Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Electronic structures for M-*pigments*

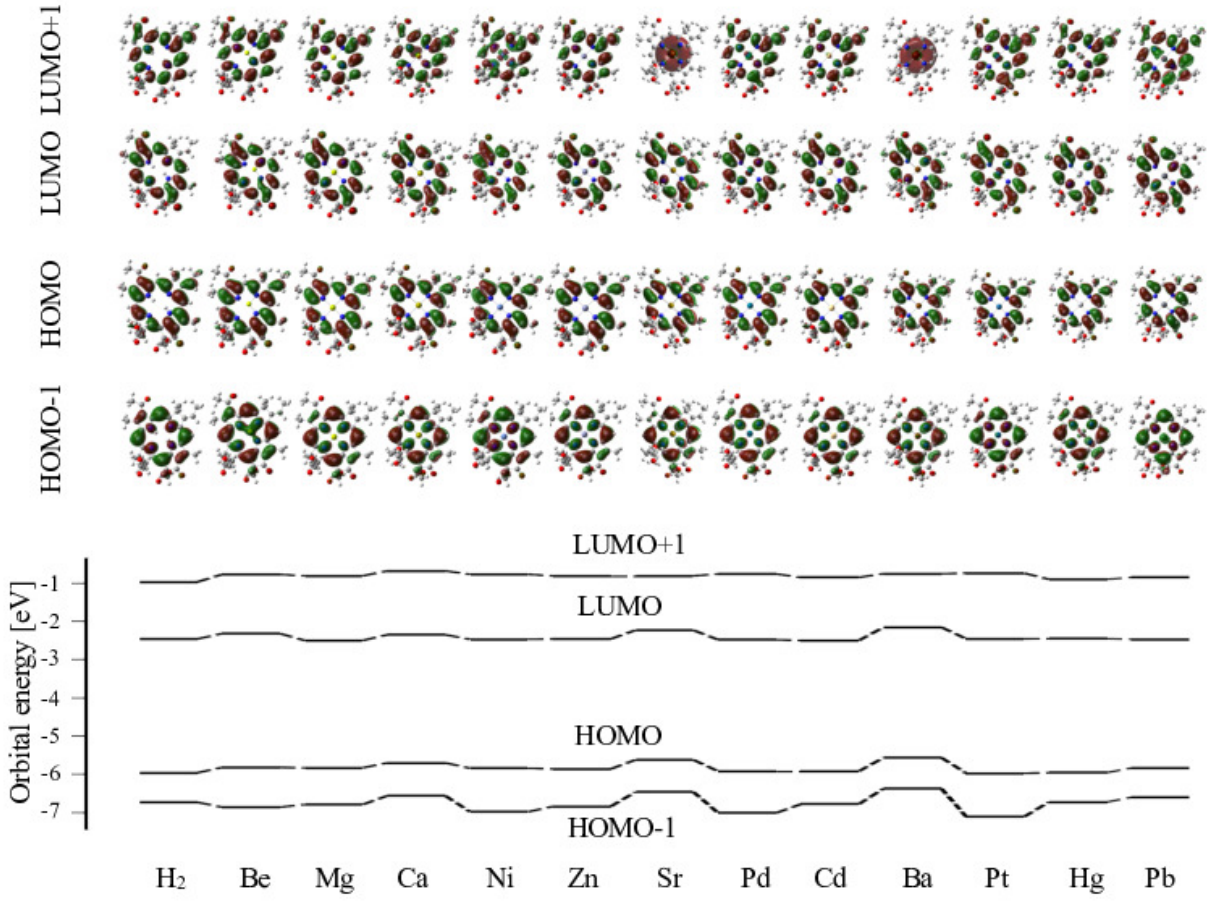

Fig. S1: Profiles of the HOMO-1, HOMO, LUMO and LUMO+1 of the M-Bchl *b* series in a vacuum. Red (green) indicates a positive (negative) sign of the molecular orbital wave function.

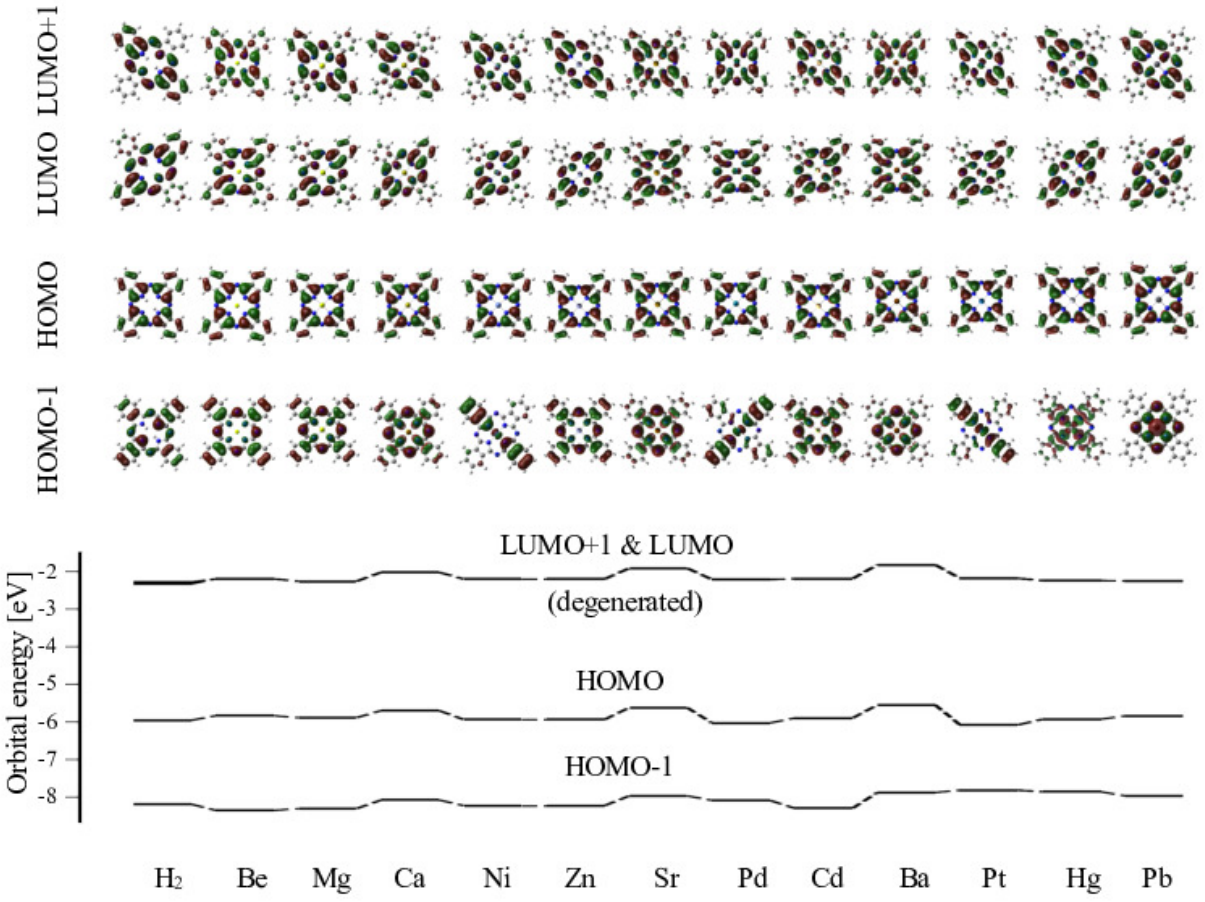

Fig. S2: Profiles of the HOMO-1, HOMO, LUMO and LUMO+1 of the M-Pht series in a vacuum.

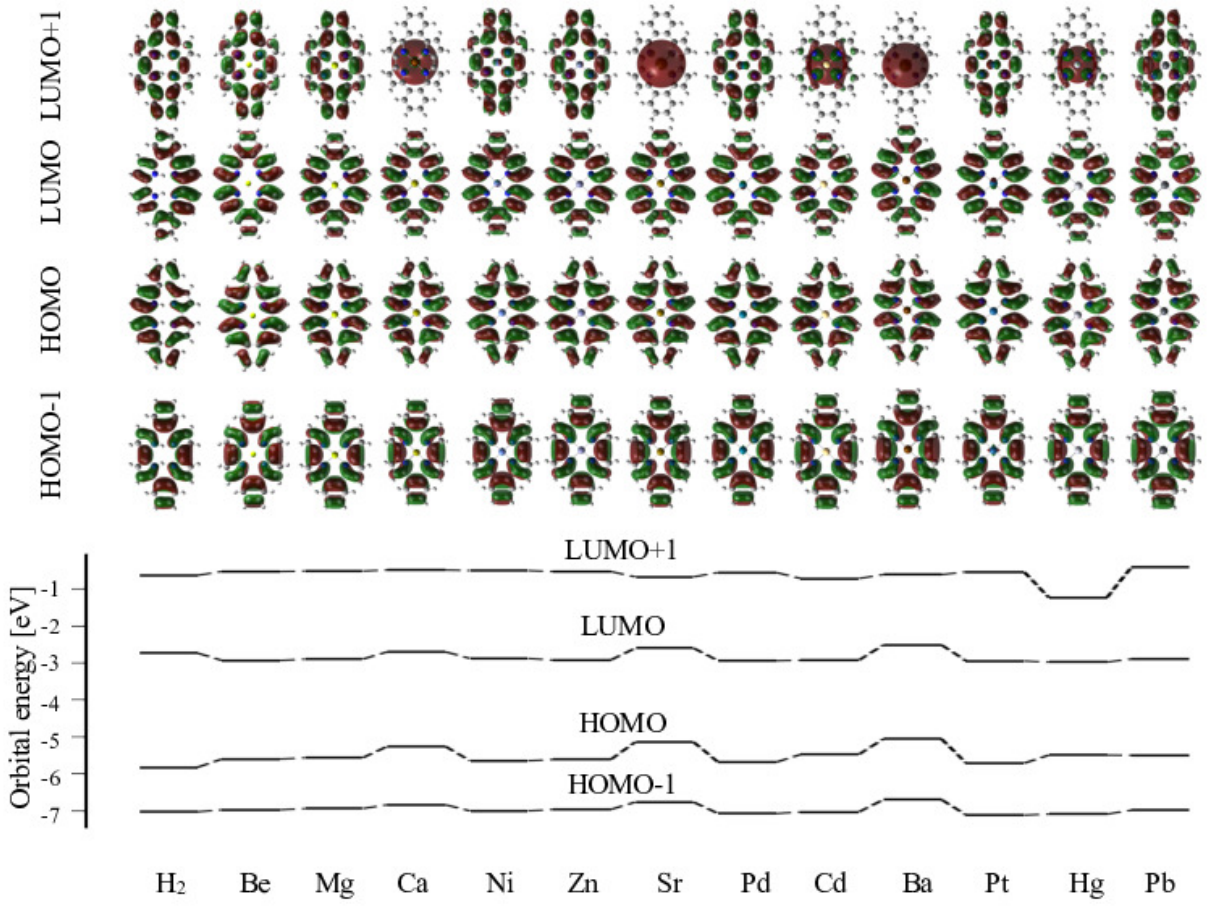

Fig. S3: Profiles of the HOMO-1, HOMO, LUMO and LUMO+1 for the M-*m*DBPc series in a vacuum.

Table S1: Wavelengths and oscillator strengths of the low-lying excited states corresponding to Q_y and Q_x bands for the (a) M-Bchl *b*, (b) M-Pht and (c) M-*m*DBPc series in a vacuum, water, methanol and benzene. Legend: $\Delta\lambda_i^J$; the estimated difference of wavelengths from the first excited state for each pigment in a vacuum, f_i^J; the oscillator strength, $i = 1$; Q_y and $i = 2$; Q_x, where $i = 1$ and $i = 2$ basically correspond to the first and second excited states. Values with $\dagger k$ are associated with the kth excited state and $J = B$, P and D indicate the M-Bchl *b*, M-Pht and M-*m*DBPc series, respectively.

	Bchlb				Pht				mDBPc			
	$\Delta\lambda_1^B$	f_1^B	$\Delta\lambda_2^B$	f_2^B	$\Delta\lambda_1^P$	f_1^P	$\Delta\lambda_2^P$	f_2^P	$\Delta\lambda_1^D$	f_1^D	$\Delta\lambda_2^D$	f_2^D
H_2	0.00	0.3223	-183.26	0.0556	0.00	0.4703	-14.27	0.5109	0.00	0.1581	-279.95	0.1613
(water)	+30.84	0.4326	-179.34	0.0911	+25.63	0.6207	+20.8	0.6629	+11.04	0.1982	-280.17	0.2764
(methanol)	+30.67	0.4314	-179.33	0.0906	+25.35	0.6190	+20.22	0.6611	+11.87	0.1981	-279.90	0.2747
(benzene)	+42.78	0.4730	-176.31	0.1063	+36.35	0.6757	+26.67	0.7129	+43.41	0.2244	-271.38	0.3253
Be	0.00	0.3122	-215.43	0.0329	+1.18	0.4654	+1.16	0.4654	+181.84	0.1829	-246.98	0.2057
(water)	+22.07	0.4152	-212.36	0.0668	+28.94	0.6127	+28.92	0.6127	+267.03	0.2398	-236.22	0.3343
(methanol)	+22.40	0.4139	-212.41	0.0660	+28.67	0.6108	+28.65	0.6108	+265.87	0.2391	-236.33	0.3324
(benzene)	+40.89	0.4488	-210.96	0.0720	+36.02	0.6872	+39.53	0.6591	+39.50	0.6591	-230.86	0.3861
Mg	+34.02	0.3599	-173.91	0.0554	-1.06	0.4828	-1.07	0.4828	+166.93	0.1920	-245.96	0.1996
(water)	+66.66	0.4801	-159.94	0.1064	+23.6	0.6411	+23.59	0.6411	+254.83	0.2502	-234.97	0.3308
(methanol)	+66.81	0.4783	-160.50	0.1052	+23.46	0.6390	+23.45	0.6390	+253.56	0.2495	-235.11	0.3288
(benzene)	+87.13	0.5141	-163.89	0.1110	+36.02	0.6872	+36.01	0.6872	+287.11	0.2723	-229.92	0.3793
Ca	+28.43	0.3574	-159.61	0.0651	-6.14	0.4670	-6.19	0.4670	+268.37	0.1643	-263.04	0.1919
(water)	+63.83	0.4894	-143.56	0.1200	+13.84	0.6303	+13.78	0.6303	-	-	-	-
(methanol)	+63.59	0.4874	-144.07	0.1188	+13.84	0.6303	+13.78	0.6303	-	-	-	-
(benzene)	+79.50	0.5187	-147.94	0.1259	+26.5	0.6739	+26.44	0.6740	+412.63	0.2321	-248.92	0.3792
Ni	$+28.64^{\dagger 2}$	$0.3459^{\dagger 2}$	$-202.79^{\dagger 5}$	$0.0336^{\dagger 5}$	$-20.68^{\dagger}$	$0.4706^{\dagger}$	$-20.69^{\dagger}$	$0.4706^{\dagger 2}$	+162.74	0.1676	$-257.34^{\dagger 4}$	$0.1917^{\dagger 4}$
(water)	$+61.58^{\dagger 2}$	$0.4494^{\dagger 2}$	$-199.80^{\dagger 5}$	$0.0645^{\dagger 5}$	+5.45	0.6185	+5.44	0.6185	+234.38	0.2187	$-248.57^{\dagger 3}$	$0.3012^{\dagger 3}$
(methanol)	$+61.64^{\dagger 2}$	$0.4483^{\dagger 2}$	$-199.84^{\dagger 5}$	$0.0640^{\dagger 5}$	+5.14	0.6168	+5.13	0.6168	+233.53	0.2183	$-248.62^{\dagger 3}$	$0.3000^{\dagger 3}$
(benzene)	$+75.76^{\dagger 4}$	$0.4800^{\dagger 4}$	$-185.63^{\dagger 7}$	$0.0952^{\dagger 7}$	+13.76	0.6691	+13.75	0.6690	+264.66	0.2420	$-243.29^{\dagger 3}$	$0.3552^{\dagger 3}$
Zn	+14.80	0.3540	-191.68	0.0486	-12.53	0.4923	-12.54	0.4923	+167.08	0.1858	-246.92	0.2060
(water)	+46.84	0.4720	-180.22	0.0959	+12.97	0.6506	+12.95	0.6505	+250.27	0.2441	-235.82	0.3353
(methanol)	+46.90	0.4703	-180.67	0.0947	+12.76	0.6486	+12.75	0.6485	+249.09	0.2434	-235.96	0.3333
(benzene)	+64.19	0.5072	-183.26	0.0998	+23.82	0.6988	+23.8	0.6987	+282.24	0.2661	-230.66	0.3857
Sr	+17.68	0.3612	-163.74	0.0664	-13.09	0.4700	-13.13	0.4700	+288.75	0.1583	-268.85	0.1924
(water)	-	-	-	-	+9.11	0.6296	+9.08	0.6296	-	-	-	-
(methanol)	-	-	-	-	+8.87	0.6277	+8.84	0.6276	-	-	-	-
(benzene)	-	-	-	-	+19.93	0.6763	+19.89	0.6763	+438.57	0.2240	-254.41	0.3796
Pd	-0.81	0.3670	-211.18	0.0439	-7.28	0.4606	-7.29	0.4607	+169.43	0.1721	-259.58	0.1797
(water)	+33.63	0.4782	-207.83	0.0780	+15.51	0.6122	+15.5	0.6123	+243.01	0.2251	-251.57	0.2838
(methanol)	+33.44	0.4770	-207.87	0.0774	+15.36	0.6108	+15.35	0.6109	+242.12	0.2247	-251.61	0.2828
(benzene)	+47.15	0.5200	-206.31	0.0861	+26.88	0.6645	+26.88	0.6646	+273.30	0.2506	-246.54	0.3370
Cd	+5.45	0.3639	-177.99	0.0620	-17.13	0.4809	-17.16	0.4809	+268.08	0.1673	-260.86	0.2122
(water)	+41.70	0.4904	-160.60	0.1157	+5.51	0.6392	+5.47	0.6392	+371.35	0.2201	-249.52	0.3560
(methanol)	+41.48	0.4885	-161.32	0.1145	+5.37	0.6373	+5.33	0.6372	+369.59	0.2194	-249.76	0.3530
(benzene)	+55.06	0.5255	-166.67	0.1216	+16.99	0.6878	+16.95	0.6875	+409.54	0.2378	-245.70	0.3975
Ba	-	-	-	-	-15.74	0.4657	-15.75	0.4657	+297.70	0.1527	-271.53	0.1898
(water)	-	-	-	-	-	-	-	-	-	-	-	-
(methanol)	-	-	-	-	+16.42	0.6711	+16.41	0.6711	+417.63	0.1996	-258.54	0.3548
(benzene)	-	-	-	-	-	-	-	-	+448.71	0.2176	-256.91	0.3749
Pt	-24.42	0.3842	-231.30	0.0325	-57.71	0.5031	-57.71	0.5031	+157.92	0.1734	$-266.39^{\dagger 4}$	$0.1754^{\dagger 4}$
(water)	+8.72	0.4980	-228.49	0.0552	-35.86	0.6601	-35.87	0.6601	+228.45	0.2270	$-259.16^{\dagger 4}$	$0.2753^{\dagger 4}$
(methanol)	+8.46	0.4967	-228.53	0.0550	-36.08	0.6583	-36.1	0.6583	+227.59	0.2266	$-259.18^{\dagger 4}$	$0.2743^{\dagger 4}$
(benzene)	+20.56	0.5410	-227.44	0.0667	-28.33	0.7165	-28.35	0.7165	+257.33	0.2537	$-254.28^{\dagger 4}$	$0.3281^{\dagger 4}$
Hg	-5.49	0.3262	-155.81	0.0412	-7.28	0.4606	-7.29	0.4607	+314.35	0.1534	-262.70	0.2173
(water)	+25.67	0.4460	-92.73	0.0242	+15.51	0.6122	+15.5	0.6123	+418.79	0.2050	$-251.40^{\dagger 3}$	$0.3599^{\dagger 3}$
(methanol)	+25.46	0.4444	-96.67	0.0251	+15.37	0.6118	+15.36	0.6118	+417.03	0.2048	$-251.68^{\dagger 3}$	$0.3569^{\dagger 3}$
(benzene)	+37.30	0.4806	-136.53	0.0601	+26.88	0.6645	+26.88	0.6646	+460.85	0.2207	$-247.76^{\dagger 3}$	$0.4026^{\dagger 3}$
Pb	+48.94	0.2909	-110.12	0.0543	+31.17	0.3925	+31.15	0.3925	+289.64	0.1381	-250.51	0.2051
(water)	+68.88	0.3907	-101.00	0.0876	+55.08	0.5345	+55.05	0.5344	+382.63	0.1818	-238.09	0.3418
(methanol)	+69.42	0.3895	-101.23	0.0871	+54.85	0.5325	+54.82	0.5325	+69.42	0.3895	-101.23	0.0871
(benzene)	+91.56	0.4244	-100.85	0.0965	+66.09	0.5743	+66.06	0.5742	+91.56	0.4244	-100.85	0.0965

Pb binding to thiol groups

Assuming the appearance of prebiotic amino acids with binding between amino acids or peptides via disulfide bonds, the extent of bonding with Pb^{2+} was evaluated by quantum chemistry calculations. The binding energies between a cystine (the disulfide form of cysteine; that is, two cysteines bonded together) and Pb or Mg were estimated based on the formula $E_{bindc} = E(M + Cystine)$ -$E(M^{2+})$ - $E(Cystine)$ with M=Mg and Pb. Structural optimizations of the cystine, Mg+cystine and Pb+cystine were performed using the UCAM-B3LYP/Def2tzvp functional in a vacuum. The optimized structures for Mg+cystine and Pb+cystine are presented in Figures. S1(a) and (b), respectively. Subsequently, the E_{bindc} values were determined with the UCAM-B3LYP/def2tzvp and UMP2(Full)/def2tzvp functionals for comparison. The E_{bindc} of Mg+cystine was found to be higher (-589.169 kcal/mol using UMP2(Full)) than that of Pb-cystine for all conditions as shown in Table S2, contrary to our expectation. These results indicated that the slight difference between different metal ions might not have a significant effect on disulfide or thiol bond formation (the results for thiol bonds are not included herein, but the same tendency was observed).

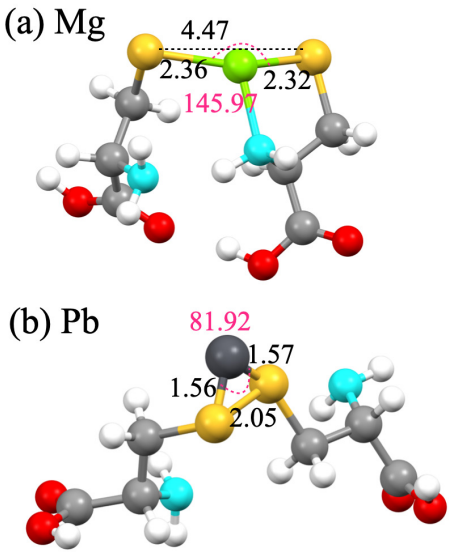

Fig. S4: Structures of cystine with (a) Mg and (b) Pb as optimized in a vacuum at the UCAM-B3LYP/def2tzvp level. The distances between atoms are shown in Å and the angles between the metal and two sulfur atoms are shown in magenta.

Table S2: Binding energies, E_{bindc}, for cystine with Mg or Pb in a vacuum (kcal/mol), as determined from the equation $E_{bindc} = E(M + Cystine)$ -$E(M^{2+})$ - $E(Cystine)$. Structures were optimized in vacuum at the UCAM-B3LYP/def2tzvp level, and the energies were evaluated using the UCAM-B3LYP/def2tzvp and UMP2(Full)/def2tzvp functionals for comparison purposes.

Mg		Pb	
UCAM-B3LYP	UMP2(Full)	UCAM-B3LYP	UMP2(Full)
-628.579	-589.169	-484.080	-431.473

Optimized atomic coordinates for M-Bchls *b*

All the structures below were optimized in vacuum at B3LYP-D3/Def2tzvp level using the Gaussian 16 software.

H_2-Bchl *b* (Bacteriopheophytin *b*)

Be-Bchl *b*

Be -1.238387 0.333933 -0.084612
C 2.455631 0.791051 -0.085108
C -0.026985 -3.044814 -0.877298
C -4.188341 -0.620304 0.078061
C -1.695300 3.414294 0.332829
N 1.085362 -1.035784 -0.419497
C 2.329612 -0.549548 -0.325171
C 3.395222 -1.615334 -0.502725
C 2.544513 -2.813546 -1.002815

C 1.132130 -2.314112 -0.755363
C 2.782511 -3.143114 -2.480160
C 4.188044 -1.893500 0.786377
C 3.306766 -2.165753 2.000626
C 4.098279 -2.493686 3.239654
O 5.295042 -2.590690 3.313922
O 3.284044 -2.680431 4.308116
N -1.853936 -1.347546 -0.321609
C -1.329449 -2.617720 -0.652865
C -2.375708 -3.598522 -0.710543
C -3.548807 -2.959481 -0.396506
C -3.217661 -1.574669 -0.194076
C -2.178491 -5.029981 -1.105141
C -4.906427 -3.539219 -0.274024
O -5.911765 -2.910110 -0.553082
C -5.054533 -4.954578 0.260263
N -2.689262 1.240629 0.157196
C -3.932513 0.709330 0.208790
C -5.005660 1.760705 0.355650
C -4.177871 3.003174 0.577692
C -2.787442 2.603719 0.342718
C -5.887843 1.830857 -0.904493
C -4.609076 4.211024 0.954177
C -6.025419 4.586323 1.251274
N -0.013694 1.599684 0.040234
C -0.389157 2.954434 0.207235
C 0.731522 3.825513 0.288419
C 1.822970 2.996484 0.190899
C 1.365013 1.666300 0.036755
C 0.713058 5.308182 0.455097
C 3.271769 3.055512 0.189552
O 4.011598 4.007644 0.296821
C 3.747695 1.580223 0.030631
C 4.669430 1.402493 -1.160694
O 5.750340 0.873263 -1.122521
O 4.111674 1.889127 -2.281555
C 4.900691 1.778242 -3.476816
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H -5.211153 -0.955276 0.118071
H -1.834773 4.476666 0.465757
H 4.118426 -1.316033 -1.263830
H 2.744772 -3.711023 -0.410539
H 2.119405 -3.941387 -2.818796
H 2.596675 -2.265395 -3.103099
H 3.813382 -3.464953 -2.641185
H 4.848163 -2.746354 0.614660
H 4.846046 -1.049211 0.995683
H 2.668772 -1.308169 2.230463
H 2.617721 -2.997552 1.828170
H -1.734702 -5.615682 -0.295016
H -3.117357 -5.501634 -1.379267
H -1.516570 -5.113823 -1.967790
H -5.940457 -4.977695 0.893738
H -5.233872 -5.640224 -0.571496
H -4.186604 -5.300017 0.818277
H -6.629919 2.623511 -0.809820
H -5.276284 2.040497 -1.783621
H -6.406231 0.885203 -1.066128
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H -5.638073 1.536136 1.218988
H -6.087984 5.132302 2.196569
H -6.427800 5.252275 0.480518
H -6.683093 3.719829 1.316551
H 1.730923 5.694208 0.463283
H 0.166931 5.795520 -0.356847
H 0.229934 5.599396 1.391910
H 4.327601 1.302001 0.912012
H 4.301823 2.226399 -4.264751
H 5.843704 2.311306 -3.359185
H 5.109281 0.731710 -3.700172
H 3.851712 -2.886628 5.067216

Mg-Bchl b (Bchl b)

Mg -0.796243 0.168526 -0.128344
C 2.627848 0.546223 -0.150788
C -0.387322 -3.159277 -0.701606
C -4.160912 -0.169221 -0.053645
C -1.129526 3.586504 0.436095
N 0.910211 -1.116940 -0.381302
C 2.229714 -0.760522 -0.325665
C 3.129258 -1.977892 -0.412111
C 2.150782 -3.066570 -0.905243
C 0.792804 -2.441229 -0.635931
C 2.327791 -3.384699 -2.395155
C 3.797989 -2.304969 0.936848
C 2.820163 -2.416904 2.101487
C 3.494242 -2.770186 3.401661
O 4.667558 -2.983580 3.558787
O 2.599379 -2.826845 4.419019
N -2.061073 -1.401003 -0.324899
C -1.706644 -2.705834 -0.548704
C -2.886107 -3.527353 -0.612349
C -3.968682 -2.677617 -0.430694
C -3.425520 -1.341989 -0.263082
C -2.873537 -5.001712 -0.867631
C -5.409002 -3.007561 -0.404382
O -6.267250 -2.160751 -0.592758
C -5.839126 -4.432838 -0.111386
N -2.404960 1.516234 0.146663
C -3.695589 1.124155 0.122187
C -4.632231 2.309191 0.268257
C -3.661983 3.426665 0.590947
C -2.314010 2.865729 0.383674
C -5.426188 2.554461 -1.027464
C -3.964652 4.655092 1.021502
C -5.338173 5.184179 1.286490
N 0.425734 1.744051 0.071253
C 0.169187 3.087047 0.294112
C 1.406389 3.827700 0.370779
C 2.401945 2.878731 0.190672
C 1.758527 1.632579 0.013506
C 1.553120 5.293808 0.599779
C 3.841766 2.666191 0.132651
O 4.758470 3.446415 0.244755
C 4.043441 1.117217 -0.097098
C 4.832727 0.825984 -1.359059
O 5.734297 0.030194 -1.437171
O 4.370626 1.537526 -2.399627
C 5.037999 1.326420 -3.654007
H -0.265775 -4.215000 -0.901056
H -5.232528 -0.293924 -0.052425
H -1.216196 4.650124 0.611969
H 3.930697 -1.817685 -1.134271
H 2.268707 -3.991366 -0.334596
H 1.580871 -4.102783 -2.737101
H 2.222938 -2.477959 -2.995214
H 3.318894 -3.803358 -2.580914
H 4.350798 -3.240942 0.831916
H 4.545334 -1.544837 1.165623
H 2.277480 -1.480256 2.255521
H 2.049862 -3.171578 1.919668
H -3.077159 -5.571629 0.042532
H -3.623717 -5.289295 -1.603486
H -1.908043 -5.331309 -1.246178
H -6.886845 -4.417510 0.181017
H -5.742667 -5.046184 -1.009971
H -5.236635 -4.894430 0.670655
H -6.059077 3.436812 -0.931013
H -4.744700 2.715351 -1.864656
H -6.058477 1.696999 -1.260893
H -3.152739 5.348537 1.217659
H -5.335825 2.138462 1.087435
H -5.379551 5.673722 2.263462
H -5.618640 5.941975 0.547223
H -6.098824 4.404226 1.266157
H 2.605487 5.571952 0.621580
H 1.062893 5.869910 -0.189896

H 1.098831 5.595939 1.547460
H 4.631363 0.721875 0.731754
H 4.544326 1.986071 -4.362169
H 6.095015 1.576422 -3.567671
H 4.942841 0.286116 -3.966016
H 3.093021 -3.055846 5.222096

Ca-Bchl *b*

Ca -0.744964 0.328074 -1.378026
C 2.704739 0.336015 -0.237130
C -0.517819 -3.191694 -0.807521
C -4.096579 0.060814 -0.238854
C -0.846848 3.638406 0.250756
N 0.936399 -1.222754 -0.704093
C 2.242581 -0.955182 -0.440288
C 3.029117 -2.245081 -0.253549
C 2.042128 -3.304256 -0.803550
C 0.716252 -2.557694 -0.779604
C 2.396227 -3.757311 -2.224834
C 3.417199 -2.485985 1.218767
C 2.246835 -2.391065 2.192485
C 2.658471 -2.618611 3.623117
O 3.777040 -2.824006 4.016801
O 1.591427 -2.563120 4.457536
N -2.111329 -1.324679 -0.627651
C -1.820959 -2.657409 -0.682401
C -3.035326 -3.419229 -0.531600
C -4.063749 -2.495429 -0.373627
C -3.449796 -1.176904 -0.432776
C -3.102270 -4.914015 -0.563781
C -5.504502 -2.739907 -0.169094
O -6.338807 -1.871937 -0.374794
C -5.969446 -4.096034 0.328739
N -2.273726 1.706674 -0.231999
C -3.567815 1.341368 -0.112283
C -4.434470 2.548645 0.213222
C -3.387751 3.608146 0.507783
C -2.086950 3.008488 0.141121
C -5.346955 2.910662 -0.971587
C -3.598505 4.818601 1.033484
C -4.917054 5.381839 1.460325
N 0.612763 1.758428 -0.290553
C 0.427820 3.066780 0.108360
C 1.701517 3.665483 0.454716
C 2.630552 2.651964 0.279182
C 1.919596 1.502538 -0.156360
C 1.930578 5.054608 0.945949
C 4.033719 2.299369 0.435234
O 4.982185 2.968921 0.775722
C 4.135987 0.766765 0.087209
C 5.080680 0.485453 -1.064523
O 5.858555 -0.434467 -1.104166
O 4.911190 1.362355 -2.068811
C 5.752141 1.172425 -3.217229
H -0.459933 -4.271088 -0.858272
H -5.166912 -0.010503 -0.116016
H -0.864100 4.671865 0.570736
H 3.953152 -2.224573 -0.833321
H 2.008224 -4.182983 -0.155145
H 1.645245 -4.445134 -2.617499
H 2.453928 -2.898241 -2.897689
H 3.365012 -4.260935 -2.237273
H 3.879637 -3.472383 1.297589
H 4.188836 -1.777241 1.517293
H 1.766940 -1.409472 2.142159
H 1.456238 -3.108831 1.958862
H -3.253518 -5.335871 0.433255
H -3.920304 -5.268081 -1.190668
H -2.183665 -5.342665 -0.960210
H -6.989108 -3.992547 0.693503
H -5.968265 -4.818830 -0.490081
H -5.326330 -4.488526 1.116292
H -5.930772 3.805264 -0.753780

H -4.749443 3.107219 -1.864105
H -6.034368 2.092907 -1.192392
H -2.743517 5.469079 1.190058
H -5.056239 2.349230 1.089742
H -4.844622 5.808079 2.464893
H -5.232551 6.196391 0.799664
H -5.709617 4.634188 1.467502
H 2.990048 5.223266 1.131890
H 1.586819 5.795788 0.219035
H 1.385922 5.240973 1.875846
H 4.549159 0.249858 0.953075
H 5.491871 1.971549 -3.905996
H 6.802184 1.237673 -2.933557
H 5.567085 0.197683 -3.669518
H 1.924705 -2.705619 5.357280

Ni-Bchl *b*

Ni -0.701534 0.266599 -0.178542
C 2.682079 0.558441 0.097710
C -0.309494 -2.948449 -1.156263
C -4.013110 -0.145969 0.109480
C -1.028940 3.642053 0.250651
N 0.906119 -0.964604 -0.452949
C 2.234615 -0.686521 -0.214838
C 3.101274 -1.912224 -0.360692
C 2.201840 -2.809092 -1.219919
C 0.832130 -2.229704 -0.940955
C 2.542702 -2.719631 -2.712882
C 3.492963 -2.508703 1.004399
C 2.311602 -2.828172 1.914570
C 2.738440 -3.384034 3.248155
O 3.870752 -3.553570 3.617670
O 1.665836 -3.684553 4.020772
N -1.916345 -1.252254 -0.434229
C -1.592971 -2.516640 -0.857583
C -2.753638 -3.359344 -0.894615
C -3.810048 -2.582276 -0.462584
C -3.267281 -1.261926 -0.217954
C -2.737982 -4.784084 -1.350654
C -5.226114 -2.962236 -0.277080
O -6.123763 -2.136360 -0.245569
C -5.576865 -4.427644 -0.092426
N -2.231450 1.516717 0.101177
C -3.524861 1.131103 0.192154
C -4.470961 2.303665 0.320074
C -3.512285 3.447438 0.494426
C -2.174406 2.890596 0.253148
C -5.354674 2.439768 -0.933797
C -3.811009 4.701705 0.847395
C -5.178024 5.224415 1.155733
N 0.486445 1.747792 0.078679
C 0.247065 3.112151 0.201062
C 1.473209 3.844665 0.357132
C 2.461273 2.878152 0.352231
C 1.815269 1.636816 0.173201
C 1.609703 5.321602 0.509033
C 3.895993 2.649188 0.440207
O 4.807939 3.427109 0.593195
C 4.093946 1.085084 0.298271
C 5.038317 0.759329 -0.842140
O 6.048747 0.112989 -0.739838
O 4.589818 1.269841 -2.002379
C 5.412700 1.029368 -3.154781
H -0.185626 -3.955091 -1.526893
H -5.075846 -0.285588 0.217975
H -1.121838 4.712399 0.359282
H 4.028292 -1.672057 -0.882153
H 2.250064 -3.853736 -0.904063
H 1.830474 -3.287232 -3.313509
H 2.516898 -1.680580 -3.048810
H 3.543687 -3.114694 -2.898224
H 4.077366 -3.415298 0.831178
H 4.161972 -1.815215 1.516359

H 1.705706 -1.938727 2.108766
H 1.626286 -3.549666 1.462447
H -2.663302 -5.477300 -0.507939
H -3.640246 -5.038692 -1.902719
H -1.892635 -4.980584 -2.008105
H -6.539299 -4.482605 0.412125
H -5.678892 -4.909519 -1.067730
H -4.822593 -4.972807 0.473439
H -5.993276 3.319826 -0.857710
H -4.732898 2.546463 -1.824290
H -5.987098 1.560675 -1.060566
H -3.006128 5.423560 0.939947
H -5.113196 2.173793 1.195452
H -5.167558 5.801361 2.084489
H -5.528212 5.903823 0.371344
H -5.917089 4.430356 1.259462
H 2.660294 5.597032 0.584383
H 1.175339 5.852303 -0.342258
H 1.098803 5.678553 1.407729
H 4.566417 0.711888 1.207656
H 4.908925 1.522242 -3.981643
H 6.407450 1.447928 -3.004930
H 5.501956 -0.041022 -3.342261
H 2.006018 -4.027124 4.862174

Zn-Bchl *b*

Zn -0.771781 0.147208 -0.120152
C 2.658368 0.571953 -0.147087
C -0.278788 -3.167730 -0.702754
C -4.120637 -0.245674 -0.042177
C -1.169258 3.544463 0.443174
N 0.990349 -1.124120 -0.379509
C 2.297815 -0.743604 -0.323368
C 3.222616 -1.941992 -0.412804
C 2.262839 -3.050559 -0.901015
C 0.895464 -2.444475 -0.635231
C 2.445694 -3.375152 -2.388528
C 3.903748 -2.253379 0.933333
C 2.933114 -2.386569 2.101848
C 3.621787 -2.713725 3.401181
O 4.803528 -2.874843 3.558051
O 2.730434 -2.812297 4.418261
N -1.977701 -1.421346 -0.317952
C -1.596783 -2.720931 -0.547857
C -2.761520 -3.560919 -0.613508
C -3.858342 -2.734909 -0.426231
C -3.346316 -1.388949 -0.255328
C -2.723688 -5.033295 -0.878508
C -5.291075 -3.098959 -0.394001
O -6.169449 -2.282640 -0.618028
C -5.686373 -4.522359 -0.045725
N -2.418326 1.473702 0.159220
C -3.696399 1.058519 0.137040
C -4.656059 2.224458 0.288082
C -3.703723 3.360828 0.602556
C -2.347745 2.819933 0.394737
C -5.464664 2.450778 -1.001641
C -4.023217 4.587028 1.026321
C -5.403474 5.097432 1.292851
N 0.418884 1.711931 0.072344
C 0.129859 3.052031 0.297905
C 1.350533 3.816024 0.375664
C 2.366127 2.891157 0.195331
C 1.756273 1.628821 0.015885
C 1.466401 5.284622 0.606951
C 3.811492 2.720951 0.139741
O 4.703316 3.529126 0.254378
C 4.057182 1.180710 -0.090723
C 4.854802 0.910078 -1.352277
O 5.773102 0.133763 -1.430536
O 4.378950 1.614239 -2.391240
C 5.050870 1.419745 -3.646025
H -0.155740 -4.222998 -0.902748

H -5.187127 -0.407688 -0.043633
H -1.256874 4.607844 0.619617
H 4.016708 -1.765639 -1.139361
H 2.395170 -3.969462 -0.324006
H 1.710844 -4.107719 -2.726081
H 2.325776 -2.474213 -2.994391
H 3.443479 -3.778844 -2.571547
H 4.477188 -3.176719 0.826618
H 4.634820 -1.476614 1.158709
H 2.365330 -1.464431 2.253733
H 2.182682 -3.162322 1.926534
H -2.823371 -5.612163 0.043784
H -3.527069 -5.342883 -1.544631
H -1.786426 -5.329019 -1.346264
H -6.714369 -4.509707 0.310609
H -5.646103 -5.148376 -0.940140
H -5.032554 -4.967521 0.703280
H -6.115820 3.319327 -0.902062
H -4.793059 2.624450 -1.844181
H -6.080120 1.579484 -1.228998
H -3.220497 5.293293 1.214969
H -5.348956 2.041472 1.113809
H -5.448603 5.592551 2.266821
H -5.697911 5.846049 0.549712
H -6.152200 4.305862 1.280527
H 2.512926 5.584308 0.622122
H 0.958708 5.851756 -0.178048
H 1.012908 5.574753 1.558723
H 4.653369 0.799678 0.738920
H 4.543344 2.070162 -4.352888
H 6.102324 1.691889 -3.558883
H 4.977592 0.378274 -3.959942
H 3.234016 -3.019126 5.221174

Sr-Bchl *b*

Sr -0.703998 0.358980 -1.653571
C 2.753197 0.288739 -0.168180
C -0.483886 -3.213304 -0.750825
C -4.038471 0.064174 -0.162347
C -0.772337 3.615225 0.335293
N 0.988959 -1.257908 -0.681872
C 2.285764 -1.000404 -0.376616
C 3.051730 -2.295192 -0.136499
C 2.075075 -3.351684 -0.708714
C 0.756142 -2.591697 -0.728775
C 2.467882 -3.815882 -2.115970
C 3.371476 -2.516316 1.355568
C 2.160325 -2.394747 2.275199
C 2.509320 -2.589856 3.726899
O 3.610687 -2.778109 4.174494
O 1.406062 -2.525460 4.512184
N -2.064928 -1.331274 -0.588274
C -1.782150 -2.665666 -0.621106
C -2.995594 -3.421181 -0.430010
C -4.016579 -2.491080 -0.267683
C -3.397150 -1.176046 -0.363740
C -3.068236 -4.916173 -0.429141
C -5.452452 -2.726553 -0.027486
O -6.290819 -1.864574 -0.243803
C -5.909281 -4.066226 0.521129
N -2.217897 1.711262 -0.186610
C -3.507077 1.343597 -0.035885
C -4.365130 2.544067 0.337823
C -3.309648 3.595139 0.630949
C -2.019133 2.999207 0.221080
C -5.305129 2.932608 -0.816389
C -3.505150 4.794494 1.186941
C -4.812086 5.351943 1.655764
N 0.676399 1.736778 -0.255944
C 0.496854 3.033234 0.182561
C 1.768541 3.610028 0.573987
C 2.690292 2.593340 0.389645
C 1.976502 1.462448 -0.094144

C 1.999014 4.978912 1.118732
C 4.084825 2.224622 0.572459
O 5.031961 2.878789 0.946563
C 4.180083 0.698779 0.198533
C 5.149090 0.427361 -0.934629
O 5.924202 -0.495049 -0.969225
O 5.007052 1.317976 -1.932462
C 5.877151 1.139627 -3.060418
H -0.436405 -4.294166 -0.778453
H -5.105671 -0.007182 -0.013742
H -0.777523 4.638183 0.688099
H 3.999774 -2.294060 -0.676729
H 2.015469 -4.225713 -0.055984
H 1.722865 -4.499468 -2.527248
H 2.553658 -2.960827 -2.791223
H 3.432312 -4.327730 -2.097506
H 3.820226 -3.505570 1.470474
H 4.135565 -1.810186 1.678407
H 1.687511 -1.412792 2.181651
H 1.376824 -3.114192 2.024151
H -3.177767 -5.317553 0.581930
H -3.913140 -5.279959 -1.013135
H -2.168549 -5.356251 -0.855670
H -6.914845 -3.945178 0.918416
H -5.943714 -4.808421 -0.279546
H -5.241979 -4.445394 1.294807
H -5.883343 3.822364 -0.565959
H -4.728550 3.149148 -1.718260
H -5.998030 2.119929 -1.039120
H -2.644855 5.439272 1.338290
H -4.966042 2.326262 1.224398
H -4.716276 5.753537 2.668556
H -5.139159 6.183248 1.022105
H -5.607029 4.606810 1.662689
H 3.058290 5.137600 1.314546
H 1.658637 5.748762 0.420631
H 1.452364 5.130163 2.053938
H 4.567634 0.161965 1.063975
H 5.638751 1.948963 -3.745312
H 6.919688 1.196649 -2.748597
H 5.700907 0.171636 -3.530578
H 1.700796 -2.644906 5.428552

Pd-Bchl *b*

Pd -0.688706 0.190868 -0.122237
C 2.733521 0.470607 -0.107815
C -0.376807 -3.141548 -0.751462
C -4.056351 -0.086215 -0.070991
C -0.929591 3.586629 0.452871
N 0.931367 -1.114307 -0.376771
C 2.267403 -0.802243 -0.288047
C 3.121826 -2.047354 -0.352464
C 2.140344 -3.073157 -0.941803
C 0.795262 -2.432996 -0.665218
C 2.347555 -3.286801 -2.446368
C 3.679301 -2.431992 1.031622
C 2.617426 -2.575546 2.116891
C 3.201415 -2.932606 3.458973
O 4.370200 -3.063998 3.712513
O 2.229920 -3.094044 4.390271
N -1.997035 -1.356234 -0.347230
C -1.674575 -2.661698 -0.585646
C -2.871207 -3.456447 -0.652462
C -3.931174 -2.587777 -0.454788
C -3.354151 -1.267577 -0.278810
C -2.882632 -4.928098 -0.921066
C -5.378583 -2.879709 -0.421250
O -6.218058 -2.002982 -0.549998
C -5.842900 -4.307026 -0.199010
N -2.227589 1.522876 0.142191
C -3.532535 1.172864 0.104096
C -4.429935 2.384039 0.239008
C -3.439476 3.460520 0.604090

C -2.106480 2.874701 0.393777
C -5.173202 2.671948 -1.078196
C -3.715718 4.682006 1.069801
C -5.080683 5.236240 1.327356
N 0.581550 1.718871 0.097142
C 0.350498 3.063545 0.314410
C 1.602821 3.773995 0.397375
C 2.576237 2.803651 0.226539
C 1.903596 1.574803 0.046157
C 1.773790 5.236923 0.627687
C 4.009908 2.546327 0.184455
O 4.948274 3.298115 0.305800
C 4.166666 0.989663 -0.042793
C 4.952621 0.675745 -1.302081
O 5.831720 -0.144967 -1.376181
O 4.513999 1.400146 -2.343021
C 5.175832 1.168834 -3.597061
H -0.267674 -4.193294 -0.973224
H -5.131099 -0.170689 -0.071422
H -1.005499 4.649928 0.629634
H 3.976829 -1.895719 -1.011685
H 2.217996 -4.037514 -0.433927
H 1.590153 -3.956019 -2.857129
H 2.282947 -2.336059 -2.980132
H 3.331727 -3.719484 -2.636769
H 4.231052 -3.369569 0.932160
H 4.412687 -1.688409 1.344860
H 2.050190 -1.649087 2.243996
H 1.873531 -3.336904 1.868776
H -3.073870 -5.502517 -0.010942
H -3.651549 -5.199289 -1.642940
H -1.930003 -5.267118 -1.322952
H -6.888707 -4.279368 0.099005
H -5.765548 -4.876140 -1.128081
H -5.250543 -4.822977 0.556168
H -5.778467 3.574041 -0.986551
H -4.460216 2.820944 -1.890825
H -5.826094 1.839472 -1.342734
H -2.891289 5.348186 1.303242
H -5.162978 2.221329 1.032967
H -5.131881 5.684511 2.323467
H -5.323290 6.032121 0.615310
H -5.861506 4.479591 1.256405
H 2.831381 5.492939 0.662382
H 1.305872 5.822180 -0.168692
H 1.314635 5.548493 1.569889
H 4.734702 0.573849 0.789609
H 4.701084 1.841315 -4.305970
H 6.239414 1.388863 -3.510167
H 5.050891 0.131294 -3.907581
H 2.668976 -3.310937 5.227660

Cd-Bchl *b*

Cd -0.738480 0.164400 -0.406885
C 2.722122 0.470823 -0.210749
C -0.362878 -3.216595 -0.674504
C -4.114194 -0.134042 -0.051888
C -1.009484 3.598695 0.363732
N 1.032699 -1.214386 -0.486806
C 2.335370 -0.854747 -0.379210
C 3.211294 -2.101025 -0.369270
C 2.214782 -3.212870 -0.808235
C 0.856900 -2.541532 -0.641272
C 2.438194 -3.663089 -2.256419
C 3.851225 -2.361636 1.007037
C 2.854619 -2.353230 2.161245
C 3.495146 -2.651700 3.491684
O 4.656312 -2.903033 3.680561
O 2.585288 -2.607147 4.496005
N -2.068174 -1.454643 -0.399127
C -1.698236 -2.758293 -0.546336
C -2.894367 -3.564649 -0.516418
C -3.968458 -2.692451 -0.342146

C -3.417478 -1.345248 -0.269300
C -2.900618 -5.052658 -0.676002
C -5.407979 -3.005960 -0.236938
O -6.261190 -2.143006 -0.370228
C -5.846968 -4.426025 0.065172
N -2.383390 1.595143 0.053112
C -3.658725 1.178493 0.100918
C -4.575439 2.374628 0.324133
C -3.572690 3.492125 0.593755
C -2.234848 2.922783 0.316499
C -5.455210 2.637536 -0.910018
C -3.844885 4.723432 1.034601
C -5.196502 5.264850 1.376644
N 0.560846 1.783880 -0.119135
C 0.298561 3.097281 0.198695
C 1.562683 3.785216 0.395291
C 2.541838 2.816353 0.207139
C 1.882110 1.598165 -0.092742
C 1.744546 5.221096 0.753065
C 3.975406 2.552852 0.251194
O 4.905499 3.290310 0.479584
C 4.145487 1.010629 -0.040455
C 4.997072 0.737872 -1.265815
O 5.818430 -0.140887 -1.345017
O 4.684946 1.564466 -2.275325
C 5.413663 1.370978 -3.498345
H -0.262211 -4.287134 -0.796843
H -5.185055 -0.255931 0.012625
H -1.067901 4.653194 0.601000
H 4.025445 -2.005016 -1.088815
H 2.297040 -4.085442 -0.155198
H 1.690764 -4.397809 -2.560469
H 2.369860 -2.811628 -2.937164
H 3.427160 -4.111477 -2.370305
H 4.364656 -3.324851 0.974391
H 4.629181 -1.621824 1.194641
H 2.353139 -1.385264 2.246643
H 2.052222 -3.081958 2.015741
H -3.135256 -5.561355 0.262035
H -3.636549 -5.376553 -1.411752
H -1.930812 -5.417468 -1.008407
H -6.897272 -4.403415 0.346995
H -5.738632 -5.053870 -0.821640
H -5.255151 -4.876765 0.861976
H -6.075007 3.522395 -0.764897
H -4.832507 2.800237 -1.791467
H -6.107730 1.785495 -1.105180
H -3.017765 5.412072 1.178463
H -5.220307 2.205719 1.190621
H -5.174803 5.763090 2.349798
H -5.515854 6.018217 0.648803
H -5.961881 4.490136 1.410278
H 2.802113 5.456445 0.860306
H 1.323268 5.876951 -0.013959
H 1.241825 5.462528 1.693662
H 4.669205 0.562056 0.803792
H 5.040610 2.127395 -4.183114
H 6.481948 1.500034 -3.327174
H 5.234626 0.371046 -3.894056
H 3.058179 -2.804360 5.319727

Ba-Bchl *b*

Ba -0.683104 0.390147 -1.837607
C 2.792064 0.257063 -0.077865
C -0.443709 -3.236864 -0.667440
C -3.989219 0.044609 -0.035861
C -0.723640 3.585807 0.479954
N 1.034123 -1.287586 -0.610196
C 2.325073 -1.032069 -0.288865
C 3.085076 -2.327311 -0.027882
C 2.115523 -3.383488 -0.612353
C 0.798250 -2.620022 -0.647441
C 2.524674 -3.846051 -2.015347

C 3.373685 -2.541543 1.471659
C 2.144063 -2.414448 2.365921
C 2.464918 -2.595785 3.825718
O 3.558386 -2.771908 4.297296
O 1.345639 -2.534038 4.588262
N -2.019083 -1.348792 -0.495221
C -1.738747 -2.683311 -0.527581
C -2.950160 -3.438633 -0.319283
C -3.968122 -2.507974 -0.146310
C -3.347640 -1.193258 -0.252287
C -3.023591 -4.933645 -0.311961
C -5.400319 -2.742730 0.112612
O -6.243392 -1.885400 -0.105261
C -5.848695 -4.076402 0.683206
N -2.175682 1.697347 -0.063967
C -3.459642 1.323308 0.102966
C -4.315389 2.514151 0.514008
C -3.257280 3.561335 0.811507
C -1.972811 2.974590 0.368951
C -5.273315 2.922766 -0.618077
C -3.445164 4.749111 1.394191
C -4.745180 5.295852 1.894252
N 0.717734 1.713989 -0.161392
C 0.541548 3.000388 0.308251
C 1.813237 3.565395 0.717418
C 2.731985 2.550739 0.514765
C 2.015942 1.431337 0.003767
C 2.045052 4.919255 1.298162
C 4.124079 2.177010 0.698966
O 5.070922 2.824028 1.087110
C 4.217887 0.658064 0.301340
C 5.190392 0.402595 -0.832156
O 5.969836 -0.515716 -0.875640
O 5.047406 1.303714 -1.821415
C 5.923139 1.141560 -2.947106
H -0.401077 -4.318097 -0.690094
H -5.054197 -0.031288 0.126291
H -0.721179 4.600631 0.855622
H 4.043384 -2.331185 -0.549874
H 2.047626 -4.258000 0.038861
H 1.783634 -4.527972 -2.436621
H 2.619821 -2.989758 -2.687974
H 3.488269 -4.359085 -1.986870
H 3.819330 -3.530477 1.600916
H 4.130979 -1.834148 1.807477
H 1.671169 -1.434403 2.254204
H 1.366844 -3.137328 2.105700
H -3.102937 -5.332021 0.703267
H -3.885611 -5.298825 -0.869278
H -2.137172 -5.375635 -0.763800
H -6.844087 -3.948119 1.103363
H -5.906399 -4.824072 -0.111107
H -5.164661 -4.453075 1.443241
H -5.850149 3.805973 -0.342366
H -4.710443 3.158792 -1.523913
H -5.967351 2.112665 -0.846763
H -2.582893 5.391321 1.545530
H -4.902311 2.277801 1.405143
H -4.634748 5.674649 2.914356
H -5.081597 6.141046 1.284274
H -5.539887 4.550421 1.896250
H 3.105685 5.075073 1.489056
H 1.696096 5.707750 0.625606
H 1.506855 5.042324 2.242430
H 4.601514 0.106425 1.159085
H 5.684768 1.957593 -3.624140
H 6.964144 1.199305 -2.630266
H 5.753381 0.178105 -3.428995
H 1.623198 -2.643146 5.511238

Pt-Bchl *b*

Pt -0.625053 0.179697 -0.114533
C 2.799236 0.435943 -0.098792

C -0.343605 -3.154558 -0.743051
C -3.998592 -0.071550 -0.070295
C -0.836121 3.573407 0.464258
N 0.970993 -1.129053 -0.367453
C 2.316036 -0.829716 -0.274528
C 3.154232 -2.084076 -0.327001
C 2.171166 -3.096375 -0.933808
C 0.829713 -2.452966 -0.657603
C 2.386654 -3.291996 -2.439859
C 3.682273 -2.475837 1.067008
C 2.599707 -2.614401 2.132505
C 3.158969 -2.965046 3.486790
O 4.323761 -3.079507 3.765920
O 2.169812 -3.141114 4.396393
N -1.951134 -1.360442 -0.339600
C -1.639854 -2.671019 -0.577290
C -2.841640 -3.453785 -0.645146
C -3.896000 -2.576123 -0.450730
C -3.310326 -1.261401 -0.274156
C -2.863312 -4.925811 -0.911290
C -5.345572 -2.855054 -0.421650
O -6.177020 -1.967098 -0.526355
C -5.824303 -4.282672 -0.236143
N -2.148718 1.513571 0.147879
C -3.463238 1.180177 0.105758
C -4.343641 2.401365 0.237569
C -3.343738 3.463526 0.615966
C -2.016094 2.869311 0.404722
C -5.070977 2.705376 -1.085195
C -3.610947 4.682919 1.092426
C -4.972045 5.247751 1.347240
N 0.665374 1.702643 0.103715
C 0.443159 3.049470 0.324337
C 1.700749 3.749656 0.408257
C 2.668318 2.773181 0.234773
C 1.987267 1.551230 0.052275
C 1.880646 5.210790 0.643000
C 4.099528 2.499074 0.195564
O 5.046944 3.238687 0.319313
C 4.238736 0.939055 -0.032019
C 5.020914 0.615921 -1.291348
O 5.887337 -0.218079 -1.366342
O 4.593830 1.348835 -2.330865
C 5.251531 1.109113 -3.585594
H -0.238234 -4.206485 -0.966054
H -5.074244 -0.144700 -0.073349
H -0.909150 4.636717 0.642915
H 4.022308 -1.942305 -0.970975
H 2.240632 -4.067026 -0.437069
H 1.626989 -3.950527 -2.863484
H 2.331565 -2.333999 -2.961572
H 3.369018 -3.728927 -2.629772
H 4.229883 -3.416723 0.975791
H 4.414062 -1.737281 1.395607
H 2.030720 -1.687057 2.245688
H 1.859892 -3.375959 1.873726
H -3.095133 -5.495392 -0.007872
H -3.609753 -5.188235 -1.659848
H -1.901789 -5.278967 -1.277887
H -6.877212 -4.253033 0.035164
H -5.724125 -4.839063 -1.170578
H -5.255395 -4.812976 0.527265
H -5.665630 3.614592 -0.994518
H -4.348556 2.848920 -1.890425
H -5.731717 1.882251 -1.359416
H -2.781756 5.338954 1.337424
H -5.086035 2.245547 1.024022
H -5.026091 5.683831 2.348605
H -5.201170 6.055085 0.643667
H -5.760176 4.500362 1.260943
H 2.939720 5.459956 0.680961
H 1.418502 5.801126 -0.153030
H 1.421074 5.522726 1.584870
H 4.800878 0.516411 0.800837
H 4.786850 1.789838 -4.293284

H 6.318398 1.312614 -3.498793
H 5.110364 0.074062 -3.897414
H 2.593511 -3.350806 5.243472

Hg-Bchl *b*

Hg -0.714639 0.160812 -0.613320
C 2.768230 0.494116 -0.190535
C -0.208392 -3.241960 -0.664442
C -4.058522 -0.244231 0.021988
C -1.066720 3.540562 0.410230
N 1.167775 -1.247599 -0.472331
C 2.447769 -0.852571 -0.345971
C 3.359263 -2.076302 -0.306448
C 2.388525 -3.225926 -0.724309
C 1.015213 -2.569954 -0.612020
C 2.653684 -3.733166 -2.145821
C 4.007645 -2.296305 1.072358
C 3.013961 -2.274449 2.228922
C 3.660588 -2.539366 3.563452
O 4.825078 -2.773404 3.754570
O 2.752638 -2.485711 4.569024
N -1.966053 -1.490937 -0.459168
C -1.548440 -2.792401 -0.557476
C -2.718397 -3.626589 -0.447926
C -3.811729 -2.785477 -0.253344
C -3.315648 -1.417024 -0.247758
C -2.685975 -5.119568 -0.551828
C -5.230683 -3.151402 -0.055703
O -6.128751 -2.345452 -0.236038
C -5.587699 -4.551783 0.406316
N -2.415398 1.542417 0.156247
C -3.667931 1.087229 0.208957
C -4.618319 2.252395 0.472447
C -3.638463 3.403115 0.713592
C -2.292679 2.864910 0.406880
C -5.553285 2.492048 -0.724304
C -3.930191 4.629790 1.153771
C -5.284386 5.140244 1.531497
N 0.553684 1.761552 -0.194982
C 0.241680 3.054428 0.194947
C 1.483122 3.753164 0.456874
C 2.490530 2.817587 0.261456
C 1.883021 1.593324 -0.112276
C 1.624703 5.169450 0.902049
C 3.927770 2.601020 0.370625
O 4.816228 3.365451 0.667133
C 4.162979 1.079283 0.048075
C 5.066838 0.859118 -1.150535
O 5.897681 -0.010966 -1.226252
O 4.788935 1.718785 -2.141723
C 5.565368 1.571769 -3.341879
H -0.109954 -4.315824 -0.757030
H -5.118973 -0.425961 0.114091
H -1.113003 4.590743 0.669681
H 4.169325 -1.974210 -1.030178
H 2.471376 -4.068723 -0.033010
H 1.926618 -4.494326 -2.434382
H 2.585639 -2.913296 -2.864288
H 3.652487 -4.168047 -2.218964
H 4.533478 -3.253287 1.060681
H 4.777361 -1.543189 1.239680
H 2.501454 -1.310786 2.295824
H 2.218685 -3.014099 2.100026
H -2.733512 -5.596470 0.430805
H -3.519908 -5.500586 -1.138670
H -1.771365 -5.460429 -1.033700
H -6.594136 -4.524416 0.818546
H -5.586087 -5.238291 -0.443289
H -4.887724 -4.937362 1.146835
H -6.198796 3.353015 -0.550724
H -4.971244 2.681167 -1.628002
H -6.182311 1.618347 -0.900591
H -3.115662 5.339093 1.268108

H -5.222514 2.059293 1.363275
H -5.246180 5.648401 2.498973
H -5.645039 5.877808 0.806798
H -6.027543 4.346059 1.595746
H 2.676027 5.425301 1.022538
H 1.183015 5.859381 0.177899
H 1.119592 5.337661 1.857164
H 4.667696 0.625159 0.900736
H 5.213874 2.349669 -4.013827
H 6.625408 1.700313 -3.125186
H 5.407917 0.585320 -3.778414
H 3.229982 -2.660489 5.395232

Pb-Bchl *b*

Pb -0.660509 -0.076951 1.150134
C 2.657670 0.856249 -0.240800
C 0.069034 -3.133498 -0.762316
C -4.024297 -0.559557 -0.122359
C -1.434831 3.487343 0.366331
N 1.202450 -1.043754 -0.251067
C 2.441834 -0.495336 -0.379528
C 3.466836 -1.564198 -0.709028
C 2.570434 -2.752770 -1.134036
C 1.189091 -2.319599 -0.661382
C 2.600582 -2.995620 -2.647412
C 4.398917 -1.865487 0.478388
C 3.661184 -2.176726 1.775924
C 4.585762 -2.553057 2.904498
O 5.776473 -2.703239 2.828349
O 3.901317 -2.719557 4.063796
N -1.789089 -1.578296 -0.283402
C -1.288643 -2.802534 -0.637110
C -2.382015 -3.698214 -0.928496
C -3.547729 -2.971130 -0.752373
C -3.150530 -1.628422 -0.358500
C -2.216929 -5.111428 -1.392569
C -4.945227 -3.417180 -0.936176
O -5.848568 -2.632831 -1.173906
C -5.273675 -4.892543 -0.794831
N -2.507588 1.299556 0.294713
C -3.725808 0.779273 0.096900
C -4.777512 1.875671 0.026712
C -3.956855 3.107290 0.362378
C -2.549759 2.664989 0.363237
C -5.427307 1.947892 -1.365958
C -4.413782 4.331041 0.641981
C -5.850179 4.743703 0.701744
N 0.332331 1.788287 0.159317
C -0.092351 3.107740 0.219238
C 1.030107 3.993561 0.043521
C 2.125146 3.157446 -0.122794
C 1.655061 1.825855 -0.047694
C 0.994335 5.484222 0.008115
C 3.559896 3.139880 -0.357022
O 4.348949 4.048242 -0.476257
C 3.969554 1.615291 -0.417480
C 4.694862 1.304065 -1.711556
O 5.799968 0.831986 -1.788513
O 3.933668 1.605126 -2.778018
C 4.526477 1.361057 -4.063004
H 0.275600 -4.147638 -1.074691
H -5.069570 -0.793793 -0.249055
H -1.621193 4.552261 0.399895
H 4.101004 -1.254809 -1.540517
H 2.871474 -3.673827 -0.626393
H 1.914808 -3.793735 -2.935024
H 2.307230 -2.090951 -3.184558
H 3.605662 -3.274911 -2.969778
H 5.041645 -2.707437 0.212556
H 5.068126 -1.018304 0.635797
H 3.062008 -1.324730 2.106890
H 2.952476 -3.001354 1.654688
H -2.369078 -5.823122 -0.576504

H -2.926322 -5.363158 -2.179209
H -1.219204 -5.285104 -1.791112
H -6.329308 -4.981550 -0.546267
H -5.107027 -5.401561 -1.747037
H -4.664530 -5.387927 -0.039761
H -6.144621 2.767187 -1.415368
H -4.666057 2.115603 -2.129686
H -5.945521 1.017292 -1.599846
H -3.692459 5.112048 0.862770
H -5.556357 1.694102 0.773214
H -6.049764 5.312988 1.613718
H -6.107998 5.399086 -0.136990
H -6.530773 3.892878 0.677629
H 2.002515 5.885110 -0.083071
H 0.406450 5.846134 -0.840141
H 0.540302 5.895141 0.913684
H 4.682683 1.424740 0.385799
H 3.783004 1.671950 -4.791718
H 5.442195 1.940888 -4.175032
H 4.759956 0.302421 -4.180270
H 4.547039 -2.965907 4.744579

Optimized atomic coordinates for M-Phts

H_2-Pht (Pht)

N -0.000039 2.022334 -0.000000
C 1.142383 2.784449 -0.000000
C -1.142162 2.784299 -0.000000
C 0.704286 4.164946 -0.000000
N 2.387915 2.374406 -0.000000
C -0.704263 4.164894 -0.000000
C 1.421157 5.358265 -0.000000
C -1.421325 5.358070 -0.000000
N -2.387937 2.374395 -0.000000
C 2.754859 1.096007 -0.000000
C -2.754758 1.095993 -0.000000
C 4.163410 -0.699867 0.000000
C 4.163411 0.699898 -0.000000
C 2.754859 -1.095978 0.000000
C 5.349287 -1.419606 0.000000
C 5.349287 1.419637 -0.000000
N 1.949581 0.000015 -0.000000
N 2.387918 -2.374377 0.000000
C -4.163379 -0.699899 0.000000
C -4.163379 0.699869 -0.000000
C -2.754758 -1.096022 0.000000
C -5.349195 -1.419631 0.000000
C -5.349195 1.419600 -0.000000
N -1.949496 -0.000015 0.000000
N -2.387934 -2.374423 0.000000
C 1.142388 -2.784434 0.000000
C -0.704241 -4.164904 0.000000
C 0.704308 -4.164937 0.000000
C -1.142157 -2.784314 0.000000
C -1.421288 -5.358088 0.000000
C 1.421194 -5.358247 0.000000
N -0.000043 -2.022334 0.000000
C -0.702980 6.543279 -0.000000
C 0.702618 6.543355 -0.000000
C -6.540808 -0.700175 0.000000
C -6.540809 0.700144 -0.000000
C 0.702670 -6.543346 0.000000
C -0.702928 -6.543288 0.000000
C 6.540849 0.700206 -0.000000
C 6.540849 -0.700175 0.000000
H 2.502623 5.347495 -0.000000
H -2.502789 5.347041 -0.000000
H 5.339742 -2.501381 0.000000
H 5.339742 2.501412 -0.000000
H -5.339707 -2.501405 0.000000
H -5.339708 2.501374 -0.000000
H -2.502752 -5.347073 0.000000
H 2.502659 -5.347463 0.000000

H -1.230315 7.488683 -0.000000
H 1.229844 7.488823 -0.000000
H -7.485580 -1.229073 0.000000
H -7.485580 1.229042 -0.000000
H 1.229909 -7.488807 0.000000
H -1.230251 -7.488699 0.000000
H 7.485655 1.229043 -0.000000
H 7.485655 -1.229012 0.000000
H 0.000008 1.012572 -0.000000
H -0.000007 -1.012572 0.000000

Be-Pht

N -1.591245 0.995404 0.000334
C -2.881635 0.506892 0.000274
C -1.716539 2.369386 0.000279
C -3.847878 1.584863 0.000095
N -3.256289 -0.750153 0.000378
C -3.108593 2.766650 0.000098
C -5.239790 1.600304 -0.000173
C -3.731333 4.011572 -0.000165
N -0.750158 3.256327 0.000385
C -2.369331 -1.716538 0.000263
C 0.506884 2.881577 0.000267
C -1.584850 -3.847915 0.000065
C -2.766662 -3.108574 0.000067
C -0.506891 -2.881650 0.000260
C -1.600333 -5.239785 -0.000213
C -4.011556 -3.731287 -0.000207
N -0.995346 -1.591311 0.000330
N 0.750171 -3.256347 0.000373
C 2.766647 3.108570 0.000071
C 1.584852 3.847844 0.000073
C 2.369401 1.716529 0.000263
C 4.011564 3.731326 -0.000207
C 1.600273 5.239750 -0.000201
N 0.995361 1.591251 0.000325
N 3.256327 0.750168 0.000380
C 1.716546 -2.369432 0.000270
C 3.847865 -1.584829 0.000094
C 3.108579 -2.766648 0.000091
C 2.881613 -0.506883 0.000277
C 5.239760 -1.600266 -0.000168
C 3.731342 -4.011546 -0.000178
N 1.591248 -0.995356 0.000337
C -5.118021 4.030902 -0.000421
C -5.863751 2.838844 -0.000426
C 4.030874 5.118013 -0.000471
C 2.838807 5.863727 -0.000467
C 5.118042 -4.030861 -0.000432
C 5.863746 -2.838811 -0.000426
C -4.030917 -5.118010 -0.000476
C -2.838916 -5.863740 -0.000480
H -5.802831 0.676954 -0.000179
H -3.147295 4.921785 -0.000157
H -0.677031 -5.802909 -0.000216
H -4.921800 -3.147295 -0.000203
H 4.921790 3.147308 -0.000210
H 0.676914 5.802774 -0.000194
H 5.802820 -0.676927 -0.000161
H 3.147353 -4.921792 -0.000185
H -5.641076 4.978829 -0.000628
H -6.944975 2.894548 -0.000641
H 4.978795 5.641078 -0.000693
H 2.894499 6.944951 -0.000684
H 5.641068 -4.978803 -0.000647
H 6.944972 -2.894458 -0.000634
H -4.978893 -5.640975 -0.000694
H -2.894566 -6.944966 -0.000702
Be 0.000245 0.000046 0.000191

Mg-Pht

N 0.630228 -1.899290 -0.000476
C 1.940892 -2.291969 -0.000206
C -0.185841 -2.997916 -0.000427
C 1.985490 -3.748939 -0.000116
N 3.015603 -1.512838 -0.000080
C 0.649782 -4.192295 -0.000249
C 3.040611 -4.653522 0.000074
C 0.345092 -5.548299 -0.000194
N -1.512867 -3.015623 -0.000479
C 2.997830 -0.185880 0.000013
C -2.292055 -1.941195 -0.000489
C 3.748938 1.985470 0.000108
C 4.192242 0.649791 0.000018
C 2.291909 1.941021 0.000161
C 4.653522 3.040565 0.000104
C 5.548205 0.345026 -0.000078
N 1.899216 0.630222 0.000089
N 1.512848 3.015581 0.000188
C -4.192228 -0.649787 -0.000140
C -3.749019 -1.985547 -0.000223
C -2.997705 0.185606 -0.000352
C -5.548194 -0.344909 0.000135
C -4.653766 -3.040549 -0.000033
N -1.899292 -0.630271 -0.000683
N -3.015607 1.512865 -0.000230
C 0.185651 2.997604 0.000120
C -1.985534 3.748993 -0.000098
C -0.649797 4.192160 0.000042
C -1.941304 2.291966 -0.000112
C -3.040509 4.653726 -0.000227
C -0.344860 5.548081 0.000059
N -0.630262 1.899214 0.000010
C 1.401619 -6.449982 0.000006
C 2.733045 -6.008027 0.000138
C -6.450015 -1.401309 0.000326
C -6.008219 -2.732799 0.000243
C -1.401254 6.449953 -0.000046
C -2.732723 6.008201 -0.000186
C 6.449945 1.401537 -0.000058
C 6.008040 2.732951 0.000031
H 4.064238 -4.303616 0.000167
H -0.684569 -5.880010 -0.000305
H 4.303644 4.064199 0.000155
H 5.879868 -0.684648 -0.000165
H -5.879752 0.684801 0.000196
H -4.304003 -4.064226 -0.000101
H -4.064194 4.303993 -0.000353
H 0.684857 5.879608 0.000149
H 1.198154 -7.513384 0.000060
H 3.532045 -6.738656 0.000289
H -7.513391 -1.197716 0.000542
H -6.738957 -3.531701 0.000398
H -1.197616 7.513321 -0.000025
H -3.531620 6.738945 -0.000269
H 7.513338 1.198027 -0.000118
H 6.738689 3.531934 0.000038
Mg 0.000122 0.000146 0.001743

Ca-Pht

N -2.021380 -0.165250 0.429741
C -2.687141 -1.340171 0.216653
C -2.869350 0.885083 0.217448
C -4.088774 -1.040186 -0.063297
N -2.178064 -2.566382 0.170760
C -4.203554 0.361400 -0.062966
C -5.185458 -1.848585 -0.336684
C -5.417076 0.980826 -0.336112
N -2.566902 2.178356 0.172360
C -0.884742 -2.869218 0.215536
C -1.340083 2.687043 0.217372
C 1.040388 -4.088791 -0.064477

C -0.361339 -4.203356 -0.064562
C 1.340369 -2.687362 0.215371
C 1.848647 -5.185795 -0.337111
C -0.980816 -5.416947 -0.337383
N 0.165668 -2.021279 0.427673
N 2.566812 -2.178138 0.170327
C 0.361199 4.203294 -0.064124
C -1.040362 4.088543 -0.063707
C 0.885154 2.869253 0.216731
C 0.980460 5.416643 -0.338480
C -1.848925 5.185004 -0.337505
N -0.165701 2.021273 0.430014
N 2.177994 2.566653 0.171415
C 2.869622 -0.885258 0.215805
C 4.088769 1.040419 -0.063203
C 4.203717 -0.361236 -0.063581
C 2.687147 1.339818 0.216451
C 5.185535 1.849120 -0.335470
C 5.417552 -0.980273 -0.336375
N 2.021296 0.165511 0.428208
C -6.516185 0.170323 -0.592621
C -6.401752 -1.227503 -0.592870
C 0.169819 6.515573 -0.595359
C -1.227998 6.401139 -0.594865
C 6.516635 -0.169477 -0.591772
C 6.402013 1.228378 -0.591314
C -0.170430 -6.516236 -0.593191
C 1.227458 -6.402029 -0.593021
H -5.084716 -2.925671 -0.348167
H -5.492731 2.059976 -0.347242
H 2.925772 -5.085307 -0.348173
H -2.059980 -5.492466 -0.348726
H 2.059602 5.492304 -0.350161
H -2.926009 5.084210 -0.348410
H 5.084655 2.926205 -0.346337
H 5.493424 -2.059411 -0.347971
H -7.477904 0.621930 -0.801386
H -7.277237 -1.829429 -0.801797
H 0.621309 7.477156 -0.805018
H -1.830024 7.276472 -0.804147
H 7.478550 -0.620813 -0.800210
H 7.277543 1.830525 -0.799396
H -0.622118 -7.477967 -0.801702
H 1.829305 -7.277701 -0.801371
Ca -0.000025 -0.000092 1.485441

Ni-Pht

N -1.926762 0.003287 -0.000220
C -2.739197 -1.104533 -0.000196
C -2.735559 1.113780 -0.000286
C -4.129831 -0.691873 -0.000041
N -2.375236 -2.367301 -0.000148
C -4.127495 0.705717 -0.000104
C -5.319045 -1.412367 0.000182
C -5.314286 1.430209 0.000056
N -2.367391 2.375290 -0.000313
C -1.113697 -2.735417 -0.000101
C -1.104647 2.739236 -0.000309
C 0.691892 -4.129815 0.000015
C -0.705728 -4.127440 -0.000038
C 1.104538 -2.739136 -0.000025
C 1.412334 -5.319012 0.000115
C -1.430241 -5.314162 0.000008
N -0.003214 -1.926746 0.000083
N 2.367335 -2.375229 -0.000011
C 0.705700 4.127369 -0.000090
C -0.691875 4.129792 -0.000124
C 1.113695 2.735399 -0.000254
C 1.430305 5.314094 0.000130
C -1.412276 5.319088 0.000061
N 0.003152 1.926641 -0.000286
N 2.375247 2.367324 -0.000216
C 2.735430 -1.113658 -0.000044

C 4.129897 0.691894 -0.000050
C 4.127479 -0.705724 0.000024
C 2.739266 1.104590 -0.000161
C 5.319158 1.412264 0.000023
C 5.314159 -1.430308 0.000172
N 1.926820 -0.003173 0.000009
C -6.502817 0.712999 0.000233
C -6.505175 -0.691161 0.000294
C 0.713204 6.502680 0.000267
C -0.690970 6.505141 0.000234
C 6.502785 -0.713190 0.000199
C 6.505245 0.690933 0.000126
C -0.713047 -6.502751 0.000066
C 0.691066 -6.505150 0.000118
H -5.309359 -2.493888 0.000224
H -5.301010 2.511689 0.000006
H 2.493855 -5.309430 0.000147
H -2.511721 -5.300903 -0.000039
H 2.511782 5.300667 0.000153
H -2.493797 5.309515 0.000031
H 5.309664 2.493787 -0.000042
H 5.300788 -2.511787 0.000222
H -7.447360 1.242109 0.000327
H -7.451499 -1.217075 0.000433
H 1.242371 7.447190 0.000406
H -1.216807 7.451508 0.000347
H 7.447274 -1.242394 0.000279
H 7.451591 1.216809 0.000151
H -1.242221 -7.447258 0.000070
H 1.216989 -7.451470 0.000160
Ni -0.000064 0.000120 0.000066

Zn-Pht

N 1.998230 -0.085787 -0.001629
C 2.829235 0.999840 -0.000848
C 2.733309 -1.238986 -0.001025
C 4.206781 0.523269 -0.000071
N 2.483405 2.278957 -0.000617
C 4.146559 -0.881911 -0.000172
C 5.426922 1.188469 0.000806
C 5.305362 -1.649007 0.000598
N 2.278991 -2.483415 -0.000941
C 1.238959 2.733057 -0.000640
C 1.000104 -2.829300 -0.001048
C -0.523257 4.206647 0.000158
C 0.881875 4.146367 0.000092
C -1.000010 2.829098 -0.000525
C -1.188416 5.426774 0.000896
C 1.649047 5.305078 0.000760
N 0.085730 1.998006 -0.001147
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C 0.523276 -4.206739 -0.000100
C -1.238705 -2.733075 -0.000940
C -1.649172 -5.305052 0.000928
C 1.188295 -5.426999 0.000798
N -0.085791 -1.998089 -0.001776
N -2.483452 -2.278918 -0.000740
C -2.733093 1.238716 -0.000591
C -4.206836 -0.523269 -0.000054
C -4.146454 0.881874 0.000051
C -2.829343 -1.000186 -0.000770
C -5.427055 -1.188278 0.000572
C -5.305079 1.649170 0.000787
N -1.998167 0.085829 -0.001238
C 6.523688 -0.981895 0.001444
C 6.583740 0.419616 0.001547
C -0.982240 -6.523464 0.001791
C 0.419279 -6.583693 0.001727
C -6.523540 0.982239 0.001396
C -6.583780 -0.419230 0.001290
C 0.981982 6.523469 0.001481
C -0.419488 6.583584 0.001548

H 5.463352 2.269626 0.000915
H 5.249217 -2.729319 0.000547
H -2.269567 5.463259 0.000968
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H 2.269447 -5.463589 0.000781
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H 7.445357 -1.549990 0.002047
H 7.550620 0.906798 0.002225
H -1.550450 -7.445060 0.002537
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H -7.550724 -0.906289 0.001786
H 1.550136 7.445102 0.002009
H -0.906641 7.550480 0.002125
Zn 0.000024 -0.000003 -0.001170

Sr-Pht

N -0.123275 -2.028750 0.357912
C 0.943801 -2.848308 0.122980
C -1.281021 -2.713376 0.120132
C 0.450629 -4.187486 -0.191443
N 2.230442 -2.518199 0.076430
C -0.952549 -4.102411 -0.193196
C 1.096321 -5.379611 -0.495668
C -1.736780 -5.207828 -0.499220
N -2.518183 -2.229980 0.071498
C 2.714053 -1.281192 0.125976
C -2.848158 -0.943308 0.119585
C 4.187815 0.450181 -0.188622
C 4.102659 -0.952979 -0.189460
C 2.849110 0.943597 0.127317
C 5.379433 1.095629 -0.495264
C 5.207493 -1.737416 -0.496990
N 2.029832 -0.123316 0.364436
N 2.518773 2.230041 0.078766
C -4.102427 0.953754 -0.191330
C -4.187674 -0.449415 -0.192032
C -2.712954 1.281513 0.120816
C -5.208250 1.738670 -0.494198
C -5.380357 -1.094432 -0.495601
N -2.028129 0.123299 0.355377
N -2.229587 2.518747 0.073607
C 1.281693 2.713624 0.125949
C -0.448919 4.187541 -0.192077
C 0.954228 4.102231 -0.190255
C -0.943044 2.848859 0.122898
C -1.093703 5.379245 -0.499831
C 1.739359 5.207048 -0.496138
N 0.123350 2.029469 0.362010
C -1.089680 -6.404086 -0.784565
C 0.310156 -6.488956 -0.782830
C -6.404991 1.092236 -0.778930
C -6.490030 -0.307613 -0.779624
C 1.093152 6.402947 -0.784964
C -0.306664 6.488039 -0.786782
C 6.403336 -1.090551 -0.784658
C 6.488288 0.309255 -0.783819
H 2.176932 -5.431424 -0.507376
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H 5.128437 -2.816356 -0.510720
H -5.129131 2.817620 -0.506591
H -5.432377 -2.175010 -0.509161
H -2.174270 5.431291 -0.514362
H 2.818309 5.127810 -0.507768
H -1.672495 -7.286185 -1.018539
H 0.782699 -7.435030 -1.015574
H -7.287397 1.675545 -1.010499
H -7.436529 -0.779596 -1.011773
H 1.676685 7.284574 -1.018932
H -0.778528 7.433798 -1.022160

H 7.284979 -1.673583 -1.019806
H 7.433977 0.781665 -1.018389
Sr -0.003036 -0.001159 1.703257

Pd-Pht

N 0.052637 -1.988129 -0.000075
C 1.193851 -2.742467 -0.000128
C -1.047094 -2.801779 -0.000127
C 0.811846 -4.146573 0.000008
N 2.442981 -2.316985 -0.000129
C -0.591281 -4.183702 0.000006
C 1.561489 -5.316065 0.000126
C -1.278034 -5.391186 0.000122
N -2.317000 -2.442990 -0.000129
C 2.801779 -1.047084 -0.000135
C -2.742484 -1.193869 -0.000136
C 4.146586 0.811851 -0.000005
C 4.183699 -0.591279 -0.000008
C 2.742494 1.193884 -0.000135
C 5.316081 1.561481 0.000110
C 5.391172 -1.278042 0.000104
N 1.988125 0.052664 -0.000086
N 2.317017 2.443007 -0.000128
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C -4.146584 -0.811850 -0.000007
C -2.801787 1.047077 -0.000134
C -5.391199 1.278028 0.000098
C -5.316079 -1.561495 0.000105
N -1.988146 -0.052645 -0.000084
N -2.442977 2.316988 -0.000128
C 1.047094 2.801788 -0.000126
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C 1.278021 5.391188 0.000123
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C -6.560570 0.527750 0.000183
C -6.523484 -0.874088 0.000187
C 0.527731 6.560560 0.000215
C -0.874098 6.523464 0.000219
C 6.560557 -0.527771 0.000190
C 6.523486 0.874058 0.000193
H 2.642431 -5.277298 0.000120
H -2.359508 -5.409631 0.000114
H 5.277336 2.642422 0.000105
H 5.409613 -2.359516 0.000096
H -5.409640 2.359503 0.000091
H -5.277310 -2.642436 0.000101
H -2.642442 5.277286 0.000126
H 2.359495 5.409646 0.000115
H -1.031004 -7.519079 0.000282
H 1.427328 -7.454037 0.000285
H -7.519092 1.030998 0.000248
H -7.454050 -1.427331 0.000254
H 1.030982 7.519080 0.000286
H -1.427358 7.454021 0.000291
H 7.519069 -1.031040 0.000257
H 7.454052 1.427302 0.000262
Pd 0.000016 0.000011 -0.000133

Cd-Pht

N -2.053182 0.168595 0.326940
C -2.882075 -0.888664 0.134091
C -2.698612 1.347016 0.133960
C -4.213665 -0.358090 -0.125508
N -2.562686 -2.173734 0.089433
C -4.098936 1.040490 -0.125582
C -5.427072 -0.972872 -0.379988

C -5.195948 1.844780 -0.380058
N -2.173804 2.562716 0.089443
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C -0.888805 2.882076 0.134258
C 0.358030 -4.213563 -0.125625
C -1.040514 -4.098757 -0.125702
C 0.888728 -2.882034 0.134179
C 0.972770 -5.426937 -0.380303
C -1.844871 -5.195662 -0.380365
N -0.168526 -2.053089 0.327290
N 2.173794 -2.562839 0.089468
C 1.040491 4.098868 -0.124890
C -0.358079 4.213679 -0.124859
C 1.346911 2.698466 0.134226
C 1.844880 5.195918 -0.378957
C -0.972768 5.427225 -0.378998
N 0.168510 2.053013 0.326881
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C 4.098872 -1.040566 -0.125710
C 2.882082 0.888676 0.134125
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C 5.195810 -1.844893 -0.380311
N 2.053182 -0.168741 0.327148
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C -6.524288 -0.164761 -0.618634
C 1.226471 6.410302 -0.617201
C -0.164576 6.524450 -0.617231
C 6.410091 -1.226412 -0.619033
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H 2.053738 -5.503789 -0.389062
H -2.923882 -5.095141 -0.389237
H 2.923887 5.095374 -0.387766
H -2.053736 5.504092 -0.387765
H 5.503855 2.053727 -0.388980
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H 7.289866 -1.828706 -0.813765
H 7.490347 0.615529 -0.813716
H -1.828741 -7.289694 -0.813913
H 0.615489 -7.490245 -0.813880
Cd 0.000103 -0.000063 0.947044

Ba-Pht

N 1.652359 -1.184328 0.238175
C 2.911122 -0.717145 -0.008281
C 1.614624 -2.526473 -0.008586
C 3.781009 -1.845106 -0.337269
N 3.317597 0.547616 -0.055881
C 2.962425 -2.987508 -0.337341
C 5.130539 -1.930779 -0.656478
C 3.477482 -4.237834 -0.656560
N 0.547615 -3.317819 -0.056658
C 2.526325 1.614644 -0.007964
C -0.717070 -2.911291 -0.008630
C 1.845115 3.780997 -0.337146
C 2.987465 2.962343 -0.337035
C 0.717082 2.911281 -0.007935
C 1.930869 5.130410 -0.656827
C 4.237799 3.477188 -0.656517
N 1.184189 1.652532 0.238851
N -0.547646 3.317846 -0.055637
C -2.987566 -2.962273 -0.337022
C -1.845237 -3.780944 -0.337497
C -2.526274 -1.614600 -0.008033

C -4.238029 -3.477113 -0.656019
C -1.931126 -5.130381 -0.657087
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C -2.962358 2.987560 -0.336961
C -2.911183 0.717168 -0.007949
C -5.130345 1.930838 -0.656924
C -3.477262 4.237866 -0.656457
N -1.652453 1.184376 0.238947
C 4.831945 -4.325144 -0.955686
C 5.648707 -3.185228 -0.955693
C -4.325554 -4.831485 -0.955497
C -3.185709 -5.648348 -0.956073
C -4.831621 4.325189 -0.956081
C -5.648393 3.185289 -0.956362
C 4.325198 4.831557 -0.956073
C 3.185343 5.648393 -0.956274
H 5.749120 -1.043228 -0.670516
H 2.835968 -5.108948 -0.670648
H 1.043365 5.749055 -0.671044
H 5.108857 2.835596 -0.670463
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H -1.043636 -5.749039 -0.671581
H -5.748927 1.043291 -0.671195
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H 5.266088 -5.286681 -1.199731
H 6.698782 -3.287155 -1.199708
H -5.287203 -5.265478 -1.199363
H -3.287800 -6.698340 -1.200374
H -5.265654 5.286727 -1.200315
H -6.698373 3.287211 -1.200787
H 5.286754 5.265547 -1.200309
H 3.287316 6.698380 -1.200649
Ba 0.000047 -0.000112 1.854164

Pt-Pht

N 0.603109 -1.899412 -0.000043
C 1.912472 -2.308243 0.000060
C -0.230541 -2.988719 0.000066
C 1.931279 -3.762316 -0.000009
N 2.990980 -1.549279 0.000060
C 0.592940 -4.187248 -0.000003
C 2.975234 -4.678497 -0.000028
C 0.268674 -5.537837 -0.000013
N -1.549300 -2.991035 0.000067
C 2.988609 -0.230498 0.000064
C -2.308269 -1.912548 0.000070
C 3.762307 1.931290 0.000006
C 4.187208 0.592924 0.000009
C 2.308218 1.912489 0.000062
C 4.678505 2.975199 0.000002
C 5.537754 0.268601 0.000008
N 1.899365 0.603159 -0.000045
N 1.549308 2.991050 0.000058
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C -3.762316 -1.931303 -0.000001
C -2.988706 0.230509 0.000069
C -5.537821 -0.268663 -0.000010
C -4.678534 -2.975240 -0.000018
N -1.899385 -0.603156 -0.000036
N -2.990992 1.549264 0.000067
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C -0.268645 5.537777 -0.000009
N -0.603093 1.899388 -0.000043
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C 2.649901 -6.029437 -0.000014
C -6.453696 -1.313656 -0.000002

C -6.029461 -2.649873 -0.000006
C -1.313663 6.453656 0.000008
C -2.649853 6.029413 0.000009
C 6.453653 1.313606 0.000030
C 6.029452 2.649806 0.000027
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H -0.765233 -5.855647 -0.000004
H 4.341759 4.003096 0.000005
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H -4.003120 4.341725 -0.000002
H 0.765271 5.855561 -0.000007
H 1.095516 -7.514058 0.000010
H 3.439778 -6.769759 -0.000002
H -7.514065 -1.095471 0.000013
H -6.769795 -3.439741 0.000007
H -1.095470 7.514023 0.000026
H -3.439745 6.769721 0.000028
H 7.514014 1.095380 0.000055
H 6.769787 3.439672 0.000050
Pt 0.000021 0.000057 -0.000047

Hg-Pht

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C 4.189635 0.730194 -0.242316
N 2.373983 2.401765 -0.031227
C 4.197886 -0.681315 -0.242528
C 5.350068 1.450349 -0.493800
C 5.366656 -1.387757 -0.494304
N 2.401780 -2.374017 -0.031718
C 1.113239 2.823186 0.012946
C 1.145984 -2.809989 0.012421
C -0.730251 4.189507 -0.242078
C 0.681255 4.197748 -0.242476
C -1.146001 2.810003 0.013589
C -1.450430 5.349779 -0.494232
C 1.387673 5.366345 -0.495119
N -0.011988 2.075045 0.197177
N -2.401775 2.373958 -0.030148
C -0.681424 -4.197749 -0.242323
C 0.730080 -4.189547 -0.242634
C -1.113239 -2.823117 0.012975
C -1.388005 -5.366408 -0.494227
C 1.450104 -5.349913 -0.494810
N 0.012122 -2.074895 0.196321
N -2.374044 -2.401764 -0.030647
C -2.823228 1.113194 0.013737
C -4.189634 -0.730143 -0.241950
C -4.197819 0.681371 -0.241822
C -2.810133 -1.146023 0.013494
C -5.349938 -1.450178 -0.494350
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C 0.738423 -6.520406 -0.730789
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C -6.520368 -0.738513 -0.730718
C 0.662377 6.528396 -0.731368
C -0.738903 6.520225 -0.730913
H 5.332868 2.532007 -0.502719
H 5.362106 -2.469541 -0.503626
H -2.532088 5.332575 -0.503032
H 2.469455 5.361774 -0.504614
H -2.469791 -5.361809 -0.503157
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H -5.332790 -2.531834 -0.503565
H -5.361788 2.469711 -0.503230
H 7.457094 -1.186027 -0.920884

H 7.442726 1.273238 -0.920409
H -1.186511 -7.456707 -0.921585
H 1.272762 -7.442421 -0.922037
H -7.456591 1.186409 -0.922004
H -7.442336 -1.272873 -0.922133
H 1.185910 7.456518 -0.922965
H -1.273366 7.442168 -0.922161
Hg 0.000106 -0.000029 0.957065

Pb-Pht

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C -2.707572 1.278126 -0.111234
C -4.185042 -0.457349 -0.371252
N -2.516978 -2.237056 -0.137752
C -4.102535 0.945426 -0.370938
C -5.387416 -1.105507 -0.627866
C -5.220590 1.730230 -0.627210
N -2.237194 2.517010 -0.137143
C -1.278033 -2.707278 -0.111628
C -0.951630 2.838691 -0.110827
C 0.457492 -4.184931 -0.370799
C -0.945285 -4.102317 -0.370920
C 0.951607 -2.838569 -0.111406
C 1.105617 -5.387416 -0.626919
C -1.730078 -5.220396 -0.627102
N -0.118128 -2.007373 0.070653
N 2.237178 -2.516881 -0.137084
C 0.945346 4.102317 -0.370154
C -0.457444 4.184886 -0.370525
C 1.278042 2.707448 -0.110285
C 1.730199 5.220324 -0.626615
C -1.105518 5.387264 -0.627458
N 0.118105 2.007517 0.072096
N 2.517025 2.237225 -0.136272
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C 4.102426 -0.945187 -0.370286
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C 5.220406 -1.730050 -0.626732
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C 1.081191 6.424834 -0.865584
C -0.319504 6.507281 -0.866019
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C 6.507616 0.319629 -0.864990
C -1.081014 -6.425063 -0.865319
C 0.319635 -6.507551 -0.865243
H -5.438334 -2.185974 -0.638095
H -5.144478 2.809218 -0.636878
H 2.186084 -5.438435 -0.636825
H -2.809062 -5.144210 -0.637096
H 2.809186 5.144118 -0.636228
H -2.185987 5.438196 -0.637780
H 5.438659 2.186134 -0.636269
H 5.144153 -2.809023 -0.636796
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H -7.462087 -0.792241 -1.060220
H 1.662689 7.317322 -1.059429
H -0.792143 7.461821 -1.060225
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Pb -0.000042 -0.000116 1.343596

Optimized atomic coordinates for M-mDBPcs

H_2-mDBPc (cis-mDBPc)

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C -0.70891500 -2.42666700 0.25999500
C 0.70896900 -2.42665300 0.26014000
C 1.59199300 -3.50389700 0.48497000
C 2.87841000 -3.01604700 0.35901900
C 2.79859800 -1.63053600 0.06047000
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C 2.83118600 3.02313400 0.40627700
C 1.56338000 3.48753700 0.51207400
C 0.69470500 2.37047500 0.20906400
C -0.69474600 2.37039100 0.20911400
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H -1.29989700 -4.51495300 0.71490600
H 1.30003400 -4.51469900 0.71594900
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H -7.20156500 1.31946300 -0.76121300
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H 7.23500200 -1.18578300 -0.77576200
H 5.18140200 -2.41556500 -0.43936800
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Be-mDBPc

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N -1.356623 -1.456167 0.049053
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C 0.705863 2.583374 -0.386266
C 1.660871 3.542133 -0.825366
C 2.892622 2.969794 -0.635431
C 2.684699 1.649291 -0.090661
C 2.684512 -1.649206 -0.090715
C 2.892766 -2.970120 -0.634690
C 1.661161 -3.542280 -0.825718
C 0.705793 -2.583114 -0.388110
C -0.705841 -2.583110 -0.388091
C -1.661222 -3.542309 -0.825607

C -2.892819 -2.970158 -0.634508
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H 1.445286 4.510875 -1.246383
H 3.842308 3.402618 -0.901730
H 3.842730 -3.403058 -0.899788
H 1.445725 -4.511148 -1.246523
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C -3.747348 -0.724061 0.253839
C -3.747540 0.724049 0.253276
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H -7.015752 -1.253826 1.175834
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H -4.980893 2.446010 0.628137
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C 4.973058 -1.367503 0.585992
C 6.125374 -0.700128 0.906944
C 6.125683 0.699776 0.906057
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H 7.015764 -1.253902 1.175679
H 7.016352 1.253496 1.173986
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Mg-*m*DBPc

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N -1.356623 -1.456167 0.049053
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C -2.892587 2.969749 -0.635616
C -1.660836 3.542115 -0.825450
C -0.705844 2.583360 -0.386304
C 0.705863 2.583374 -0.386266
C 1.660871 3.542133 -0.825366
C 2.892622 2.969794 -0.635431
C 2.684699 1.649291 -0.090661
C 2.684512 -1.649206 -0.090715
C 2.892766 -2.970120 -0.634690
C 1.661161 -3.542280 -0.825718
C 0.705793 -2.583114 -0.388110
C -0.705841 -2.583110 -0.388091
C -1.661222 -3.542309 -0.825607
C -2.892819 -2.970158 -0.634508
C -2.684533 -1.649204 -0.090633
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H -1.445240 4.510850 -1.246475
H 1.445286 4.510875 -1.246383
H 3.842308 3.402618 -0.901730
H 3.842730 -3.403058 -0.899788
H 1.445725 -4.511148 -1.246523
H -1.445803 -4.511199 -1.246370
H -3.842802 -3.403119 -0.899499
C -6.125692 0.699833 0.905991
C -6.125371 -0.700071 0.907030
C -4.973051 -1.367466 0.586132
C -3.747348 -0.724061 0.253839
C -3.747540 0.724049 0.253276
C -4.973614 1.367320 0.584401
H -7.016366 1.253575 1.173854
H -7.015752 -1.253826 1.175834
H -4.979839 -2.446103 0.631175
H -4.980893 2.446010 0.628137
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C 3.747340 -0.724081 0.253776

C 4.973058 -1.367503 0.585992
C 6.125374 -0.700128 0.906944
C 6.125683 0.699776 0.906057
C 4.973600 1.367285 0.584537
H 4.979862 -2.446144 0.630937
H 7.015764 -1.253902 1.175679
H 7.016352 1.253496 1.173986
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Mg 0.000066 0.000398 0.383967

Ca-*m*DBPc

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C -1.627263 -3.362413 1.099045
C -0.706155 -2.482703 0.455229
C 0.706168 -2.482701 0.455232
C 1.627278 -3.362408 1.099052
C 2.876508 -2.838068 0.882981
C 2.704524 -1.623100 0.127736
C 2.704537 1.623155 0.127447
C 2.876525 2.838297 0.882419
C 1.627304 3.362724 1.098343
C 0.706154 2.482715 0.455004
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C -1.627334 3.362716 1.098324
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C -2.704541 1.623138 0.127422
H -3.810202 -3.211665 1.271030
H -1.373551 -4.239475 1.672592
H 1.373569 -4.239469 1.672600
H 3.810232 -3.211730 1.270913
H 3.810254 3.212108 1.270193
H 1.373628 4.239993 1.671588
H -1.373671 4.239988 1.671570
H -3.810296 3.212128 1.270078
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C -3.784943 -0.722032 -0.234418
C -5.014953 -1.371075 -0.521163
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H -7.075812 1.251542 -1.054504
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C 6.175584 0.699754 -0.815466
C 6.175588 -0.699944 -0.815248
C 5.014948 -1.371059 -0.521151
H 5.019919 2.451854 -0.543762
H 7.075805 1.251552 -1.054526
H 7.075812 -1.251814 -1.054130
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Ca 0.000009 -0.000088 -1.265808

Ni-*m*DBPc

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C 0.696222 -2.539202 0.664247

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C 2.880214 -2.943834 0.603198
C 2.622567 -1.597326 0.149871
C 2.622540 1.597351 0.149608
C 2.880195 2.943945 0.602680
C 1.683993 3.520961 0.929471
C 0.696221 2.539267 0.664000
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C -1.683995 3.520962 0.929467
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H 1.509749 -4.512598 1.313508
H 3.853331 -3.393011 0.703801
H 3.853311 3.393161 0.703121
H 1.509757 4.512793 1.312855
H -1.509759 4.512794 1.312849
H -3.853312 3.393162 0.703110
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C -3.645331 -0.717054 -0.350723
C -4.800059 -1.370922 -0.866062
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H -6.728118 1.252475 -1.759778
H -4.797079 2.448928 -0.916311
H -4.797213 -2.449045 -0.915704
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C 5.888431 0.700856 -1.357024
C 5.888473 -0.701021 -1.356843
C 4.800059 -1.370922 -0.866060
H 4.797081 2.448928 -0.916299
H 6.728121 1.252476 -1.759765
H 6.728199 -1.252695 -1.759437
H 4.797212 -2.449044 -0.915705
Ni 0.000002 -0.000013 0.064894

Zn-mDBPc

N -1.345034 -1.464595 0.018561
N 1.345033 -1.464596 0.018562
N 1.345013 1.464462 0.018867
N -1.345017 1.464455 0.018876
C -2.676872 -1.650216 0.126682
C -2.896656 -2.980526 0.645645
C -1.670858 -3.561594 0.845880
C -0.704936 -2.599306 0.440939
C 0.704936 -2.599308 0.440939
C 1.670858 -3.561596 0.845876
C 2.896656 -2.980534 0.645625
C 2.676871 -1.650217 0.126679
C 2.676871 1.650246 0.126494
C 2.896677 2.980732 0.645001
C 1.670882 3.561752 0.845407
C 0.704934 2.599262 0.441020
C -0.704940 2.599260 0.441022
C -1.670889 3.561752 0.845399
C -2.896683 2.980733 0.644988
C -2.676874 1.650243 0.126493
H -3.851976 -3.414968 0.887921
H -1.466610 -4.539510 1.250987
H 1.466611 -4.539513 1.250981
H 3.851979 -3.414981 0.887888
H 3.852021 3.415339 0.886888
H 1.466664 4.539782 1.250254
H -1.466673 4.539785 1.250239
H -3.852027 3.415343 0.886865
C -6.096968 -0.700055 -0.931538
C -6.096924 0.699951 -0.931778
C -4.951111 1.367033 -0.589532

C -3.731376 0.723797 -0.233290
C -3.731398 -0.723804 -0.233128
C -4.951182 -1.367090 -0.589107
H -6.981949 -1.253982 -1.217195
H -6.981867 1.253835 -1.217635
H -4.957393 2.445352 -0.636631
H -4.957511 -2.445422 -0.635885
C 3.731397 -0.723802 -0.233128
C 3.731374 0.723800 -0.233286
C 4.951111 1.367036 -0.589522
C 6.096925 0.699954 -0.931766
C 6.096970 -0.700052 -0.931530
C 4.951181 -1.367087 -0.589104
H 4.957393 2.445355 -0.636618
H 6.981869 1.253839 -1.217618
H 6.981951 -1.253978 -1.217185
H 4.957511 -2.445420 -0.635883
Zn 0.000006 -0.000038 -0.298856

Sr-*m*DBPc

N -1.403333 -1.451496 -0.029011
N 1.403333 -1.451496 -0.029009
N 1.403317 1.451348 -0.029067
N -1.403317 1.451349 -0.029070
C -2.708042 -1.617300 0.256369
C -2.872159 -2.811199 1.046652
C -1.619234 -3.323659 1.267612
C -0.706113 -2.458261 0.590348
C 0.706112 -2.458261 0.590349
C 1.619232 -3.323660 1.267614
C 2.872158 -2.811200 1.046657
C 2.708042 -1.617300 0.256374
C 2.708058 1.617326 0.256084
C 2.872197 2.811500 1.045943
C 1.619266 3.323974 1.266867
C 0.706116 2.458295 0.590012
C -0.706117 2.458295 0.590011
C -1.619269 3.323974 1.266864
C -2.872199 2.811500 1.045938
C -2.708059 1.617326 0.256079
H -3.802194 -3.174351 1.453469
H -1.356684 -4.181316 1.866088
H 1.356681 -4.181317 1.866090
H 3.802192 -3.174353 1.453474
H 3.802254 3.174855 1.452529
H 1.356747 4.181838 1.865060
H -1.356751 4.181838 1.865057
H -3.802257 3.174854 1.452522
C -6.183896 -0.699980 -0.683049
C -6.183891 0.699797 -0.683227
C -5.022208 1.371514 -0.392256
C -3.791930 0.721706 -0.111038
C -3.791929 -0.721748 -0.110886
C -5.022209 -1.371626 -0.391921
H -7.085487 -1.251534 -0.917721
H -7.085480 1.251295 -0.918042
H -5.026824 2.452760 -0.409463
H -5.026821 -2.452876 -0.408865
C 3.791929 -0.721748 -0.110880
C 3.791931 0.721706 -0.111031
C 5.022208 1.371515 -0.392249
C 6.183892 0.699798 -0.683218
C 6.183897 -0.699979 -0.683041
C 5.022210 -1.371625 -0.391914
H 5.026825 2.452760 -0.409455
H 7.085481 1.251296 -0.918033
H 7.085489 -1.251533 -0.917713
H 5.026822 -2.452876 -0.408859
Sr 0.000001 -0.000088 -1.434827

Pd-*m*DBPc

N -1.319808 -1.478426 0.108207
N 1.319808 -1.478426 0.108208
N 1.319805 1.478417 0.108083
N -1.319805 1.478417 0.108081
C -2.655379 -1.652204 0.141288
C -2.898320 -3.010457 0.581844
C -1.691045 -3.617893 0.794832
C -0.699370 -2.648941 0.484877
C 0.699370 -2.648941 0.484878
C 1.691044 -3.617894 0.794833
C 2.898319 -3.010457 0.581845
C 2.655378 -1.652204 0.141290
C 2.655372 1.652230 0.141026
C 2.898318 3.010572 0.581311
C 1.691047 3.618021 0.794279
C 0.699369 2.648993 0.484567
C -0.699369 2.648993 0.484566
C -1.691048 3.618021 0.794276
C -2.898319 3.010573 0.581305
C -2.655372 1.652230 0.141022
H -3.865638 -3.449878 0.754336
H -1.512426 -4.621495 1.144150
H 1.512425 -4.621496 1.144150
H 3.865638 -3.449878 0.754338
H 3.865640 3.450043 0.753656
H 1.512432 4.621681 1.143432
H -1.512433 4.621681 1.143429
H -3.865641 3.450044 0.753647
C -6.024401 -0.699978 -1.059927
C -6.024381 0.699829 -1.060088
C -4.894884 1.365450 -0.667506
C -3.692904 0.722502 -0.251521
C -3.692915 -0.722533 -0.251381
C -4.894918 -1.365541 -0.667206
H -6.894268 -1.254844 -1.386949
H -6.894231 1.254644 -1.387243
H -4.899160 2.442750 -0.722345
H -4.899221 -2.442853 -0.721811
C 3.692915 -0.722533 -0.251378
C 3.692904 0.722502 -0.251516
C 4.894886 1.365450 -0.667499
C 6.024383 0.699829 -1.060081
C 6.024402 -0.699978 -1.059921
C 4.894918 -1.365541 -0.667202
H 4.899162 2.442750 -0.722336
H 6.894234 1.254645 -1.387233
H 6.894270 -1.254844 -1.386943
H 4.899221 -2.442853 -0.721809
Pd -0.000000 -0.000012 -0.059552

Cd-*m*DBPc

N -1.385414 -1.520928 -0.055435
N 1.385413 -1.520928 -0.055435
N 1.385405 1.520887 -0.055632
N -1.385407 1.520887 -0.055634
C -2.697005 -1.650308 0.206974
C -2.887005 -2.879206 0.938536
C -1.649370 -3.440757 1.133884
C -0.707602 -2.571118 0.508064
C 0.707602 -2.571118 0.508064
C 1.649370 -3.440756 1.133884
C 2.887006 -2.879211 0.938527
C 2.697005 -1.650308 0.206974
C 2.697007 1.650347 0.206685
C 2.887017 2.879406 0.937975
C 1.649380 3.440976 1.133259
C 0.707601 2.571190 0.507661
C -0.707603 2.571190 0.507661
C -1.649382 3.440974 1.133260
C -2.887019 2.879405 0.937975
C -2.697008 1.650346 0.206685

H -3.826001 -3.242307 1.323414
H -1.416935 -4.337255 1.685838
H 1.416936 -4.337255 1.685839
H 3.826004 -3.242315 1.323398
H 3.826023 3.242606 1.322737
H 1.416956 4.337590 1.685030
H -1.416958 4.337587 1.685033
H -3.826024 3.242604 1.322737
C -6.153307 -0.699315 -0.735824
C -6.153303 0.699183 -0.735965
C -4.993030 1.368667 -0.439123
C -3.761244 0.723799 -0.146877
C -3.761245 -0.723823 -0.146741
C -4.993035 -1.368744 -0.438851
H -7.051293 -1.252533 -0.979461
H -7.051286 1.252355 -0.979715
H -4.998937 2.448990 -0.467798
H -4.998944 -2.449073 -0.467313
C 3.761244 -0.723822 -0.146740
C 3.761243 0.723800 -0.146875
C 4.993031 1.368668 -0.439115
C 6.153306 0.699184 -0.735953
C 6.153309 -0.699315 -0.735812
C 4.993036 -1.368743 -0.438844
H 4.998938 2.448991 -0.467789
H 7.051290 1.252356 -0.979699
H 7.051296 -1.252532 -0.979445
H 4.998945 -2.449072 -0.467305
Cd -0.000000 -0.000077 -0.830138

Ba-*m*DBPc

N -1.407760 -1.440901 0.119192
N 1.407760 -1.440900 0.119194
N 1.407736 1.440690 0.119222
N -1.407736 1.440690 0.119219
C -2.710895 -1.611691 0.407274
C -2.870032 -2.799359 1.209017
C -1.614456 -3.301957 1.434742
C -0.705834 -2.437271 0.747716
C 0.705832 -2.437271 0.747717
C 1.614454 -3.301957 1.434745
C 2.870030 -2.799359 1.209021
C 2.710894 -1.611691 0.407278
C 2.710917 1.611703 0.406993
C 2.870086 2.799703 1.208230
C 1.614503 3.302309 1.433943
C 0.705839 2.437278 0.747423
C -0.705840 2.437278 0.747422
C -1.614506 3.302309 1.433939
C -2.870089 2.799704 1.208224
C -2.710918 1.611703 0.406988
H -3.798299 -3.162092 1.620542
H -1.346510 -4.151625 2.042249
H 1.346507 -4.151626 2.042251
H 3.798297 -3.162092 1.620547
H 3.798384 3.162688 1.619463
H 1.346600 4.152228 2.041119
H -1.346604 4.152228 2.041116
H -3.798387 3.162689 1.619456
C -6.189422 -0.700141 -0.533858
C -6.189417 0.699927 -0.534053
C -5.027674 1.372041 -0.243448
C -3.797746 0.721477 0.036685
C -3.797743 -0.721535 0.036843
C -5.027674 -1.372175 -0.243083
H -7.091564 -1.251377 -0.767332
H -7.091556 1.251102 -0.767685
H -5.032094 2.453455 -0.258166
H -5.032088 -2.453594 -0.257514
C 3.797743 -0.721535 0.036849
C 3.797745 0.721477 0.036692
C 5.027674 1.372041 -0.243439
C 6.189418 0.699928 -0.534042

C 6.189423 -0.700140 -0.533847
C 5.027675 -1.372175 -0.243075
H 5.032095 2.453455 -0.258156
H 7.091557 1.251103 -0.767671
H 7.091566 -1.251376 -0.767319
H 5.032089 -2.453594 -0.257506
Ba 0.000001 -0.000042 -1.558153

Pt-*m*DBPc

N -1.306723 -1.498879 0.138993
N 1.306723 -1.498878 0.138995
N 1.306722 1.498885 0.138828
N -1.306721 1.498886 0.138826
C -2.644981 -1.662454 0.148616
C -2.900971 -3.026699 0.564438
C -1.702311 -3.649498 0.779411
C -0.698142 -2.686326 0.498310
C 0.698142 -2.686325 0.498311
C 1.702311 -3.649498 0.779412
C 2.900970 -3.026699 0.564440
C 2.644982 -1.662453 0.148619
C 2.644975 1.662480 0.148352
C 2.900970 3.026797 0.563940
C 1.702314 3.649618 0.778865
C 0.698141 2.686387 0.497973
C -0.698141 2.686388 0.497972
C -1.702314 3.649619 0.778861
C -2.900970 3.026798 0.563934
C -2.644974 1.662481 0.148346
H -3.873092 -3.461252 0.720456
H -1.537472 -4.661087 1.111640
H 1.537471 -4.661086 1.111641
H 3.873092 -3.461252 0.720459
H 3.873095 3.461382 0.719841
H 1.537479 4.661257 1.110944
H -1.537480 4.661258 1.110939
H -3.873095 3.461384 0.719833
C -5.989628 -0.699825 -1.103326
C -5.989607 0.699670 -1.103491
C -4.866234 1.363928 -0.692897
C -3.669804 0.723147 -0.254813
C -3.669815 -0.723179 -0.254671
C -4.866270 -1.364023 -0.692594
H -6.853241 -1.255566 -1.445066
H -6.853200 1.255357 -1.445368
H -4.870018 2.440835 -0.750692
H -4.870088 -2.440943 -0.750150
C 3.669816 -0.723180 -0.254667
C 3.669805 0.723147 -0.254807
C 4.866236 1.363928 -0.692890
C 5.989609 0.699670 -1.103483
C 5.989629 -0.699825 -1.103321
C 4.866271 -1.364024 -0.692590
H 4.870021 2.440835 -0.750682
H 6.853202 1.255357 -1.445359
H 6.853242 -1.255566 -1.445062
H 4.870088 -2.440943 -0.750149
Pt -0.000001 -0.000005 -0.012439

Hg-*m*DBPc

N -1.387947 -1.539954 0.049516
N 1.387947 -1.539953 0.049521
N 1.387940 1.539922 0.049330
N -1.387940 1.539923 0.049329
C -2.697028 -1.649622 0.324003
C -2.887616 -2.856680 1.091260
C -1.651102 -3.419170 1.294501
C -0.707711 -2.573198 0.638114
C 0.707710 -2.573198 0.638116
C 1.651100 -3.419174 1.294499
C 2.887614 -2.856676 1.091273

C 2.697029 -1.649624 0.324006
C 2.697034 1.649682 0.323720
C 2.887629 2.856901 1.090722
C 1.651114 3.419421 1.293879
C 0.707711 2.573287 0.637722
C -0.707711 2.573287 0.637722
C -1.651114 3.419422 1.293877
C -2.887629 2.856900 1.090723
C -2.697035 1.649684 0.323718
H -3.826774 -3.202239 1.492068
H -1.419451 -4.299594 1.872103
H 1.419449 -4.299600 1.872096
H 3.826769 -3.202232 1.492088
H 3.826793 3.202562 1.491425
H 1.419473 4.299969 1.871295
H -1.419473 4.299970 1.871294
H -3.826793 3.202561 1.491429
C -6.145191 -0.699091 -0.646474
C -6.145190 0.698969 -0.646614
C -4.986701 1.368906 -0.341535
C -3.757320 0.723476 -0.043865
C -3.757319 -0.723478 -0.043732
C -4.986701 -1.368967 -0.341267
H -7.041812 -1.252213 -0.895251
H -7.041810 1.252043 -0.895502
H -4.991992 2.449483 -0.366942
H -4.991990 -2.449550 -0.366463
C 3.757320 -0.723480 -0.043728
C 3.757320 0.723474 -0.043862
C 4.986700 1.368905 -0.341530
C 6.145191 0.698970 -0.646606
C 6.145194 -0.699090 -0.646465
C 4.986703 -1.368968 -0.341260
H 4.991990 2.449483 -0.366938
H 7.041811 1.252044 -0.895494
H 7.041815 -1.252212 -0.895240
H 4.991994 -2.449550 -0.366455
Hg -0.000000 -0.000071 -0.816936

Pb-*m*DBPc

N -1.362793 -1.415393 0.288710
N 1.362946 -1.415269 0.289125
N 1.362936 1.415268 0.288986
N -1.362798 1.415417 0.288550
C -2.688159 -1.602013 0.452973
C -2.889228 -2.831326 1.176466
C -1.651040 -3.348916 1.461027
C -0.702972 -2.451142 0.888757
C 0.703070 -2.451200 0.888870
C 1.651127 -3.349006 1.461087
C 2.889344 -2.831224 1.177010
C 2.688248 -1.602028 0.453282
C 2.688243 1.602102 0.453012
C 2.889345 2.831443 1.176499
C 1.651132 3.349267 1.460513
C 0.703067 2.451310 0.888548
C -0.702976 2.451254 0.888443
C -1.651045 3.349138 1.460543
C -2.889233 2.831476 1.176114
C -2.688163 1.602072 0.452773
H -3.841942 -3.220209 1.497081
H -1.423183 -4.236716 2.028559
H 1.423284 -4.236950 2.028373
H 3.842005 -3.220039 1.497900
H 3.842011 3.220344 1.497269
H 1.423299 4.237331 2.027616
H -1.423187 4.237035 2.027920
H -3.841944 3.220399 1.496689
C -6.096130 -0.700392 -0.708201
C -6.096133 0.700300 -0.708287
C -4.958035 1.373494 -0.342241
C -3.751549 0.720016 0.022002
C -3.751547 -0.720011 0.022092

C -4.958030 -1.373538 -0.342072
H -6.979657 -1.250703 -1.005408
H -6.979661 1.250572 -1.005562
H -4.960055 2.454182 -0.367425
H -4.960046 -2.454229 -0.367121
C 3.751679 -0.719995 0.022504
C 3.751672 0.720001 0.022369
C 4.958127 1.373483 -0.342031
C 6.096208 0.700292 -0.708084
C 6.096219 -0.700406 -0.707936
C 4.958143 -1.373536 -0.341750
H 4.960136 2.454159 -0.367322
H 6.979734 1.250533 -1.005426
H 6.979753 -1.250697 -1.005159
H 4.960165 -2.454218 -0.366820
Pb -0.000135 -0.000078 -1.067371

Optimized atomic coordinates for M-Chls *a*

H_2-Chl *a* (Pheophytin *a*)

O -3.099223 -4.466060 -0.018776
O -5.238508 -2.144419 -0.898853
O -3.607381 -1.560703 -2.334340
O -7.280479 2.684264 1.719887
O -5.847693 1.573430 3.045135
N -0.688655 1.014723 -0.155136
N 0.596153 -1.714450 0.203738
N 2.092904 2.054878 -0.099467
N 3.153155 -0.713329 0.298762
C -3.066449 1.199741 -0.302133
C -2.426776 2.565571 -0.645177
C -1.845050 0.310677 -0.145140
C -1.857656 -1.060054 -0.018041
C -3.940915 1.229216 0.959765
C -0.949622 2.303395 -0.382206
C -3.060004 -1.991382 -0.020006
C -0.727076 -1.877639 0.103585
C -2.682423 3.007494 -2.090079
C -1.007274 -3.262123 0.136323
C -2.444758 -3.452303 0.023912
C -5.248976 1.977953 0.735747
C 0.001919 3.319137 -0.413024
C 0.191028 -3.957797 0.264253
C 1.209860 -2.957556 0.309404
C -3.966354 -1.860735 -1.223909
C 1.381461 3.207753 -0.268008
C 0.395190 -5.433361 0.325241
C -6.117193 2.033457 1.967063
C 2.589931 -3.085215 0.436911
C 2.330465 4.285588 -0.287858
C 3.499044 -2.029896 0.444520
C 3.440157 2.310118 -0.007761
C 3.591280 3.743270 -0.150681
C 4.942011 -2.169273 0.615628
C 4.305896 -0.016270 0.367605
C 5.448424 -0.905112 0.571800
C 4.427036 1.376263 0.234302
C 1.961973 5.720406 -0.474899
C 5.679364 -3.464262 0.755782
C 6.871876 -0.465449 0.683529
C 4.842036 4.495253 -0.156950
C -6.172692 -2.167003 -1.991088
C 5.954850 -4.143855 -0.594253
C 5.992808 4.123867 -0.719615
H -3.669655 0.839568 -1.140126
H -2.785903 3.347634 0.030137
H -3.384912 1.686586 1.781329
H -4.172769 0.214914 1.283379
H -3.669052 -1.898840 0.881186
H -3.749464 3.166542 -2.260007
H -2.337809 2.243603 -2.789792
H -2.159044 3.937151 -2.319117
H -5.835114 1.510644 -0.061368

H -5.079968 3.007906 0.408894
H -0.369779 4.322899 -0.571154
H 1.001058 -5.715912 1.189356
H -0.562966 -5.945913 0.390004
H 0.913493 -5.795218 -0.566979
H 2.976849 -4.089931 0.540526
H 5.423455 1.779161 0.337202
H 1.260118 6.053090 0.293829
H 1.480815 5.880964 -1.443511
H 2.836828 6.366749 -0.434656
H 5.111643 -4.146511 1.394804
H 6.626595 -3.292336 1.271930
H 7.214979 0.016060 -0.236762
H 7.535270 -1.307727 0.878240
H 7.006475 0.257204 1.492739
H 4.801389 5.468410 0.323613
H -7.790428 2.684324 2.545195
H -6.218414 -1.191339 -2.475410
H -5.876300 -2.914619 -2.726188
H -7.131929 -2.422857 -1.549844
H 6.482203 -5.090380 -0.457268
H 6.565279 -3.500956 -1.231033
H 5.023784 -4.345325 -1.126983
H 6.864999 4.762531 -0.672339
H 6.094903 3.193740 -1.263139
H 1.141197 -0.861535 0.228430
H 1.683198 1.135612 -0.052073

Mg-Chl a (Chl a)

O -3.281319 -4.449342 0.014016
O -5.345406 -2.193855 -0.948671
O -3.727660 -1.501059 -2.349929
O -7.134747 2.929327 1.854099
O -5.664937 1.830566 3.148598
N -0.708827 0.977700 -0.191070
N 0.461432 -1.689736 0.171694
N 2.089606 1.986734 -0.099197
N 3.102847 -0.729639 0.301007
C -3.074157 1.238186 -0.317932
C -2.389894 2.566899 -0.715654
C -1.898230 0.294598 -0.179733
C -1.964459 -1.069541 -0.051578
C -3.889334 1.333185 0.981307
C -0.923479 2.290896 -0.423183
C -3.186424 -1.972078 -0.040860
C -0.846353 -1.912809 0.081966
C -2.608749 2.932433 -2.188623
C -1.156605 -3.292629 0.149055
C -2.597326 -3.454835 0.038107
C -5.178820 2.123592 0.796452
C 0.039392 3.286145 -0.446384
C 0.044516 -3.971960 0.297255
C 1.055255 -2.939974 0.312821
C -4.083770 -1.846895 -1.251002
C 1.429182 3.159262 -0.288455
C 0.268564 -5.441617 0.410744
C -5.978965 2.254374 2.067692
C 2.433096 -3.090126 0.455870
C 2.372949 4.254048 -0.330632
C 3.385164 -2.066382 0.461849
C 3.436080 2.269366 -0.023355
C 3.625429 3.706013 -0.190553
C 4.811074 -2.240892 0.640611
C 4.284825 -0.059991 0.368836
C 5.370820 -0.989208 0.585043
C 4.425513 1.332428 0.224896
C 2.007651 5.686318 -0.542251
C 5.511234 -3.554947 0.798676
C 6.812348 -0.611409 0.699124
C 4.883883 4.441916 -0.219620
C -6.265067 -2.236014 -2.052020
C 5.815583 -4.233394 -0.545560
C 6.033433 4.042174 -0.767081

H -3.728153 0.887325 -1.120447
H -2.740258 3.393662 -0.092389
H -3.280606 1.790647 1.764635
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H -3.801455 -1.853616 0.853672
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H -2.276119 2.119810 -2.837426
H -2.054842 3.832387 -2.459210
H -5.821886 1.653702 0.046297
H -4.989169 3.135179 0.426250
H -0.327857 4.288827 -0.622859
H 0.805790 -5.691689 1.329322
H -0.681377 -5.973458 0.412233
H 0.867435 -5.815142 -0.424409
H 2.801593 -4.100186 0.579787
H 5.429677 1.717533 0.323486
H 1.284612 6.025862 0.203773
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H 2.879187 6.336731 -0.485820
H 4.905807 -4.226017 1.413679
H 6.444163 -3.408608 1.347637
H 7.183574 -0.169881 -0.230061
H 7.435693 -1.476852 0.921565
H 6.972017 0.125414 1.490384
H 4.854199 5.431609 0.227887
H -7.600114 2.978758 2.703920
H -6.352178 -1.253256 -2.515960
H -5.925864 -2.952567 -2.799545
H -7.215886 -2.546804 -1.628101
H 6.318290 -5.191434 -0.396962
H 6.459465 -3.601020 -1.159596
H 4.897124 -4.412525 -1.107349
H 6.911421 4.674085 -0.738229
H 6.128380 3.094821 -1.281372
Mg 1.255421 0.150161 0.052218

Zn-Chl *a*

O -3.302767 -4.466589 0.008995
O -5.402043 -2.236259 -0.927914
O -3.808059 -1.508735 -2.338918
O -7.247113 2.883894 1.823473
O -5.799770 1.755235 3.117606
N -0.793739 0.976384 -0.190951
N 0.410018 -1.668248 0.153643
N 2.009297 1.966865 -0.095813
N 3.064877 -0.728327 0.297767
C -3.158163 1.226795 -0.320260
C -2.478798 2.563716 -0.700092
C -1.975946 0.290595 -0.180591
C -2.026854 -1.073526 -0.055945
C -3.988390 1.304236 0.970077
C -1.011044 2.285210 -0.416725
C -3.238861 -1.988629 -0.038570
C -0.898358 -1.899323 0.069692
C -2.705039 2.954396 -2.165118
C -1.193832 -3.282536 0.137633
C -2.632822 -3.462602 0.032809
C -5.277647 2.093661 0.779333
C -0.044151 3.274225 -0.437754
C 0.010976 -3.952533 0.281509
C 1.015552 -2.916133 0.294913
C -4.148916 -1.868204 -1.239605
C 1.341244 3.138208 -0.282245
C 0.244559 -5.420653 0.396177
C -6.096330 2.201602 2.040888
C 2.390430 -3.076238 0.440775
C 2.281723 4.234425 -0.324303
C 3.346993 -2.061836 0.454098
C 3.356469 2.255815 -0.021232
C 3.535691 3.692493 -0.187481
C 4.773866 -2.233272 0.635428
C 4.239540 -0.053793 0.368952
C 5.329376 -0.980224 0.584691

C 4.360660 1.336619 0.226158
C 1.911049 5.665751 -0.533409
C 5.474519 -3.547222 0.790355
C 6.768422 -0.595159 0.702087
C 4.791058 4.434695 -0.218259
C -6.331878 -2.283419 -2.022566
C 5.775417 -4.224392 -0.555307
C 5.936645 4.047763 -0.782515
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H -4.240510 0.301490 1.314963
H -3.846265 -1.878257 0.862210
H -3.766058 3.131419 -2.353726
H -2.371984 2.154720 -2.829546
H -2.155387 3.860972 -2.422209
H -5.908671 1.633456 0.013042
H -5.086194 3.111348 0.427379
H -0.403905 4.280418 -0.608556
H 0.766021 -5.668403 1.324485
H -0.701710 -5.958690 0.379840
H 0.861425 -5.788289 -0.428255
H 2.748778 -4.090137 0.562477
H 5.357985 1.739274 0.322976
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H 2.782856 6.316630 -0.489549
H 4.869984 -4.218645 1.406043
H 6.408660 -3.401427 1.337383
H 7.139053 -0.151053 -0.226140
H 7.395775 -1.457479 0.925465
H 6.922071 0.142245 1.494014
H 4.760839 5.417959 0.243068
H -7.725299 2.917274 2.666938
H -6.438043 -1.298414 -2.477667
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H -7.273720 -2.611603 -1.591815
H 6.277355 -5.183134 -0.408771
H 6.418728 -3.591931 -1.169815
H 4.855755 -4.401914 -1.115631
H 6.811926 4.683444 -0.754246
H 6.030654 3.107574 -1.310053
Zn 1.215327 0.144319 0.048020

Pb-Chl *a*

O 3.652374 4.301171 0.569461
O 5.693116 2.132516 -0.675105
O 4.103760 1.718153 -2.213102
O 6.963831 -3.115667 2.577989
O 5.366693 -1.932995 3.623991
N 0.995057 -0.990471 -0.403518
N -0.178094 1.714394 0.058556
N -1.850296 -1.944602 -0.096230
N -2.874202 0.822284 0.274442
C 3.333805 -1.324309 -0.195588
C 2.660234 -2.640020 -0.659316
C 2.177136 -0.341339 -0.243675
C 2.250550 1.020764 -0.073596
C 3.940325 -1.430093 1.213210
C 1.181726 -2.317282 -0.500751
C 3.493221 1.870650 0.121719
C 1.142722 1.878309 0.073213
C 2.991198 -3.002563 -2.111609
C 1.495506 3.215909 0.391522
C 2.944234 3.338156 0.397471
C 5.222921 -2.252537 1.229736
C 0.190008 -3.284028 -0.455871
C 0.318093 3.914283 0.604436
C -0.732907 2.942988 0.402204
C 4.431355 1.885541 -1.065159
C -1.184766 -3.123497 -0.201233
C 0.150262 5.340120 1.006441
C 5.818721 -2.390802 2.607965

C -2.097730 3.124719 0.618807
C -2.103646 -4.218536 0.025419
C -3.081514 2.130299 0.624323
C -3.166567 -2.216715 0.190848
C -3.342013 -3.664603 0.244613
C -4.429840 2.278058 1.133119
C -3.997253 0.126070 0.584303
C -4.997663 1.028164 1.111742
C -4.135937 -1.269522 0.488322
C -1.731011 -5.664615 -0.001100
C -5.045753 3.564950 1.587723
C -6.361097 0.619169 1.567725
C -4.572958 -4.403927 0.498723
C 6.654770 2.291583 -1.730947
C -5.560021 4.423318 0.422161
C -5.795582 -4.092571 0.063491
H 4.113096 -1.012752 -0.897499
H 2.937535 -3.476106 -0.013665
H 3.206297 -1.868109 1.893334
H 4.156369 -0.438328 1.608195
H 4.070650 1.600577 1.007583
H 4.058405 -3.208011 -2.220699
H 2.735322 -2.177695 -2.779870
H 2.436914 -3.885526 -2.433440
H 5.984117 -1.802987 0.584808
H 5.067846 -3.261988 0.838700
H 0.533221 -4.307104 -0.540056
H -0.275543 5.418374 2.010787
H 1.111682 5.850991 1.005479
H -0.524117 5.868373 0.327988
H -2.410100 4.119566 0.907814
H -5.102413 -1.661899 0.768126
H -0.958937 -5.889167 0.739457
H -1.333521 -5.953694 -0.977997
H -2.588458 -6.304031 0.202981
H -4.316815 4.139656 2.165461
H -5.869855 3.355999 2.272898
H -6.921676 0.135653 0.763211
H -6.943825 1.476032 1.903751
H -6.309130 -0.092991 2.395468
H -4.458845 -5.316877 1.076666
H 7.296464 -3.164922 3.487999
H 6.721051 1.382321 -2.328802
H 6.372192 3.121775 -2.377742
H 7.600287 2.496908 -1.236667
H -5.995200 5.356994 0.784766
H -6.324063 3.887109 -0.143820
H -4.750565 4.669035 -0.267558
H -6.646777 -4.715831 0.304477
H -5.981664 -3.229901 -0.562976
Pb -1.194373 0.033114 -1.219392

Optimized atomic coordinates for M-BChls *a*

H_2-Bchl *a* (Bacteriopheophytin *a*)

C 2.459476 0.484854 -0.259048
C -0.641479 -3.122255 -0.687421
C -4.273137 0.115336 -0.216623
C -1.160726 3.787719 0.101963
N 0.714420 -1.130804 -0.434747
C 2.027905 -0.819461 -0.394998
C 2.917177 -2.048041 -0.486105
C 1.901726 -3.140223 -0.892319
C 0.569840 -2.445021 -0.648044
C 2.050702 -3.572142 -2.355740
C 3.666814 -2.345801 0.824982
C 2.761367 -2.416949 2.049903
C 3.519353 -2.697349 3.320916
O 4.713457 -2.804608 3.426124
O 2.680877 -2.815346 4.379234
N -2.256774 -1.284137 -0.407492
C -1.931865 -2.609046 -0.556199
C -3.159481 -3.340606 -0.560778

C -4.196776 -2.420110 -0.425300
C -3.610319 -1.102719 -0.344284
C -3.235153 -4.825649 -0.726937
C -5.653101 -2.678995 -0.364980
O -6.470458 -1.809640 -0.613912
C -6.145075 -4.054241 0.044089
N -2.464408 1.748012 -0.081208
C -3.758464 1.402139 -0.117030
C -4.680252 2.613378 -0.084649
C -3.706836 3.754668 0.272934
C -2.354886 3.089167 0.073405
C -5.381153 2.819122 -1.432641
C -3.877595 4.309783 1.701020
C -3.664187 3.284121 2.813695
N 0.320846 1.863887 -0.105751
C 0.118240 3.230114 0.006642
C 1.396052 3.867230 0.016223
C 2.327091 2.837144 -0.086873
C 1.638614 1.608814 -0.159871
C 1.649806 5.333630 0.110436
C 3.757118 2.573074 -0.143821
O 4.692924 3.335364 -0.133000
C 3.891380 0.994089 -0.213285
C 4.738578 0.612305 -1.408142
O 4.317322 0.402958 -2.517858
O 6.036019 0.560710 -1.073722
C 6.953384 0.318108 -2.153747
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H -0.575429 -4.190781 -0.837587
H -5.348797 0.034422 -0.223085
H -1.213841 4.862535 0.216108
H 3.661832 -1.911196 -1.272505
H 1.996067 -4.024849 -0.256109
H 3.021473 -4.044917 -2.518948
H 1.272839 -4.283503 -2.638824
H 1.977278 -2.707615 -3.018438
H 4.204812 -3.290181 0.713909
H 4.432997 -1.588394 0.994301
H 2.216850 -1.479175 2.193766
H 1.989900 -3.184264 1.947498
H -3.461125 -5.327399 0.216979
H -4.008066 -5.109987 -1.439758
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H -6.096855 -4.739030 -0.805254
H -5.551410 -4.483385 0.850871
H -7.184965 -3.963123 0.350104
H -5.443866 2.485102 0.686558
H -3.820154 4.589005 -0.424516
H -4.647370 2.950243 -2.231199
H -6.005933 1.961654 -1.686399
H -6.015376 3.707810 -1.402101
H -3.176335 5.138602 1.836324
H -4.881234 4.739520 1.779166
H -3.801060 3.745295 3.793096
H -4.367767 2.452883 2.739578
H -2.655863 2.867753 2.777255
H 1.239190 5.862356 -0.754016
H 1.184546 5.761523 1.002220
H 2.719639 5.530387 0.152181
H 4.420699 0.694546 0.693276
H 7.941810 0.322635 -1.703181
H 6.746588 -0.644860 -2.620767
H 6.869056 1.103649 -2.904138
H -1.572315 -0.545231 -0.394331
H -0.447265 1.209841 -0.116229

Mg-Bchl *a* (Bchl *a*)

C 2.549447 0.437613 -0.258438
C -0.710790 -3.072815 -0.677187
C -4.276449 0.194403 -0.209811
C -1.001974 3.750353 0.108414
N 0.722627 -1.113159 -0.431764
C 2.061854 -0.842880 -0.386450

C 2.881181 -2.114978 -0.455235
C 1.827240 -3.159048 -0.888860
C 0.515817 -2.433673 -0.639788
C 1.969333 -3.557851 -2.363063
C 3.576236 -2.444613 0.878611
C 2.632165 -2.470177 2.075669
C 3.332671 -2.806398 3.366229
O 4.507372 -3.030952 3.498261
O 2.463838 -2.828326 4.406296
N -2.262748 -1.190571 -0.389595
C -1.996305 -2.525914 -0.548304
C -3.228458 -3.268131 -0.579456
C -4.251697 -2.339275 -0.447566
C -3.620116 -1.036236 -0.343521
C -3.315001 -4.750752 -0.762104
C -5.710919 -2.570706 -0.414450
O -6.510572 -1.679616 -0.650173
C -6.236232 -3.947815 -0.053339
N -2.407264 1.758238 -0.080489
C -3.725249 1.460573 -0.105646
C -4.573696 2.718042 -0.062010
C -3.544145 3.804762 0.316615
C -2.219124 3.098452 0.085779
C -5.250265 2.977037 -1.413798
C -3.678279 4.319879 1.763907
C -3.490255 3.251995 2.840820
N 0.433133 1.794601 -0.119672
C 0.269670 3.163385 0.003736
C 1.550048 3.822651 0.028473
C 2.480791 2.796169 -0.078693
C 1.755901 1.587074 -0.163702
C 1.794821 5.289478 0.140112
C 3.901738 2.494166 -0.130837
O 4.864893 3.221998 -0.114703
C 3.994368 0.902443 -0.205550
C 4.833999 0.496968 -1.396415
O 4.406007 0.251973 -2.497134
O 6.135002 0.465905 -1.073257
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H -0.660659 -4.141475 -0.833975
H -5.354167 0.143789 -0.219136
H -1.034360 4.825168 0.236354
H 3.654661 -2.016704 -1.218894
H 1.888981 -4.061626 -0.274998
H 2.925088 -4.058307 -2.532009
H 1.169131 -4.234206 -2.667672
H 1.931175 -2.674344 -3.003379
H 4.072678 -3.413139 0.784490
H 4.370114 -1.721091 1.068912
H 2.140558 -1.502682 2.211105
H 1.821300 -3.191548 1.944109
H -3.563849 -5.259736 0.172576
H -4.077716 -5.022710 -1.491061
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H -5.916862 2.156609 -1.682486
H -5.835846 3.898260 -1.376929
H -2.945718 5.117739 1.916523
H -4.665187 4.781963 1.867055
H -3.603522 3.684900 3.835910
H -4.221036 2.446640 2.746235
H -2.495224 2.806651 2.782111
H 1.392579 5.825307 -0.724324
H 1.314893 5.707575 1.029095
H 2.862585 5.494352 0.198128
H 4.514593 0.589581 0.702069
H 8.037610 0.235436 -1.714211
H 6.846531 -0.769244 -2.596511
H 6.944811 0.972957 -2.924142

Zn-Bchl *a*

Zn -0.865827 0.269016 -0.249025
C 2.585553 0.447468 -0.252896
C -0.610174 -3.093646 -0.673773
C -4.238596 0.120469 -0.184145
C -1.030848 3.708393 0.114684
N 0.800174 -1.133622 -0.426862
C 2.130183 -0.842672 -0.383032
C 2.972005 -2.099930 -0.457899
C 1.932030 -3.161610 -0.885033
C 0.612223 -2.451425 -0.636780
C 2.076886 -3.567099 -2.356844
C 3.682128 -2.417095 0.870675
C 2.746795 -2.460526 2.074188
C 3.464382 -2.773807 3.361076
O 4.647818 -2.950661 3.488402
O 2.600985 -2.834585 4.403935
N -2.182486 -1.217757 -0.374042
C -1.893367 -2.550513 -0.539673
C -3.114134 -3.309010 -0.568781
C -4.150424 -2.399721 -0.427631
C -3.545287 -1.085773 -0.322993
C -3.179581 -4.791775 -0.760134
C -5.604995 -2.661216 -0.383409
O -6.424878 -1.798786 -0.651731
C -6.098537 -4.034549 0.034444
N -2.415856 1.717810 -0.062968
C -3.723881 1.399243 -0.081133
C -4.593884 2.641478 -0.031729
C -3.577194 3.746811 0.332315
C -2.244452 3.056134 0.099135
C -5.291329 2.884335 -1.375548
C -3.709279 4.272105 1.775847
C -3.500517 3.215286 2.859913
N 0.431987 1.755827 -0.120276
C 0.239633 3.124564 0.006361
C 1.507081 3.804561 0.034176
C 2.456765 2.797930 -0.071568
C 1.760715 1.572451 -0.160218
C 1.724710 5.275303 0.151762
C 3.885152 2.533200 -0.119752
O 4.827483 3.287737 -0.101695
C 4.018005 0.946625 -0.192419
C 4.875906 0.557719 -1.375758
O 4.461625 0.293024 -2.477050
O 6.174962 0.566376 -1.044288
C 7.099247 0.326337 -2.118480
H 3.123078 -3.029871 5.197900
H -0.561089 -4.162043 -0.831540
H -5.314033 0.035281 -0.191130
H -1.060259 4.783281 0.241425
H 3.737447 -1.987053 -1.227609
H 2.006548 -4.059425 -0.265580
H 3.039146 -4.055165 -2.525005
H 1.285737 -4.256637 -2.655716
H 2.024423 -2.688139 -3.002316
H 4.196093 -3.376105 0.772702
H 4.463711 -1.679022 1.055929
H 2.233316 -1.504309 2.209588
H 1.951916 -3.200700 1.950891
H -3.318645 -5.315508 0.189638
H -4.003166 -5.077440 -1.412123
H -2.265564 -5.175184 -1.209922
H -6.104349 -4.705117 -0.828005
H -5.476271 -4.487241 0.805447
H -7.122436 -3.931974 0.388072
H -5.358279 2.536284 0.741896
H -3.681076 4.599206 -0.343912
H -4.556102 2.996215 -2.175700
H -5.946793 2.051513 -1.633468
H -5.892523 3.795235 -1.334341
H -2.986093 5.080587 1.917185

H -4.701271 4.722534 1.881555
H -3.611179 3.655131 3.852235
H -4.222876 2.401033 2.777711
H -2.501299 2.780160 2.797033
H 1.277045 5.811506 -0.689515
H 1.272838 5.673527 1.064430
H 2.789613 5.501065 0.170812
H 4.537963 0.646975 0.719913
H 8.087544 0.386384 -1.671550
H 6.931798 -0.659109 -2.553406
H 6.981680 1.082706 -2.894002

Pb-Bchl *a*

Pb -0.758620 0.418664 -1.436386
C 2.736073 0.257870 -0.129030
C -0.593571 -3.139459 -0.651688
C -4.075890 0.215288 0.045167
C -0.726580 3.671592 0.392072
N 0.921430 -1.239373 -0.557276
C 2.237435 -1.011764 -0.335101
C 3.000345 -2.320921 -0.225037
C 1.958916 -3.344890 -0.740878
C 0.661523 -2.557496 -0.652942
C 2.233663 -3.790321 -2.181931
C 3.482068 -2.608058 1.209458
C 2.377479 -2.524014 2.258016
C 2.881090 -2.778107 3.654504
O 4.026352 -2.969703 3.971355
O 1.868354 -2.762218 4.554410
N -2.102446 -1.202706 -0.356501
C -1.853489 -2.546682 -0.446665
C -3.079582 -3.272722 -0.250726
C -4.073857 -2.324998 -0.047012
C -3.435298 -1.023941 -0.133194
C -3.191679 -4.764639 -0.288869
C -5.509250 -2.540513 0.232277
O -6.343742 -1.675515 0.021754
C -5.962320 -3.864559 0.820426
N -2.225828 1.801189 -0.029423
C -3.524583 1.479881 0.140510
C -4.338762 2.718651 0.470559
C -3.245476 3.745696 0.847701
C -1.975442 3.076679 0.341109
C -5.184289 3.154892 -0.731521
C -3.172851 4.054407 2.356395
C -2.862117 2.843860 3.236246
N 0.653396 1.699084 -0.083533
C 0.518022 3.038681 0.241685
C 1.813311 3.616840 0.502134
C 2.711287 2.573403 0.333971
C 1.963467 1.422598 -0.014349
C 2.095107 5.024484 0.905679
C 4.119532 2.220183 0.409402
O 5.090570 2.903033 0.630843
C 4.176991 0.655147 0.136412
C 5.122480 0.362052 -1.008304
O 4.801888 0.274967 -2.167542
O 6.381724 0.231532 -0.565432
C 7.389110 0.064504 -1.576770
H 2.259088 -2.917356 5.428657
H -0.590957 -4.217864 -0.732535
H -5.144010 0.154955 0.187360
H -0.702148 4.711589 0.691915
H 3.877069 -2.300205 -0.876425
H 1.925111 -4.228629 -0.099315
H 3.181250 -4.330224 -2.240736
H 1.441940 -4.445584 -2.548939
H 2.294537 -2.924943 -2.845232
H 3.934044 -3.602338 1.233689
H 4.279201 -1.915394 1.479338
H 1.904460 -1.537621 2.255610
H 1.568043 -3.231583 2.062255
H -3.210786 -5.195744 0.715916

H -4.098940 -5.086500 -0.797301
H -2.351455 -5.212126 -0.816903
H -6.090489 -4.601332 0.024087
H -5.249187 -4.269397 1.537602
H -6.928707 -3.709848 1.295885
H -5.005571 2.525248 1.313289
H -3.405906 4.689425 0.318953
H -4.548048 3.359957 -1.595759
H -5.896954 2.378179 -1.012292
H -5.741654 4.064292 -0.495702
H -2.409850 4.821563 2.516403
H -4.126203 4.499770 2.657460
H -2.820664 3.133189 4.287457
H -3.620756 2.065271 3.138062
H -1.899288 2.402661 2.972091
H 1.719326 5.734121 0.163863
H 1.613693 5.268526 1.856988
H 3.166922 5.180348 1.016616
H 4.589725 0.208203 1.042547
H 8.331134 -0.009331 -1.040746
H 7.202752 -0.839960 -2.156056
H 7.395885 0.922391 -2.248656