

Int1

Pd	0.057257	-0.559010	0.214920	C	5.145172	-2.890905	-2.298888
Br	-1.881379	-3.323028	0.134593	H	5.813664	-3.629025	-2.734145
P	2.231981	0.244313	-0.454936	C	5.598084	-1.589064	-2.064309
P	-1.353922	0.887213	-1.118057	H	6.618838	-1.313837	-2.316928
C	3.240316	1.084033	0.845033	C	4.742842	-0.640795	-1.503861
C	3.153961	2.468199	1.067589	H	5.109492	0.364760	-1.314685
H	2.538957	3.090751	0.425295	C	-1.243253	2.647924	-0.555435
C	3.849668	3.066361	2.121014	C	-1.732419	3.724002	-1.316553
H	3.773395	4.140212	2.271922	H	-2.215030	3.540472	-2.272842
C	4.640910	2.294373	2.971958	C	-1.625488	5.033871	-0.849327
H	5.183143	2.761246	3.789725	H	-2.009160	5.854371	-1.450124
C	4.729656	0.915438	2.764782	C	-1.032956	5.290254	0.390626
H	5.344481	0.304027	3.420342	H	-0.952039	6.311251	0.754198
C	4.033432	0.316181	1.715870	C	-0.551707	4.231068	1.160806
H	4.117925	-0.756384	1.563850	H	-0.095014	4.420579	2.128474
C	3.421223	-0.980687	-1.167205	C	-0.655927	2.918953	0.689708
C	2.979162	-2.290108	-1.405934	H	-0.277757	2.091424	1.285493
H	1.958493	-2.560802	-1.146026	C	-3.181340	0.617743	-1.236877
C	3.835155	-3.240140	-1.969928	C	-3.658373	-0.490165	-1.960077
H	3.477444	-4.250820	-2.147657	H	-2.962664	-1.144033	-2.479581

C	-5.020730	-0.783510	-2.001240	C	3.021213	-3.709315	-1.635883
H	-5.368060	-1.643259	-2.568197	H	2.691564	-4.744944	-1.658822
C	-5.932855	0.013524	-1.304761	C	3.859692	-3.218231	-2.638281
H	-6.993624	-0.220347	-1.329147	H	4.186972	-3.867785	-3.445574
C	-5.469828	1.102784	-0.566794	C	4.274163	-1.885271	-2.595090
H	-6.168150	1.721531	-0.009926	H	4.928822	-1.492261	-3.368734
C	-4.106322	1.403531	-0.532029	C	3.856992	-1.050687	-1.557095
H	-3.766882	2.254519	0.049185	H	4.195419	-0.018742	-1.533479
C	-1.128462	-1.937354	1.433603	C	3.794859	0.723795	1.089523
C	-2.036803	-1.330435	2.366196	C	3.578355	2.108516	1.115839
C	-1.533769	-0.864937	3.575416	H	2.588615	2.498168	0.896346
H	-2.234963	-0.370770	4.241944	C	4.626603	2.985175	1.411622
C	-0.181365	-1.026571	3.931644	H	4.444328	4.056392	1.425583
C	0.683628	-1.672984	3.067855	C	5.900381	2.486558	1.683240
H	1.714548	-1.858728	3.359047	H	6.715711	3.167740	1.912414
C	0.238595	-2.155054	1.805103	C	6.128254	1.107015	1.656565
H	0.830626	-2.904752	1.290805	H	7.120221	0.714273	1.864739
H	0.170782	-0.670970	4.895690	C	5.083899	0.231957	1.361762
C	-3.476733	-1.126358	2.080670	H	5.273817	-0.837793	1.333815
O	-4.253624	-0.605454	2.865566	C	-2.146007	-2.189599	0.669863
H	-3.824977	-1.473427	1.091335	C	-3.016582	-3.025246	1.391608
C	-0.867098	0.970466	-2.945169	H	-3.482733	-2.666455	2.305377
H	-0.826410	2.020005	-3.260651	C	-3.310123	-4.311315	0.939049
H	-1.698772	0.517573	-3.494122	H	-3.985777	-4.943371	1.509571
C	0.435335	0.238734	-3.328799	C	-2.740113	-4.784365	-0.246413
H	0.354546	-0.047373	-4.386424	H	-2.968976	-5.786888	-0.598405
H	0.500940	-0.700847	-2.766842	C	-1.881191	-3.962859	-0.976375
C	1.748258	1.031012	-3.191986	H	-1.438331	-4.320021	-1.902378
H	1.699925	1.903450	-3.859604	C	-1.586242	-2.674410	-0.521415
H	2.559402	0.400816	-3.577032	H	-0.915869	-2.038154	-1.092434
C	2.151379	1.548769	-1.797658	C	-3.348376	0.361667	1.337803
H	3.122262	2.054146	-1.875780	C	-3.429874	1.587560	2.023959
H	1.429063	2.296542	-1.450583	H	-2.550543	1.994509	2.518746
				C	-4.623648	2.304890	2.067437
				H	-4.665724	3.248223	2.605538
TS1				C	-5.756176	1.822310	1.406969
				H	-6.683158	2.388352	1.427466
Pd	0.161410	0.486443	0.031934	C	-5.683454	0.618480	0.708032
Br	0.433102	3.025779	-1.154134	H	-6.555439	0.241323	0.180469
P	2.361845	-0.396265	0.762294	C	-4.490855	-0.107576	0.672887
P	-1.704016	-0.482137	1.240441	H	-4.453701	-1.041135	0.121440
C	3.020102	-1.535822	-0.537706	C	-0.673098	1.234847	-1.834019
C	2.602028	-2.875675	-0.597521	C	-2.054711	1.401216	-2.086367
H	1.939337	-3.276943	0.164283	C	-2.644133	0.605893	-3.079434

H	-3.712550	0.727353	-3.234696	C	3.562947	-3.118149	-2.077854
C	-1.894279	-0.290838	-3.837827	H	3.190785	-4.109872	-2.319516
C	-0.512358	-0.372550	-3.637704	C	4.894112	-2.786045	-2.331980
H	0.094664	-1.028726	-4.256668	H	5.563294	-3.517884	-2.776997
C	0.115437	0.421506	-2.673262	C	5.368920	-1.512745	-2.006083
H	1.195697	0.422110	-2.580171	H	6.406800	-1.251389	-2.195615
H	-2.373162	-0.891056	-4.605988	C	4.512119	-0.574595	-1.431025
C	-2.904113	2.379041	-1.365990	H	4.892919	0.409122	-1.169650
O	-4.073400	2.587425	-1.642117	C	-1.295593	2.634303	-0.295887
H	-2.402526	2.939791	-0.557085	C	-1.804122	3.730509	-1.015357
C	2.382521	-1.484091	2.309325	H	-2.331510	3.573509	-1.952363
H	2.868831	-0.900594	3.099576	C	-1.656520	5.028405	-0.527532
H	3.016824	-2.357955	2.122260	H	-2.053812	5.865934	-1.094675
C	0.973712	-1.903588	2.760105	C	-1.004146	5.250809	0.688974
H	1.055889	-2.722181	3.487658	H	-0.890186	6.263127	1.067296
H	0.428689	-2.319182	1.904748	C	-0.502862	4.170616	1.415390
C	0.179315	-0.733325	3.381441	H	0.007768	4.333643	2.360176
H	0.589346	0.218088	3.021002	C	-0.647912	2.869341	0.926153
H	0.323276	-0.734596	4.470658	H	-0.249732	2.028726	1.488902
C	-1.323717	-0.739016	3.075145	C	-3.315831	0.651003	-0.894157
H	-1.793185	-1.668533	3.417686	C	-3.860188	-0.406484	-1.642491
H	-1.810882	0.079081	3.615968	H	-3.207711	-1.067353	-2.205994
				C	-5.235513	-0.633589	-1.652338
				H	-5.639970	-1.453548	-2.239727
				C	-6.088276	0.183121	-0.906297
				H	-7.160261	0.005774	-0.914909
				C	-5.554692	1.221945	-0.143849
				H	-6.208877	1.857992	0.446491
				C	-4.177405	1.454115	-0.134133
				H	-3.780112	2.266951	0.464306
				C	-1.784425	-1.456621	1.141060
				C	-2.332978	-2.637917	0.591798
				C	-3.380672	-3.311292	1.251674
				H	-3.773275	-4.229375	0.816557
				C	-3.911976	-2.816331	2.435246
				C	-3.382062	-1.638665	2.972115
				H	-3.782315	-1.239857	3.901930
				C	-2.330252	-0.973246	2.334557
				H	-1.921022	-0.078382	2.795374
				H	-4.721823	-3.337212	2.938326
				C	-1.875364	-3.218496	-0.676267
				O	-1.090305	-2.721083	-1.475641
				H	-2.333469	-4.204176	-0.914487
				C	1.875159	1.564373	-1.910200
Int2							
Pd	-0.133360	-0.576090	0.324573				
Br	1.184379	-2.174607	1.892550				
P	1.998701	0.346886	-0.497165				
P	-1.485336	0.898642	-0.895483				
C	2.984858	1.278943	0.751740				
C	3.637309	0.569952	1.776429				
H	3.566033	-0.511806	1.813802				
C	4.356604	1.250403	2.758130				
H	4.854830	0.685840	3.541561				
C	4.432928	2.645200	2.740868				
H	4.994415	3.172027	3.507980				
C	3.781791	3.358028	1.734253				
H	3.834085	4.443581	1.710485				
C	3.061943	2.681197	0.746276				
H	2.563283	3.260271	-0.023533				
C	3.170748	-0.901750	-1.173053				
C	2.702465	-2.183575	-1.496910				
H	1.673956	-2.455090	-1.280558				

H	1.171875	2.345598	-1.598842	C	0.617377	-1.369407	3.567085
H	2.849553	2.048263	-2.047300	H	1.252273	-0.952177	4.343957
C	1.428593	0.948935	-3.247468	C	0.224428	-2.708189	3.627667
H	1.365052	1.767977	-3.978217	H	0.553224	-3.334835	4.452108
H	2.214956	0.276309	-3.609441	C	-0.598973	-3.237527	2.631544
C	0.098387	0.179844	-3.249092	H	-0.915596	-4.275703	2.677363
H	-0.101987	-0.117236	-4.286865	C	-1.027819	-2.429350	1.578010
H	0.183981	-0.754093	-2.684154	H	-1.680743	-2.839195	0.810570
C	-1.126325	0.968855	-2.747387	C	-1.074273	1.649868	0.565981
H	-1.058492	2.023344	-3.041070	C	-0.403203	2.621446	-0.193199
H	-2.026382	0.574004	-3.225896	H	0.139253	2.346366	-1.091364
				C	-0.421640	3.961785	0.196992
				H	0.103926	4.700280	-0.401596
				C	-1.110794	4.349305	1.346012
				H	-1.127974	5.393343	1.645679
Int3				C	-1.786445	3.390970	2.105000
Pd	-3.105990	-0.900111	-0.960149	H	-2.333880	3.685907	2.995652
Br	-4.891141	-2.015729	-2.318753	C	-1.773883	2.051859	1.718254
P	5.023076	-0.632218	-1.223143	H	-2.314386	1.320174	2.310870
P	-1.156776	-0.104934	0.040960	C	-4.243422	-0.090542	0.459967
C	6.624254	-1.070718	-0.391567	C	-4.838267	1.166260	0.274852
C	6.933926	-2.436905	-0.259389	C	-5.680154	1.675209	1.281755
H	6.226781	-3.189264	-0.603071	H	-6.129696	2.649307	1.110692
C	8.143538	-2.850148	0.296807	C	-5.924910	0.950988	2.440988
H	8.356700	-3.911498	0.395226	C	-5.327346	-0.303257	2.607734
C	9.083166	-1.903888	0.713730	H	-5.517065	-0.884337	3.506963
H	10.029577	-2.223787	1.141270	C	-4.485577	-0.827660	1.620929
C	8.800251	-0.546189	0.566088	H	-4.036735	-1.804677	1.763965
H	9.527343	0.198918	0.879222	H	-6.580297	1.350789	3.209683
C	7.582614	-0.132210	0.019138	C	-4.618604	1.993692	-0.940131
H	7.382155	0.929196	-0.084473	O	-5.081343	3.108306	-1.095957
C	4.919761	1.205706	-0.996979	H	-3.987293	1.522366	-1.721732
C	4.902744	1.994337	-2.158634	C	0.184533	-0.328383	-1.237178
H	4.961152	1.510344	-3.130489	H	-0.086945	0.349714	-2.054805
C	4.807868	3.386394	-2.082722	H	0.039411	-1.339340	-1.638632
H	4.797406	3.978410	-2.994075	C	1.656438	-0.131458	-0.800483
C	4.725947	4.012615	-0.838648	H	2.191189	0.366131	-1.618182
H	4.650771	5.095015	-0.775686	H	1.719485	0.554455	0.053195
C	4.744217	3.242625	0.327838	C	2.364792	-1.451438	-0.460775
H	4.685602	3.725850	1.299839	H	2.371532	-2.089929	-1.355035
C	4.841902	1.852969	0.248538	H	1.783459	-1.987400	0.299920
H	4.871104	1.271155	1.165996	C	3.803647	-1.291724	0.058072
C	-0.627756	-1.084877	1.502513	H	3.818126	-0.685380	0.972313
C	0.195804	-0.559742	2.511041	H	4.186754	-2.279683	0.338845
H	0.500238	0.481438	2.478439				

Int4

P 4.508372 -0.423693 0.140276
C 6.225244 -1.093748 -0.078819
C 7.370007 -0.295670 -0.223258
H 7.275073 0.783603 -0.283990
C 8.640534 -0.873514 -0.294245
H 9.513079 -0.235236 -0.409216
C 8.792224 -2.258018 -0.221847
H 9.780764 -2.705515 -0.279572
C 7.662309 -3.064623 -0.064315
H 7.767310 -4.144349 0.004487
C 6.396174 -2.487137 0.017108
H 5.531682 -3.130984 0.166051
C 4.697302 1.367406 -0.305609
C 5.112830 1.830043 -1.566558
H 5.368796 1.120154 -2.348598
C 5.219477 3.196204 -1.828800
H 5.544978 3.534467 -2.809281
C 4.913764 4.127710 -0.832306
H 5.000665 5.191829 -1.036364
C 4.502364 3.685112 0.425340
H 4.266864 4.402749 1.207142
C 4.394458 2.315916 0.683840
H 4.063294 1.977731 1.662324
P -1.157615 -0.267570 0.051478
C -0.921906 -2.071301 0.323012
C -0.918806 -2.616141 1.616597
H -0.975383 -1.966239 2.483666
C -0.848433 -3.997827 1.804951
H -0.850230 -4.400357 2.813964
C -0.788023 -4.854693 0.706275
H -0.737443 -5.929965 0.853773
C -0.810336 -4.323780 -0.585336
H -0.780598 -4.983914 -1.447872
C -0.883535 -2.944942 -0.776265
H -0.925418 -2.555368 -1.788365
C -0.420232 0.547657 1.534799
C 0.806964 0.139635 2.087035
H 1.352271 -0.696662 1.661786
C 1.335965 0.791101 3.202274
H 2.282379 0.455944 3.617976

C 0.646125 1.857001 3.784652
H 1.052900 2.355788 4.660603
C -0.572919 2.269497 3.244346
H -1.123039 3.086880 3.704744
C -1.106194 1.622318 2.126445
H -2.050875 1.951909 1.702369
Pd -3.257107 0.552821 -0.435557
C -4.031577 -1.276418 -0.790601
C -4.176454 -1.667638 -2.131732
C -4.528560 -2.138964 0.207703
C -4.788082 -2.877912 -2.467676
H -3.827910 -1.014054 -2.928037
C -5.140405 -3.359295 -0.137888
C -5.269769 -3.732875 -1.468214
H -4.895038 -3.153402 -3.515229
H -5.510266 -3.988373 0.667373
H -5.746831 -4.672998 -1.733208
C -4.428543 -1.789226 1.641135
O -4.799774 -2.495293 2.564747
H -3.974248 -0.792972 1.838038
O -4.950341 1.729907 -0.868093
C -4.325087 2.847896 -0.660921
O -4.827707 3.989073 -0.775760
O -3.032499 2.701185 -0.302053
K -2.697331 5.210025 -0.279604
C -0.059122 0.230193 -1.384159
H -0.394888 1.253828 -1.589924
H -0.398062 -0.365368 -2.241391
C 1.476596 0.211669 -1.277776
H 1.862443 0.790849 -2.129349
H 1.787229 0.762880 -0.382835
C 2.130460 -1.176915 -1.300211
H 1.750796 -1.734405 -2.168452
H 1.827584 -1.754494 -0.419303
C 3.666848 -1.151576 -1.384748
H 4.034632 -2.181260 -1.461661
H 3.994940 -0.635833 -2.295952

TS2

P -5.206366 0.247755 0.163907
C -7.047584 0.438454 0.222455
C -7.811582 -0.621258 0.748781

H	-7.316837	-1.549908	1.023075	C	4.757211	1.909642	-0.422996
C	-9.844395	0.680524	0.568507	C	4.692009	2.246670	-3.186048
H	-10.919596	0.773393	0.700350	H	3.037007	0.884263	-3.168800
C	-9.102288	1.744311	0.056764	C	5.682514	2.762536	-1.057651
H	-9.597809	2.673482	-0.215898	C	5.655695	2.935034	-2.434111
C	-7.720127	1.623876	-0.116496	H	4.658622	2.369860	-4.267626
H	-7.168868	2.466151	-0.522924	H	6.409033	3.277898	-0.434406
C	-4.983836	-1.234489	-0.920949	H	6.371043	3.591469	-2.924470
C	-5.889674	-1.633476	-1.920111	C	4.823957	1.796013	1.051463
H	-6.825159	-1.095891	-2.051879	O	5.597660	2.416934	1.766379
C	-5.596687	-2.721297	-2.742986	H	4.088905	1.089208	1.490480
H	-6.308374	-3.023526	-3.508913	C	3.810392	-1.628633	-0.301737
C	-4.387156	-3.410935	-2.598152	N	4.608256	-1.609643	-1.751812
H	-4.157398	-4.246025	-3.256342	N	4.681242	-1.789238	-2.854994
C	-3.475957	-3.020153	-1.617328	C	3.514585	-3.028470	-0.033486
H	-2.511300	-3.499517	-1.482454	C	2.549612	-3.751859	-0.766540
C	-3.785351	-1.950273	-0.773245	C	4.269167	-3.663007	1.064574
H	-3.052263	-1.690329	-0.015015	C	2.243688	-5.072305	-0.466247
P	0.683742	1.577437	0.185693	H	1.998373	-3.236056	-1.550815
C	0.863231	3.425226	0.112616	C	3.856511	-5.030163	1.368841
C	0.055357	4.287799	0.876270	C	2.913347	-5.701352	0.616179
H	-0.639311	3.876329	1.601550	H	1.489024	-5.606432	-1.035966
C	0.144782	5.672142	0.725830	H	4.389449	-5.527108	2.177253
H	-0.487366	6.320244	1.328423	H	2.678328	-6.739431	0.855194
C	1.041410	6.222615	-0.192914	O	-0.039165	-1.645684	-1.586393
H	1.113996	7.301655	-0.306878	C	-0.019158	-1.905497	-0.355026
C	1.845088	5.378640	-0.959091	O	-0.811267	-2.708820	0.265769
H	2.552160	5.793764	-1.672726	O	0.896453	-1.303079	0.448705
C	1.758049	3.992280	-0.807759	K	1.064317	-3.337231	1.938567
H	2.393609	3.349686	-1.406072	O	5.163808	-3.073926	1.717289
C	0.227037	1.279747	1.950548	H	4.619927	-1.287609	0.347138
C	-0.670077	0.262519	2.320767	C	-0.809901	1.321279	-0.899645
H	-1.143286	-0.357683	1.569938	H	-0.796446	0.259296	-1.178296
C	-0.920848	-0.001623	3.669590	H	-0.541728	1.866221	-1.816276
H	-1.635866	-0.778045	3.932997	C	-2.195271	1.764492	-0.411427
C	-0.264820	0.719181	4.670388	H	-2.467397	1.206578	0.490586
H	-0.462727	0.508067	5.718828	H	-2.195936	2.827024	-0.131499
C	0.650221	1.710584	4.312986	C	-3.252878	1.521079	-1.504852
H	1.179708	2.271525	5.079125	H	-3.089687	0.532276	-1.948887
C	0.892603	1.987277	2.965923	H	-3.099542	2.246482	-2.316701
H	1.610486	2.760529	2.708391	C	-4.714077	1.626241	-1.029671
Pd	2.375705	-0.050635	-0.376314	H	-5.385670	1.613704	-1.898039
C	3.775833	1.205068	-1.160178	H	-4.867462	2.580697	-0.507298
C	3.774070	1.403058	-2.558067	C	-9.190478	-0.506516	0.912503

H	-9.756485	-1.344632	1.312536	H	0.158040	-3.474225	5.692923
				C	-0.402502	-3.917548	3.655826
				H	-0.646615	-4.957666	3.858759
Int5				C	-0.548077	-3.415186	2.362060
				H	-0.903792	-4.074400	1.574870
P	5.398803	0.745956	0.460181	Pd	-2.755242	-0.306408	0.249380
C	7.170488	0.202950	0.408863	C	-3.567508	-1.210339	-1.402805
C	8.150359	1.122436	0.829589	C	-3.429537	-0.626964	-2.680820
H	7.852664	2.131758	1.104931	C	-4.244590	-2.453704	-1.354330
C	9.894804	-0.532396	0.559795	C	-3.906805	-1.247705	-3.836377
H	10.942601	-0.816012	0.618530	H	-2.936708	0.337327	-2.777735
C	8.936131	-1.459563	0.153552	C	-4.726892	-3.080330	-2.520451
H	9.233465	-2.472050	-0.109375	C	-4.558676	-2.486985	-3.763227
C	7.588200	-1.095184	0.075688	H	-3.774777	-0.761209	-4.802216
H	6.864340	-1.835571	-0.249282	H	-5.233332	-4.036161	-2.410432
C	5.385487	2.081224	-0.830308	H	-4.932510	-2.968528	-4.664289
C	6.207504	2.081494	-1.969717	C	-4.467133	-3.142106	-0.063404
H	6.927026	1.280058	-2.114685	O	-4.998292	-4.237360	0.064210
C	6.117120	3.104989	-2.913479	H	-4.107606	-2.578681	0.823431
H	6.762110	3.090884	-3.789057	C	-4.391843	0.829179	0.361627
C	5.197489	4.142949	-2.738648	C	-4.625240	2.086406	-0.168804
H	5.125573	4.938022	-3.476718	C	-3.669051	2.713624	-1.051387
C	4.373631	4.154987	-1.612706	C	-5.865964	2.840731	0.207631
H	3.655056	4.957628	-1.468326	C	-3.839133	3.984356	-1.534875
C	4.473176	3.135215	-0.662762	H	-2.771208	2.147814	-1.275383
H	3.834837	3.156500	0.217050	C	-5.950970	4.215463	-0.312946
P	-0.563459	-1.399317	0.388529	C	-5.002779	4.735526	-1.148975
C	0.088657	-2.736275	-0.728017	H	-3.105765	4.430480	-2.201866
C	1.163511	-3.575917	-0.384675	H	-6.835556	4.782132	-0.031292
H	1.603852	-3.509302	0.605262	H	-5.126162	5.746870	-1.538430
C	1.662550	-4.509182	-1.294851	O	-1.267657	2.413000	0.974444
H	2.492577	-5.151072	-1.007622	C	-1.726198	1.847611	2.043766
C	1.096788	-4.622160	-2.567288	O	-1.990398	2.509546	3.103492
H	1.482845	-5.352795	-3.274459	O	-1.966849	0.539870	2.036408
C	0.027762	-3.797938	-2.919934	K	-2.937238	4.259501	1.554617
H	-0.429706	-3.883735	-3.902410	O	-6.763420	2.378488	0.926350
C	-0.473665	-2.865545	-2.008179	H	-5.198832	0.477076	1.011252
H	-1.313936	-2.239599	-2.289946	C	0.662984	-0.022749	0.107646
C	-0.241931	-2.074879	2.070907	H	0.220818	0.851669	0.602859
C	0.184774	-1.241533	3.117029	H	0.559546	0.190771	-0.964963
H	0.367248	-0.190826	2.931290	C	2.151211	-0.242556	0.467111
C	0.334725	-1.747864	4.408950	H	2.493503	0.599697	1.081729
H	0.662859	-1.085019	5.205556	H	2.282987	-1.131629	1.097161
C	0.046176	-3.085494	4.683328	C	3.050730	-0.367601	-0.772789

H	2.960116	0.542084	-1.381141	C	-0.495021	3.240888	0.579084
H	2.679904	-1.190614	-1.397223	H	-1.484060	2.937528	0.906309
C	4.536263	-0.640896	-0.473724	C	0.208302	0.254103	-2.167370
H	5.072303	-0.842543	-1.410639	C	0.473702	-1.076356	-2.537651
H	4.618451	-1.540316	0.151562	H	0.422405	-1.868134	-1.797183
C	9.495103	0.764631	0.896074	C	0.765448	-1.400065	-3.864886
H	10.232412	1.496449	1.217483	H	0.965335	-2.437432	-4.122973
				C	0.786149	-0.407671	-4.849604
				H	1.017711	-0.661698	-5.882144
				C	0.510558	0.915353	-4.494709
				H	0.522259	1.698709	-5.249660
				C	0.222314	1.240990	-3.167088
				H	0.006906	2.274244	-2.909899
				Pd	-2.729932	-0.001862	-0.107207
				C	-3.535559	1.226381	1.310745
				C	-3.332981	0.934057	2.681063
				C	-4.138574	2.481331	1.022990
				C	-3.695174	1.822042	3.688877
				H	-2.903980	-0.026155	2.955495
				C	-4.514435	3.373692	2.046489
				C	-4.292328	3.054802	3.377095
				H	-3.520315	1.553645	4.729573
				H	-4.972529	4.315720	1.755687
				H	-4.581652	3.742590	4.168446
				C	-4.374596	2.897103	-0.374992
				O	-4.829179	3.979596	-0.722334
				H	-4.090768	2.132999	-1.129866
				C	-4.626793	-0.358965	0.374947
				C	-5.122754	-1.454250	1.057643
				C	-4.260615	-2.475060	1.605868
				C	-6.606038	-1.588347	1.213230
				C	-4.763280	-3.541719	2.294318
				H	-3.193187	-2.400271	1.403366
				C	-7.058684	-2.751504	1.979792
				C	-6.181919	-3.663867	2.486757
				H	-4.101099	-4.313239	2.678113
				H	-8.133038	-2.849221	2.117218
				H	-6.560892	-4.519514	3.046967
				O	-1.176691	-2.805066	-0.106775
				C	-1.790901	-2.713238	-1.206826
				O	-1.857487	-3.639372	-2.097289
				O	-2.401214	-1.547164	-1.543795
				K	-3.200046	-2.326564	-3.705773
				C	4.318915	-1.796280	1.190831
TS3							
P	5.458579	-0.384762	1.691540				
C	7.087332	-1.284251	1.642769				
C	8.052949	-1.146931	0.634477				
H	7.859964	-0.496401	-0.212773				
C	9.263911	-1.841161	0.703193				
H	9.997201	-1.720218	-0.090920				
C	9.531941	-2.689496	1.777960				
H	10.473463	-3.230695	1.828393				
C	8.582387	-2.832317	2.792918				
H	8.781877	-3.484539	3.639814				
C	7.380415	-2.128333	2.729433				
H	6.659610	-2.231362	3.538328				
C	5.571840	0.708109	0.197625				
C	5.363734	0.293851	-1.128369				
H	5.118578	-0.741336	-1.344792				
C	5.458848	1.200286	-2.186350				
H	5.280722	0.860939	-3.203488				
C	5.776411	2.538104	-1.939010				
H	5.848473	3.243093	-2.763305				
C	5.992017	2.965221	-0.627356				
H	6.235234	4.005242	-0.424204				
C	5.881513	2.058743	0.428988				
H	6.026608	2.402594	1.450285				
P	-0.366772	0.636338	-0.452510				
C	0.296132	2.342337	-0.153475				
C	1.569542	2.764415	-0.577738				
H	2.197699	2.095849	-1.158320				
C	2.036749	4.043315	-0.272527				
H	3.027068	4.344505	-0.605275				
C	1.239667	4.925494	0.461872				
H	1.603793	5.922812	0.698411				
C	-0.026336	4.521283	0.885877				
H	-0.659297	5.200953	1.450767				

H	4.637334	-2.631155	1.828397	C	-2.009964	2.224868	-3.010492
H	4.506076	-2.118087	0.158309	H	-2.764260	2.992159	-3.168883
C	2.818400	-1.536885	1.417635	C	-1.545924	1.463661	-4.084294
H	2.288558	-2.488912	1.279725	H	-1.933639	1.639718	-5.085333
H	2.655168	-1.242918	2.463855	C	-0.582206	0.474521	-3.866554
C	2.184235	-0.490387	0.487067	H	-0.217547	-0.124374	-4.697671
H	2.427090	-0.744775	-0.553004	C	-0.074287	0.248861	-2.586772
H	2.625555	0.496126	0.677641	H	0.665173	-0.530645	-2.405984
C	0.662423	-0.442673	0.665887	C	-0.470014	1.879435	1.309843
H	0.195575	-1.432004	0.540140	C	-1.143931	1.535209	2.494605
H	0.405718	-0.106058	1.679958	H	-1.357445	0.496100	2.719591
O	-7.421183	-0.780284	0.733668	C	-1.545055	2.517145	3.403116
H	-5.417571	0.278756	-0.024328	H	-2.067062	2.223743	4.310918
				C	-1.278765	3.862950	3.147920
				H	-1.588817	4.627399	3.856586
				C	-0.592423	4.217510	1.984434
Int6				H	-0.350506	5.258201	1.785522
P	-5.381079	-0.326175	-0.491967	C	-0.186269	3.237825	1.078773
C	-7.033075	-1.003379	-1.012116	H	0.387063	3.533857	0.207689
C	-8.193378	-0.915363	-0.226055	Pd	2.568369	0.341635	0.011701
H	-8.133686	-0.514359	0.780735	C	4.446254	1.123879	-1.094707
C	-9.429552	-1.344690	-0.715949	C	4.800765	0.748982	-2.438569
H	-10.311125	-1.269710	-0.083275	C	3.468685	2.207636	-0.943296
C	-9.535985	-1.870455	-2.003583	C	4.198401	1.317245	-3.527905
H	-10.497407	-2.207778	-2.382598	H	5.593251	0.022491	-2.572093
C	-8.394116	-1.950467	-2.804599	C	2.851189	2.746770	-2.125006
H	-8.462031	-2.348628	-3.814235	C	3.180112	2.304577	-3.375374
C	-7.163087	-1.512981	-2.317735	H	4.511878	1.023686	-4.527382
H	-6.292927	-1.562974	-2.968336	H	2.145402	3.558709	-1.982224
C	-5.571697	-0.187137	1.349529	H	2.702192	2.729940	-4.253822
C	-5.901292	-1.263230	2.191926	C	3.408155	3.057367	0.267987
H	-6.092513	-2.244547	1.765799	O	2.698005	4.053277	0.377142
C	-5.995157	-1.088968	3.572701	H	4.086888	2.779146	1.094169
H	-6.248289	-1.934026	4.208481	C	5.733799	-0.750429	0.167251
C	-5.758112	0.167189	4.138743	C	5.771525	-1.803971	-0.770468
H	-5.824441	0.300800	5.215667	C	6.509304	-0.856633	1.421338
C	-5.431921	1.245845	3.316697	C	6.577004	-2.929181	-0.598947
H	-5.238163	2.224455	3.747880	H	5.095727	-1.775887	-1.620675
C	-5.342093	1.067824	1.933343	C	7.354814	-2.032550	1.527145
H	-5.075579	1.908666	1.298371	C	7.388105	-3.017741	0.554129
P	0.179825	0.602225	0.147312	H	6.564666	-3.729176	-1.333892
C	-0.544817	1.011206	-1.499958	H	7.964198	-2.109200	2.425864
C	-1.515078	1.998299	-1.723117	H	8.036434	-3.884425	0.688436
H	-1.891027	2.590614	-0.894908	O	1.574691	-2.172738	-1.198093

C	2.113957	-2.538196	-0.113636	C	4.963296	3.695299	0.801907
O	2.397699	-3.729351	0.232883	H	4.687805	4.273745	1.679744
O	2.437482	-1.586225	0.816836	C	4.919341	2.299213	0.850608
K	4.331865	-3.007988	1.750348	H	4.598778	1.803160	1.762774
C	-0.676340	-0.975616	0.628466	C	-0.328368	-1.926674	0.618872
H	-0.274833	-1.229384	1.615284	C	-0.343870	-2.602080	1.852539
H	-0.231480	-1.705222	-0.058637	H	-0.470511	-2.043162	2.772414
C	-2.220701	-1.039260	0.604079	C	-0.264317	-3.996448	1.899741
H	-2.664508	-0.057901	0.812133	H	-0.295508	-4.495972	2.864074
H	-2.549393	-1.690821	1.427354	C	-0.177254	-4.740641	0.720426
C	-2.795019	-1.594631	-0.708819	H	-0.105235	-5.825855	0.759883
H	-2.286277	-2.540113	-0.941025	C	-0.199929	-4.077682	-0.513266
H	-2.562975	-0.912788	-1.533823	H	-0.154180	-4.645208	-1.440662
C	-4.309498	-1.868957	-0.679548	C	-0.287254	-2.682688	-0.569643
H	-4.555887	-2.599074	0.102545	H	-0.398339	-2.192269	-1.534958
H	-4.606326	-2.322358	-1.632888	C	0.431217	0.509544	2.023484
C	4.901239	0.431909	0.068368	C	1.661726	-0.062659	2.387355
H	4.907285	0.974477	1.012470	H	2.044169	-0.924033	1.848563
O	6.417757	-0.011995	2.353708	C	2.399286	0.450026	3.456572

TS4

Pd	-2.888546	0.646019	0.778414	H	3.343897	-0.015377	3.728659
P	-0.554696	-0.090312	0.581075	C	1.918344	1.547723	4.174593
P	5.115418	-0.315688	-0.126640	H	2.488804	1.944836	5.011519
C	6.783876	-0.891477	-0.710982	C	0.696309	2.121687	3.821235
C	7.931449	-0.082038	-0.677683	H	0.305344	2.966635	4.382280
H	7.846495	0.961674	-0.392504	C	-0.048552	1.604986	2.758475
C	9.186205	-0.596030	-1.013885	H	-1.008897	2.047434	2.513845
H	10.056585	0.055556	-0.984491	C	-3.876181	2.230162	-1.535404
C	9.325751	-1.932526	-1.388552	C	-4.513242	2.604321	-2.727191
H	10.301883	-2.330978	-1.653350	C	-3.695614	3.207485	-0.542687
C	8.197411	-2.755762	-1.411082	C	-4.935056	3.921944	-2.919814
H	8.290464	-3.802302	-1.691486	H	-4.664265	1.858154	-3.502423
C	6.946913	-2.243332	-1.067412	C	-4.084777	4.535231	-0.746384
H	6.088683	-2.911303	-1.070048	C	-4.712813	4.894787	-1.937758
C	5.252479	1.528759	-0.273803	H	-5.436380	4.194067	-3.846664
C	5.635548	2.194849	-1.451194	H	-3.916484	5.255978	0.049234
H	5.904668	1.621227	-2.334513	H	-5.043853	5.918603	-2.097331
C	5.685130	3.587844	-1.500677	C	-3.131554	2.736249	0.762812
H	5.981052	4.086217	-2.420726	O	-2.733423	3.494539	1.630607
C	5.347103	4.341690	-0.372887	H	-4.157005	1.614664	1.161330
H	5.377204	5.427619	-0.414226	C	-3.842564	-0.351495	-1.836845
				C	-5.197260	-0.668430	-1.655079
				C	-2.950285	-1.304929	-2.501887
				C	-5.746505	-1.881260	-2.075947
				H	-5.828577	0.052576	-1.139061

C	-3.555387	-2.552638	-2.900273	C	-5.875709	3.683632	0.825479
C	-4.907243	-2.821309	-2.702258	H	-6.203295	4.395971	1.578912
H	-6.801449	-2.093629	-1.920908	C	-5.371851	4.138667	-0.396880
H	-2.915361	-3.263701	-3.421333	H	-5.303580	5.205503	-0.594226
H	-5.323840	-3.766641	-3.055037	C	-4.946480	3.220124	-1.355980
O	-2.622847	-0.424385	2.805578	H	-4.533371	3.561787	-2.300597
C	-3.261226	-1.481807	2.367924	C	-5.028823	1.849600	-1.095641
O	-3.275664	-2.599189	2.951345	H	-4.681158	1.141502	-1.843153
O	-3.838425	-1.328323	1.190369	P	-0.002562	-0.575204	-0.479182
K	-3.433112	-3.525666	0.232715	C	-0.792399	-2.224999	-0.793666
C	0.372988	0.570967	-0.904654	C	-2.122944	-2.401403	-1.214795
H	0.049178	1.620176	-0.920345	H	-2.747912	-1.538720	-1.424190
H	-0.105341	0.097830	-1.771650	C	-2.662506	-3.679541	-1.369046
C	1.909187	0.543524	-0.993322	H	-3.695169	-3.790070	-1.691659
H	2.340357	0.946217	-0.069486	C	-1.882129	-4.807814	-1.103726
H	2.196280	1.248995	-1.787776	H	-2.302271	-5.803798	-1.224970
C	2.537124	-0.818551	-1.317347	C	-0.559753	-4.648103	-0.688945
H	2.033859	-1.239531	-2.198531	H	0.059915	-5.519142	-0.489764
H	2.355387	-1.525534	-0.499749	C	-0.018420	-3.368733	-0.540685
C	4.047171	-0.766829	-1.616262	H	1.017093	-3.252495	-0.241446
H	4.253141	-0.084622	-2.451044	C	-0.728641	0.532929	-1.760186
H	4.379861	-1.761633	-1.935231	C	-0.797534	1.917135	-1.518787
C	-3.237632	0.887932	-1.331152	H	-0.464233	2.323505	-0.569995
H	-2.214309	0.941475	-1.709505	C	-1.238954	2.791032	-2.512877
O	-1.716982	-1.057133	-2.718363	H	-1.268141	3.857147	-2.303630
				C	-1.614953	2.306683	-3.767525
				H	-1.953630	2.990852	-4.542651
				C	-1.526512	0.937104	-4.027409
				H	-1.797557	0.546959	-5.006070
				C	-1.080442	0.060367	-3.037319
				H	-1.003787	-0.998611	-3.262932
				Pd	2.623345	-0.302226	-0.090697
				C	5.337588	-1.457539	0.135430
				C	6.589817	-1.870077	0.616312
				C	4.681341	-2.282767	-0.789411
				C	7.160985	-3.060428	0.162852
				H	7.107455	-1.247282	1.339520
				C	5.262710	-3.461621	-1.270298
				C	6.507272	-3.858057	-0.786194
				H	8.129852	-3.369696	0.550598
				H	4.713413	-4.059835	-1.992326
				H	6.961105	-4.785967	-1.127234
				C	3.314390	-1.843625	-1.185680
				O	2.662903	-2.375562	-2.061091

Int7

P	-5.531729	-0.455510	0.406707
C	-7.274499	-0.776026	0.967129
C	-8.350643	0.062451	0.631457
H	-8.163553	0.995663	0.109747
C	-9.662859	-0.279893	0.966448
H	-10.475733	0.391473	0.699148
C	-9.932759	-1.470227	1.642234
H	-10.953792	-1.734292	1.905876
C	-8.876189	-2.323565	1.968812
H	-9.070485	-3.259757	2.486896
C	-7.567537	-1.984175	1.626784
H	-6.765847	-2.676972	1.871329
C	-5.526257	1.377088	0.127880
C	-5.947946	2.315631	1.086160
H	-6.341308	1.974039	2.040281

H	2.513650	-1.445346	0.988652	H	8.930445	3.417057	2.536904
C	5.018378	0.509743	1.745570	C	7.471049	2.098167	1.667085
C	4.838345	-0.159745	2.970148	H	6.648667	2.770187	1.900566
C	5.571102	1.856291	1.728340	C	5.536594	-1.324920	0.167824
C	5.175747	0.416746	4.188380	C	5.977030	-2.244838	1.135750
H	4.404089	-1.158802	2.947678	H	6.352367	-1.886123	2.090873
C	5.906636	2.411453	3.009092	C	5.947103	-3.615888	0.883172
C	5.712784	1.718585	4.190925	H	6.288600	-4.313759	1.643915
H	5.013725	-0.119833	5.120364	C	5.468135	-4.092839	-0.340863
H	6.324134	3.416925	3.012651	H	5.433195	-5.162353	-0.532243
H	5.977784	2.189710	5.138085	C	5.024694	-3.192980	-1.309436
O	1.725270	1.655333	0.677680	H	4.630802	-3.552353	-2.255653
C	2.172127	2.286233	-0.366580	C	5.063962	-1.819033	-1.056966
O	2.088466	3.529948	-0.542851	H	4.702140	-1.125987	-1.811854
O	2.786171	1.517466	-1.272388	P	-0.023706	0.462205	-0.495541
K	4.561400	3.466113	-1.265063	C	0.689399	2.144577	-0.803370
C	-0.773241	0.000565	1.127394	C	2.011707	2.373781	-1.223588
H	-0.195399	0.904713	1.343965	H	2.668550	1.536384	-1.437496
H	-0.450398	-0.738222	1.872860	C	2.501230	3.673028	-1.368177
C	-2.292699	0.256609	1.227237	H	3.528413	3.826048	-1.690625
H	-2.700470	0.498693	0.238866	C	1.678255	4.768174	-1.093475
H	-2.454358	1.158423	1.835181	H	2.059504	5.780366	-1.207949
C	-3.087169	-0.896074	1.859423	C	0.364049	4.555203	-0.676175
H	-2.663903	-1.108251	2.852279	H	-0.287349	5.400215	-0.466902
H	-2.956175	-1.809010	1.267864	C	-0.126745	3.254870	-0.537916
C	-4.591169	-0.618037	2.037474	H	-1.153998	3.093945	-0.227519
H	-4.749552	0.277180	2.652821	C	0.752208	-0.624273	-1.762394
H	-5.049151	-1.456054	2.576162	C	0.852779	-2.004559	-1.509348
C	4.724152	-0.126041	0.456358	H	0.517111	-2.410775	-0.560954
H	4.971607	0.577293	-0.342814	C	1.331951	-2.872418	-2.490640
O	5.783459	2.506652	0.639794	H	1.388446	-3.936087	-2.274608
				C	1.711329	-2.385424	-3.743547
				H	2.077995	-3.065408	-4.509439
TS5				C	1.589008	-1.020998	-4.014834
				H	1.860031	-0.631006	-4.993430
P	5.489200	0.508797	0.435346	C	1.106392	-0.149439	-3.037116
C	7.217330	0.879786	1.009955	H	0.998077	0.904531	-3.272166
C	8.318947	0.069415	0.688261	Pd	-2.492662	0.108841	-0.256073
H	8.162335	-0.870367	0.168414	C	-5.170168	1.569201	0.014029
C	9.618007	0.448220	1.035045	C	-6.372915	2.157221	0.434790
H	10.451313	-0.202021	0.778747	C	-4.477638	2.162299	-1.056158
C	9.848862	1.647951	1.708652	C	-6.870814	3.287704	-0.213742
H	10.859666	1.940331	1.981621	H	-6.912295	1.712213	1.265028
C	8.766569	2.473957	2.020858	C	-4.991633	3.281760	-1.723719

C	-6.188321	3.852898	-1.299178	H	7.516547	-1.618675	-0.498426
H	-7.804298	3.731306	0.127344	C	9.209471	-0.743315	0.490506
H	-4.423696	3.695098	-2.552643	H	9.895985	-1.502724	0.123176
H	-6.583556	4.736237	-1.795869	C	9.676676	0.282996	1.311725
C	-3.156822	1.574812	-1.443029	H	10.726630	0.330899	1.589315
O	-2.538560	1.944417	-2.423030	C	8.781359	1.253908	1.767231
H	-3.061986	0.976510	0.952025	H	9.131751	2.065477	2.400612
C	-5.081889	-0.195457	1.899248	C	7.435818	1.192510	1.406566
C	-4.957011	0.564859	3.072373	H	6.762829	1.972881	1.754648
C	-5.715085	-1.502253	1.940191	C	4.871771	-1.512641	-0.560941
C	-5.440101	0.121368	4.299852	C	5.078032	-2.669814	0.210179
H	-4.455547	1.531514	3.010286	H	5.470848	-2.585174	1.220156
C	-6.196581	-1.922077	3.224536	C	4.788722	-3.932677	-0.305772
C	-6.062490	-1.138701	4.358795	H	4.947550	-4.816480	0.307166
H	-5.323213	0.728043	5.194748	C	4.282408	-4.061800	-1.602409
H	-6.678016	-2.897358	3.273928	H	4.043659	-5.045686	-1.997880
H	-6.441077	-1.507983	5.312463	C	4.073249	-2.923634	-2.380468
O	-1.709521	-1.769788	0.654156	H	3.663895	-3.011381	-3.382928
C	-2.161069	-2.537581	-0.310239	C	4.369860	-1.660232	-1.862688
O	-2.141615	-3.796215	-0.248770	H	4.190156	-0.776166	-2.468911
O	-2.705384	-1.905424	-1.335722	P	-0.392060	1.038092	-0.377094
K	-4.677232	-3.578506	-0.805749	C	0.561995	2.619848	-0.449394
C	0.738998	-0.078227	1.124589	C	1.800852	2.754051	-1.097663
H	0.182622	-0.996407	1.341149	H	2.229283	1.912511	-1.632771
H	0.389074	0.658029	1.860122	C	2.492932	3.966201	-1.064406
C	2.263900	-0.291942	1.239997	H	3.450666	4.051112	-1.571912
H	2.686633	-0.535302	0.258303	C	1.959650	5.060004	-0.378584
H	2.443666	-1.181553	1.860566	H	2.498436	6.004452	-0.355227
C	3.021146	0.889714	1.864570	C	0.731533	4.935874	0.273457
H	2.583799	1.101583	2.851336	H	0.307269	5.782098	0.807885
H	2.870353	1.792057	1.261382	C	0.034137	3.726696	0.235959
C	4.530646	0.655220	2.057275	H	-0.923876	3.630621	0.741097
H	4.708687	-0.230976	2.680206	C	0.015961	0.147285	-1.934730
H	4.959991	1.509454	2.593944	C	0.074705	-1.258669	-1.946003
C	-4.638252	0.289780	0.579457	H	-0.104745	-1.834229	-1.039484
H	-4.827579	-0.516237	-0.136961	C	0.298032	-1.937394	-3.146796
O	-5.860530	-2.232976	0.890817	H	0.337001	-3.023830	-3.139491
				C	0.454274	-1.235955	-4.343527
				H	0.623605	-1.771142	-5.275318
Int8				C	0.367634	0.157965	-4.341363
				H	0.462884	0.714335	-5.270722
P	5.167396	0.211383	0.051478	C	0.143636	0.844926	-3.148106
C	6.943166	0.150703	0.598594	H	0.056664	1.926342	-3.163662
C	7.859337	-0.808539	0.137205	Pd	-2.604734	1.442874	0.206885

C	-4.455274	-1.138248	-1.345117				
C	-5.564440	-1.945108	-1.654163	TS6			
C	-4.465271	0.198251	-1.805554				
C	-6.671056	-1.452069	-2.341318	P	-5.608827	-0.072864	-0.405973
H	-5.546104	-2.987532	-1.344703	C	-5.296857	1.663021	0.169992
C	-5.575968	0.680730	-2.521233	C	-4.548712	1.830541	1.346359
C	-6.682140	-0.123575	-2.772396	H	-4.207485	0.958642	1.899130
H	-7.516804	-2.104956	-2.546899	C	-4.224572	3.107860	1.811801
H	-5.545470	1.705365	-2.878460	H	-3.631516	3.214590	2.715993
H	-7.538276	0.275887	-3.311545	C	-4.657283	4.235804	1.114172
C	-3.334588	1.206363	-1.631422	H	-4.406335	5.230113	1.475171
O	-3.050038	1.938445	-2.564149	C	-5.411091	4.083421	-0.053387
H	-2.449780	-1.046047	-0.595523	H	-5.749036	4.959813	-0.601724
C	-3.441733	-2.378606	0.729865	C	-5.724466	2.808103	-0.523464
C	-4.652559	-2.475154	1.410215	H	-6.309871	2.700319	-1.432802
C	-2.216005	-2.908007	1.320941	C	-7.303050	0.073904	-1.143627
C	-4.761599	-3.100079	2.670399	C	-8.351994	0.564697	-0.342803
H	-5.545760	-2.049658	0.958573	H	-8.134348	0.931697	0.657299
C	-2.368634	-3.535007	2.609914	C	-9.663415	0.600083	-0.812607
C	-3.606344	-3.648286	3.246293	H	-10.452534	0.993330	-0.175888
H	-5.728174	-3.180899	3.161438	C	-9.965603	0.130077	-2.094044
H	-1.472462	-3.965268	3.054428	H	-10.988917	0.153396	-2.460319
H	-3.671263	-4.165120	4.204952	C	-8.941077	-0.371817	-2.895875
O	-4.387509	1.940417	1.239342	H	-9.161559	-0.741474	-3.894702
C	-3.806021	1.866997	2.416995	C	-7.624466	-0.398763	-2.426654
O	-4.425482	1.784708	3.498106	H	-6.846361	-0.791875	-3.073769
O	-2.476289	1.742154	2.364446	P	0.176214	-1.350017	0.742581
K	-3.129942	-0.592176	3.423077	C	-0.735354	-0.991987	2.326149
C	0.392043	0.034948	0.982601	C	-2.000046	-1.515400	2.651553
H	-0.199585	-0.892199	1.008901	H	-2.475333	-2.236271	1.992515
H	0.154682	0.589330	1.900087	C	-2.652530	-1.135985	3.827345
C	1.893751	-0.316740	0.911686	H	-3.627622	-1.557304	4.063704
H	2.211719	-0.407142	-0.133668	C	-2.049401	-0.222547	4.696979
H	2.019111	-1.321688	1.338092	H	-2.555718	0.072850	5.613995
C	2.816740	0.653636	1.663635	C	-0.790902	0.296439	4.388141
H	2.454012	0.750890	2.697688	H	-0.305977	0.997988	5.062606
H	2.754681	1.654093	1.221257	C	-0.129688	-0.084929	3.215792
C	4.291616	0.213499	1.724297	H	0.861623	0.321137	2.997447
H	4.380289	-0.771687	2.200049	C	-0.198749	-3.131168	0.389964
H	4.849044	0.917732	2.353503	C	-0.145537	-3.591699	-0.939898
C	-3.263391	-1.771014	-0.653888	H	0.070547	-2.891979	-1.741295
H	-2.864875	-2.564914	-1.305973	C	-0.313766	-4.944835	-1.235324
O	-1.083363	-2.801897	0.739454	H	-0.269268	-5.275548	-2.270983
				C	-0.527782	-5.873281	-0.213249

H	-0.658874	-6.927772	-0.445878	H	-4.639550	-1.149036	-2.364208
C	-0.558241	-5.433390	1.111315	H	-4.920439	0.565766	-2.700430
H	-0.711250	-6.145434	1.919819	C	4.470723	1.308115	-3.303435
C	-0.393104	-4.079133	1.409246	H	5.256807	1.704030	-3.956346
H	-0.414535	-3.756864	2.446170	O	2.207003	0.952487	-1.744544
Pd	2.297463	-0.645919	0.869380				
C	4.944717	0.029298	-2.629420				
C	6.289844	-0.361864	-2.728703	P			
C	4.070384	-0.723183	-1.811871				
C	6.767305	-1.489140	-2.056265	C	-2.385584	-1.052342	-1.364139
H	6.963067	0.221688	-3.355566	C	-1.043345	-1.161533	-1.912897
C	4.552195	-1.867572	-1.163643	C	-3.132628	0.121508	-1.800530
C	5.887806	-2.247208	-1.274673	C	-0.545179	-0.281304	-2.856843
H	7.812209	-1.777589	-2.150390	H	-0.478812	-2.058703	-1.669166
H	3.860973	-2.417264	-0.530440	C	-2.596222	0.969843	-2.799572
H	6.243433	-3.127533	-0.745539	C	-1.334337	0.800913	-3.333775
C	2.587099	-0.418194	-1.742975	H	0.440526	-0.465758	-3.282279
O	1.777602	-1.189251	-2.254609	H	-3.222846	1.800279	-3.113392
H	3.588431	1.110306	-3.925140	H	-0.949997	1.473940	-4.095812
C	4.129719	2.299902	-2.212237	C	-4.391166	0.564924	-1.228663
C	4.912102	3.418959	-1.906826	O	-5.113042	1.455452	-1.645381
C	3.049230	1.978764	-1.374382	C	-4.186805	-2.361029	-0.140222
C	4.639595	4.184740	-0.765288	C	-4.651249	-3.676468	0.128111
H	5.738943	3.686923	-2.564055	C	-5.136880	-1.325903	0.047300
C	2.782572	2.719476	-0.223025	C	-5.965519	-3.939725	0.497081
C	3.593693	3.814968	0.086115	H	-3.944156	-4.497848	0.022564
H	5.257593	5.048319	-0.530351	C	-6.462561	-1.585850	0.381839
H	2.014395	2.384961	0.465359	C	-6.893331	-2.896393	0.612084
H	3.423799	4.350399	1.014051	H	-6.273689	-4.966611	0.688171
O	4.173182	0.194693	1.361521	H	-7.131670	-0.738081	0.502009
C	4.005336	1.186298	2.279601	H	-7.924107	-3.094465	0.896269
O	5.044716	1.907236	2.510888	C	-2.848934	-2.117692	-0.589225
O	2.863696	1.364002	2.793036	H	-2.159236	-2.953285	-0.473988
K	6.124162	1.271209	0.328292	O	-4.722668	0.002445	0.034620
C	-0.867882	-0.435189	-0.522093	Pd	0.720857	0.034126	-0.391499
H	-0.312111	-0.526598	-1.462119	P	2.319498	-1.421959	0.438962
H	-0.769994	0.615799	-0.220432	P	0.505993	2.064117	0.726915
C	-2.347035	-0.793957	-0.704081	C	2.006433	-3.252167	0.518632
H	-2.863667	-0.743860	0.261194	C	1.149955	-3.789367	1.496264
H	-2.446504	-1.830145	-1.054778	H	0.732643	-3.146815	2.266320
C	-3.040207	0.154540	-1.695223	C	0.806259	-5.142121	1.488447
H	-2.517254	0.110135	-2.660998	H	0.139823	-5.529751	2.255273
H	-2.932410	1.187315	-1.340268	C	1.305610	-5.991194	0.499239
C	-4.530534	-0.136730	-1.951870	H	1.034177	-7.043845	0.490429

C	2.146073	-5.469927	-0.487164	H	-2.190421	0.972473	0.854694
H	2.536858	-6.117759	-1.268769	C	1.119560	3.561209	-0.186605
C	2.487838	-4.117475	-0.480049	C	2.100111	4.446985	0.285133
H	3.140613	-3.730641	-1.257728	H	2.553731	4.293518	1.259743
C	4.074909	-1.385108	-0.181632	C	2.513211	5.538208	-0.485987
C	4.386856	-0.514723	-1.235917	H	3.278552	6.209723	-0.102242
H	3.591296	0.090231	-1.665600	C	1.945754	5.766981	-1.739150
C	5.692460	-0.421237	-1.726954	H	2.265262	6.616521	-2.338402
H	5.913601	0.258708	-2.546150	C	0.968950	4.890667	-2.222360
C	6.706777	-1.199455	-1.167992	H	0.523563	5.056077	-3.200551
H	7.723090	-1.129407	-1.548763	C	0.569102	3.793753	-1.460798
C	6.410660	-2.072827	-0.117109	H	-0.170937	3.100455	-1.855994
H	7.196593	-2.684014	0.321150	C	1.593417	2.033473	2.260802
C	5.106391	-2.163935	0.370327	H	1.070613	1.359841	2.950292
H	4.885303	-2.856228	1.178824	H	1.604323	3.013095	2.755685
C	-1.068374	2.712501	1.468582	C	3.031731	1.531724	1.979683
C	-1.144580	3.955150	2.120811	H	3.751079	2.279619	2.340703
H	-0.265151	4.592248	2.182601	H	3.196382	1.455630	0.898443
C	-2.347986	4.394192	2.671477	C	3.415621	0.187778	2.629603
H	-2.394490	5.360561	3.169847	H	3.381166	0.301725	3.723942
C	-3.495360	3.600403	2.569334	H	4.465168	-0.014947	2.379428
H	-4.437003	3.950558	2.986471	C	2.580459	-1.060776	2.276854
C	-3.434650	2.368669	1.917896	H	3.038635	-1.930215	2.767313
H	-4.318842	1.750781	1.796311	H	1.569289	-0.962160	2.688366
C	-2.224617	1.926207	1.373232				