.84303	5.26320	8.86381	0.02864	0.00132	0.00000
5 h	0.00427	0.99146	0.00407	0.00020	0.00000	0.00000
6 p	0.84303	5.26320	8.86381	0.02864	0.00132	0.00000
7 h	0.00427	0.99146	0.00407	0.00020	0.00000	0.00000
8 h	0.01781	0.97743	0.00456	0.00020	0.00000	0.00000
9 h	0.01781	0.97743	0.00456	0.00020	0.00000	0.00000
10 b	-0.69123	2.92385	2.76043	0.00601	0.00094	0.00000
11 h	0.02907	0.96892	0.00187	0.00015	0.00000	0.00000
12 h	0.01549	0.98265	0.00174	0.00012	0.00000	0.00000
13 h	0.01385	0.98415	0.00188	0.00012	0.00000	0.00000
14 b	-0.69123	2.92385	2.76043	0.00601	0.00094	0.00000
15 h	0.01549	0.98265	0.00174	0.00012	0.00000	0.00000
16 h	0.01385	0.98415	0.00188	0.00012	0.00000	0.00000
17 h	0.02907	0.96892	0.00187	0.00015	0.00000	0.00000

(7-H)2Ca C2-symmetry E(B3LYP/TZVPP) = -2231.611600836

coordinates:

Ca	0.0000000	0.0000000	-0.4374471
P	3.0999203	-1.1357305	-0.5747952
H	3.2832669	-2.4876159	-0.2324401
H	4.4567520	-0.7519498	-0.7639787
P	2.6096466	1.3034663	1.2398364
H	2.4652353	1.3810276	2.6377642
H	3.9647152	1.7245625	1.1231617
C	2.3749300	-0.4186113	0.8819273
H	2.5611315	-1.0361109	1.7552448
P	-3.0999203	1.1357305	-0.5747952
H	-4.4567520	0.7519498	-0.7639787
H	-3.2832669	2.4876159	-0.2324401
P	-2.6096466	-1.3034663	1.2398364
H	-3.9647152	-1.7245625	1.1231617
H	-2.4652353	-1.3810276	2.6377642
C	-2.3749300	0.4186113	0.8819273
H	-2.5611315	1.0361109	1.7552448
B	-1.3495586	-2.4428474	0.3150312
H	-0.2792898	-2.0935430	0.7843233
H	-1.4425745	-2.1408337	-0.8546559
H	-1.5678936	-3.6026781	0.5192592
B	-2.0157943	0.9464372	-2.1714952
H	-1.0279816	1.6130660	-1.9182989
H	-2.5964232	1.3613782	-3.1324498
H	-1.7507625	-0.2346063	-2.2544515
B	1.3495586	2.4428474	0.3150312
H	1.4425745	2.1408337	-0.8546559
H	1.5678936	3.6026781	0.5192592
H	0.2792898	2.0935430	0.7843233
B	2.0157943	-0.9464372	-2.1714952
H	2.5964232	-1.3613782	-3.1324498
H	1.7507625	0.2346063	-2.2544515
H	1.0279816	-1.6130660	-1.9182989

vibrational modes:

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.85	1.59516	YES	YES
8	b	36.20	0.30074	YES	YES
9	a	41.12	0.04407	YES	YES
10	a	72.77	0.09142	YES	YES
11	b	81.68	2.72937	YES	YES
12	a	105.18	0.00459	YES	YES
13	a	119.22	1.09690	YES	YES
14	b	120.68	14.71271	YES	YES
15	a	159.77	4.01308	YES	YES
16	b	161.40	19.85190	YES	YES
17	b	175.55	1.89735	YES	YES
18	a	180.29	5.88847	YES	YES
19	b	189.61	16.67264	YES	YES
20	a	203.60	0.24437	YES	YES
21	b	215.25	45.29487	YES	YES
22	a	235.15	24.47662	YES	YES
23	b	239.97	80.84973	YES	YES

24	a	314.84	3.30195	YES	YES
25	b	315.42	16.08350	YES	YES
26	b	340.04	44.78979	YES	YES
27	a	342.71	11.07143	YES	YES
28	b	360.12	58.04065	YES	YES
29	a	376.03	0.04370	YES	YES
30	a	428.11	0.30823	YES	YES
31	b	429.93	3.58192	YES	YES
32	b	430.79	0.16155	YES	YES
33	a	431.57	2.42793	YES	YES
34	b	552.79	33.29871	YES	YES
35	a	554.47	0.00050	YES	YES
36	b	576.99	1.56490	YES	YES
37	a	578.20	0.08996	YES	YES
38	b	631.83	47.48672	YES	YES
39	a	632.12	14.06899	YES	YES
40	b	679.04	48.48463	YES	YES
41	a	679.07	2.55816	YES	YES
42	b	716.71	1.81311	YES	YES
43	a	716.76	0.25492	YES	YES
44	b	729.61	18.98793	YES	YES
45	a	729.89	8.06183	YES	YES
46	a	754.56	14.03323	YES	YES
47	b	754.95	41.85935	YES	YES
48	a	818.74	15.19086	YES	YES
49	b	818.91	6.51256	YES	YES
50	a	890.46	110.05808	YES	YES
51	b	892.77	168.96986	YES	YES
52	a	910.46	42.35912	YES	YES
53	b	914.04	137.69433	YES	YES
54	a	938.00	0.39414	YES	YES
55	b	939.93	2.34138	YES	YES
56	b	940.61	35.95406	YES	YES
57	a	940.96	23.98569	YES	YES
58	a	968.68	114.50453	YES	YES
59	b	968.86	129.83493	YES	YES
60	b	1083.60	4.31708	YES	YES
61	a	1084.17	4.06655	YES	YES
62	b	1089.14	162.74148	YES	YES
63	a	1090.84	49.90435	YES	YES
64	b	1110.80	3.57652	YES	YES
65	a	1110.90	19.19079	YES	YES
66	b	1112.12	20.25404	YES	YES
67	a	1112.27	0.87913	YES	YES
68	b	1178.38	3.31680	YES	YES
69	a	1178.51	0.45715	YES	YES
70	a	1188.50	0.26946	YES	YES
71	b	1188.57	9.55885	YES	YES
72	b	1196.67	1.71401	YES	YES
73	a	1197.17	0.36203	YES	YES
74	b	1225.73	45.29366	YES	YES
75	a	1226.08	23.36032	YES	YES
76	b	1232.48	65.47488	YES	YES
77	a	1234.13	2.74876	YES	YES
78	b	2332.26	134.44824	YES	YES
79	a	2332.51	25.31904	YES	YES
80	b	2341.44	319.62024	YES	YES
81	a	2342.28	2.77613	YES	YES
82	a	2384.63	4.99833	YES	YES
83	b	2385.67	192.53134	YES	YES
84	b	2396.28	296.71095	YES	YES
85	a	2398.28	5.64242	YES	YES
86	b	2438.10	56.70932	YES	YES

87	a	2438.75	7.24578	YES	YES
88	a	2458.50	0.16934	YES	YES
89	b	2459.49	12.48670	YES	YES
90	a	2467.95	89.28420	YES	YES
91	b	2468.25	12.85563	YES	YES
92	a	2472.45	62.57027	YES	YES
93	b	2474.21	91.23001	YES	YES
94	b	2560.56	263.22942	YES	YES
95	a	2560.80	53.91277	YES	YES
96	b	2566.28	110.54100	YES	YES
97	a	2568.42	110.70101	YES	YES
98	b	3126.98	0.28695	YES	YES
99	a	3126.98	0.38491	YES	YES

atomic populations:

atom		charge	n(s)	n(p)	n(d)	n(f)	n(g)
1	ca	1.75037	6.15691	12.00048	0.09223	0.00000	0.00000
2	p	0.86067	5.21408	8.88843	0.03544	0.00138	0.00000
3	h	0.01281	0.98365	0.00339	0.00016	0.00000	0.00000
4	h	-0.02967	1.02573	0.00379	0.00015	0.00000	0.00000
5	p	0.86562	5.21163	8.88574	0.03562	0.00139	0.00000
6	h	0.00572	0.99077	0.00336	0.00016	0.00000	0.00000
7	h	-0.03339	1.02945	0.00379	0.00015	0.00000	0.00000
8	c	-1.36009	3.26041	4.08054	0.01722	0.00192	0.00000
9	h	0.25721	0.74062	0.00191	0.00026	0.00000	0.00000
10	p	0.86067	5.21408	8.88843	0.03544	0.00138	0.00000
11	h	-0.02967	1.02573	0.00379	0.00015	0.00000	0.00000
12	h	0.01281	0.98365	0.00339	0.00016	0.00000	0.00000
13	p	0.86562	5.21163	8.88574	0.03562	0.00139	0.00000
14	h	-0.03339	1.02945	0.00379	0.00015	0.00000	0.00000
15	h	0.00572	0.99077	0.00336	0.00016	0.00000	0.00000
16	c	-1.36009	3.26041	4.08054	0.01722	0.00192	0.00000
17	h	0.25721	0.74062	0.00191	0.00026	0.00000	0.00000
18	b	-0.75314	2.91347	2.83111	0.00750	0.00106	0.00000
19	h	-0.02366	1.02119	0.00240	0.00007	0.00000	0.00000
20	h	0.00391	0.99395	0.00206	0.00008	0.00000	0.00000
21	h	0.04417	0.95409	0.00161	0.00013	0.00000	0.00000
22	b	-0.75386	2.91535	2.82989	0.00757	0.00105	0.00000
23	h	-0.01686	1.01417	0.00262	0.00007	0.00000	0.00000
24	h	0.04839	0.94982	0.00165	0.00014	0.00000	0.00000
25	h	-0.00300	1.00068	0.00225	0.00008	0.00000	0.00000
26	b	-0.75314	2.91347	2.83111	0.00750	0.00106	0.00000
27	h	0.00391	0.99395	0.00206	0.00008	0.00000	0.00000
28	h	0.04417	0.95409	0.00161	0.00013	0.00000	0.00000
29	h	-0.02366	1.02119	0.00240	0.00007	0.00000	0.00000
30	b	-0.75386	2.91535	2.82989	0.00757	0.00105	0.00000
31	h	0.04839	0.94982	0.00165	0.00014	0.00000	0.00000
32	h	-0.00300	1.00068	0.00225	0.00008	0.00000	0.00000
33	h	-0.01686	1.01417	0.00262	0.00007	0.00000	0.00000

7-Ca Cs symmetry E(B3LYP/TZVPP) = -1453.943380094

coordinates:

C	-0.7316155	-0.4223414	0.0000000
P	-1.0513446	0.0180840	-1.5989913
H	-1.8421844	1.1879802	-1.7882206
H	-1.8535404	-0.8885661	-2.3511147
P	-1.0513446	0.0180840	1.5989913
H	-1.8535404	-0.8885661	2.3511147
H	-1.8421844	1.1879802	1.7882206
Ca	1.5055081	-0.1197000	0.0000000
B	0.6806733	0.2837183	-2.5105232
H	0.5892083	0.5063259	-3.6817681
H	1.3341726	-0.7381915	-2.2939178
H	1.2056306	1.2298929	-1.9145275
B	0.6806733	0.2837183	2.5105232
H	1.2056306	1.2298929	1.9145275
H	1.3341726	-0.7381915	2.2939178
H	0.5892083	0.5063259	3.6817681

vibrational modes:

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a'	57.66	3.95671	YES	YES
8	a"	129.25	1.64363	YES	YES
9	a'	166.74	16.44748	YES	YES
10	a'	197.69	39.58380	YES	YES
11	a"	198.36	6.59060	YES	YES
12	a'	329.62	1.26666	YES	YES
13	a"	371.13	73.34401	YES	YES
14	a'	415.61	0.58679	YES	YES
15	a"	417.36	1.80711	YES	YES
16	a'	471.24	9.30240	YES	YES
17	a"	481.78	0.13454	YES	YES
18	a'	494.29	31.80464	YES	YES
19	a'	542.47	48.36228	YES	YES
20	a"	563.56	6.01342	YES	YES
21	a'	627.45	15.76260	YES	YES
22	a"	729.65	8.80146	YES	YES
23	a'	745.44	16.64783	YES	YES
24	a"	769.02	9.34500	YES	YES
25	a'	781.99	28.69470	YES	YES
26	a"	870.24	14.59001	YES	YES
27	a'	883.58	8.21761	YES	YES
28	a"	913.39	251.45394	YES	YES
29	a'	938.20	43.36668	YES	YES
30	a"	1085.76	47.30410	YES	YES
31	a'	1087.71	26.91778	YES	YES
32	a"	1121.94	155.00942	YES	YES
33	a'	1134.56	92.95046	YES	YES
34	a'	1209.10	1.23977	YES	YES
35	a"	1209.66	0.32611	YES	YES
36	a"	1223.59	40.04418	YES	YES
37	a'	1234.13	18.64371	YES	YES
38	a"	1239.10	462.78001	YES	YES
39	a"	2266.10	53.40555	YES	YES
40	a'	2273.73	158.99133	YES	YES

41	a"	2290.15	15.94659	YES	YES
42	a'	2291.79	181.38046	YES	YES
43	a"	2303.34	199.62508	YES	YES
44	a'	2310.84	258.29807	YES	YES
45	a"	2317.31	150.96102	YES	YES
46	a'	2327.17	306.11446	YES	YES
47	a"	2572.19	267.12029	YES	YES
48	a'	2573.26	8.39099	YES	YES

atomic populations:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 c	-1.66521	3.27520	4.36205	0.02374	0.00421	0.00000
2 p	0.89279	5.16821	8.89483	0.04258	0.00158	0.00000
3 h	-0.04587	1.04209	0.00365	0.00013	0.00000	0.00000
4 h	-0.04677	1.04311	0.00354	0.00012	0.00000	0.00000
5 p	0.89279	5.16821	8.89483	0.04258	0.00158	0.00000
6 h	-0.04677	1.04311	0.00354	0.00012	0.00000	0.00000
7 h	-0.04587	1.04209	0.00365	0.00013	0.00000	0.00000
8 ca	1.68354	6.14936	11.99785	0.16924	0.00000	0.00000
9 b	-0.72951	2.92788	2.79321	0.00723	0.00119	0.00000
10 h	0.04107	0.95693	0.00182	0.00018	0.00000	0.00000
11 h	-0.05863	1.05573	0.00281	0.00008	0.00000	0.00000
12 h	-0.06225	1.05931	0.00287	0.00008	0.00000	0.00000
13 b	-0.72951	2.92788	2.79321	0.00723	0.00119	0.00000
14 h	-0.06225	1.05931	0.00287	0.00008	0.00000	0.00000
15 h	-0.05863	1.05573	0.00281	0.00008	0.00000	0.00000
16 h	0.04107	0.95693	0.00182	0.00018	0.00000	0.00000

(7-Ca)2 D2 symmetry E(B3LYP/TZVPP) = -2908.002901301

coordinates:

C	0.0000000	0.0000000	1.8534264
P	-0.9074290	-1.1965770	2.7320232
H	-1.4456759	-0.7168528	3.9558808
H	-0.1186894	-2.2538692	3.2624735
P	0.9074290	1.1965770	2.7320232
H	1.4456759	0.7168528	3.9558808
H	0.1186894	2.2538692	3.2624735
Ca	1.6856035	0.0000000	0.0000000
Ca	-1.6856035	0.0000000	0.0000000
C	0.0000000	0.0000000	-1.8534264
P	-0.9074290	1.1965770	-2.7320232
H	-0.1186894	2.2538692	-3.2624735
H	-1.4456759	0.7168528	-3.9558808
P	0.9074290	-1.1965770	-2.7320232
H	0.1186894	-2.2538692	-3.2624735
H	1.4456759	-0.7168528	-3.9558808
B	2.3819379	-1.9532223	-1.6853982
H	2.8901121	-2.8673412	-2.2636115
H	1.9083930	-2.2985804	-0.6112299
H	3.1764121	-1.0321220	-1.5234624
B	-2.3819379	1.9532223	-1.6853982
H	-2.8901121	2.8673412	-2.2636115
H	-1.9083930	2.2985804	-0.6112299
H	-3.1764121	1.0321220	-1.5234624
B	2.3819379	1.9532223	1.6853982
H	1.9083930	2.2985804	0.6112299
H	3.1764121	1.0321220	1.5234624
H	2.8901121	2.8673412	2.2636115
B	-2.3819379	-1.9532223	1.6853982
H	-1.9083930	-2.2985804	0.6112299
H	-3.1764121	-1.0321220	1.5234624
H	-2.8901121	-2.8673412	2.2636115

vibrational modes:

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b2	39.24	0.67056	YES	YES
8	a	41.21	0.00000	NO	YES
9	b2	66.73	3.98291	YES	YES
10	b3	80.14	7.53064	YES	YES
11	b1	87.96	4.69273	YES	YES
12	a	106.27	0.00000	NO	YES
13	b1	107.73	2.13757	YES	YES
14	b3	121.26	4.46635	YES	YES
15	a	138.59	0.00000	NO	YES
16	b3	167.53	1.98171	YES	YES
17	b2	187.16	10.98411	YES	YES
18	a	198.37	0.00000	NO	YES
19	b1	217.25	34.93285	YES	YES
20	b2	226.22	7.17547	YES	YES
21	b2	260.17	0.18981	YES	YES
22	a	278.72	0.00000	NO	YES
23	b1	279.55	16.65048	YES	YES

24	b3	292.63	80.03319	YES	YES
25	a	350.26	0.00000	NO	YES
26	b2	373.65	70.70563	YES	YES
27	b3	373.68	0.01202	YES	YES
28	b1	378.16	143.37299	YES	YES
29	b1	422.26	8.96216	YES	YES
30	b2	423.05	2.21004	YES	YES
31	b3	425.95	3.82703	YES	YES
32	a	426.14	0.00000	NO	YES
33	b1	460.00	0.34440	YES	YES
34	a	460.72	0.00000	NO	YES
35	b2	476.21	6.85768	YES	YES
36	b3	478.10	13.63271	YES	YES
37	b1	562.52	75.50393	YES	YES
38	a	564.72	0.00000	NO	YES
39	b3	573.00	11.75697	YES	YES
40	b2	573.20	3.66876	YES	YES
41	b1	667.83	125.93972	YES	YES
42	a	680.35	0.00000	NO	YES
43	b3	738.92	27.60205	YES	YES
44	b2	739.25	16.58432	YES	YES
45	a	756.57	0.00000	NO	YES
46	b1	757.69	1.40086	YES	YES
47	b2	765.23	2.30403	YES	YES
48	b3	766.02	53.44101	YES	YES
49	b1	811.14	149.30292	YES	YES
50	a	815.03	0.00000	NO	YES
51	b2	883.54	0.90525	YES	YES
52	b3	884.05	1.78082	YES	YES
53	b1	888.65	4.17763	YES	YES
54	a	889.71	0.00000	NO	YES
55	b2	915.42	220.26967	YES	YES
56	b3	920.13	334.52906	YES	YES
57	b1	943.95	32.38336	YES	YES
58	a	944.42	0.00000	NO	YES
59	b2	1022.86	386.71345	YES	YES
60	b3	1025.27	337.51722	YES	YES
61	b2	1094.52	2.51626	YES	YES
62	b3	1095.09	51.61292	YES	YES
63	a	1097.39	0.00000	NO	YES
64	b1	1097.49	35.30647	YES	YES
65	b3	1131.08	5.00973	YES	YES
66	b2	1131.36	71.50087	YES	YES
67	b1	1148.14	150.84467	YES	YES
68	a	1151.52	0.00000	NO	YES
69	b3	1209.76	2.06743	YES	YES
70	b2	1209.85	1.73363	YES	YES
71	b1	1210.02	0.00439	YES	YES
72	a	1210.48	0.00000	NO	YES
73	b2	1239.07	75.81285	YES	YES
74	b1	1239.67	118.72703	YES	YES
75	b3	1240.10	6.61847	YES	YES
76	a	1242.00	0.00000	NO	YES
77	b2	2322.49	53.96964	YES	YES
78	b1	2324.77	110.46521	YES	YES
79	b3	2327.72	38.94115	YES	YES
80	a	2328.99	0.00000	NO	YES
81	b2	2333.22	330.33741	YES	YES
82	b3	2335.27	83.74216	YES	YES
83	b1	2336.08	185.95517	YES	YES
84	a	2338.01	0.00000	NO	YES
85	b2	2349.64	40.72733	YES	YES
86	b3	2349.70	35.16693	YES	YES

87	b1	2357.46	18.22606	YES	YES
88	a	2358.56	0.00000	NO	YES
89	b3	2361.49	171.44437	YES	YES
90	b2	2363.43	94.06349	YES	YES
91	b1	2363.63	686.68563	YES	YES
92	a	2366.98	0.00000	NO	YES
93	b1	2578.29	124.01810	YES	YES
94	b2	2578.45	262.13305	YES	YES
95	b3	2578.64	117.48557	YES	YES
96	a	2579.73	0.00000	NO	YES

atomic populations:

atom		charge	n(s)	n(p)	n(d)	n(f)	n(g)
1	c	-1.77544	3.38817	4.37070	0.01428	0.00228	0.00000
2	p	0.85925	5.18160	8.91852	0.03919	0.00144	0.00000
3	h	-0.03591	1.03213	0.00365	0.00013	0.00000	0.00000
4	h	-0.03461	1.03090	0.00358	0.00013	0.00000	0.00000
5	p	0.85925	5.18160	8.91852	0.03919	0.00144	0.00000
6	h	-0.03591	1.03213	0.00365	0.00013	0.00000	0.00000
7	h	-0.03461	1.03090	0.00358	0.00013	0.00000	0.00000
8	ca	1.74398	6.14997	11.99531	0.11074	0.00000	0.00000
9	ca	1.74398	6.14997	11.99531	0.11074	0.00000	0.00000
10	c	-1.77544	3.38817	4.37070	0.01428	0.00228	0.00000
11	p	0.85925	5.18160	8.91852	0.03919	0.00144	0.00000
12	h	-0.03461	1.03090	0.00358	0.00013	0.00000	0.00000
13	h	-0.03591	1.03213	0.00365	0.00013	0.00000	0.00000
14	p	0.85925	5.18160	8.91852	0.03919	0.00144	0.00000
15	h	-0.03461	1.03090	0.00358	0.00013	0.00000	0.00000
16	h	-0.03591	1.03213	0.00365	0.00013	0.00000	0.00000
17	b	-0.74645	2.91864	2.81903	0.00768	0.00109	0.00000
18	h	0.05135	0.94684	0.00166	0.00015	0.00000	0.00000
19	h	-0.03380	1.03113	0.00260	0.00007	0.00000	0.00000
20	h	-0.04409	1.04124	0.00278	0.00008	0.00000	0.00000
21	b	-0.74645	2.91864	2.81903	0.00768	0.00109	0.00000
22	h	0.05135	0.94684	0.00166	0.00015	0.00000	0.00000
23	h	-0.03380	1.03113	0.00260	0.00007	0.00000	0.00000
24	h	-0.04409	1.04124	0.00278	0.00008	0.00000	0.00000
25	b	-0.74645	2.91864	2.81903	0.00768	0.00109	0.00000
26	h	-0.03380	1.03113	0.00260	0.00007	0.00000	0.00000
27	h	-0.04409	1.04124	0.00278	0.00008	0.00000	0.00000
28	h	0.05135	0.94684	0.00166	0.00015	0.00000	0.00000
29	b	-0.74645	2.91864	2.81903	0.00768	0.00109	0.00000
30	h	-0.03380	1.03113	0.00260	0.00007	0.00000	0.00000
31	h	-0.04409	1.04124	0.00278	0.00008	0.00000	0.00000
32	h	0.05135	0.94684	0.00166	0.00015	0.00000	0.00000

(4-H2)Ca*THF C1 symmetry E(RI-BP86/TZVP) = -4313.829805133

coordinates:

Ca	0.2887922	-1.3373337	0.4806503
P	1.6648132	-0.1408664	3.2633049
P	-1.4808092	-0.3961317	3.2213923
P	1.5891138	0.3343523	-3.3442669
P	-1.5627825	0.3654667	-3.1245757
O	0.4087622	-3.6675195	-0.1785370
C	0.0447909	0.3640696	2.6530244
C	2.7613756	1.3179547	2.9484475
C	3.9853378	1.4035862	3.6324632
C	4.8625032	2.4607645	3.3810469
C	4.5288452	3.4439663	2.4440690
C	3.3184420	3.3570288	1.7517288
C	2.4400412	2.2964509	1.9966847
C	1.7992554	-0.3726181	5.1010907
C	1.4989560	0.6753270	5.9864764
C	1.6117265	0.4846696	7.3640560
C	2.0187202	-0.7556657	7.8706440
C	2.3098634	-1.8042454	6.9950083
C	2.2018053	-1.6147161	5.6126857
C	-2.8390180	0.6315725	2.4990231
C	-2.6105708	1.7077859	1.6326973
C	-3.6861848	2.4378637	1.1150967
C	-4.9956767	2.0962211	1.4584651
C	-5.2309490	1.0164890	2.3172349
C	-4.1599786	0.2855320	2.8326729
C	-1.8122227	-0.2153915	5.0448426
C	-2.1037882	1.0400154	5.6027627
C	-2.3524535	1.1624992	6.9710549
C	-2.3068664	0.0323896	7.7961019
C	-2.0121280	-1.2181628	7.2468947
C	-1.7682967	-1.3442137	5.8749625
C	-0.0229847	0.8143096	-3.8101796
C	2.6653934	1.7999108	-3.7164271
C	2.9027987	2.1912228	-5.0443401
C	3.6539949	3.3366102	-5.3205836
C	4.1846179	4.0973585	-4.2732803
C	3.9616883	3.7057965	-2.9496235
C	3.2056088	2.5627967	-2.6707465
C	2.2873214	-0.9533647	-4.5083316
C	1.4442659	-1.5876258	-5.4285424
C	1.9440547	-2.5822040	-6.2777814
C	3.2909131	-2.9490274	-6.2097568
C	4.1381274	-2.3196618	-5.2891156
C	3.6399163	-1.3276420	-4.4411688
C	-2.5582514	-0.6362328	-4.3497744
C	-3.1411586	-1.8578690	-3.9824302
C	-3.8379445	-2.6234592	-4.9255886
C	-3.9642063	-2.1733165	-6.2418872
C	-3.3897418	-0.9518142	-6.6150575
C	-2.6900456	-0.1913674	-5.6764373
C	-2.5845586	1.9200306	-3.0117121
C	-3.9851624	1.8628782	-2.9381870
C	-4.7314604	3.0372208	-2.8123866
C	-4.0865356	4.2785364	-2.7572725
C	-2.6913164	4.3392032	-2.8254217
C	-1.9426733	3.1637439	-2.9521761
C	0.4475219	-4.1694268	-1.5570729
C	0.7200959	-5.6684261	-1.4433375
C	0.0771461	-6.0195517	-0.0916524
C	0.4253817	-4.7987212	0.7534977

B	2.3635024	-1.6807764	2.2951378
B	-1.6591929	-2.2478222	2.6577034
B	1.9551340	-0.3071716	-1.5387773
B	-1.6271995	-0.5336601	-1.3978560
H	-0.0407658	1.4569049	2.7175897
H	4.2508175	0.6455517	4.3710402
H	5.8086038	2.5172803	3.9223029
H	5.2126684	4.2726619	2.2521024
H	3.0509274	4.1177038	1.0161194
H	1.5085080	2.2280820	1.4344387
H	1.1812462	1.6444315	5.5968105
H	1.3786258	1.3043290	8.0457369
H	2.1067239	-0.9022022	8.9487134
H	2.6275084	-2.7728659	7.3855593
H	2.4403919	-2.4281132	4.9260871
H	-1.5939068	1.9665529	1.3375588
H	-3.4968493	3.2644426	0.4286048
H	-5.8333476	2.6649597	1.0511619
H	-6.2525964	0.7385408	2.5827602
H	-4.3493249	-0.5577801	3.4992762
H	-2.1550594	1.9227388	4.9614683
H	-2.5896992	2.1405641	7.3943285
H	-2.5053994	0.1278454	8.8652333
H	-1.9782219	-2.1025649	7.8857339
H	-1.5532280	-2.3230597	5.4436129
H	-0.0740744	1.3819546	-4.7440105
H	2.5097632	1.5913842	-5.8679161
H	3.8329632	3.6309391	-6.3566021
H	4.7770486	4.9883873	-4.4892186
H	4.3864036	4.2871267	-2.1289265
H	3.0441230	2.2533397	-1.6369205
H	0.3925445	-1.2922370	-5.4702299
H	1.2790166	-3.0682026	-6.9946594
H	3.6827596	-3.7228718	-6.8727695
H	5.1909590	-2.6036260	-5.2322965
H	4.3051194	-0.8408637	-3.7251170
H	-3.0562750	-2.2062202	-2.9521255
H	-4.2880047	-3.5722989	-4.6263019
H	-4.5102590	-2.7686798	-6.9759723
H	-3.4889492	-0.5910856	-7.6408222
H	-2.2439438	0.7586967	-5.9792470
H	-4.4952299	0.8990001	-2.9854800
H	-5.8208007	2.9838269	-2.7621585
H	-4.6716934	5.1957289	-2.6656625
H	-2.1825340	5.3046526	-2.7873170
H	-0.8521176	3.1938077	-3.0146665
H	1.2242714	-3.6145205	-2.0983751
H	-0.5295420	-3.9604225	-2.0189820
H	0.2913024	-6.2274596	-2.2853774
H	1.8022741	-5.8642907	-1.4171153
H	-1.0136983	-6.1198750	-0.1944956
H	0.4691470	-6.9482132	0.3439693
H	-0.2929733	-4.5781725	1.5527637
H	1.4360502	-4.8726398	1.1856110
H	1.5012958	-2.5464174	2.3289969
H	2.5507094	-1.2525820	1.1611636
H	3.4109476	-2.0503471	2.7724784
H	-1.6691944	-2.2105474	1.4268797
H	-0.7123195	-2.8658371	3.1049112
H	-2.7302637	-2.6685487	3.0387591
H	1.5172954	-1.4492330	-1.4999631
H	1.4261743	0.4381260	-0.7213085
H	3.1602693	-0.3228842	-1.4221505

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H    -1.1048202    0.2309995   -0.5973640
H    -1.0389037   -1.6039411   -1.4974300
H    -2.7973933   -0.6957826   -1.1320089
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atomic populations:

atom		charge	n(s)	n(p)	n(d)	n(f)	n(g)
1	ca	1.77117	6.11669	11.99733	0.11481	0.00000	0.00000
2	p	1.30293	5.08721	8.57729	0.03257	0.00000	0.00000
3	p	1.29576	5.08425	8.58743	0.03256	0.00000	0.00000
4	p	1.32346	5.06812	8.57442	0.03401	0.00000	0.00000
5	p	1.32078	5.06700	8.57797	0.03425	0.00000	0.00000
6	o	-0.57307	3.64919	4.92085	0.00303	0.00000	0.00000
7	c	-1.34773	3.25885	4.08439	0.00449	0.00000	0.00000
8	c	-0.30651	3.00777	3.29511	0.00362	0.00000	0.00000
9	c	-0.19589	2.97817	3.21425	0.00347	0.00000	0.00000
10	c	-0.20640	2.98488	3.21807	0.00346	0.00000	0.00000
11	c	-0.20466	2.98807	3.21316	0.00343	0.00000	0.00000
12	c	-0.20885	2.98454	3.22088	0.00343	0.00000	0.00000
13	c	-0.20417	2.97760	3.22307	0.00349	0.00000	0.00000
14	c	-0.33791	3.01799	3.31629	0.00362	0.00000	0.00000
15	c	-0.19210	2.97784	3.21079	0.00347	0.00000	0.00000
16	c	-0.20632	2.98500	3.21786	0.00346	0.00000	0.00000
17	c	-0.20143	2.98863	3.20935	0.00345	0.00000	0.00000
18	c	-0.21141	2.98537	3.22260	0.00343	0.00000	0.00000
19	c	-0.19874	2.98099	3.21426	0.00348	0.00000	0.00000
20	c	-0.31425	3.00649	3.30412	0.00364	0.00000	0.00000
21	c	-0.20115	2.97637	3.22128	0.00350	0.00000	0.00000
22	c	-0.20409	2.98524	3.21538	0.00347	0.00000	0.00000
23	c	-0.20256	2.98804	3.21107	0.00345	0.00000	0.00000
24	c	-0.20938	2.98438	3.22154	0.00346	0.00000	0.00000
25	c	-0.19510	2.97701	3.21463	0.00346	0.00000	0.00000
26	c	-0.32651	3.02050	3.30239	0.00362	0.00000	0.00000
27	c	-0.20113	2.97800	3.21965	0.00348	0.00000	0.00000
28	c	-0.21280	2.98470	3.22465	0.00345	0.00000	0.00000
29	c	-0.20550	2.98823	3.21383	0.00344	0.00000	0.00000
30	c	-0.20641	2.98548	3.21749	0.00343	0.00000	0.00000
31	c	-0.19691	2.98080	3.21260	0.00350	0.00000	0.00000
32	c	-1.27613	3.16867	4.10344	0.00401	0.00000	0.00000
33	c	-0.30080	3.01441	3.28272	0.00367	0.00000	0.00000
34	c	-0.20570	2.97895	3.22325	0.00350	0.00000	0.00000
35	c	-0.21043	2.98496	3.22203	0.00345	0.00000	0.00000
36	c	-0.21076	2.98777	3.21958	0.00342	0.00000	0.00000
37	c	-0.21183	2.98506	3.22335	0.00342	0.00000	0.00000
38	c	-0.20075	2.98029	3.21693	0.00353	0.00000	0.00000
39	c	-0.32128	3.02974	3.28799	0.00355	0.00000	0.00000
40	c	-0.21424	2.98481	3.22589	0.00354	0.00000	0.00000
41	c	-0.21367	2.98569	3.22453	0.00345	0.00000	0.00000
42	c	-0.21318	2.98860	3.22117	0.00342	0.00000	0.00000
43	c	-0.21307	2.98622	3.22341	0.00344	0.00000	0.00000
44	c	-0.20176	2.97975	3.21852	0.00349	0.00000	0.00000
45	c	-0.31170	3.02298	3.28511	0.00361	0.00000	0.00000
46	c	-0.21038	2.98142	3.22546	0.00350	0.00000	0.00000
47	c	-0.21236	2.98566	3.22327	0.00342	0.00000	0.00000
48	c	-0.21132	2.98809	3.21982	0.00342	0.00000	0.00000
49	c	-0.21227	2.98531	3.22350	0.00346	0.00000	0.00000
50	c	-0.20269	2.97855	3.22064	0.00350	0.00000	0.00000
51	c	-0.30816	3.02288	3.28170	0.00358	0.00000	0.00000
52	c	-0.19684	2.97906	3.21429	0.00349	0.00000	0.00000
53	c	-0.21386	2.98534	3.22508	0.00344	0.00000	0.00000
54	c	-0.21538	2.98856	3.22340	0.00342	0.00000	0.00000
55	c	-0.21511	2.98551	3.22616	0.00344	0.00000	0.00000
56	c	-0.20903	2.98516	3.22033	0.00353	0.00000	0.00000
57	c	-0.10644	3.05760	3.04363	0.00521	0.00000	0.00000

58	c	-0.43857	3.07411	3.36089	0.00356	0.00000	0.00000
59	c	-0.43806	3.07366	3.36082	0.00358	0.00000	0.00000
60	c	-0.10845	3.05710	3.04613	0.00522	0.00000	0.00000
61	b	-0.82520	2.91703	2.90439	0.00379	0.00000	0.00000
62	b	-0.79222	2.90995	2.87876	0.00351	0.00000	0.00000
63	b	-0.79268	2.91063	2.87862	0.00343	0.00000	0.00000
64	b	-0.80481	2.91150	2.88985	0.00346	0.00000	0.00000
65	h	0.25468	0.74439	0.00093	0.00000	0.00000	0.00000
66	h	0.22867	0.77048	0.00085	0.00000	0.00000	0.00000
67	h	0.21777	0.78142	0.00081	0.00000	0.00000	0.00000
68	h	0.21607	0.78314	0.00079	0.00000	0.00000	0.00000
69	h	0.21738	0.78180	0.00082	0.00000	0.00000	0.00000
70	h	0.22933	0.76977	0.00090	0.00000	0.00000	0.00000
71	h	0.22418	0.77497	0.00085	0.00000	0.00000	0.00000
72	h	0.21798	0.78119	0.00083	0.00000	0.00000	0.00000
73	h	0.21541	0.78379	0.00081	0.00000	0.00000	0.00000
74	h	0.21675	0.78244	0.00081	0.00000	0.00000	0.00000
75	h	0.23680	0.76234	0.00085	0.00000	0.00000	0.00000
76	h	0.22648	0.77261	0.00091	0.00000	0.00000	0.00000
77	h	0.22532	0.77386	0.00082	0.00000	0.00000	0.00000
78	h	0.21521	0.78399	0.00080	0.00000	0.00000	0.00000
79	h	0.21603	0.78316	0.00081	0.00000	0.00000	0.00000
80	h	0.22826	0.77089	0.00084	0.00000	0.00000	0.00000
81	h	0.22278	0.77635	0.00086	0.00000	0.00000	0.00000
82	h	0.21560	0.78358	0.00082	0.00000	0.00000	0.00000
83	h	0.21472	0.78447	0.00081	0.00000	0.00000	0.00000
84	h	0.21668	0.78250	0.00082	0.00000	0.00000	0.00000
85	h	0.23595	0.76320	0.00085	0.00000	0.00000	0.00000
86	h	0.26061	0.73862	0.00077	0.00000	0.00000	0.00000
87	h	0.22222	0.77694	0.00084	0.00000	0.00000	0.00000
88	h	0.21505	0.78414	0.00081	0.00000	0.00000	0.00000
89	h	0.21401	0.78519	0.00080	0.00000	0.00000	0.00000
90	h	0.21357	0.78562	0.00081	0.00000	0.00000	0.00000
91	h	0.23308	0.76609	0.00083	0.00000	0.00000	0.00000
92	h	0.23651	0.76264	0.00085	0.00000	0.00000	0.00000
93	h	0.21455	0.78465	0.00081	0.00000	0.00000	0.00000
94	h	0.21327	0.78593	0.00080	0.00000	0.00000	0.00000
95	h	0.21480	0.78438	0.00081	0.00000	0.00000	0.00000
96	h	0.22722	0.77195	0.00083	0.00000	0.00000	0.00000
97	h	0.23369	0.76546	0.00085	0.00000	0.00000	0.00000
98	h	0.21430	0.78489	0.00081	0.00000	0.00000	0.00000
99	h	0.21439	0.78481	0.00080	0.00000	0.00000	0.00000
100	h	0.21523	0.78396	0.00081	0.00000	0.00000	0.00000
101	h	0.21925	0.77991	0.00084	0.00000	0.00000	0.00000
102	h	0.22641	0.77275	0.00084	0.00000	0.00000	0.00000
103	h	0.21476	0.78441	0.00082	0.00000	0.00000	0.00000
104	h	0.21385	0.78535	0.00080	0.00000	0.00000	0.00000
105	h	0.21478	0.78441	0.00081	0.00000	0.00000	0.00000
106	h	0.24023	0.75891	0.00086	0.00000	0.00000	0.00000
107	h	0.21461	0.78455	0.00085	0.00000	0.00000	0.00000
108	h	0.19001	0.80914	0.00085	0.00000	0.00000	0.00000
109	h	0.22962	0.76963	0.00075	0.00000	0.00000	0.00000
110	h	0.21338	0.78595	0.00067	0.00000	0.00000	0.00000
111	h	0.21329	0.78605	0.00066	0.00000	0.00000	0.00000
112	h	0.22866	0.77059	0.00075	0.00000	0.00000	0.00000
113	h	0.22283	0.77628	0.00089	0.00000	0.00000	0.00000
114	h	0.18739	0.81177	0.00084	0.00000	0.00000	0.00000
115	h	0.00880	0.99009	0.00111	0.00000	0.00000	0.00000
116	h	0.01423	0.98456	0.00121	0.00000	0.00000	0.00000
117	h	0.06071	0.93834	0.00095	0.00000	0.00000	0.00000
118	h	-0.02780	1.02658	0.00122	0.00000	0.00000	0.00000
119	h	0.03012	0.96890	0.00098	0.00000	0.00000	0.00000
120	h	0.05431	0.94476	0.00092	0.00000	0.00000	0.00000

121	h	-0.02016	1.01891	0.00124	0.00000	0.00000	0.00000
122	h	-0.00604	1.00496	0.00108	0.00000	0.00000	0.00000
123	h	0.05713	0.94193	0.00095	0.00000	0.00000	0.00000
124	h	-0.00292	1.00176	0.00116	0.00000	0.00000	0.00000
125	h	-0.01392	1.01275	0.00117	0.00000	0.00000	0.00000
126	h	0.05794	0.94115	0.00091	0.00000	0.00000	0.00000

[4-Ca*(THF)]2 C1 symmetry E(RI-BP86/TZVP) = -5222.900653281

coordinates:

Ca	-1.6748196	0.3177250	0.0329043
Ca	1.7206687	-0.2380272	0.1339525
P	-0.8464233	-1.3454801	2.7400417
P	0.6720412	1.4409120	2.7307171
P	-0.1807224	1.6284307	-2.4740783
P	0.3528058	-1.5561398	-2.5371604
O	-3.9999316	0.1898674	-0.7917197
O	4.1950886	-0.4097170	-0.0693556
C	-0.0133046	0.0071768	1.9881792
C	0.2858253	-2.8170840	2.9653067
C	-0.2445886	-4.1146235	3.0373108
C	0.6014495	-5.2152198	3.1998821
C	1.9847703	-5.0323642	3.3015869
C	2.5191715	-3.7421540	3.2367081
C	1.6718113	-2.6434412	3.0603223
C	-1.4991473	-1.1500093	4.4821721
C	-0.6936361	-1.4066575	5.6029372
C	-1.2101963	-1.2752153	6.8948230
C	-2.5384862	-0.8836692	7.0865556
C	-3.3502957	-0.6288427	5.9768590
C	-2.8356622	-0.7663055	4.6845133
C	-0.5793079	2.8216107	2.8978723
C	-1.9458220	2.5338298	3.0170832
C	-2.8862601	3.5638065	3.1239669
C	-2.4671292	4.8976133	3.0953722
C	-1.1057508	5.1933284	2.9697831
C	-0.1659589	4.1627147	2.8756362
C	1.3144344	1.3155924	4.4853036
C	0.5985671	1.8179163	5.5825718
C	1.1188924	1.7221736	6.8773250
C	2.3607192	1.1204540	7.0956382
C	3.0840435	0.6179004	6.0082590
C	2.5666072	0.7195899	4.7147660
C	0.0494999	0.0206396	-1.8080525
C	-1.1291968	1.8005601	-4.0828570
C	-0.6582339	2.5429286	-5.1776622
C	-1.4391490	2.6852249	-6.3305232
C	-2.7020448	2.0917888	-6.4040274
C	-3.1814021	1.3541462	-5.3156641
C	-2.4021532	1.2106775	-4.1649885
C	1.4270518	2.5028673	-2.8658147
C	2.5475560	1.7786172	-3.2999719
C	3.7436832	2.4356702	-3.6070163
C	3.8421034	3.8231609	-3.4562088
C	2.7369631	4.5490412	-3.0017339
C	1.5348341	3.8949905	-2.7128265
C	-1.2008990	-2.5092795	-2.9869040
C	-1.9262179	-2.2597953	-4.1643132
C	-3.0770664	-2.9956487	-4.4609879
C	-3.5187723	-3.9959200	-3.5867634
C	-2.8023277	-4.2531331	-2.4142347
C	-1.6499362	-3.5167101	-2.1171666
C	1.2869369	-1.6618278	-4.1580654
C	1.0470958	-0.7849888	-5.2287127
C	1.7483391	-0.9171372	-6.4311184
C	2.7035498	-1.9269276	-6.5815676
C	2.9525491	-2.8035165	-5.5213041
C	2.2492249	-2.6740572	-4.3194097
C	-4.9577913	1.2936983	-0.8539778

C	-6.3364851	0.6432876	-0.7670502
C	-6.1046889	-0.7024504	-1.4736854
C	-4.7030015	-1.0831346	-1.0019574
C	5.0689368	0.7577769	-0.2568934
C	6.4997021	0.2325362	-0.1288119
C	6.3624027	-1.2340006	-0.5710216
C	5.0117190	-1.6161103	0.0248673
B	-2.3587125	-1.8607969	1.6110480
B	2.1811641	2.0437287	1.6380682
B	-1.2079896	2.7064682	-1.1912408
B	1.3526240	-2.6125654	-1.2236551
H	-1.3230157	-4.2612930	2.9582186
H	0.1793141	-6.2212419	3.2441923
H	2.6435009	-5.8934494	3.4288405
H	3.5973408	-3.5919891	3.3252647
H	2.0788637	-1.6292697	3.0096200
H	0.3427237	-1.7194312	5.4692698
H	-0.5692445	-1.4798555	7.7542957
H	-2.9421643	-0.7858293	8.0961247
H	-4.3933506	-0.3373132	6.1163940
H	-3.4856346	-0.6019712	3.8237537
H	-2.2685821	1.4893273	3.0441804
H	-3.9463385	3.3249795	3.2335101
H	-3.1988971	5.7043957	3.1676602
H	-0.7738290	6.2330462	2.9387168
H	0.8943914	4.3973649	2.7711632
H	-0.3715186	2.2911652	5.4280797
H	0.5467814	2.1190252	7.7182116
H	2.7676962	1.0489488	8.1060667
H	4.0614917	0.1574828	6.1665801
H	3.1539507	0.3556224	3.8703030
H	0.3241981	3.0145202	-5.1317930
H	-1.0568262	3.2653684	-7.1728835
H	-3.3109083	2.2038342	-7.3030096
H	-4.1673529	0.8873112	-5.3642714
H	-2.7823289	0.6306335	-3.3212918
H	2.4791567	0.6947077	-3.4100226
H	4.5986671	1.8617122	-3.9709833
H	4.7772575	4.3360692	-3.6892888
H	2.8093192	5.6303069	-2.8688513
H	0.6753143	4.4640770	-2.3565711
H	-1.5861987	-1.4988120	-4.8672267
H	-3.6215981	-2.7970924	-5.3864942
H	-4.4106666	-4.5787277	-3.8252267
H	-3.1329588	-5.0356694	-1.7285986
H	-1.0884062	-3.7346976	-1.2083342
H	0.3168341	0.0187307	-5.1276328
H	1.5459506	-0.2255422	-7.2512217
H	3.2514463	-2.0294452	-7.5202273
H	3.6959458	-3.5961947	-5.6290863
H	2.4418214	-3.3664933	-3.4992406
H	-4.7383371	1.9850122	-0.0291202
H	-4.8100135	1.8281001	-1.8058284
H	-6.6233741	0.4823626	0.2828284
H	-7.1122708	1.2555142	-1.2457550
H	-6.1266608	-0.5730585	-2.5659697
H	-6.8488989	-1.4635054	-1.2048689
H	-4.1305470	-1.6681399	-1.7332703
H	-4.7150218	-1.6225934	-0.0428405
H	4.8641537	1.1685652	-1.2570108
H	4.7964436	1.5056627	0.4990241
H	6.8413449	0.2875316	0.9156165
H	7.2034855	0.8054140	-0.7468775

H	7.1755076	-1.8739950	-0.2031948
H	6.3322188	-1.3094369	-1.6681699
H	5.1072808	-1.8975312	1.0877914
H	4.4834084	-2.4140700	-0.5118852
H	-1.9020611	-2.0302101	0.4826565
H	-3.1112300	-0.8842022	1.6247927
H	-2.9372797	-2.8507229	1.9986608
H	1.7835220	2.1329263	0.4775053
H	3.0002974	1.1340314	1.7489373
H	2.6526280	3.0905561	2.0189302
H	-0.6943505	2.5398780	-0.0905823
H	-2.3439273	2.2416005	-1.2318874
H	-1.2367848	3.8732165	-1.5036615
H	0.7869029	-2.4621719	-0.1449098
H	2.4674950	-2.0968766	-1.2089671
H	1.4303714	-3.7856346	-1.5077604

atomic populations:

atom		charge	n(s)	n(p)	n(d)	n(f)	n(g)
1	ca	1.76773	6.11690	11.99621	0.11916	0.00000	0.00000
2	ca	1.76875	6.11692	11.99628	0.11804	0.00000	0.00000
3	p	1.28439	5.05819	8.62179	0.03564	0.00000	0.00000
4	p	1.28439	5.05706	8.62284	0.03571	0.00000	0.00000
5	p	1.27135	5.06149	8.63133	0.03584	0.00000	0.00000
6	p	1.27654	5.06472	8.62327	0.03546	0.00000	0.00000
7	o	-0.57633	3.65195	4.92124	0.00315	0.00000	0.00000
8	o	-0.57083	3.65159	4.91608	0.00316	0.00000	0.00000
9	c	-1.72382	3.34876	4.37143	0.00363	0.00000	0.00000
10	c	-0.30982	3.02405	3.28219	0.00358	0.00000	0.00000
11	c	-0.19769	2.97960	3.21460	0.00350	0.00000	0.00000
12	c	-0.20588	2.98594	3.21650	0.00344	0.00000	0.00000
13	c	-0.20934	2.98750	3.21841	0.00343	0.00000	0.00000
14	c	-0.21465	2.98266	3.22853	0.00345	0.00000	0.00000
15	c	-0.22380	2.97714	3.24314	0.00352	0.00000	0.00000
16	c	-0.31493	3.01822	3.29311	0.00360	0.00000	0.00000
17	c	-0.19635	2.97900	3.21384	0.00351	0.00000	0.00000
18	c	-0.20800	2.98432	3.22023	0.00345	0.00000	0.00000
19	c	-0.21110	2.98710	3.22055	0.00345	0.00000	0.00000
20	c	-0.21497	2.98373	3.22781	0.00343	0.00000	0.00000
21	c	-0.20937	2.97820	3.22766	0.00351	0.00000	0.00000
22	c	-0.31588	3.02455	3.28774	0.00360	0.00000	0.00000
23	c	-0.22972	2.97795	3.24824	0.00353	0.00000	0.00000
24	c	-0.21598	2.98311	3.22942	0.00345	0.00000	0.00000
25	c	-0.20942	2.98770	3.21829	0.00343	0.00000	0.00000
26	c	-0.20453	2.98605	3.21504	0.00344	0.00000	0.00000
27	c	-0.19636	2.97995	3.21293	0.00348	0.00000	0.00000
28	c	-0.31120	3.02030	3.28730	0.00360	0.00000	0.00000
29	c	-0.19992	2.97923	3.21719	0.00349	0.00000	0.00000
30	c	-0.20797	2.98427	3.22024	0.00345	0.00000	0.00000
31	c	-0.21406	2.98699	3.22363	0.00344	0.00000	0.00000
32	c	-0.21587	2.98368	3.22875	0.00343	0.00000	0.00000
33	c	-0.20724	2.97668	3.22705	0.00351	0.00000	0.00000
34	c	-1.71124	3.34548	4.36237	0.00340	0.00000	0.00000
35	c	-0.31832	3.02452	3.29020	0.00359	0.00000	0.00000
36	c	-0.21546	2.97992	3.23207	0.00347	0.00000	0.00000
37	c	-0.21091	2.98501	3.22245	0.00346	0.00000	0.00000
38	c	-0.21407	2.98725	3.22338	0.00344	0.00000	0.00000
39	c	-0.21615	2.98390	3.22880	0.00345	0.00000	0.00000
40	c	-0.21130	2.97793	3.22981	0.00356	0.00000	0.00000
41	c	-0.32126	3.02327	3.29438	0.00361	0.00000	0.00000
42	c	-0.21581	2.98026	3.23200	0.00355	0.00000	0.00000
43	c	-0.22433	2.98513	3.23576	0.00345	0.00000	0.00000

44	c	-0.21127	2.98793	3.21989	0.00344	0.00000	0.00000
45	c	-0.20912	2.98603	3.21964	0.00344	0.00000	0.00000
46	c	-0.20070	2.98221	3.21501	0.00348	0.00000	0.00000
47	c	-0.31285	3.02501	3.28415	0.00368	0.00000	0.00000
48	c	-0.20753	2.97963	3.22436	0.00354	0.00000	0.00000
49	c	-0.22123	2.98518	3.23260	0.00345	0.00000	0.00000
50	c	-0.21986	2.98794	3.22848	0.00344	0.00000	0.00000
51	c	-0.21673	2.98579	3.22750	0.00344	0.00000	0.00000
52	c	-0.20353	2.98265	3.21732	0.00357	0.00000	0.00000
53	c	-0.31768	3.01947	3.29461	0.00360	0.00000	0.00000
54	c	-0.21837	2.97925	3.23559	0.00352	0.00000	0.00000
55	c	-0.21171	2.98446	3.22380	0.00345	0.00000	0.00000
56	c	-0.20991	2.98763	3.21884	0.00344	0.00000	0.00000
57	c	-0.21323	2.98536	3.22444	0.00342	0.00000	0.00000
58	c	-0.20316	2.98149	3.21817	0.00351	0.00000	0.00000
59	c	-0.10346	3.05444	3.04374	0.00528	0.00000	0.00000
60	c	-0.43866	3.07367	3.36140	0.00359	0.00000	0.00000
61	c	-0.43836	3.07390	3.36088	0.00358	0.00000	0.00000
62	c	-0.11107	3.05765	3.04813	0.00528	0.00000	0.00000
63	c	-0.11213	3.05843	3.04844	0.00526	0.00000	0.00000
64	c	-0.43946	3.07489	3.36101	0.00356	0.00000	0.00000
65	c	-0.43704	3.07410	3.35935	0.00359	0.00000	0.00000
66	c	-0.10439	3.05359	3.04549	0.00531	0.00000	0.00000
67	b	-0.80554	2.90924	2.89272	0.00358	0.00000	0.00000
68	b	-0.79890	2.90872	2.88662	0.00355	0.00000	0.00000
69	b	-0.78880	2.91031	2.87495	0.00354	0.00000	0.00000
70	b	-0.82421	2.91062	2.90990	0.00369	0.00000	0.00000
71	h	0.23112	0.76803	0.00085	0.00000	0.00000	0.00000
72	h	0.21465	0.78453	0.00081	0.00000	0.00000	0.00000
73	h	0.21332	0.78587	0.00081	0.00000	0.00000	0.00000
74	h	0.20951	0.78965	0.00084	0.00000	0.00000	0.00000
75	h	0.21940	0.77970	0.00090	0.00000	0.00000	0.00000
76	h	0.22922	0.76992	0.00087	0.00000	0.00000	0.00000
77	h	0.21600	0.78317	0.00083	0.00000	0.00000	0.00000
78	h	0.21285	0.78635	0.00080	0.00000	0.00000	0.00000
79	h	0.21242	0.78676	0.00082	0.00000	0.00000	0.00000
80	h	0.22576	0.77335	0.00089	0.00000	0.00000	0.00000
81	h	0.22335	0.77576	0.00089	0.00000	0.00000	0.00000
82	h	0.21109	0.78808	0.00083	0.00000	0.00000	0.00000
83	h	0.21341	0.78579	0.00081	0.00000	0.00000	0.00000
84	h	0.21492	0.78426	0.00081	0.00000	0.00000	0.00000
85	h	0.23341	0.76573	0.00086	0.00000	0.00000	0.00000
86	h	0.22908	0.77004	0.00088	0.00000	0.00000	0.00000
87	h	0.21507	0.78410	0.00083	0.00000	0.00000	0.00000
88	h	0.21295	0.78624	0.00081	0.00000	0.00000	0.00000
89	h	0.21222	0.78696	0.00083	0.00000	0.00000	0.00000
90	h	0.22014	0.77896	0.00090	0.00000	0.00000	0.00000
91	h	0.23022	0.76890	0.00088	0.00000	0.00000	0.00000
92	h	0.21527	0.78392	0.00081	0.00000	0.00000	0.00000
93	h	0.21446	0.78473	0.00080	0.00000	0.00000	0.00000
94	h	0.21248	0.78669	0.00083	0.00000	0.00000	0.00000
95	h	0.22952	0.76964	0.00084	0.00000	0.00000	0.00000
96	h	0.23457	0.76455	0.00088	0.00000	0.00000	0.00000
97	h	0.21453	0.78464	0.00083	0.00000	0.00000	0.00000
98	h	0.21368	0.78552	0.00080	0.00000	0.00000	0.00000
99	h	0.21623	0.78297	0.00081	0.00000	0.00000	0.00000
100	h	0.23797	0.76117	0.00086	0.00000	0.00000	0.00000
101	h	0.22844	0.77069	0.00087	0.00000	0.00000	0.00000
102	h	0.21421	0.78497	0.00082	0.00000	0.00000	0.00000
103	h	0.21391	0.78528	0.00081	0.00000	0.00000	0.00000
104	h	0.21806	0.78113	0.00081	0.00000	0.00000	0.00000
105	h	0.24288	0.75629	0.00083	0.00000	0.00000	0.00000
106	h	0.23237	0.76673	0.00089	0.00000	0.00000	0.00000

107	h	0.21621	0.78298	0.00081	0.00000	0.00000	0.00000
108	h	0.21359	0.78561	0.00080	0.00000	0.00000	0.00000
109	h	0.21380	0.78539	0.00081	0.00000	0.00000	0.00000
110	h	0.23650	0.76264	0.00086	0.00000	0.00000	0.00000
111	h	0.20182	0.79733	0.00086	0.00000	0.00000	0.00000
112	h	0.19120	0.80796	0.00084	0.00000	0.00000	0.00000
113	h	0.21253	0.78680	0.00067	0.00000	0.00000	0.00000
114	h	0.22891	0.77033	0.00075	0.00000	0.00000	0.00000
115	h	0.21101	0.78832	0.00067	0.00000	0.00000	0.00000
116	h	0.23044	0.76882	0.00075	0.00000	0.00000	0.00000
117	h	0.21568	0.78346	0.00086	0.00000	0.00000	0.00000
118	h	0.20247	0.79666	0.00087	0.00000	0.00000	0.00000
119	h	0.19359	0.80556	0.00085	0.00000	0.00000	0.00000
120	h	0.21996	0.77915	0.00089	0.00000	0.00000	0.00000
121	h	0.21214	0.78718	0.00068	0.00000	0.00000	0.00000
122	h	0.22960	0.76965	0.00075	0.00000	0.00000	0.00000
123	h	0.22783	0.77141	0.00075	0.00000	0.00000	0.00000
124	h	0.21434	0.78500	0.00066	0.00000	0.00000	0.00000
125	h	0.17425	0.82491	0.00084	0.00000	0.00000	0.00000
126	h	0.21861	0.78050	0.00089	0.00000	0.00000	0.00000
127	h	-0.01174	1.01063	0.00111	0.00000	0.00000	0.00000
128	h	-0.02372	1.02266	0.00105	0.00000	0.00000	0.00000
129	h	0.04744	0.95159	0.00096	0.00000	0.00000	0.00000
130	h	-0.00999	1.00885	0.00114	0.00000	0.00000	0.00000
131	h	-0.02086	1.01975	0.00111	0.00000	0.00000	0.00000
132	h	0.04885	0.95019	0.00095	0.00000	0.00000	0.00000
133	h	-0.00048	0.99932	0.00116	0.00000	0.00000	0.00000
134	h	-0.02112	1.01994	0.00117	0.00000	0.00000	0.00000
135	h	0.04900	0.95006	0.00094	0.00000	0.00000	0.00000
136	h	0.00379	0.99516	0.00105	0.00000	0.00000	0.00000
137	h	-0.01829	1.01723	0.00106	0.00000	0.00000	0.00000
138	h	0.05352	0.94556	0.00092	0.00000	0.00000	0.00000