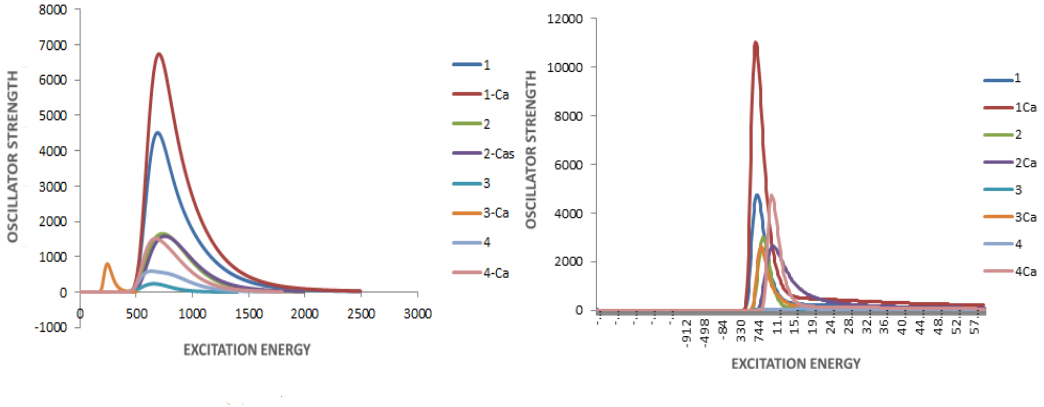
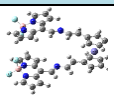
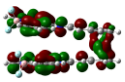
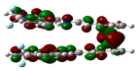
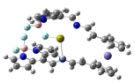
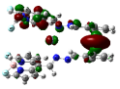
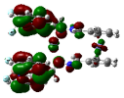
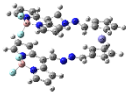
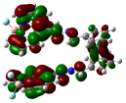
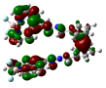
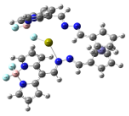
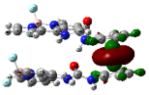
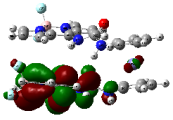
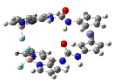
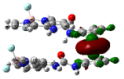
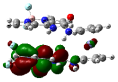
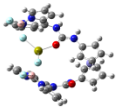
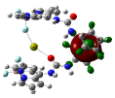
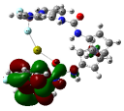
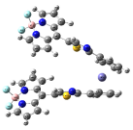
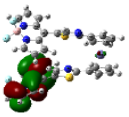
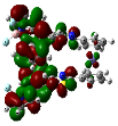
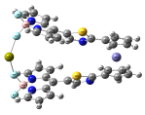
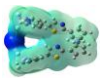
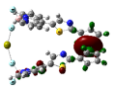
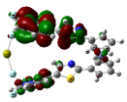
Supplementary Information

Figure S1: a) UV-Vis absorption of probe **1**, **2**, **3**, **4** and their complexes complexes b) emission spectrums of probe **1**, **2**, **3**, **4** and their complexes complexes



(a) (b)

Table S1: Geometries, ESP maps and frontier orbitals of designed BODIPY-Ferrocene based sensors and their complexes. Geometries in this table are the most stable state of structures which are found by Gaussian09 program. Red and blue regions, in ESP maps, show negatively and positively charged parts of the molecules in respect. Ca(II) ion joins to the sensor from positively charged parts. That is why colors of ESP maps in complexes are widely blue. Also energies of frontier orbitals are shown here. Energy amounts are decreased by adding metal ion to the structure and this corresponds to the stability of complexes that are formed by adding Ca(II) ion.

Structure	Geometry	ESP	HOMO	E_H (eV)	LUMO	E_L (eV)	ΔE	Reduction Potential,E0 (V)
1				-6.00		-3.65	2.35	1.23
1-Ca				-6.09		-4.20	1.89	1.27
2				-6.30		-3.78	2.52	1.24
2-Ca				-6.28		-4.04	2.24	1.29
3				-5.85		-3.24	2.61	1.23
3-Ca				-5.88		-3.86	2.02	1.27
4				-6.26		-3.65	2.61	1.24
4-Ca				-6.23		-3.80	2.43	1.31

Standard orientation of 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.718220	-1.872761	-0.562995
2	6	0	5.335626	-2.145204	-0.286755
3	6	0	4.526197	-1.345406	-1.192491
4	6	0	5.442815	-0.550824	-1.999477
5	6	0	6.784389	-0.891215	-1.622502
6	1	0	7.563889	-2.314527	-0.055301
7	1	0	4.965430	-2.835113	0.457939
8	1	0	5.150905	0.148428	-2.770847
9	1	0	7.687809	-0.473866	-2.043709
10	6	0	5.883029	2.005888	0.346362
11	6	0	4.659807	1.518458	0.963200
12	6	0	6.996738	1.351964	0.972327
13	1	0	5.932530	2.752731	-0.433996
14	6	0	5.045551	0.522570	1.954530
15	6	0	6.479052	0.438811	1.966192
16	1	0	8.039456	1.505528	0.734087
17	1	0	4.376172	-0.040400	2.589154
18	1	0	7.069686	-0.211853	2.595476
19	6	0	-1.440125	-2.690856	-0.338716
20	5	0	-4.461004	-2.711310	-0.563216
21	9	0	-5.240852	-3.468359	-1.534789
22	9	0	-5.433729	-1.992556	0.246827
23	7	0	-3.626383	-3.651162	0.303311
24	6	0	-4.099200	-4.650238	1.108557
25	6	0	-1.837504	-4.675183	1.295614
26	6	0	-3.015562	-5.305299	1.739516
27	1	0	-5.157692	-4.849791	1.196825
28	1	0	-0.830043	-4.933045	1.587670
29	1	0	-3.094024	-6.132489	2.429589
30	7	0	-3.516533	-1.742706	-1.268110
31	6	0	-2.102726	-1.743483	-1.167046
32	6	0	-3.883711	-0.734517	-2.113055
33	6	0	-1.617426	-0.685241	-1.992884
34	6	0	-2.731223	-0.057802	-2.579762
35	1	0	-4.922184	-0.543382	-2.343453
36	1	0	-0.574553	-0.442273	-2.114193
37	1	0	-2.727454	0.782521	-3.258670
38	6	0	3.083658	-1.287165	-1.287618
39	6	0	0.009077	-2.761926	-0.189335
40	7	0	0.841520	-1.962183	-0.818635
41	26	0	5.733910	-0.086790	0.044115
42	1	0	0.385895	-3.537529	0.484111
43	1	0	2.658450	-0.536171	-1.952088
44	6	0	-2.219373	-3.635131	0.393896
45	6	0	-1.469870	2.271408	0.833474
46	5	0	-4.237617	3.220023	0.047048
47	9	0	-4.933447	4.371012	0.611962
48	9	0	-5.147234	2.659998	-0.940722
49	7	0	-2.925071	3.651379	-0.599762
50	6	0	-2.791878	4.542182	-1.627284
51	6	0	-0.693908	3.881536	-1.064788
52	6	0	-1.421857	4.708340	-1.941150
53	1	0	-3.653811	5.011257	-2.080557
54	1	0	0.373782	3.746943	-1.009207
55	1	0	-1.026570	5.353554	-2.712239
56	7	0	-3.922672	2.199213	1.137684

57	6	0	-2.627810	1.775356	1.501681
58	6	0	-4.827265	1.554793	1.934741
59	6	0	-2.770554	0.834617	2.567427
60	6	0	-4.145941	0.700473	2.833489
61	1	0	-5.889663	1.725114	1.833599
62	1	0	-1.970816	0.316567	3.076144
63	1	0	-4.609455	0.068338	3.576506
64	6	0	3.333744	1.957667	0.586747
65	6	0	-0.174580	1.769830	1.278362
66	7	0	0.961841	2.116815	0.717025
67	1	0	-0.190386	1.069457	2.118714
68	1	0	3.265319	2.651494	-0.250408
69	6	0	-1.631508	3.214035	-0.221020
70	6	0	2.209194	-2.112703	-0.628056
71	6	0	2.158022	1.598086	1.195135
72	1	0	2.146227	0.912950	2.048484
73	1	0	2.572407	-2.898187	0.042221

Standard orientation of 1-Ca

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	6.634419	1.263812	-1.526115
2	6	0	5.206362	1.400415	-1.594172
3	6	0	4.725157	1.766518	-0.270107
4	6	0	5.880649	1.802837	0.613646
5	6	0	7.051098	1.512524	-0.164081
6	1	0	7.284522	0.996813	-2.347209
7	1	0	4.600975	1.275611	-2.480445
8	1	0	5.853306	2.048984	1.666248
9	1	0	8.065502	1.469849	0.205735
10	6	0	5.518671	-1.605029	1.295951
11	6	0	4.457147	-1.795296	0.319657
12	6	0	6.779427	-1.761445	0.627388
13	1	0	5.371065	-1.419327	2.350951
14	6	0	5.093442	-2.022013	-0.968106
15	6	0	6.516586	-2.018630	-0.770592
16	1	0	7.755218	-1.683878	1.085135
17	1	0	4.589325	-2.193304	-1.908404
18	1	0	7.262383	-2.161458	-1.539722
19	6	0	-1.312480	3.045474	-0.414061
20	7	0	-3.710067	3.328673	-0.944524
21	6	0	-4.524168	3.240173	-2.039052
22	6	0	-2.427617	2.727503	-2.741967
23	6	0	-3.759844	2.871214	-3.171908
24	1	0	-5.584693	3.436563	-1.970523
25	1	0	-1.584766	2.458016	-3.361569
26	1	0	-4.142208	2.733609	-4.172601
27	7	0	-2.882094	3.761112	1.346328
28	6	0	-1.565880	3.443389	0.929889
29	6	0	-2.833369	4.166799	2.650156
30	6	0	-0.700966	3.679214	2.041046
31	6	0	-1.496113	4.128601	3.112427
32	1	0	-3.727086	4.462250	3.181443
33	1	0	0.367267	3.536644	2.020735
34	1	0	-1.164282	4.405771	4.102501
35	6	0	3.372582	2.054018	0.150868
36	6	0	0.008542	2.679630	-0.911429
37	7	0	1.053974	2.528587	-0.128463

38	26	0	5.714397	-0.136058	-0.221418
39	1	0	0.093037	2.524961	-1.991064
40	1	0	3.209116	2.207117	1.217004
41	6	0	-2.393479	3.017383	-1.343008
42	6	0	-1.567346	-2.946399	-0.472829
43	5	0	-4.501377	-3.437741	0.037828
44	7	0	-3.355488	-3.801574	0.985014
45	6	0	-3.461449	-4.439684	2.187153
46	6	0	-1.248654	-4.051438	1.857092
47	6	0	-2.173998	-4.609276	2.756271
48	1	0	-4.420265	-4.749096	2.578639
49	1	0	-0.174001	-4.020964	1.955762
50	1	0	-1.962368	-5.093086	3.698420
51	7	0	-3.894168	-2.964285	-1.284491
52	6	0	-2.522729	-2.702400	-1.493249
53	6	0	-4.569101	-2.636478	-2.425696
54	6	0	-2.376993	-2.192193	-2.819668
55	6	0	-3.657717	-2.157589	-3.399924
56	1	0	-5.641507	-2.748889	-2.499574
57	1	0	-1.449526	-1.895927	-3.288518
58	1	0	-3.916126	-1.833525	-4.397222
59	6	0	3.040745	-1.795120	0.634732
60	6	0	-0.157706	-2.656531	-0.757566
61	7	0	0.709003	-2.248086	0.144072
62	1	0	0.156983	-2.817299	-1.793667
63	1	0	2.773687	-1.559610	1.663716
64	6	0	-1.987311	-3.533629	0.747612
65	6	0	2.287143	2.199553	-0.676074
66	6	0	2.053485	-2.146356	-0.243964
67	1	0	2.304530	-2.411263	-1.274446
68	1	0	2.380325	2.079271	-1.759865
69	5	0	-4.138577	3.638375	0.488248
70	9	0	-4.924739	4.856596	0.541862
71	9	0	-5.005658	2.579830	0.998787
72	9	0	-5.330434	-2.387892	0.618167
73	9	0	-5.374945	-4.574111	-0.170396
74	20	0	-0.336616	-0.229580	2.157089

Standard orientation of 2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-6.466381	-1.661102	1.147230
2	6	0	-5.138350	-2.113690	0.847706
3	6	0	-4.203348	-1.144992	1.392312
4	6	0	-4.983122	-0.082422	2.012848
5	6	0	-6.370173	-0.410862	1.869254
6	1	0	-7.383117	-2.160488	0.867839
7	1	0	-4.869776	-3.013367	0.314065
8	1	0	-4.576137	0.786504	2.511268
9	1	0	-7.201715	0.180720	2.224319
10	6	0	-5.901076	1.648272	-0.953993
11	6	0	-4.542793	1.249067	-1.282492
12	6	0	-6.791807	0.648716	-1.469661
13	1	0	-6.182636	2.546866	-0.422852
14	6	0	-4.615600	-0.019674	-1.992479
15	6	0	-5.997730	-0.377194	-2.110286

16	1	0	-7.868835	0.654556	-1.383849
17	1	0	-3.770227	-0.579854	-2.363483
18	1	0	-6.382680	-1.271624	-2.579102
19	6	0	1.436567	-3.069107	0.390571
20	5	0	4.445081	-3.334090	0.204778
21	9	0	5.334212	-3.842733	1.238475
22	9	0	5.299645	-2.985710	-0.919490
23	7	0	3.428641	-4.400366	-0.202377
24	6	0	3.705038	-5.637113	-0.711070
25	6	0	1.444708	-5.480418	-0.581094
26	6	0	2.496132	-6.333845	-0.957314
27	1	0	4.721672	-5.965831	-0.873934
28	1	0	0.390079	-5.705768	-0.641478
29	1	0	2.415644	-7.332998	-1.359143
30	7	0	3.680165	-2.110438	0.704283
31	6	0	2.269686	-1.994892	0.795294
32	6	0	4.231896	-0.942023	1.142145
33	6	0	1.983029	-0.693592	1.314139
34	6	0	3.208083	-0.040424	1.526979
35	1	0	5.303009	-0.798157	1.162438
36	1	0	0.989413	-0.315204	1.491747
37	1	0	3.365016	0.959148	1.905076
38	6	0	-2.758578	-1.168593	1.326661
39	6	0	-0.028630	-3.032050	0.445912
40	7	0	-0.697630	-2.000047	0.891947
41	26	0	-5.449321	-0.211325	-0.048255
42	1	0	-0.568362	-3.911977	0.096695
43	1	0	-2.215246	-0.298360	1.706286
44	6	0	2.027910	-4.262998	-0.106064
45	6	0	1.278400	2.744884	-0.728700
46	5	0	3.915112	3.879237	0.215689
47	9	0	4.692708	5.015958	-0.241539
48	9	0	4.666559	3.295023	1.320310
49	7	0	2.530293	4.320887	0.685212
50	6	0	2.264534	5.277073	1.621753
51	6	0	0.259805	4.417005	0.991656
52	6	0	0.865893	5.364699	1.834191
53	1	0	3.057748	5.841755	2.091245
54	1	0	-0.790620	4.202167	0.881118
55	1	0	0.375479	6.040475	2.519491
56	7	0	3.735669	2.858656	-0.907626
57	6	0	2.499038	2.317255	-1.316084
58	6	0	4.724345	2.277759	-1.648161
59	6	0	2.768179	1.368026	-2.352530
60	6	0	4.158029	1.349357	-2.557163
61	1	0	5.763553	2.537949	-1.504963
62	1	0	2.037987	0.778273	-2.886965
63	1	0	4.706473	0.749273	-3.268014
64	6	0	-3.351864	1.968657	-0.888686
65	6	0	0.054370	2.081385	-1.187058
66	7	0	-1.134803	2.412987	-0.754308
67	1	0	0.158499	1.268845	-1.905987
68	1	0	-3.467806	2.836806	-0.233325
69	6	0	1.299084	3.758772	0.264251
70	7	0	-2.100631	-2.202405	0.848189
71	7	0	-2.158247	1.600805	-1.301946

Standard orientation of 2-Ca

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.882773	1.690110	0.941068
2	6	0	-5.458372	1.743108	1.107008
3	6	0	-4.859978	1.793997	-0.215675
4	6	0	-5.937112	1.739428	-1.192293
5	6	0	-7.178374	1.690535	-0.474813
6	1	0	-7.611447	1.634864	1.737275
7	1	0	-4.917998	1.765129	2.041551
8	1	0	-5.814513	1.767978	-2.265985
9	1	0	-8.164035	1.642807	-0.914972
10	6	0	-5.938056	-1.740617	-1.190076
11	6	0	-4.860378	-1.794105	-0.214014
12	6	0	-7.178905	-1.690595	-0.471946
13	1	0	-5.816089	-1.770572	-2.263802
14	6	0	-5.458014	-1.741406	1.108953
15	6	0	-6.882498	-1.688412	0.943767
16	1	0	-8.164810	-1.643241	-0.911598
17	1	0	-4.917106	-1.762363	2.043212
18	1	0	-7.610706	-1.632034	1.740323
19	6	0	1.064021	2.771087	0.358590
20	5	0	3.985568	3.264740	-0.167227
21	9	0	4.787332	4.422931	-0.444378
22	9	0	4.966307	2.127435	-0.171950
23	7	0	3.318893	3.331321	1.192621
24	6	0	3.915739	3.613611	2.390302
25	6	0	1.729078	3.197892	2.834848
26	6	0	2.957093	3.538900	3.428800
27	1	0	4.968140	3.851203	2.454816
28	1	0	0.788441	3.067334	3.349419
29	1	0	3.149008	3.717527	4.476290
30	7	0	2.930741	3.017845	-1.227246
31	6	0	1.560036	2.754575	-0.971856
32	6	0	3.128816	2.977389	-2.579741
33	6	0	0.926605	2.546405	-2.234170
34	6	0	1.907638	2.686300	-3.232389
35	1	0	4.103248	3.155152	-3.012632
36	1	0	-0.121796	2.330365	-2.360449
37	1	0	1.771576	2.598031	-4.300213
38	6	0	-3.457805	1.903510	-0.549702
39	6	0	-0.338409	2.526113	0.706835
40	7	0	-1.250568	2.251860	-0.190491
41	26	0	-5.983472	0.000176	0.011947
42	1	0	-0.618843	2.593939	1.757698
43	1	0	-3.176064	1.859243	-1.605974
44	6	0	1.951507	3.067590	1.428454
45	6	0	1.063760	-2.770466	0.360354
46	5	0	3.985230	-3.265382	-0.164743
47	9	0	4.787039	-4.424169	-0.439238
48	9	0	4.965874	-2.128010	-0.172391
49	7	0	2.930220	-3.021006	-1.225192
50	6	0	3.128091	-2.983562	-2.577799
51	6	0	0.925980	-2.551536	-2.232860
52	6	0	1.906837	-2.693792	-3.230912
53	1	0	4.102437	-3.162379	-3.010451
54	1	0	-0.122414	-2.335621	-2.359450
55	1	0	1.770627	-2.607883	-4.298909
56	7	0	3.318756	-3.328796	1.195346

57	6	0	1.951410	-3.064505	1.430774
58	6	0	3.915757	-3.608443	2.393579
59	6	0	1.729160	-3.191702	2.837474
60	6	0	2.957242	-3.531448	3.432022
61	1	0	4.968163	-3.845912	2.458472
62	1	0	0.788588	-3.059982	3.351871
63	1	0	3.149289	-3.707743	4.479883
64	6	0	-3.458364	-1.904334	-0.548522
65	6	0	-0.338620	-2.524770	0.708274
66	7	0	-1.250997	-2.252462	-0.189431
67	1	0	-0.618829	-2.590273	1.759342
68	1	0	-3.177043	-1.861706	-1.604973
69	6	0	1.559585	-2.756990	-0.970184
70	7	0	-2.540769	2.101379	0.373646
71	7	0	-2.541026	-2.100839	0.374813
72	20	0	5.836928	-0.000362	-0.680663

Standard orientation of 3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	2.014541	5.531392	-1.426095
2	6	0	3.014980	4.566910	-1.044291
3	6	0	2.483425	3.252799	-1.328337
4	6	0	1.156323	3.402051	-1.877665
5	6	0	0.869282	4.813598	-1.931813
6	1	0	2.105448	6.604341	-1.335473
7	1	0	3.992055	4.778301	-0.632583
8	1	0	0.500998	2.598791	-2.177151
9	1	0	-0.051894	5.253376	-2.287170
10	6	0	-0.543887	4.391146	1.194109
11	6	0	0.010308	3.062144	1.314229
12	6	0	0.435069	5.315808	1.709602
13	1	0	-1.519763	4.635300	0.803474
14	6	0	1.330358	3.165852	1.891615
15	6	0	1.591209	4.562569	2.133594
16	1	0	0.321351	6.389308	1.763310
17	1	0	1.989233	2.338218	2.112793
18	1	0	2.495175	4.970613	2.562938
19	6	0	3.511251	-1.526565	-0.460527
20	5	0	3.303205	-4.483362	0.110669
21	9	0	2.574719	-4.972182	1.275561
22	9	0	3.797075	-5.661441	-0.575393
23	7	0	2.379735	-3.674610	-0.800620
24	6	0	1.363188	-4.180599	-1.555735
25	6	0	1.442919	-1.954978	-1.989719
26	6	0	0.760437	-3.142591	-2.305624
27	1	0	1.122066	-5.233979	-1.539162
28	1	0	1.237591	-0.971559	-2.379830
29	1	0	-0.066493	-3.257506	-2.990737
30	7	0	4.452346	-3.577115	0.543767
31	6	0	4.506562	-2.188245	0.321648
32	6	0	5.527129	-3.928883	1.313347
33	6	0	5.657638	-1.685258	0.989552
34	6	0	6.298882	-2.781728	1.603002
35	1	0	5.686126	-4.951834	1.623046
36	1	0	5.986431	-0.655624	1.033101
37	1	0	7.204186	-2.760749	2.191555
38	26	0	1.246370	4.232090	0.070404

39	6	0	2.459208	-2.280158	-1.044288
40	6	0	-3.373483	-0.436625	0.387897
41	5	0	-5.908678	-2.018510	-0.085622
42	9	0	-6.879722	-2.294154	0.967002
43	9	0	-6.445475	-2.630743	-1.288784
44	7	0	-5.734844	-0.513605	-0.279158
45	6	0	-6.684436	0.334736	-0.770001
46	6	0	-4.825070	1.583049	-0.408948
47	6	0	-6.155237	1.642085	-0.864036
48	1	0	-7.670397	-0.020104	-1.034593
49	1	0	-4.133069	2.405206	-0.333568
50	1	0	-6.684352	2.513920	-1.219726
51	7	0	-4.550627	-2.611049	0.271732
52	6	0	-3.389197	-1.862285	0.534647
53	6	0	-4.269242	-3.932030	0.496477
54	6	0	-2.371063	-2.767576	0.938229
55	6	0	-2.925862	-4.065802	0.906289
56	1	0	-5.021763	-4.696619	0.367403
57	1	0	-1.359185	-2.522871	1.231724
58	1	0	-2.428448	-4.991995	1.153927
59	6	0	-4.554423	0.234647	-0.038142
60	6	0	-1.888992	1.521812	1.042834
61	8	0	-2.765913	2.269305	1.544580
62	7	0	-2.159287	0.186276	0.608762
63	7	0	-0.569374	1.840927	0.881837
64	6	0	2.708325	0.841849	-0.820637
65	8	0	1.483514	0.635117	-0.611059
66	7	0	3.692740	-0.162248	-0.663966
67	7	0	3.233475	2.055256	-1.176407
68	1	0	4.231833	2.134567	-1.343903
69	1	0	4.642517	0.168739	-0.523995
70	1	0	0.062480	1.225305	0.354152
71	1	0	-1.350564	-0.428390	0.602174

Standard orientation of 3-Ca

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.330127	-2.856120	-1.846163
2	6	0	3.369931	-3.597432	-1.066698
3	6	0	2.238459	-2.730893	-0.832092
4	6	0	2.506628	-1.448258	-1.433171
5	6	0	3.800401	-1.534017	-2.068699
6	1	0	5.284196	-3.228862	-2.190165
7	1	0	3.460335	-4.624437	-0.741329
8	1	0	1.843007	-0.599046	-1.435733
9	1	0	4.284169	-0.737094	-2.615133
10	6	0	5.257670	-0.366581	0.826303
11	6	0	4.002866	-0.411526	1.539196
12	6	0	5.882135	-1.658990	0.980375
13	1	0	5.644297	0.480594	0.285044
14	6	0	3.840854	-1.727933	2.110012
15	6	0	5.013086	-2.495041	1.770246
16	1	0	6.836005	-1.947601	0.562148
17	1	0	3.004668	-2.062305	2.708506
18	1	0	5.199973	-3.519495	2.058488
19	6	0	-2.438636	-2.827403	0.618512

20	5	0	-4.877834	-1.380078	-0.018959
21	9	0	-4.202174	-0.129579	-0.533053
22	9	0	-6.275567	-1.177625	-0.115981
23	7	0	-4.357126	-2.527391	-0.872347
24	6	0	-4.801710	-3.015294	-2.066155
25	6	0	-2.776456	-3.980718	-1.677790
26	6	0	-3.850139	-3.931074	-2.586423
27	1	0	-5.745545	-2.702159	-2.489461
28	1	0	-1.889708	-4.595031	-1.745284
29	1	0	-3.953456	-4.487679	-3.506055
30	7	0	-4.387963	-1.592582	1.411931
31	6	0	-3.115842	-2.158530	1.664002
32	6	0	-4.829842	-1.014315	2.566824
33	6	0	-2.786707	-1.906886	3.027088
34	6	0	-3.872546	-1.211906	3.594274
35	1	0	-5.767641	-0.478578	2.606609
36	1	0	-1.883749	-2.219044	3.532949
37	1	0	-3.970914	-0.878032	4.616556
38	26	0	4.017087	-1.885663	0.003648
39	6	0	-3.100016	-3.106168	-0.600464
40	6	0	1.042007	3.329308	0.610556
41	5	0	-1.304575	4.219460	-0.962152
42	9	0	-2.067844	5.246626	-1.583055
43	9	0	-2.034256	2.927811	-1.272274
44	7	0	0.099546	4.095072	-1.516342
45	6	0	0.488957	4.299643	-2.809893
46	6	0	2.290097	3.467134	-1.705743
47	6	0	1.841835	3.931222	-2.958909
48	1	0	-0.199987	4.687823	-3.546535
49	1	0	3.282772	3.139564	-1.447978
50	1	0	2.422183	4.009020	-3.866463
51	7	0	-1.211691	4.356534	0.539169
52	6	0	-0.129694	3.842732	1.274356
53	6	0	-2.165923	4.796052	1.420626
54	6	0	-0.437825	3.979621	2.651141
55	6	0	-1.712832	4.587978	2.738008
56	1	0	-3.097519	5.219561	1.074310
57	1	0	0.192198	3.719194	3.491525
58	1	0	-2.242919	4.856275	3.639908
59	6	0	1.200255	3.564415	-0.792624
60	6	0	3.047737	1.822445	1.061981
61	8	0	3.945002	2.216176	0.281878
62	7	0	1.895919	2.607549	1.412075
63	7	0	3.035634	0.610078	1.696378
64	6	0	-0.142218	-2.546622	-0.125589
65	8	0	-0.442950	-1.498939	-0.782844
66	7	0	-1.077019	-3.169719	0.731318
67	7	0	1.071320	-3.163204	-0.154296
68	1	0	1.144764	-4.062063	0.313461
69	1	0	-0.744330	-3.617918	1.580309
70	1	0	2.210320	0.352283	2.228779
71	1	0	1.586576	2.495912	2.373924
72	20	0	-1.833303	0.550151	-1.258220

Standard orientation of 4-Ca

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-6.369727	1.065626	1.480112

2	6	0	-4.992347	0.877279	1.831953
3	6	0	-4.184225	1.609145	0.869832
4	6	0	-5.084899	2.224944	-0.086590
5	6	0	-6.428087	1.892773	0.296574
6	1	0	-7.218194	0.641740	1.997881
7	1	0	-4.608535	0.316218	2.670814
8	1	0	-4.799915	2.835604	-0.932081
9	1	0	-7.325294	2.195215	-0.223763
10	6	0	-4.503224	-0.783540	-1.854795
11	6	0	-4.255232	-1.626138	-0.697542
12	6	0	-5.924467	-0.659343	-2.010831
13	1	0	-3.753687	-0.345388	-2.499283
14	6	0	-5.541184	-1.991759	-0.133421
15	6	0	-6.564165	-1.402814	-0.950041
16	1	0	-6.427321	-0.090659	-2.779843
17	1	0	-5.684574	-2.616543	0.735398
18	1	0	-7.629230	-1.487439	-0.788355
19	6	0	1.026328	2.714506	0.157781
20	5	0	3.868074	3.384304	-0.544865
21	9	0	4.774581	2.195599	-0.726016
22	9	0	4.709319	4.516102	-0.787145
23	7	0	2.727250	3.272994	-1.536702
24	6	0	2.820906	3.360358	-2.898385
25	6	0	0.701218	2.698103	-2.430375
26	6	0	1.580834	3.016428	-3.482408
27	1	0	3.744674	3.644024	-3.382391
28	1	0	-0.325296	2.380765	-2.532607
29	1	0	1.364780	3.001221	-4.540334
30	7	0	3.304389	3.362144	0.860075
31	6	0	1.971325	3.017526	1.179642
32	6	0	3.957745	3.678041	2.019878
33	6	0	1.825759	3.152587	2.593417
34	6	0	3.070310	3.555319	3.113251
35	1	0	4.994043	3.985038	2.017352
36	1	0	0.911146	3.017687	3.150495
37	1	0	3.311909	3.759089	4.145816
38	26	0	-5.327148	0.117670	-0.118704
39	6	0	1.411195	2.870201	-1.204185
40	6	0	0.890429	-2.879634	0.231129
41	5	0	3.868382	-3.337270	0.326582
42	9	0	4.705914	-4.484392	0.532273
43	9	0	4.834788	-2.204755	0.131832
44	7	0	2.997854	-3.467302	-0.908853
45	6	0	3.399782	-3.873843	-2.151939
46	6	0	1.159639	-3.532199	-2.271851
47	6	0	2.286453	-3.918591	-3.021514
48	1	0	4.431508	-4.121484	-2.357894
49	1	0	0.140128	-3.487948	-2.623923
50	1	0	2.310352	-4.212226	-4.060416
51	7	0	2.988228	-3.032015	1.523514
52	6	0	1.601410	-2.759668	1.456325
53	6	0	3.399586	-2.841419	2.814211
54	6	0	1.180776	-2.367705	2.763136
55	6	0	2.303213	-2.433664	3.608902
56	1	0	4.430786	-2.985033	3.104504
57	1	0	0.184692	-2.057136	3.040488
58	1	0	2.340763	-2.206303	4.663830
59	6	0	1.600996	-3.240326	-0.946550
60	6	0	-0.299722	2.253393	0.543268
61	6	0	-2.741088	1.697504	0.896847

62	16	0	-1.834413	2.754251	-0.288633
63	7	0	-1.946871	1.080215	1.766245
64	6	0	-0.611965	1.382302	1.580547
65	6	0	-2.977842	-2.076280	-0.186586
66	6	0	-1.479776	-3.117909	1.146945
67	6	0	-0.552506	-2.665382	0.218357
68	16	0	-1.418938	-1.737614	-1.081275
69	1	0	-1.232746	-3.738863	1.997729
70	7	0	-2.805031	-2.802392	0.912824
71	1	0	0.125498	0.901201	2.208817
72	20	0	5.422243	-0.068148	-0.722239