

SUPPORTING INFORMATION

Luminescence, Singlet Oxygen Production and Optical Power Limiting of Some Diacetylide Platinum (II) Diphosphine Complexes

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1)

REPRESENTATIVE PLOT OF INPUT VS. OUTPUT ENERGY FROM OPL MEASUREMENTS

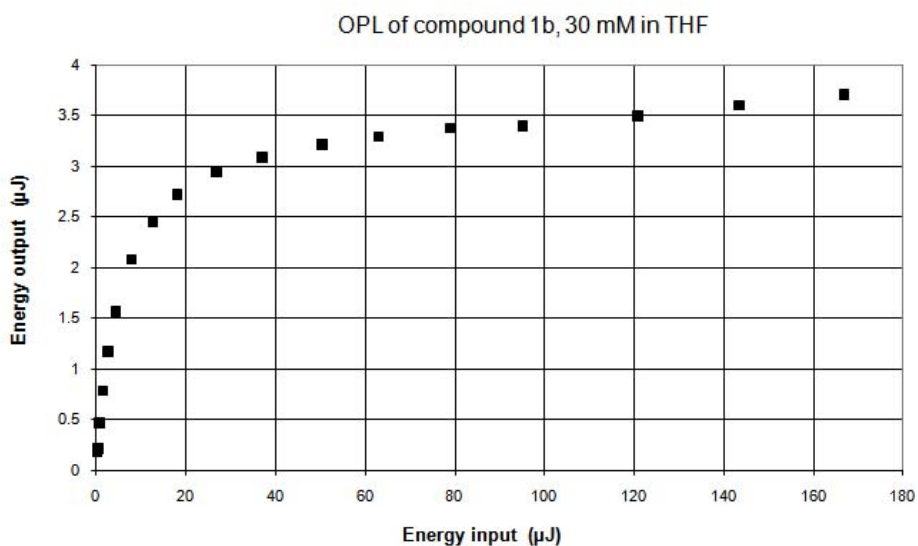
2)

DATA FOR GEOMETRY OPTIMIZATIONS AT THE RHF MPW1PW91/SDD LEVEL, USING GAUSSIAN 03 SOFTWARE.

1)

REPRESENTATIVE PLOT OF INPUT VS. OUTPUT ENERGY FROM OPL MEASUREMENTS

Compound 1b in tetrahydrofuran solution. 532 nm 5 ns laser pulses.



2)

DATA FOR GEOMETRY OPTIMIZATIONS AT THE RHF MPW1PW91/SDD LEVEL, USING GAUSSIAN 03 SOFTWARE.

The sections below show the abbreviation for each compound and conformation, and the energy and Cartesian coordinates.

1a' pl-pl-trans
HF=-3526.8483124 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	78	0	-0.000008	0.000113	0.000187
2	15	0	0.714816	2.236968	0.203778
3	15	0	-0.714831	-2.236742	-0.203405
4	6	0	1.872463	-0.685527	0.064849
5	6	0	-1.872481	0.685749	-0.064472
6	6	0	-0.001556	3.078318	1.700895
7	6	0	0.170988	3.297783	-1.225190
8	6	0	2.543035	2.546510	0.332011
9	6	0	0.001608	-3.078122	-1.700473
10	6	0	-0.171073	-3.297534	1.225607
11	6	0	-2.543045	-2.546282	-0.331718
12	6	0	3.032582	-1.125236	0.098737
13	6	0	-3.032605	1.125444	-0.098351
14	6	0	4.364307	-1.569787	0.132313
15	6	0	-4.364340	1.569964	-0.131951
16	16	0	5.721932	-0.380261	0.051969
17	6	0	4.869227	-2.859373	0.221919
18	16	0	-5.721933	0.380366	-0.052134
19	6	0	-4.869294	2.859554	-0.221305
20	6	0	6.930305	-1.714309	0.144846
21	6	0	6.288594	-2.939679	0.229088
22	6	0	-6.930342	1.714407	-0.144661
23	6	0	-6.288663	2.939816	-0.228576
24	6	0	8.305531	-1.439092	0.124188
25	6	0	-8.305561	1.439140	-0.124144
26	6	0	9.505429	-1.181526	0.103021
27	6	0	-9.505450	1.181522	-0.103141
28	6	0	10.896907	-0.882524	0.076635
29	6	0	-10.896916	0.882460	-0.076851
30	6	0	11.863556	-1.915222	0.121153
31	6	0	11.345291	0.457941	0.004254
32	6	0	-11.863609	1.915119	-0.121324
33	6	0	-11.345245	-0.458032	-0.004603
34	6	0	13.224543	-1.618479	0.093696
35	6	0	12.706423	0.753182	-0.023013
36	6	0	-13.224584	1.618314	-0.093946
37	6	0	-12.706365	-0.753334	0.022587
38	6	0	13.672734	-0.278930	0.020802
39	6	0	-13.672719	0.278739	-0.021180
40	6	0	15.066077	0.024684	-0.008529
41	6	0	16.262321	0.287082	-0.034380
42	6	0	17.656548	0.598082	-0.064549
43	6	0	18.090178	1.942133	-0.125164
44	6	0	19.455282	2.245103	-0.154015

45	6	0	20.410071	1.216343	-0.123151
46	6	0	19.988576	-0.121414	-0.063164
47	6	0	18.624893	-0.431211	-0.034014
48	6	0	-15.066050	-0.024939	0.008079
49	6	0	-16.262283	-0.287392	0.033878
50	6	0	-17.656497	-0.598458	0.063980
51	6	0	-18.090065	-1.942531	0.124542
52	6	0	-19.455156	-2.245566	0.153334
53	6	0	-20.409992	-1.216850	0.122464
54	6	0	-19.988558	0.120929	0.062530
55	6	0	-18.624889	0.430790	0.033440
56	1	0	0.358341	2.576210	2.600841
57	1	0	-1.088278	2.989844	1.662160
58	1	0	0.289412	4.132290	1.728542
59	1	0	0.630385	2.927067	-2.143357
60	1	0	0.463010	4.339623	-1.064729
61	1	0	-0.913034	3.221628	-1.321002
62	1	0	2.738475	3.619219	0.417482
63	1	0	3.040535	2.148332	-0.553331
64	1	0	2.938992	2.026100	1.205088
65	1	0	-0.358244	-2.576026	-2.600445
66	1	0	-0.289367	-4.132092	-1.728117
67	1	0	1.088328	-2.989655	-1.661688
68	1	0	-0.630506	-2.926796	2.143747
69	1	0	0.912947	-3.221386	1.321463
70	1	0	-0.463095	-4.339375	1.065154
71	1	0	-2.738482	-3.618991	-0.417198
72	1	0	-2.938962	-2.025872	-1.204813
73	1	0	-3.040583	-2.148103	0.553602
74	1	0	4.219881	-3.722365	0.281653
75	1	0	-4.219971	3.722583	-0.280745
76	1	0	6.839188	-3.868828	0.293936
77	1	0	-6.839282	3.868965	-0.293214
78	1	0	11.532508	-2.946115	0.176838
79	1	0	10.614261	1.257819	-0.030109
80	1	0	-11.532604	2.946030	-0.176908
81	1	0	-10.614181	-1.257881	0.029726
82	1	0	13.955688	-2.418336	0.127911
83	1	0	13.037605	1.784072	-0.078861
84	1	0	-13.955763	2.418142	-0.128122
85	1	0	-13.037504	-1.784243	0.078337
86	1	0	17.351354	2.735507	-0.148803
87	1	0	19.775664	3.280547	-0.200554
88	1	0	21.468285	1.453861	-0.145696
89	1	0	20.722259	-0.920205	-0.039241
90	1	0	18.297558	-1.463987	0.012407
91	1	0	-17.351205	-2.735871	0.148187
92	1	0	-19.775492	-3.281026	0.199831
93	1	0	-21.468196	-1.454418	0.144962
94	1	0	-20.722278	0.919686	0.038602
95	1	0	-18.297600	1.463583	-0.012939

la' pl-pl-cis
HF=-3526.8482832

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	78	0	0.004892	-2.466582	0.100067
2	15	0	-0.127157	-0.207904	0.768225
3	15	0	0.139241	-4.721000	-0.570914
4	6	0	1.998658	-2.451088	0.181627
5	6	0	-1.988309	-2.468357	0.011304
6	6	0	-1.136680	0.023873	2.313892
7	6	0	-0.963390	0.868592	-0.498284
8	6	0	1.472847	0.667338	1.127993
9	6	0	1.134953	-4.945995	-2.126531
10	6	0	0.995007	-5.794828	0.684932
11	6	0	-1.460316	-5.603999	-0.914625
12	6	0	3.239171	-2.447924	0.218381
13	6	0	-3.227980	-2.441798	-0.039671
14	6	0	4.641417	-2.376660	0.255110
15	6	0	-4.629624	-2.377016	-0.096908
16	16	0	5.471305	-0.779258	0.099558
17	6	0	5.581554	-3.386912	0.400158
18	16	0	-5.467420	-0.779031	0.002750
19	6	0	-5.564137	-3.394476	-0.225861
20	6	0	7.082877	-1.573897	0.241138
21	6	0	6.932400	-2.943068	0.393011
22	6	0	-7.074404	-1.583462	-0.138250
23	6	0	-6.916436	-2.955841	-0.248442
24	6	0	8.261588	-0.815352	0.187929
25	6	0	-8.256276	-0.828185	-0.129907
26	6	0	9.281011	-0.133692	0.136560
27	6	0	-9.279201	-0.149848	-0.122554
28	6	0	10.461993	0.658586	0.073407
29	6	0	-10.464416	0.638568	-0.115892
30	6	0	11.742492	0.066002	0.182386
31	6	0	10.380842	2.060680	-0.102201
32	6	0	-11.739792	0.035738	-0.228732
33	6	0	-10.392806	2.047097	0.003282
34	6	0	12.895695	0.845123	0.117329
35	6	0	11.534718	2.838444	-0.167106
36	6	0	-12.897156	0.811357	-0.223179
37	6	0	-11.550841	2.821353	0.008691
38	6	0	12.814730	2.246191	-0.059125
39	6	0	-12.825682	2.219002	-0.104549
40	6	0	13.995341	3.043699	-0.127484
41	6	0	15.007285	3.731419	-0.186562
42	6	0	16.187796	4.533370	-0.255940
43	6	0	16.095659	5.932861	-0.432440
44	6	0	17.252660	6.715712	-0.500940
45	6	0	18.519026	6.119060	-0.395089
46	6	0	18.620102	4.729860	-0.219485
47	6	0	17.466978	3.941275	-0.150164
48	6	0	-14.010521	3.013125	-0.099869
49	6	0	-15.026887	3.696826	-0.096229
50	6	0	-16.210698	4.496902	-0.091685
51	6	0	-16.126366	5.902789	0.029091
52	6	0	-17.286442	6.684056	0.033493
53	6	0	-18.548177	6.079437	-0.082017
54	6	0	-18.641491	4.683850	-0.202493
55	6	0	-17.485250	3.896796	-0.207558

56	1	0	-0.645335	-0.487208	3.143969
57	1	0	-2.119586	-0.423235	2.158721
58	1	0	-1.242053	1.086660	2.549308
59	1	0	-0.370756	0.870623	-1.414996
60	1	0	-1.065593	1.891888	-0.125993
61	1	0	-1.947470	0.452331	-0.717732
62	1	0	1.277270	1.695964	1.443974
63	1	0	2.094896	0.667354	0.231985
64	1	0	2.010307	0.132654	1.912269
65	1	0	0.631353	-4.439110	-2.951831
66	1	0	1.248491	-6.007649	-2.363609
67	1	0	2.113976	-4.487319	-1.979637
68	1	0	0.409216	-5.806774	1.605980
69	1	0	1.973826	-5.363149	0.898667
70	1	0	1.107880	-6.815638	0.308687
71	1	0	-1.265793	-6.634111	-1.226410
72	1	0	-2.002987	-5.072244	-1.697462
73	1	0	-2.073886	-5.596713	-0.012650
74	1	0	5.291505	-4.422914	0.511981
75	1	0	-5.268595	-4.432183	-0.300485
76	1	0	7.783775	-3.602852	0.495588
77	1	0	-7.764078	-3.621563	-0.343390
78	1	0	11.817928	-1.007072	0.317384
79	1	0	9.405497	2.526392	-0.187220
80	1	0	-11.807957	-1.042384	-0.320423
81	1	0	-9.421465	2.520684	0.090597
82	1	0	13.871171	0.379449	0.201869
83	1	0	11.459375	3.911536	-0.302427
84	1	0	-13.868590	0.337894	-0.310853
85	1	0	-11.482804	3.899562	0.100086
86	1	0	15.116796	6.392221	-0.514423
87	1	0	17.168729	7.788787	-0.636640
88	1	0	19.414937	6.728326	-0.448650
89	1	0	19.596214	4.263647	-0.136936
90	1	0	17.543440	2.868087	-0.014809
91	1	0	-15.151071	6.368304	0.118486
92	1	0	-17.208521	7.762106	0.126666
93	1	0	-19.446483	6.687525	-0.078374
94	1	0	-19.613994	4.211488	-0.292329
95	1	0	-17.555716	2.818688	-0.300395

la' pl-perp
HF=-3526.8481531

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	78	0	0.005621	1.466259	0.271437
2	15	0	0.290227	-0.669386	1.230623
3	15	0	-0.287046	3.594949	-0.697672
4	6	0	1.931827	1.581523	-0.237714
5	6	0	-1.921978	1.351111	0.782825
6	6	0	-0.773328	-1.961062	0.416452
7	6	0	-0.209811	-0.727803	3.021844
8	6	0	2.000784	-1.395986	1.204400

9	6	0	0.794469	4.893969	0.080599
10	6	0	0.175319	3.629870	-2.499819
11	6	0	-1.995924	4.324211	-0.645553
12	6	0	3.128453	1.668418	-0.554733
13	6	0	-3.117883	1.272142	1.102374
14	6	0	4.493901	1.719083	-0.880209
15	6	0	-4.481946	1.186001	1.431358
16	16	0	5.640371	0.511599	-0.178643
17	6	0	5.178555	2.596645	-1.708769
18	16	0	-5.629952	0.322785	0.336001
19	6	0	-5.159893	1.687346	2.532765
20	6	0	7.017734	1.269160	-1.060247
21	6	0	6.574887	2.347955	-1.808832
22	6	0	-7.002114	0.691592	1.445839
23	6	0	-6.555837	1.413840	2.540672
24	6	0	8.318091	0.758430	-0.934268
25	6	0	-8.303522	0.262845	1.144471
26	6	0	9.450266	0.300068	-0.813600
27	6	0	-9.437286	-0.115897	0.866004
28	6	0	10.764735	-0.228774	-0.676078
29	6	0	-10.755822	-0.547813	0.547354
30	6	0	11.863251	0.377974	-1.330309
31	6	0	11.002962	-1.375066	0.119108
32	6	0	-11.847676	-0.221478	1.386656
33	6	0	-11.005911	-1.311465	-0.617620
34	6	0	13.148675	-0.141662	-1.194386
35	6	0	12.288854	-1.893717	0.253995
36	6	0	-13.138336	-0.640769	1.071836
37	6	0	-12.297139	-1.730348	-0.931082
38	6	0	13.386875	-1.287429	-0.399913
39	6	0	-13.388697	-1.402733	-0.093230
40	6	0	14.703265	-1.818927	-0.261679
41	6	0	15.833945	-2.275065	-0.143301
42	6	0	17.152586	-2.807645	-0.005242
43	6	0	17.382018	-3.965829	0.772013
44	6	0	18.673899	-4.485036	0.904833
45	6	0	19.757445	-3.860483	0.267038
46	6	0	19.538962	-2.709661	-0.506768
47	6	0	18.249538	-2.185420	-0.643751
48	6	0	-14.711122	-1.829104	-0.415696
49	6	0	-15.847722	-2.192842	-0.691995
50	6	0	-17.174810	-2.614225	-1.012621
51	6	0	-17.424683	-3.387934	-2.168884
52	6	0	-18.725628	-3.796984	-2.479599
53	6	0	-19.798001	-3.443113	-1.645455
54	6	0	-19.559118	-2.675069	-0.494859
55	6	0	-18.260609	-2.262945	-0.178383
56	1	0	-0.479655	-2.062198	-0.630001
57	1	0	-1.812975	-1.633260	0.459753
58	1	0	-0.663580	-2.924460	0.922454
59	1	0	0.432758	-0.058938	3.597398
60	1	0	-0.122980	-1.745663	3.412400
61	1	0	-1.241248	-0.382301	3.104112
62	1	0	1.996624	-2.390632	1.659232
63	1	0	2.680679	-0.741439	1.751539
64	1	0	2.350862	-1.460792	0.173355
65	1	0	0.510699	5.017513	1.127445
66	1	0	0.688390	5.848666	-0.442509

67	1	0	1.830464	4.554701	0.037110
68	1	0	-0.494933	2.971404	-3.055441
69	1	0	1.195572	3.257571	-2.602178
70	1	0	0.103024	4.646224	-2.897408
71	1	0	-2.002785	5.310934	-1.117410
72	1	0	-2.321888	4.405193	0.392253
73	1	0	-2.688434	3.658975	-1.163091
74	1	0	4.673577	3.398361	-2.230537
75	1	0	-4.649960	2.238633	3.311176
76	1	0	7.250309	2.939075	-2.413027
77	1	0	-7.227985	1.734532	3.325607
78	1	0	11.693608	1.256773	-1.942128
79	1	0	10.169360	-1.848785	0.625199
80	1	0	-11.668807	0.362769	2.282247
81	1	0	-10.177628	-1.568306	-1.268304
82	1	0	13.982416	0.331990	-1.700436
83	1	0	12.458561	-2.772542	0.865850
84	1	0	-13.966853	-0.383735	1.722257
85	1	0	-12.475983	-2.314342	-1.826902
86	1	0	16.543922	-4.447073	1.263863
87	1	0	18.837093	-5.374610	1.503962
88	1	0	20.758481	-4.265116	0.371569
89	1	0	20.372818	-2.223069	-1.001625
90	1	0	18.079130	-1.296595	-1.241106
91	1	0	-16.595401	-3.660347	-2.812305
92	1	0	-18.904553	-4.390361	-3.370018
93	1	0	-20.806014	-3.761618	-1.888743
94	1	0	-20.384080	-2.398775	0.153264
95	1	0	-18.074483	-1.669587	0.709981

la' perp-perp-trans
HF=-3526.8480878

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	78	0	0.008356	0.177014	0.069643
2	15	0	0.327295	-1.537901	-1.517652
3	15	0	-0.312507	1.892752	1.655333
4	6	0	-1.864851	-0.407068	0.441491
5	6	0	1.884466	0.755153	-0.295855
6	6	0	1.740329	-2.670142	-1.087787
7	6	0	0.766528	-0.879463	-3.201620
8	6	0	-1.104362	-2.683059	-1.825113
9	6	0	-1.730700	3.018708	1.226018
10	6	0	-0.746620	1.235502	3.341105
11	6	0	1.115527	3.043449	1.958992
12	6	0	-3.029772	-0.758185	0.682657
13	6	0	3.056071	1.093252	-0.523139
14	6	0	-4.358402	-1.145445	0.928843
15	6	0	4.395742	1.453414	-0.749159
16	16	0	-5.726924	-0.210437	0.210866
17	6	0	-4.847057	-2.200533	1.685241
18	16	0	5.730481	0.362526	-0.209144
19	6	0	4.921272	2.582798	-1.359285

20	6	0	-6.920335	-1.317273	0.986500
21	6	0	-6.265922	-2.295627	1.717341
22	6	0	6.961947	1.513473	-0.849288
23	6	0	6.342371	2.616129	-1.414739
24	6	0	-8.298419	-1.126226	0.806097
25	6	0	8.331482	1.232816	-0.732044
26	6	0	-9.500975	-0.948010	0.637132
27	6	0	9.524636	0.969282	-0.616314
28	6	0	-10.896748	-0.747641	0.441633
29	6	0	10.907888	0.662986	-0.477068
30	6	0	-11.844951	-1.596496	1.060792
31	6	0	-11.368417	0.304934	-0.378501
32	6	0	11.901798	1.570339	-0.914681
33	6	0	11.320218	-0.559030	0.106013
34	6	0	-13.210462	-1.400535	0.866362
35	6	0	-12.734248	0.499683	-0.572096
36	6	0	13.254382	1.267624	-0.773197
37	6	0	12.672952	-0.860505	0.246595
38	6	0	-13.681993	-0.349241	0.045922
39	6	0	13.666537	0.046866	-0.189634
40	6	0	-15.080294	-0.150775	-0.153914
41	6	0	-16.281365	0.017832	-0.325781
42	6	0	-17.682459	0.213054	-0.526664
43	6	0	-18.151214	1.256166	-1.357500
44	6	0	-19.523481	1.443821	-1.552290
45	6	0	-20.450605	0.597279	-0.923977
46	6	0	-19.994093	-0.441267	-0.096995
47	6	0	-18.623198	-0.634385	0.101908
48	6	0	15.051292	-0.262265	-0.043104
49	6	0	16.239947	-0.529134	0.084926
50	6	0	17.625853	-0.841855	0.236616
51	6	0	18.026031	-2.077301	0.795003
52	6	0	19.383227	-2.380899	0.943292
53	6	0	20.363270	-1.460771	0.538631
54	6	0	19.975047	-0.231343	-0.017034
55	6	0	18.619499	0.078383	-0.168204
56	1	0	1.524655	-3.174688	-0.144166
57	1	0	2.643550	-2.070392	-0.967028
58	1	0	1.889024	-3.414278	-1.875425
59	1	0	-0.061450	-0.277285	-3.580324
60	1	0	0.969741	-1.700256	-3.895289
61	1	0	1.648430	-0.244303	-3.105482
62	1	0	-0.835495	-3.433217	-2.574273
63	1	0	-1.963184	-2.104488	-2.168063
64	1	0	-1.381748	-3.171818	-0.890160
65	1	0	-1.518381	3.523104	0.281549
66	1	0	-1.881985	3.763085	2.012946
67	1	0	-2.631142	2.414427	1.106792
68	1	0	0.083743	0.636171	3.719100
69	1	0	-1.627008	0.597903	3.247285
70	1	0	-0.950877	2.056707	4.033979
71	1	0	0.846082	3.792357	2.709193
72	1	0	1.387702	3.533686	1.023276
73	1	0	1.977690	2.468022	2.298824
74	1	0	-4.186100	-2.882871	2.202359
75	1	0	4.285183	3.362210	-1.756445
76	1	0	-6.806172	-3.060176	2.259897
77	1	0	6.908812	3.425279	-1.856533

78	1	0	-11.495983	-2.406280	1.691580
79	1	0	-10.651722	0.961893	-0.858254
80	1	0	11.598486	2.509688	-1.363040
81	1	0	10.567956	-1.262337	0.444934
82	1	0	-13.927307	-2.057714	1.345737
83	1	0	-13.083196	1.309347	-1.203134
84	1	0	14.006751	1.971176	-1.111589
85	1	0	12.976343	-1.799655	0.695435
86	1	0	-17.433770	1.909055	-1.842169
87	1	0	-19.870837	2.247913	-2.192396
88	1	0	-21.514372	0.744963	-1.076695
89	1	0	-20.706238	-1.098298	0.390975
90	1	0	-18.268927	-1.436233	0.740218
91	1	0	17.267733	-2.786866	1.107086
92	1	0	19.677764	-3.332348	1.373335
93	1	0	21.415287	-1.698509	0.654707
94	1	0	20.728339	0.483310	-0.331311
95	1	0	18.317888	1.027578	-0.597098

la' perp-perp-cis
HF=-3526.8480738

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	78	0	0.006808	-2.444646	0.024328
2	15	0	0.200868	-2.596065	-2.321362
3	15	0	-0.184414	-2.268700	2.368673
4	6	0	-1.988516	-2.419979	-0.062468
5	6	0	2.002470	-2.447100	0.110009
6	6	0	1.193083	-4.069104	-2.876562
7	6	0	1.097311	-1.139510	-3.054665
8	6	0	-1.376501	-2.708844	-3.298564
9	6	0	-1.042771	-0.705663	2.899585
10	6	0	-1.208101	-3.629285	3.118963
11	6	0	1.394776	-2.284384	3.349790
12	6	0	-3.228025	-2.395898	-0.100363
13	6	0	3.242204	-2.433200	0.145712
14	6	0	-4.631559	-2.336622	-0.152871
15	6	0	4.645888	-2.373507	0.195094
16	16	0	-5.478441	-0.745489	-0.037662
17	6	0	-5.557452	-3.360880	-0.285810
18	16	0	5.489684	-0.782249	0.059199
19	6	0	5.573826	-3.394271	0.339313
20	6	0	-7.080153	-1.561836	-0.176737
21	6	0	-6.913681	-2.931802	-0.298944
22	6	0	7.093106	-1.593815	0.206160
23	6	0	6.929385	-2.962446	0.345491
24	6	0	-8.267501	-0.814917	-0.154617
25	6	0	8.278204	-0.843727	0.171862
26	6	0	-9.294634	-0.143376	-0.133119
27	6	0	9.301485	-0.166800	0.138645
28	6	0	-10.484651	0.637523	-0.107868
29	6	0	10.485486	0.622614	0.098646
30	6	0	-11.757305	0.028040	-0.215323

31	6	0	-10.420513	2.045097	0.025926
32	6	0	11.763432	0.025069	0.209830
33	6	0	10.409355	2.027656	-0.054425
34	6	0	-12.919338	0.796287	-0.189862
35	6	0	-11.583217	2.811985	0.051247
36	6	0	12.919077	0.802323	0.169170
37	6	0	11.565622	2.803520	-0.094925
38	6	0	-12.855368	2.202917	-0.055955
39	6	0	12.843118	2.206353	0.015773
40	6	0	-14.045099	2.989317	-0.029707
41	6	0	-15.065754	3.666219	-0.006688
42	6	0	-16.254464	4.458521	0.020921
43	6	0	-16.177553	5.863390	0.157593
44	6	0	-17.342356	6.637127	0.184883
45	6	0	-18.601554	6.025892	0.076790
46	6	0	-18.687517	4.631265	-0.059400
47	6	0	-17.526514	3.851722	-0.087377
48	6	0	14.026061	3.002248	-0.026536
49	6	0	15.040375	3.687989	-0.063775
50	6	0	16.221708	4.490504	-0.108208
51	6	0	16.131492	5.892521	-0.264622
52	6	0	17.289155	6.676162	-0.308502
53	6	0	18.554304	6.077835	-0.197615
54	6	0	18.653467	4.686139	-0.041849
55	6	0	17.499666	3.896747	0.002784
56	1	0	0.688710	-4.983947	-2.559829
57	1	0	2.173797	-4.025516	-2.400900
58	1	0	1.303703	-4.069334	-3.964653
59	1	0	0.524965	-0.230195	-2.862317
60	1	0	1.226187	-1.269754	-4.132957
61	1	0	2.071292	-1.051141	-2.571108
62	1	0	-1.155731	-2.762339	-4.368482
63	1	0	-1.995690	-1.835798	-3.088425
64	1	0	-1.930606	-3.595648	-2.987812
65	1	0	-0.452697	0.155589	2.581043
66	1	0	-1.164191	-0.684513	3.986320
67	1	0	-2.019163	-0.661842	2.415033
68	1	0	-0.717455	-4.588615	2.943884
69	1	0	-2.183327	-3.638557	2.630119
70	1	0	-1.329292	-3.470641	4.194307
71	1	0	1.177934	-2.199259	4.418465
72	1	0	2.026957	-1.454932	3.030150
73	1	0	1.933377	-3.212088	3.151608
74	1	0	-5.252416	-4.395163	-0.369960
75	1	0	5.270966	-4.427945	0.437706
76	1	0	-7.756763	-3.603139	-0.395380
77	1	0	7.773797	-3.631036	0.449124
78	1	0	-11.819694	-1.049423	-0.318300
79	1	0	-9.451284	2.523727	0.109119
80	1	0	11.835048	-1.050305	0.327575
81	1	0	9.435945	2.497180	-0.140663
82	1	0	-13.888671	0.317749	-0.273283
83	1	0	-11.520850	3.889512	0.154042
84	1	0	13.892587	0.332864	0.255504
85	1	0	11.494055	3.878954	-0.212583
86	1	0	-15.204206	6.334020	0.241274
87	1	0	-17.270061	7.714460	0.290150
88	1	0	-19.503563	6.628109	0.098242

89	1	0	-19.658035	4.153787	-0.143579
90	1	0	-17.591305	2.774365	-0.192339
91	1	0	15.153576	6.353192	-0.350454
92	1	0	17.206669	7.751180	-0.428882
93	1	0	19.450723	6.687748	-0.231986
94	1	0	19.628621	4.218611	0.044555
95	1	0	17.574656	2.821634	0.122856

lb' perp-perp-trans
HF=-3526.843524

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-0.106589	-0.224731	-2.337721
2	6	0	1.494347	-0.125624	-3.277470
3	78	0	-0.000160	-0.002475	0.004932
4	15	0	0.106308	0.219447	2.347593
5	6	0	-0.858448	-1.840101	-2.874994
6	6	0	1.987363	0.231552	-0.025834
7	6	0	-1.188376	1.063141	-3.134251
8	6	0	7.464484	0.894536	-0.084372
9	6	0	6.891987	-0.394317	0.029599
10	6	0	5.508553	-0.560311	0.047318
11	6	0	4.635530	0.551454	-0.047698
12	6	0	5.215030	1.839243	-0.162761
13	6	0	3.217662	0.380093	-0.027521
14	6	0	6.598019	2.008794	-0.180714
15	6	0	8.878210	1.064614	-0.100656
16	6	0	10.095995	1.215358	-0.115682
17	6	0	11.490594	1.367472	-0.131937
18	6	0	12.239457	2.529864	-0.233427
19	6	0	13.645086	2.319782	-0.217506
20	6	0	14.019221	0.990456	-0.102893
21	16	0	12.567438	-0.070125	-0.007080
22	6	0	-1.987698	-0.236386	0.035516
23	6	0	-3.218051	-0.384479	0.036683
24	6	0	-7.465306	-0.895715	0.090207
25	6	0	-6.891664	0.393309	-0.015590
26	6	0	-5.508099	0.558205	-0.032337
27	6	0	-4.636052	-0.554896	0.055552
28	6	0	-5.216677	-1.842876	0.162672
29	6	0	-6.599827	-2.011338	0.179563
30	6	0	-8.879187	-1.064594	0.105644
31	6	0	-10.097002	-1.215186	0.119834
32	6	0	0.858271	1.834625	2.885286
33	6	0	-1.494601	0.120120	3.287360
34	6	0	-11.491782	-1.365869	0.134306
35	6	0	-12.242051	-2.526434	0.245884
36	6	0	-13.647428	-2.315158	0.224301
37	6	0	-14.019914	-0.986653	0.095453
38	16	0	-12.566853	0.071667	-0.005271
39	6	0	1.188077	-1.068680	3.143743
40	6	0	15.309179	0.438649	-0.056679
41	6	0	-15.309175	-0.434029	0.040478

42	6	0	16.427618	-0.062252	-0.010252
43	6	0	17.730355	-0.641779	0.039802
44	6	0	18.883998	0.170664	-0.049421
45	6	0	20.158156	-0.403689	0.000789
46	6	0	20.304703	-1.792963	0.140317
47	6	0	19.163991	-2.606689	0.229507
48	6	0	17.886552	-2.039899	0.180168
49	6	0	-16.427533	0.066989	-0.006477
50	6	0	-17.729109	0.648816	-0.060187
51	6	0	-17.882246	2.047780	-0.195565
52	6	0	-19.158446	2.617054	-0.248089
53	6	0	-20.300969	1.805048	-0.166930
54	6	0	-20.157474	0.414963	-0.032378
55	6	0	-18.884562	-0.161893	0.020857
56	1	0	1.967752	0.837213	-3.081075
57	1	0	1.312931	-0.242453	-4.349722
58	1	0	2.168177	-0.907743	-2.925060
59	1	0	-0.227278	-2.662600	-2.533269
60	1	0	-1.840957	-1.932857	-2.409771
61	1	0	-0.953561	-1.878681	-3.963975
62	1	0	-1.263077	0.891494	-4.211921
63	1	0	-0.766110	2.052728	-2.949524
64	1	0	-2.177700	1.011507	-2.677451
65	1	0	7.544527	-1.257483	0.103863
66	1	0	5.082295	-1.553689	0.134956
67	1	0	4.561231	2.701341	-0.237604
68	1	0	7.023153	3.002687	-0.269083
69	1	0	11.776635	3.503728	-0.316943
70	1	0	14.373645	3.116098	-0.287701
71	1	0	-7.543439	1.257517	-0.084273
72	1	0	-5.080976	1.551746	-0.113663
73	1	0	-4.563637	-2.705995	0.232228
74	1	0	-7.025840	-3.005394	0.261629
75	1	0	1.840921	1.927285	2.420337
76	1	0	0.953094	1.873043	3.974300
77	1	0	0.227333	2.657274	2.543499
78	1	0	-2.168482	0.902251	2.935072
79	1	0	-1.967953	-0.842716	3.090831
80	1	0	-1.313175	0.236822	4.359625
81	1	0	-11.780397	-3.499874	0.340149
82	1	0	-14.376987	-3.110033	0.300183
83	1	0	1.262724	-0.897395	4.221472
84	1	0	2.177422	-1.016876	2.687008
85	1	0	0.765832	-2.058209	2.958662
86	1	0	18.769467	1.243567	-0.157194
87	1	0	21.036159	0.229692	-0.068596
88	1	0	21.294292	-2.235470	0.179054
89	1	0	19.271283	-3.680779	0.337225
90	1	0	17.004708	-2.667153	0.249032
91	1	0	-16.999006	2.673718	-0.258159
92	1	0	-19.263372	3.691744	-0.352112
93	1	0	-21.289587	2.249507	-0.208050
94	1	0	-21.036890	-0.217096	0.030845
95	1	0	-18.772401	-1.235437	0.124689

lb' pl-perp
HF=-3526.842815

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-0.035226	2.661056	-0.078787
2	6	0	-1.695187	3.496659	-0.126058
3	78	0	-0.000024	0.315330	-0.273331
4	15	0	0.032873	-2.030736	-0.463296
5	6	0	0.736733	3.258977	1.505655
6	6	0	-1.994576	0.216430	-0.404931
7	6	0	0.943442	3.509218	-1.415378
8	6	0	-7.490530	-0.039910	-0.816206
9	6	0	-6.856382	-0.101681	0.447013
10	6	0	-5.467966	-0.042432	0.550812
11	6	0	-4.651459	0.080647	-0.600375
12	6	0	-5.292439	0.141347	-1.862444
13	6	0	-3.228486	0.143824	-0.493692
14	6	0	-6.680542	0.082607	-1.969720
15	6	0	-8.909433	-0.097599	-0.922295
16	6	0	-10.131880	-0.145003	-1.018705
17	6	0	-11.530942	-0.198818	-1.108769
18	6	0	-12.333891	-0.136398	-2.237301
19	6	0	-13.726488	-0.218258	-1.965692
20	6	0	-14.036272	-0.345888	-0.620947
21	16	0	-12.536457	-0.368295	0.374936
22	6	0	1.994318	0.420776	-0.145247
23	6	0	3.227809	0.511743	-0.063344
24	6	0	7.489708	0.788550	0.215141
25	6	0	6.859521	-0.449181	-0.054448
26	6	0	5.472031	-0.537357	-0.144662
27	6	0	4.649699	0.603339	0.029550
28	6	0	5.288499	1.839141	0.298609
29	6	0	6.675550	1.932263	0.389983
30	6	0	8.907531	0.879553	0.307954
31	6	0	10.129202	0.963667	0.388403
32	6	0	-0.756895	-2.637580	-2.035376
33	6	0	1.692463	-2.868078	-0.429499
34	6	0	11.527178	1.041057	0.476628
35	6	0	12.324129	2.149431	0.718944
36	6	0	13.717371	1.870315	0.741857
37	6	0	14.033701	0.539692	0.518101
38	16	0	12.539680	-0.432296	0.264104
39	6	0	-0.934627	-2.874376	0.884233
40	6	0	-15.298150	-0.449386	-0.014831
41	6	0	15.298116	-0.068417	0.474972
42	6	0	-16.394251	-0.539472	0.527766
43	6	0	-17.672825	-0.642379	1.152545
44	6	0	-18.855707	-0.601584	0.378950
45	6	0	-20.106942	-0.701892	0.995221
46	6	0	-20.201333	-0.844285	2.388760
47	6	0	-19.031571	-0.885660	3.164161
48	6	0	-17.776622	-0.785981	2.555343
49	6	0	16.396669	-0.612048	0.434770
50	6	0	17.678226	-1.237526	0.389615
51	6	0	17.792139	-2.622734	0.129837
52	6	0	19.050036	-3.232090	0.086448

53	6	0	20.212767	-2.474791	0.300488
54	6	0	20.108323	-1.098768	0.559025
55	6	0	18.854092	-0.482077	0.603983
56	1	0	-2.189741	3.260121	-1.069114
57	1	0	-1.578984	4.579579	-0.025544
58	1	0	-2.316461	3.110499	0.683152
59	1	0	0.137809	2.912136	2.349913
60	1	0	1.735933	2.828077	1.585578
61	1	0	0.793673	4.351211	1.521441
62	1	0	0.979925	4.588678	-1.242538
63	1	0	0.477794	3.309596	-2.382403
64	1	0	1.952267	3.093786	-1.421233
65	1	0	-7.465097	-0.195393	1.339770
66	1	0	-4.994334	-0.089546	1.525296
67	1	0	-4.682551	0.236569	-2.754183
68	1	0	-7.153333	0.131522	-2.944617
69	1	0	-11.918549	-0.033462	-3.230513
70	1	0	-14.491956	-0.184946	-2.729098
71	1	0	7.471191	-1.334281	-0.191399
72	1	0	5.004050	-1.493156	-0.352729
73	1	0	4.678278	2.725392	0.435556
74	1	0	7.144729	2.887954	0.596973
75	1	0	-1.766701	-2.228141	-2.091960
76	1	0	-0.793636	-3.730595	-2.053286
77	1	0	-0.181951	-2.276333	-2.890165
78	1	0	2.299988	-2.491056	-1.253494
79	1	0	2.197921	-2.622105	0.505396
80	1	0	1.572521	-3.951650	-0.517392
81	1	0	11.903964	3.133775	0.874185
82	1	0	14.478704	2.618396	0.916782
83	1	0	-0.957993	-3.956109	0.724048
84	1	0	-1.949319	-2.473328	0.881059
85	1	0	-0.473169	-2.656848	1.849346
86	1	0	-18.781157	-0.491554	-0.697232
87	1	0	-21.007638	-0.669260	0.391468
88	1	0	-21.173232	-0.921949	2.864156
89	1	0	-19.098862	-0.995434	4.241291
90	1	0	-16.872387	-0.817744	3.152956
91	1	0	16.893357	-3.206419	-0.035291
92	1	0	19.125076	-4.295608	-0.113764
93	1	0	21.186960	-2.950576	0.266184
94	1	0	21.003526	-0.509007	0.725165
95	1	0	18.771801	0.580569	0.803598

lb' pl-pl-trans
HF=-3526.8421706

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-0.166480	-2.331402	0.265358
2	6	0	-1.872184	-3.059809	0.396050
3	78	0	0.000086	0.001420	0.004770
4	15	0	0.166769	2.334265	-0.255331
5	6	0	0.619625	-3.268109	-1.137444

6	6	0	-1.987418	0.233204	0.033214
7	6	0	0.712675	-2.950938	1.784041
8	6	0	-7.464860	0.907501	0.102775
9	6	0	-6.890015	-0.379225	-0.022903
10	6	0	-5.506630	-0.542510	-0.040563
11	6	0	-4.633482	0.568442	0.065666
12	6	0	-5.216882	1.853638	0.190475
13	6	0	-3.216009	0.397585	0.047605
14	6	0	-6.599764	2.021846	0.209229
15	6	0	-8.878595	1.075137	0.121197
16	6	0	-10.096582	1.224379	0.137729
17	6	0	-11.491376	1.374082	0.154487
18	6	0	-12.241713	2.531751	0.292850
19	6	0	-13.646921	2.320889	0.266626
20	6	0	-14.019347	0.995568	0.107293
21	16	0	-12.566108	-0.059807	-0.018797
22	6	0	1.987573	-0.230445	-0.023322
23	6	0	3.216123	-0.395184	-0.037204
24	6	0	7.464572	-0.908702	-0.089851
25	6	0	6.890698	0.381213	0.003603
26	6	0	5.507453	0.545733	0.020377
27	6	0	4.633470	-0.567093	-0.054636
28	6	0	5.215904	-1.855444	-0.147474
29	6	0	6.598636	-2.024925	-0.165224
30	6	0	8.878174	-1.077568	-0.107079
31	6	0	10.096059	-1.227788	-0.122254
32	6	0	-0.613282	3.270008	1.151493
33	6	0	1.872345	3.061831	-0.392187
34	6	0	11.490769	-1.378411	-0.137666
35	6	0	12.240540	-2.539103	-0.251665
36	6	0	13.645859	-2.328239	-0.231736
37	6	0	14.018943	-0.999901	-0.101831
38	16	0	12.566232	0.058523	0.002977
39	6	0	-0.718166	2.955691	-1.769859
40	6	0	-15.308583	0.444323	0.041051
41	6	0	15.308436	-0.447816	-0.048879
42	6	0	-16.427292	-0.054583	-0.018394
43	6	0	-17.729293	-0.633981	-0.087307
44	6	0	-18.884156	0.173504	0.028294
45	6	0	-20.157481	-0.400645	-0.040158
46	6	0	-20.302099	-1.784919	-0.224494
47	6	0	-19.160339	-2.593786	-0.340183
48	6	0	-17.883682	-2.027237	-0.272719
49	6	0	16.427317	0.051953	-0.001070
50	6	0	17.729458	0.632445	0.054763
51	6	0	17.884126	2.029159	0.211665
52	6	0	19.160881	2.596832	0.266741
53	6	0	20.302480	1.785647	0.166772
54	6	0	20.157586	0.397944	0.010665
55	6	0	18.884157	-0.177352	-0.045236
56	1	0	-2.388878	-2.612628	1.246355
57	1	0	-1.813497	-4.144836	0.521157
58	1	0	-2.433202	-2.818239	-0.507823
59	1	0	0.080976	-3.048534	-2.061211
60	1	0	1.650226	-2.927337	-1.245238
61	1	0	0.595442	-4.344759	-0.945870
62	1	0	0.700358	-4.044031	1.820337
63	1	0	0.220222	-2.550516	2.672298

64	1	0	1.740843	-2.586787	1.760161
65	1	0	-7.541247	-1.242532	-0.105979
66	1	0	-5.081066	-1.535023	-0.138715
67	1	0	-4.566929	2.718010	0.273794
68	1	0	-7.026342	3.014278	0.306291
69	1	0	-11.780044	3.502684	0.410064
70	1	0	-14.376723	3.113517	0.361343
71	1	0	7.542608	1.246004	0.062499
72	1	0	5.082690	1.540747	0.093433
73	1	0	4.565246	-2.721298	-0.206494
74	1	0	7.024441	-3.019805	-0.237388
75	1	0	-1.643545	2.929435	1.263081
76	1	0	-0.589632	4.346824	0.960792
77	1	0	-0.070966	3.049465	2.072880
78	1	0	2.436987	2.818817	0.509036
79	1	0	2.385096	2.615314	-1.245235
80	1	0	1.813795	4.147030	-0.515861
81	1	0	11.778406	-3.512194	-0.347130
82	1	0	14.375265	-3.123025	-0.309963
83	1	0	-0.704792	4.048788	-1.805507
84	1	0	-1.746612	2.592638	-1.741776
85	1	0	-0.229966	2.555297	-2.660476
86	1	0	-18.771026	1.242520	0.170559
87	1	0	-21.036349	0.228881	0.049881
88	1	0	-21.291059	-2.227388	-0.277237
89	1	0	-19.266308	-3.663955	-0.482630
90	1	0	-17.001022	-2.650710	-0.361975
91	1	0	17.001582	2.654410	0.288850
92	1	0	19.267036	3.669665	0.387336
93	1	0	21.291527	2.228960	0.209861
94	1	0	21.036329	-0.233392	-0.067136
95	1	0	18.770841	-1.249032	-0.165626

le' perp-perp
HF= -2885.3321236

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-20.687057	0.111043	-0.608198
2	6	0	-19.290965	0.132047	-0.690729
3	6	0	-18.502606	-0.118443	0.455477
4	6	0	-19.149014	-0.389637	1.682969
5	6	0	-20.545437	-0.409245	1.758731
6	6	0	-21.320469	-0.159288	0.615132
7	6	0	-17.076052	-0.097018	0.376023
8	6	0	-15.853046	-0.079491	0.310425
9	6	0	-14.428356	-0.059533	0.237391
10	6	0	-13.642192	-0.294255	1.389469
11	6	0	-12.250698	-0.275149	1.318994
12	6	0	-11.590836	-0.020979	0.093549
13	6	0	-12.377651	0.214204	-1.058298
14	6	0	-13.769333	0.195440	-0.987590
15	6	0	-10.166753	-0.002182	0.023846
16	6	0	-8.942371	0.012794	-0.029862

17	6	0	-7.517192	0.029155	-0.085214
18	6	0	-6.745486	-0.157399	1.085489
19	6	0	-5.352841	-0.142961	1.032129
20	6	0	-4.668480	0.057430	-0.192094
21	6	0	-5.446131	0.243668	-1.361123
22	6	0	-6.839252	0.230536	-1.309846
23	6	0	-3.240563	0.068382	-0.241983
24	6	0	-2.001874	0.059786	-0.273734
25	6	0	20.537306	-0.378178	1.785633
26	6	0	19.141276	-0.362295	1.702097
27	6	0	18.501000	-0.093881	0.470776
28	6	0	19.295032	0.157605	-0.671275
29	6	0	20.690717	0.140401	-0.580947
30	6	0	21.318027	-0.127148	0.646152
31	6	0	17.074883	-0.076274	0.383427
32	6	0	15.852166	-0.062124	0.311403
33	6	0	14.427793	-0.046563	0.231420
34	6	0	13.773671	0.193818	-0.999126
35	6	0	12.382260	0.208701	-1.076196
36	6	0	11.590900	-0.015926	0.074624
37	6	0	12.245883	-0.256182	1.305482
38	6	0	13.637042	-0.271390	1.382345
39	6	0	10.167061	-0.000445	-0.000650
40	6	0	8.942757	0.010503	-0.057365
41	6	0	7.517542	0.020705	-0.113501
42	6	0	6.838196	0.199389	-1.340872
43	6	0	5.444915	0.207366	-1.391417
44	6	0	4.668639	0.038288	-0.218847
45	6	0	5.354520	-0.139157	1.008080
46	6	0	6.747159	-0.148366	1.060705
47	6	0	3.240567	0.045904	-0.265949
48	6	0	2.001773	0.065999	-0.287074
49	78	0	-0.000157	0.065331	-0.293248
50	15	0	0.097061	-2.272092	-0.559536
51	15	0	-0.095829	2.402280	-0.024152
52	6	0	1.020485	-2.789992	-2.090004
53	6	0	-1.517925	-3.187045	-0.666977
54	6	0	1.012528	-3.113113	0.825644
55	6	0	-1.068187	3.247003	-1.367361
56	6	0	1.520141	3.320924	0.020446
57	6	0	-0.957898	2.910609	1.544827
58	1	0	-21.281254	0.304877	-1.494934
59	1	0	-18.800072	0.340858	-1.634824
60	1	0	-18.548761	-0.582254	2.565284
61	1	0	-21.029916	-0.618655	2.706573
62	1	0	-22.403399	-0.174897	0.676506
63	1	0	-14.136407	-0.490540	2.334383
64	1	0	-11.658266	-0.456576	2.208651
65	1	0	-11.883465	0.410809	-2.003073
66	1	0	-14.361578	0.377328	-1.877405
67	1	0	-7.252063	-0.313323	2.031819
68	1	0	-4.772666	-0.288325	1.936912
69	1	0	-4.938751	0.397513	-2.307310
70	1	0	-7.418121	0.374747	-2.215704
71	1	0	21.017059	-0.585458	2.736359
72	1	0	18.536627	-0.555781	2.581218
73	1	0	18.808832	0.364316	-1.618272
74	1	0	21.289320	0.335065	-1.464508

75	1	0	22.400642	-0.139840	0.713560
76	1	0	14.369459	0.367777	-1.888145
77	1	0	11.891857	0.394492	-2.025141
78	1	0	11.649880	-0.429595	2.194380
79	1	0	14.127473	-0.456646	2.331455
80	1	0	7.416004	0.331117	-2.249316
81	1	0	4.936507	0.346124	-2.339360
82	1	0	4.775504	-0.268628	1.916006
83	1	0	7.254827	-0.285687	2.009325
84	1	0	1.093791	-3.879929	-2.145034
85	1	0	2.017648	-2.348560	-2.056829
86	1	0	0.498154	-2.413241	-2.971400
87	1	0	-1.339420	-4.260521	-0.777857
88	1	0	-2.087579	-2.813205	-1.518982
89	1	0	-2.101473	-2.995984	0.234587
90	1	0	1.095109	-4.187570	0.638016
91	1	0	0.479547	-2.944993	1.763378
92	1	0	2.005834	-2.668056	0.900781
93	1	0	-1.148007	4.319818	-1.169528
94	1	0	-2.061649	2.797660	-1.407085
95	1	0	-0.571402	3.087452	-2.326273
96	1	0	1.345123	4.391886	0.157675
97	1	0	2.058269	3.147411	-0.912581
98	1	0	2.132381	2.933690	0.835995
99	1	0	-1.045502	3.999440	1.600956
100	1	0	-0.390815	2.544491	2.402781
101	1	0	-1.948922	2.454539	1.556889

1e' pl-perp
HF=-2885.3313299

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-20.582449	-1.310578	0.645225
2	6	0	-19.184714	-1.290312	0.599277
3	6	0	-18.496648	-0.099984	0.270879
4	6	0	-19.244794	1.066031	-0.009700
5	6	0	-20.642399	1.039030	0.037986
6	6	0	-21.317378	-0.147677	0.365141
7	6	0	-17.068705	-0.076537	0.223814
8	6	0	-15.844590	-0.057930	0.184981
9	6	0	-14.418735	-0.038515	0.140551
10	6	0	-13.719853	1.151246	-0.169594
11	6	0	-12.327063	1.169700	-0.212011
12	6	0	-11.578957	-0.000960	0.054708
13	6	0	-12.278593	-1.191058	0.364028
14	6	0	-13.671247	-1.209390	0.406248
15	6	0	-10.153771	0.016488	0.013316
16	6	0	-8.928613	0.028019	-0.019339
17	6	0	-7.502895	0.037517	-0.053156
18	6	0	-6.789764	1.228729	-0.322296
19	6	0	-5.396269	1.235412	-0.350582
20	6	0	-4.651032	0.054596	-0.112097
21	6	0	-5.371803	-1.135338	0.155283
22	6	0	-6.765013	-1.145353	0.184735

23	6	0	-3.222462	0.062050	-0.136675
24	6	0	-1.982552	0.062436	-0.155035
25	6	0	20.593350	-0.323067	1.567825
26	6	0	19.195921	-0.310814	1.511396
27	6	0	18.531049	-0.087516	0.284090
28	6	0	19.302161	0.122142	-0.881873
29	6	0	20.699375	0.108877	-0.818586
30	6	0	21.351162	-0.113356	0.404777
31	6	0	17.103437	-0.073969	0.224903
32	6	0	15.879486	-0.062949	0.178062
33	6	0	14.453713	-0.050336	0.127707
34	6	0	13.773386	0.160455	-1.094060
35	6	0	12.380639	0.172538	-1.141998
36	6	0	11.613843	-0.024940	0.030353
37	6	0	12.295119	-0.235495	1.252352
38	6	0	13.687628	-0.248305	1.300001
39	6	0	10.188795	-0.011778	-0.015332
40	6	0	8.963546	-0.001688	-0.047849
41	6	0	7.537631	0.008270	-0.078734
42	6	0	6.837362	0.189696	-1.294018
43	6	0	5.443574	0.198355	-1.320789
44	6	0	4.686946	0.027835	-0.135332
45	6	0	5.393760	-0.151939	1.079389
46	6	0	6.787156	-0.162482	1.108023
47	6	0	3.259089	0.038397	-0.159909
48	6	0	2.020575	0.047114	-0.172250
49	78	0	0.024619	0.056727	-0.170856
50	15	0	-0.052628	-2.281421	-0.431604
51	15	0	-0.032401	2.394884	0.091028
52	6	0	1.563644	-3.188602	-0.573147
53	6	0	-1.006654	-2.811330	-1.939340
54	6	0	-0.927232	-3.122440	0.980245
55	6	0	-0.944024	3.244076	-1.292059
56	6	0	1.593638	3.290981	0.185084
57	6	0	-0.937593	2.927099	1.627777
58	1	0	-21.099031	-2.230337	0.898466
59	1	0	-18.615474	-2.187648	0.815283
60	1	0	-18.721908	1.981871	-0.262127
61	1	0	-21.205491	1.940526	-0.179238
62	1	0	-22.401389	-0.165944	0.401453
63	1	0	-14.282273	2.055122	-0.375222
64	1	0	-11.802162	2.087885	-0.450477
65	1	0	-11.716099	-2.094767	0.569860
66	1	0	-14.196147	-2.127560	0.645038
67	1	0	-7.342146	2.143653	-0.507073
68	1	0	-4.864369	2.157515	-0.558544
69	1	0	-4.820672	-2.050533	0.342663
70	1	0	-7.298307	-2.066419	0.393501
71	1	0	21.091966	-0.495625	2.515759
72	1	0	18.609018	-0.472611	2.408751
73	1	0	18.797174	0.293962	-1.825996
74	1	0	21.280134	0.271444	-1.720390
75	1	0	22.434906	-0.123187	0.451147
76	1	0	14.350011	0.313385	-1.999453
77	1	0	11.870096	0.335017	-2.084550
78	1	0	11.718302	-0.388313	2.157542
79	1	0	14.198138	-0.411068	2.242612
80	1	0	7.399644	0.322024	-2.212087

81	1	0	4.918913	0.337384	-2.259793
82	1	0	4.830126	-0.283334	1.996661
83	1	0	7.310779	-0.302376	2.047586
84	1	0	1.387340	-4.262994	-0.678585
85	1	0	2.166214	-2.993237	0.314764
86	1	0	2.112774	-2.813546	-1.437849
87	1	0	-1.092463	-3.901146	-1.977731
88	1	0	-0.492814	-2.453771	-2.833702
89	1	0	-1.997883	-2.357339	-1.900805
90	1	0	-1.034487	-4.193719	0.786597
91	1	0	-1.908667	-2.661506	1.101233
92	1	0	-0.354293	-2.972095	1.897202
93	1	0	-1.040372	4.315199	-1.092036
94	1	0	-1.930679	2.787933	-1.385662
95	1	0	-0.398949	3.094077	-2.225927
96	1	0	1.428621	4.366302	0.298917
97	1	0	2.166463	3.094218	-0.722062
98	1	0	2.167104	2.908807	1.030647
99	1	0	-1.019487	4.017120	1.669042
100	1	0	-0.397133	2.568201	2.505735
101	1	0	-1.930952	2.476053	1.619858

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HF=-2885.3308582

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	20.662035	0.965865	-0.401236
2	6	0	19.263928	1.004395	-0.388714
3	6	0	18.518544	-0.162323	-0.103754
4	6	0	19.209905	-1.364995	0.167845
5	6	0	20.608100	-1.396772	0.153692
6	6	0	21.340266	-0.233146	-0.130602
7	6	0	17.090114	-0.127879	-0.090722
8	6	0	15.865574	-0.101111	-0.079725
9	6	0	14.439224	-0.072966	-0.066940
10	6	0	13.695922	-1.240077	0.225760
11	6	0	12.302829	-1.213680	0.238113
12	6	0	11.598420	-0.019114	-0.041932
13	6	0	12.342369	1.148084	-0.334351
14	6	0	13.735628	1.121550	-0.346578
15	6	0	10.172847	0.005744	-0.029588
16	6	0	8.947322	0.022438	-0.018511
17	6	0	7.521351	0.036895	-0.004670
18	6	0	6.788214	-1.135976	0.290689
19	6	0	5.394790	-1.121837	0.303846
20	6	0	4.668901	0.062156	0.024046
21	6	0	5.409605	1.233186	-0.271077
22	6	0	6.803203	1.222425	-0.285815
23	6	0	3.240625	0.074751	0.039054
24	6	0	2.001410	0.098600	0.053519
25	6	0	-20.662311	0.915888	-0.481274
26	6	0	-19.264786	0.963181	-0.449087
27	6	0	-18.516735	-0.194715	-0.136484

28	6	0	-19.204828	-1.397556	0.142562
29	6	0	-20.602451	-1.438138	0.108590
30	6	0	-21.337280	-0.283247	-0.203139
31	6	0	-17.088851	-0.151537	-0.103985
32	6	0	-15.864734	-0.117584	-0.077050
33	6	0	-14.438826	-0.081113	-0.047165
34	6	0	-13.693037	-1.235450	0.286944
35	6	0	-12.300302	-1.201349	0.313818
36	6	0	-11.598784	-0.011614	0.007233
37	6	0	-12.345260	1.143074	-0.325644
38	6	0	-13.738140	1.108876	-0.352254
39	6	0	-10.173488	0.020487	0.030860
40	6	0	-8.948132	0.043206	0.048089
41	6	0	-7.522256	0.064777	0.063944
42	6	0	-6.784007	-1.086710	0.423965
43	6	0	-5.390636	-1.066914	0.433478
44	6	0	-4.669958	0.101917	0.084470
45	6	0	-5.415722	1.252510	-0.271554
46	6	0	-6.809335	1.236029	-0.282479
47	6	0	-3.241594	0.115276	0.088082
48	6	0	-2.002137	0.102480	0.086040
49	78	0	-0.000304	0.102119	0.072642
50	15	0	-0.093656	2.435750	0.353724
51	15	0	0.093216	-2.232080	-0.208619
52	6	0	-1.026054	3.285823	-1.014497
53	6	0	1.520815	3.354054	0.441228
54	6	0	-0.991906	2.942804	1.902571
55	6	0	0.974952	-2.737284	-1.767540
56	6	0	-1.520740	-3.152922	-0.279235
57	6	0	1.040420	-3.082008	1.149477
58	1	0	21.222971	1.868041	-0.621219
59	1	0	18.738530	1.929745	-0.597477
60	1	0	18.642782	-2.262916	0.386957
61	1	0	21.127196	-2.326017	0.363446
62	1	0	22.424650	-0.260333	-0.141026
63	1	0	14.224447	-2.161825	0.441721
64	1	0	11.743568	-2.114683	0.463677
65	1	0	11.813834	2.069747	-0.550320
66	1	0	14.294783	2.022713	-0.572093
67	1	0	7.325419	-2.052663	0.508610
68	1	0	4.847602	-2.029721	0.533789
69	1	0	4.873038	2.149631	-0.490787
70	1	0	7.352028	2.129462	-0.514920
71	1	0	-21.225333	1.811329	-0.722431
72	1	0	-18.741886	1.888610	-0.663696
73	1	0	-18.635616	-2.288743	0.382733
74	1	0	-21.119042	-2.367438	0.324204
75	1	0	-22.421216	-0.317258	-0.228938
76	1	0	-14.219343	-2.153559	0.522903
77	1	0	-11.739067	-2.092738	0.570529
78	1	0	-11.818938	2.060991	-0.562010
79	1	0	-14.299258	2.000304	-0.609382
80	1	0	-7.317351	-1.991711	0.694027
81	1	0	-4.838460	-1.957278	0.713454
82	1	0	-4.883918	2.157939	-0.543402
83	1	0	-7.362062	2.126876	-0.560499
84	1	0	-1.128648	4.355058	-0.807842
85	1	0	-2.009689	2.821591	-1.098608

86	1	0	-0.490929	3.144190	-1.955411
87	1	0	1.342120	4.422514	0.592490
88	1	0	2.071799	3.195831	-0.486983
89	1	0	2.118189	2.953880	1.261628
90	1	0	-1.089476	4.031114	1.953122
91	1	0	-0.438893	2.584741	2.773011
92	1	0	-1.978479	2.477194	1.898659
93	1	0	1.075376	-3.825307	-1.818589
94	1	0	1.960016	-2.268531	-1.775808
95	1	0	0.410349	-2.381652	-2.631511
96	1	0	-1.342066	-4.220317	-0.437926
97	1	0	-2.130009	-2.749850	-1.089361
98	1	0	-2.059304	-3.000595	0.657225
99	1	0	1.144800	-4.150408	0.939447
100	1	0	0.512641	-2.944534	2.095174
101	1	0	2.023032	-2.614516	1.226897
