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SUPPORTING INFORMATION

Title: Revisiting O–O Bond Formation through Outer-Sphere Water Molecules versus Bimolecular Mechanisms in Water-Oxidation Catalysis (WOC) by Cp*Ir Based Complexes

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Table S1. xyz coordinate data sets and absolute energies in a.u. for DFT optimized complexes.

Supporting Information

6	O	1.512312	-1.161570	-0.097005	H	-1.572723	4.682452	-0.661064
2water Energy E= -152.759617877 A.U.	H	1.520708	-0.177173	-0.052585	H	0.239347	3.028645	-0.860553
O	H	2.128729	-1.462052	0.572740	C	-1.336804	-2.587031	-0.384643
H	O	-1.168776	-1.502616	-0.085073	C	-2.521122	-3.272079	-0.129382
H	H	-0.184579	-1.537869	-0.086762	C	-3.665970	-2.580894	0.245822
O	H	-1.461319	-2.122790	0.584648	C	-3.635748	-1.198234	0.336158
H	O	-1.513332	1.162269	0.091692	C	-2.457735	-0.504405	0.069807
H	H	-2.124773	1.460125	-0.583781	C	-1.285518	-1.206301	-0.256220
H	H	-1.521117	0.177808	0.050391	H	-4.585668	-3.118365	0.447346
9	H				H	-0.461608	-3.136714	-0.710432
3water Energy E= -229.155683272 A.U.	H				H	-2.551295	-4.350857	-0.240654
O	Ir	0.406449	-0.113979	-0.484485	H	-4.539408	-0.656366	0.595702
H	C	1.107791	-0.309461	1.679192	C	3.593855	-1.040430	-1.080643
H	C	1.528832	0.988402	1.314532	C	1.144682	2.245630	2.008249
O	C	1.800422	-1.233071	0.806309	C	0.218203	-0.680976	2.813575
H	C	2.532983	0.887866	0.277676	C	1.810363	-2.713384	0.959446
H	C	2.714750	-0.471181	-0.024236	C	3.268172	2.037408	-0.316853
O	C	-3.315244	1.888037	0.139785	O	0.517599	-0.683353	-2.188962
H	C	-3.048842	3.230265	-0.083544	H	0.805632	-0.905415	3.710215
H	C	-1.772324	3.637122	-0.452141	H	-0.468931	0.129825	3.056798
H	C	-0.750471	2.701350	-0.560117	H	-0.384972	-1.557487	2.573270
12	C	-0.997232	1.355986	-0.310648	H	2.593133	-3.001677	1.670025
4water Energy E= -305.552494159 A.U.	C	-2.302995	0.940430	0.009827	H	0.859986	-3.080794	1.344418
O	H	-4.324009	1.575092	0.387317	H	2.013116	-3.216733	0.013947
H	H	-3.844845	3.960844	0.008356	H	4.438940	-0.383067	-1.286849
H	H				H	3.990312	-2.013540	-0.785803

H	3.022679	-1.167954	-2.009210	H	-1.618229	5.258622	0.447060	C	0.059624	-3.741697	1.145898
H	3.689604	1.782989	-1.288885	H	0.798769	4.699581	0.446364	C	-1.966908	-0.746142	-2.487759
H	2.619584	2.904633	-0.450848	H	1.535815	2.385129	0.236172	C	1.174238	-0.808022	-2.939729
H	4.089822	2.348347	0.337354	C	-2.652103	-1.521135	-1.037364	C	2.420428	-2.772118	-0.796163
H	1.212382	3.112165	1.351291	C	-4.032309	-1.483717	-1.207602	C	-2.630966	-2.460056	0.109476
H	0.124326	2.200056	2.387755	C	-4.745495	-0.330237	-0.906367	O	-0.438213	-0.143281	1.951553
H	1.816910	2.416861	2.855859	C	-4.074045	0.798942	-0.466824	O	-4.589360	0.282166	-0.541638

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L1_CAT_T Energy E= -1031.03191887 A.U.

lr	0.404343	-0.001888	-0.472460
C	1.315668	-0.651397	1.571394
C	1.387017	0.765762	1.508700
C	2.158503	-1.189074	0.532625
C	2.260847	1.126897	0.425127
C	2.728959	-0.086236	-0.171007
C	-3.511344	1.564481	0.224488
C	-3.383404	2.941486	0.118847
C	-2.155229	3.501148	-0.206400
C	-1.047098	2.683038	-0.406478
C	-1.158259	1.305833	-0.278508
C	-2.409492	0.738737	0.016327
H	-4.479662	1.132867	0.455331
H	-4.246304	3.578582	0.277410
H	-2.058869	4.576196	-0.314670
H	-0.097894	3.131095	-0.681097
C	-1.068639	-2.676780	-0.405795
C	-2.182637	-3.486039	-0.201679
C	-3.405980	-2.916620	0.124578
C	-3.523127	-1.538479	0.227806
C	-2.415084	-0.721643	0.017254
C	-1.168663	-1.298722	-0.278679
H	-4.273402	-3.546888	0.285729
H	-0.124186	-3.132784	-0.682003
H	-2.094530	-4.561959	-0.308533
H	-4.487909	-1.098923	0.458429
C	3.698864	-0.178066	-1.297110
C	0.763310	1.723557	2.462525
C	0.601020	-1.456156	2.601015
C	2.504432	-2.625377	0.347738
C	2.726476	2.503176	0.098420
O	0.390367	-0.002083	-2.284459
H	1.280411	-1.722424	3.417214
H	-0.236219	-0.903676	3.027361
H	0.198566	-2.377985	2.178820
H	3.403864	-2.879428	0.919651
H	1.703273	-3.276681	0.697572
H	2.701369	-2.864054	-0.698420
H	3.576067	0.648067	-1.998325
H	4.726092	-0.147386	-0.919368
H	3.575694	-1.106177	-1.855491
H	2.939602	2.616457	-0.965442
H	1.983799	3.252233	0.375010
H	3.645815	2.739568	0.646073
H	0.398588	2.617610	1.955032
H	-0.083546	1.276405	2.982469
H	1.495208	2.034142	3.215210

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L1_R_S Energy E= -1260.22584972 A.U.

lr	0.024792	-0.381323	-0.199188
C	-0.027226	-0.881730	2.009057
C	1.232226	-0.241905	1.833077
C	0.001346	-2.077332	1.212153
C	2.077390	-1.070833	1.004497
C	1.324958	-2.191980	0.617389
C	-2.240347	3.226179	0.170270
C	-1.297480	4.228554	0.337455
C	0.055807	3.916533	0.342307
C	0.472756	2.595362	0.216251
C	-0.467285	1.582407	0.070036
C	-1.836419	1.902594	0.016862
H	-3.294322	3.479628	0.129156

H	-1.618229	5.258622	0.447060
H	0.798769	4.699581	0.446364
H	1.535815	2.385129	0.236172
C	-2.652103	-1.521135	-1.037364
C	-4.032309	-1.483717	-1.207602
C	-4.745495	-0.330237	-0.906367
C	-4.074045	0.798942	-0.466824
C	-2.689391	0.774262	-0.311403
C	-1.976191	-0.407363	-0.560210
H	-5.821832	-0.306715	-1.033880
H	-2.107484	-2.419795	-1.303051
H	-4.549192	-2.356948	-1.591115
H	-4.627616	1.709580	-0.263039
C	1.814708	-3.320016	-0.219340
C	1.700748	0.960860	2.566228
C	-1.117133	-0.469079	2.936119
C	-1.017009	-3.158853	1.260407
C	3.503245	-0.820408	0.668762
O	0.300918	-0.564106	-1.996147
O	3.877249	2.445784	0.134330
H	4.581130	3.094124	0.085729
H	3.691120	2.184199	-0.794657
O	3.156133	1.650654	-2.363656
H	2.264286	1.952297	-2.555360
H	3.122440	0.679182	-2.514672
O	2.740148	-1.030197	-2.698623
H	1.764470	-0.939442	-2.455420
H	2.761316	-1.356731	-3.600361
H	-0.978803	-0.920815	3.924080
H	-1.138651	0.613757	3.061748
H	-2.093861	-0.773289	2.558587
H	-0.821717	-3.797259	2.128752
H	-2.024929	-2.757033	1.354260
H	-0.986589	-3.789714	0.372162
H	2.406351	-4.010218	0.391396
H	0.992024	-3.886512	-0.656024
H	2.448651	-2.956454	-1.030143
H	3.738990	-1.192756	-0.329627
H	3.754084	0.240528	0.705699
H	4.148940	-1.343756	1.383647
H	2.474631	1.500255	2.018819
H	0.883338	1.648626	2.780112
H	2.127755	0.640055	3.523316

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L1_R_T Energy E= -1260.22954800 A.U.

lr	0.137654	-0.421207	0.242325
C	0.447429	-1.412058	-1.786462
C	-0.977066	-1.385827	-1.582923
C	1.006926	-2.312251	-0.817065
C	-1.278326	-2.189078	-0.449722
C	-0.045912	-2.767880	0.024679
C	0.807076	3.650714	-0.893522
C	-0.427191	4.126090	-1.309680
C	-1.540494	3.296724	-1.266158
C	-1.419886	1.984147	-0.816837
C	-0.184838	1.495945	-0.412647
C	0.937493	2.341102	-0.437416
H	1.669570	4.308610	-0.914396
H	-0.522123	5.146502	-1.663980
H	-2.509114	3.666097	-1.586828
H	-2.299596	1.351559	-0.792626
C	3.036913	-0.226926	1.183147
C	4.262812	0.412549	1.338696
C	4.439065	1.703635	0.859465
C	3.385479	2.365775	0.247566
C	2.152154	1.736264	0.098564
C	1.984736	0.415254	0.545940
H	5.395471	2.200945	0.976162
H	2.907672	-1.229423	1.576149
H	5.077124	-0.097405	1.842103
H	3.522614	3.384572	-0.099259

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L1_TS Energy E= -1260.16801555 A.U.

lr	-0.560833	-0.020768	0.069130
C	-2.223784	0.516671	-1.263292
C	-2.606682	1.030744	0.034209
C	-2.168376	-0.916954	-1.172727
C	-2.702770	-0.078477	0.913350
C	-2.450523	-1.291192	0.180810
C	3.005819	1.974572	-1.267303
C	2.790606	3.331099	-1.060983
C	1.589974	3.761865	-0.518464
C	0.601598	2.833104	-0.192241
C	0.784277	1.463186	-0.402355
C	2.022470	1.044424	-0.944776
H	3.952657	1.645134	-1.682866
H	3.563138	4.047666	-1.317007
H	1.415791	4.819301	-0.348638
H	-0.329289	3.192254	0.235777
C	1.044877	-2.510034	-0.736607
C	2.170218	-3.180230	-1.213197
C	3.283636	-2.462403	-1.632304
C	3.264980	-1.076212	-1.567397
C	2.139900	-0.405464	-1.093534
C	0.996899	-1.117494	-0.668229
H	4.161261	-2.979481	-2.003849
H	0.199448	-3.096407	-0.389964
H	2.175351	-4.264831	-1.254593
H	4.138731	-0.517659	-1.887841
C	-2.633150	-2.674187	0.705662
C	-2.969534	2.443890	0.337153
C	-2.116890	1.320002	-2.513844
C	-1.978635	-1.849648	-2.316592
C	-3.004078	-0.032347	2.370880
O	0.336335	-0.278543	1.892053
O	0.977782	1.034516	2.464020
H	1.096398	1.548225	1.628192
H	1.925462	0.719097	2.797683
O	3.198843	0.162203	3.169073
H	3.392985	0.080278	4.105320
H	3.129029	-0.764073	2.789870
O	2.438126	-2.061364	2.134092

H 1.594486 -1.594200 1.948558
H 2.711066 -2.403817 1.274758
H -3.156660 0.990177 2.716115
H -3.908040 -0.604121 2.599660
H -2.177446 -0.460201 2.944998
H -2.335993 -2.747318 1.753076
H -3.681907 -2.985916 0.636333
H -2.042542 -3.398806 0.142930
H -1.387783 -1.392255 -3.109998
H -1.466516 -2.763114 -2.013695
H -2.950591 -2.130510 -2.735808
H -1.503993 0.810431 -3.257303
H -3.106546 1.492310 -2.950764
H -1.657105 2.290822 -2.323777
H -2.474381 3.135752 -0.345309
H -4.048558 2.598889 0.226505
H -2.698033 2.727556 1.355448

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L1_P Energy E= -1260.19169960 A.U.

Ir 0.574787 -0.018770 0.073235
C -2.140471 0.184409 -1.353942
C -2.519823 1.087196 -0.274667
C -2.270431 -1.171421 -0.844061
C -2.700261 0.314568 0.886818
C -2.547191 -1.092890 0.535670
C 2.890567 2.123763 -1.304345
C 2.696390 3.449057 -0.938075
C 1.553347 3.808145 -0.240753
C 0.595262 2.843404 0.068601
C 0.750595 1.507559 -0.309853
C 1.939517 1.157491 -0.991921
H 3.798057 1.846240 -1.830837
H 3.443201 4.195296 -1.185592
H 1.401661 4.838112 0.065072
H -0.288385 3.147797 0.620523
C 1.066955 -2.430327 -0.925629
C 2.171493 -3.039118 -1.521085
C 3.220903 -2.264535 -1.996620
C 3.166842 -0.884969 -1.857419
C 2.066966 -0.276002 -1.258308
C 0.977808 -1.043292 -0.788725
H 4.079859 -2.732427 -2.464376
H 0.266796 -3.062481 -0.554119
H 2.206314 -4.119953 -1.613977
H 3.996753 -0.282728 -2.212975
C -2.773741 -2.225356 1.477232
C -2.748581 2.548535 -0.431381
C -2.017578 0.558072 -2.791377
C -2.199636 -2.397730 -1.682008
C -3.050973 0.799078 2.250532
O 0.438153 -0.303651 2.022087
O 1.278323 0.767487 2.498104
H 1.326218 1.331785 1.698175
H 2.980320 0.168384 3.132475
O 3.740026 -0.423472 3.266954
H 3.934272 -0.406456 4.205853
H 2.940389 -1.790086 2.421207
O 2.154964 -2.207381 2.011933
H 1.093461 -1.084286 1.983902
H 2.365546 -2.407449 1.090554
H -4.102181 0.593618 2.479369
H -2.444063 0.303807 3.011174
H -2.891290 1.873119 2.347236
H -3.845053 -2.393821 1.633022
H -2.343471 -3.153058 1.098953
H -2.327881 -2.027668 2.453578
H -3.138939 -2.522780 -2.231198
H -1.390696 -2.341504 -2.410789
H -2.048332 -3.293790 -1.079646
H -3.000166 0.590058 -3.275617
H -1.552794 1.538050 -2.903480
H -1.398512 -0.160323 -3.329531

H -3.750789 2.725850 -0.836431
H -2.681218 3.076463 0.520751
H -2.029947 2.997790 -1.117066

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L2_CAT_S Energy E= -1047.47146088 A.U.

Ir 0.418101 -0.138563 -0.428916
C 1.281775 -0.359939 1.697045
C 1.511405 0.985214 1.352299
C 1.969953 -1.190313 0.718699
C 2.312226 1.020999 0.140566
C 2.646816 -0.318131 -0.212398
C -3.309381 1.862502 0.125304
C -3.058324 3.204315 -0.105702
C -1.778731 3.621357 -0.447709
C -0.736306 2.704967 -0.513445
C -0.965099 1.362391 -0.247429
C -2.273400 0.935577 0.042563
H -4.321326 1.539144 0.340259
H -3.866770 3.922830 -0.047136
H -1.590356 4.665264 -0.670512
H 0.250102 3.048767 -0.798071
C -1.393139 -2.527973 -0.375168
C -2.554170 -3.242430 -0.162247
C -3.699442 -2.553183 0.212802
C -3.655473 -1.176945 0.330810
C -2.463830 -0.503475 0.088428
N -1.350677 -1.202340 -0.221559
H -4.625469 -3.085564 0.394022
H -0.475960 -3.001299 -0.697776
H -2.556859 -4.315288 -0.301694
H -4.544386 -0.618257 0.591538
C 3.498505 -0.751312 -1.348730
C 1.107730 2.169226 2.149377
C 0.562324 -0.867545 2.894428
C 2.133682 -2.665317 0.797819
C 2.883011 2.240323 -0.490966
O 0.475598 -0.891914 -2.060860
H 1.268305 -1.033295 3.714129
H -0.189812 -0.159913 3.241677
H 0.066083 -1.817550 2.693155
H 2.992866 -2.898150 1.436144
H 1.263738 -3.149566 1.241953
H 2.318394 -3.102884 -0.182954
H 4.078844 0.080800 -1.745040
H 4.194537 -1.530610 -1.032911
H 2.871950 -1.145860 -2.156768
H 2.900242 2.164124 -1.577958
H 2.335771 3.139461 -0.212218
H 3.914610 2.373621 -0.149450
H 0.867006 3.027508 1.523864
H 0.244962 1.959472 2.780259
H 1.938880 2.456441 2.801732

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L2_CAT_T Energy E= -1047.48246866 A.U.

Ir 0.407406 -0.019070 -0.404399
C 1.457356 -0.566058 1.592733
C 1.504956 0.838036 1.436071
C 2.200529 -1.178852 0.505440
C 2.214010 1.124224 0.204612
C 2.684399 -0.135018 -0.327499
C -3.519995 1.549577 0.209690
C -3.400979 2.924310 0.118098
C -2.165380 3.493641 -0.162790
C -1.041167 2.692738 -0.328072
C -1.140508 1.315763 -0.209397
C -2.396857 0.739985 0.037252
H -4.492772 1.112140 0.402650
H -4.273121 3.553054 0.248724
H -2.076682 4.569350 -0.264077
H -0.093803 3.157385 -0.573596
C -1.145485 -2.629844 -0.331567

C -2.238691 -3.455674 -0.193606
C -3.474314 -2.877091 0.073356
C -3.573738 -1.504825 0.176378
C -2.438389 -0.712518 0.022489
N -1.243202 -1.301002 -0.211336
H -4.355884 -3.496432 0.188258
H -0.161507 -3.019531 -0.556867
H -2.122724 -4.525737 -0.302353
H -4.530382 -1.036799 0.364632
C 3.548017 -0.282489 -1.527183
C 0.997396 1.857698 2.389898
C 0.852463 -1.312521 2.728791
C 2.529221 -2.625572 0.393303
C 2.659119 2.467570 -0.255422
O 0.301129 -0.051384 -2.220450
H 1.629951 -1.584595 3.449057
H 0.107629 -0.716719 3.254615
H 0.376837 -2.237339 2.399440
H 3.461390 -2.837214 0.926903
H 1.758794 -3.253860 0.841725
H 2.669195 -2.933804 -0.643093
H 3.282877 0.437110 -2.302122
H 4.591654 -0.104134 -1.250012
H 3.481283 -1.281675 -1.955723
H 2.700225 2.533713 -1.342633
H 2.007059 3.258335 0.113323
H 3.663925 2.671317 0.128401
H 0.586548 2.726223 1.875452
H 0.220708 1.455652 3.039146
H 1.820105 2.201535 3.024375

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L2_R_2w Energy E= -1200.27206021 A.U.

Ir 0.242006 -0.317913 -0.181689
C 0.324709 -1.290196 1.903855
C 0.927794 -0.030706 2.072020
C 1.094421 -2.020336 0.909268
C 2.071316 0.058763 1.180461
C 2.193032 -1.179368 0.485319
O 2.931965 2.567181 -1.639774
C -2.733614 2.706822 0.221449
C -2.034284 3.892892 0.371812
C -0.645580 3.891023 0.343331
C 0.058485 2.697207 0.229181
C -0.637163 1.502037 0.132529
C -2.041005 1.506798 0.081742
H -3.816498 2.726468 0.177293
H -2.573722 4.826644 0.475026
H -0.101196 4.826416 0.402017
H 1.139868 2.718167 0.162192
C -2.150203 -1.881999 -1.119240
C -3.485996 -2.179708 -1.295833
C -4.431774 -1.230521 -0.931616
C -4.013980 -0.009844 -0.436380
C -2.654546 0.245441 -0.294647
N -1.756825 -0.714237 -0.606907
H -5.488877 -1.436476 -1.049927
H -1.363844 -2.566990 -1.406973
H -3.772337 -3.132641 -1.720575
H -4.733487 0.754364 -0.174172
O 0.500772 -0.631799 -1.946444
C 3.293507 -1.563547 -0.433506
C 0.543555 3.006581 3.066487
C -0.831244 -1.836743 2.660998
C 0.903640 -3.448309 0.545837
C 3.072478 1.153464 1.167576
H 3.486643 3.247737 -2.025293
H 2.877930 1.853869 -2.308445
O 2.712173 0.312239 -3.173116
H 1.915531 -0.122491 -2.796605
H 2.624046 0.260570 -4.127011
H 4.084448 -2.068312 0.130012

H 2.945114 -2.242945 -1.211540
H 3.723156 -0.692760 -0.927338
H 4.019264 0.766962 1.558282
H 3.255585 1.548026 0.162528
H 2.765539 1.979892 1.807295
H 0.669638 2.009647 2.675505
H -0.490799 0.889063 3.388945
H 1.183484 0.900882 3.949082
H -0.472448 -2.394711 3.531446
H -1.487706 -1.045545 3.021665
H -1.424005 -2.523062 2.055742
H 1.476338 -4.073697 1.239307
H -0.139532 -3.754532 0.622534
H 1.260638 -3.659017 -0.461751

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L2_R_T_2w Energy E= -1200.27911670 A.U.

lr 0.178052 -0.337376 -0.228254
C 0.256936 -2.217258 1.137906
C 0.500423 -1.028036 1.902875
C 1.287832 -2.361265 0.161147
C 1.721708 -0.443540 1.415385
C 2.179987 -1.238406 0.308048
O 3.632954 2.383152 -0.520551
C -2.340800 3.012963 0.601919
C -1.491252 4.064967 0.891317
C -0.115831 3.883378 0.815434
C 0.423359 2.642792 0.488981
C -0.420633 1.572790 0.243435
C -1.811628 1.767339 0.262610
H -3.412967 3.171427 0.623026
H -1.899640 5.033385 1.153485
H 0.550553 4.718039 1.001752
H 1.499558 2.539589 0.402604
C -2.479152 -1.504028 -1.111655
C -3.842632 -1.568374 -1.289033
C -4.613818 -0.485899 -0.879340
C -3.996843 0.622336 -0.336982
C -2.610921 0.645390 -0.193437
N -1.887354 -0.436689 -0.562792
H -5.690764 -0.505403 -0.997193
H -1.824987 -2.308960 -1.419952
H -4.286310 -2.444580 -1.742526
H -4.579044 1.482266 -0.034697
O 0.536343 0.080865 -1.976348
C 3.445131 -1.035439 -0.444198
C -0.256665 -0.585954 3.107555
C -0.845957 -3.179297 1.392609
C 1.475084 -3.491285 -0.786676
C 2.479929 0.659023 2.052592
H 4.421848 2.927605 -0.554285
H 3.340201 2.272483 -1.447117
O 2.606080 1.736702 -2.976075
H 1.805771 1.216387 -2.804834
H 2.426627 2.266924 -3.755137
H 4.237190 -1.631843 0.020905
H 3.352904 -1.360798 -1.480909
H 3.755231 0.010287 -0.436520
H 3.185976 0.218570 2.765308
H 3.049569 1.235394 1.321993
H 1.828053 1.332366 2.607577
H 0.171944 -1.032255 4.009886
H -0.223301 0.497429 3.221109
H -1.304264 -0.884282 3.057874
H -0.551938 -3.851077 2.205301
H -1.762351 -2.677200 1.703437
H -1.064112 -3.799491 0.523803
H 2.183368 -4.214339 -0.368898
H 0.543736 -4.023470 -0.980408
H 1.880060 -3.152617 -1.740607

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L2_TS_2w Energy E= -1200.23114774 A.U.

lr 0.485314 0.009742 0.106321
C 1.962381 0.587949 -1.437901
C 2.041845 -0.825955 -1.255635
C 2.392731 1.219199 -0.197630
C 2.403750 -1.084483 0.111743
C 2.657955 0.195258 0.740612
O -0.903406 -1.398811 2.478260
C -3.353329 -1.270789 -1.297252
C -3.300569 -2.652587 -1.368187
C -2.139035 -3.315539 -0.995322
C -1.024030 -2.596765 -0.574374
C -1.040977 -1.202595 -0.515888
C -2.240674 -0.549589 -0.866863
H -4.270006 -0.761971 -1.573487
H -4.165264 -3.212102 -1.703733
H -2.097410 -4.398364 -1.035263
H -0.129905 -3.140397 -0.287983
C -0.952619 2.686450 0.068432
C -1.969313 3.585534 -0.178041
C -3.157768 3.109851 -0.716159
C -3.287979 1.758676 -0.966893
C -2.228956 0.896087 -0.695062
N -1.067448 1.382658 -0.201917
H -3.975901 3.786975 -0.930922
H -0.010300 3.002113 0.495080
H -1.827773 4.633660 0.050648
H -4.209595 1.363930 -1.373119
O -0.148233 -0.005246 1.982708
C 3.106272 0.361108 2.147471
C 1.850873 -1.848374 -2.317173
C 1.709203 1.300652 -2.720428
C 2.636927 2.676899 -0.019217
C 2.716759 -2.409333 0.715475
H -1.295531 -1.693364 1.632296
H -1.632201 -0.992879 3.045483
O -2.705552 -0.232204 3.904190
H -3.079412 -0.580893 4.718129
H -2.506729 0.695763 4.057315
H 3.787861 -2.620197 0.634804
H 2.451029 -2.439641 1.772582
H 2.188418 -3.218411 0.210723
H 4.141579 0.024879 2.255364
H 3.055334 1.401343 2.466652
H 2.487079 -0.229841 2.824651
H 3.663070 2.921172 -0.311407
H 1.978208 3.278926 -0.646294
H 2.509277 2.990970 1.017536
H 2.655287 1.527000 -3.222032
H 1.107190 0.698952 -3.400676
H 1.187904 2.245187 -2.560198
H 2.812381 -2.047612 -2.800692
H 1.481940 -2.791700 -1.916933
H 1.153292 -1.512061 -3.083341

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L2_P_2w Energy E= -1200.26719743 A.U.

lr 0.191222 -0.290743 -0.126082
C -0.224701 -1.739931 1.621879
C 0.503021 -0.681565 2.194650
C 0.599375 -2.325050 0.577690
C 1.782902 -0.567545 1.509879
C 1.864501 -1.619224 0.554738
O 3.411826 1.057593 -1.232729
C -2.662406 2.811639 0.515982
C -1.982878 3.811935 1.190212
C -0.638545 3.651589 1.499822
C 0.019852 2.469621 1.182376
C -0.662568 1.445058 0.544527
C -2.005381 1.631546 0.175247
H -3.695890 2.968717 0.229337
H -2.494099 4.731066 1.449532

H -0.095413 4.452862 1.987555
H 1.072622 2.367029 1.413834
C -1.976961 -1.257532 -1.969218
C -3.239990 -1.334503 -2.519871
C -4.198173 -0.415538 -2.113875
C -3.856389 0.564524 -1.201342
C -2.564177 0.607157 -0.690265
N -1.666305 -0.331064 -1.060509
H -5.201660 -0.453658 -2.520604
H -1.178622 -1.926361 -2.261189
H -3.458602 -2.094065 -3.258597
H -4.580359 1.307434 -0.894363
O 0.836708 -0.077690 -1.797996
C 3.050814 -1.958174 -0.268042
C 0.092749 0.108690 3.380380
C -1.556508 -2.245858 2.046722
C 0.286666 -3.573473 -0.165970
C 2.899013 0.346844 1.862735
H 2.615081 0.738011 -1.682181
H 3.878030 1.624849 -1.867682
O 4.755669 2.655128 -3.126820
H 5.514751 2.354800 -3.631200
H 4.771360 3.613710 -3.164405
H 3.687566 -0.224795 2.362648
H 3.324114 0.799628 0.962295
H 2.580518 1.128635 2.551080
H 3.689438 -2.651251 0.289370
H 2.765481 -2.439673 -1.203464
H 3.625836 -1.062711 -0.510613
H 0.613168 -4.435334 0.425758
H -0.783388 -3.688057 -0.340213
H 0.806081 -3.614813 -1.123021
H -1.436130 -3.074337 2.751561
H -2.141172 -1.471382 2.541979
H -2.134816 -2.618255 1.200288
H 0.468436 -0.389883 4.280096
H 0.503395 1.116534 3.368061
H -0.990570 0.184412 3.466859

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L2_R_S_4w Energy E= -1353.07037516 A.U.

lr -0.225951 -0.394385 -0.053429
C -0.854890 -1.082166 2.037028
C 0.059933 -0.037983 2.270122
C -0.158046 -2.115070 1.287536
C 1.336730 -0.388140 1.670863
C 1.212588 -1.683770 1.097297
C -2.606695 3.125797 -0.379579
C -1.753335 4.178872 -0.093766
C -0.414722 3.932891 0.180983
C 0.072412 2.630739 0.242985
C -0.791838 1.572075 0.014123
C -2.127639 1.818722 -0.347916
H -3.632891 3.330125 -0.662892
H -2.124761 5.196195 -0.122793
H 0.267082 4.759231 0.346168
H 1.135040 2.478815 0.410985
C -2.573520 -1.546231 -1.534740
C -3.866011 -1.611905 -2.013456
C -4.684274 -0.498656 -1.872531
C -4.176734 0.649188 -1.294472
C -2.860478 0.668850 -0.846043
N -2.104001 -0.445959 -0.943063
H -5.707304 -0.521684 -2.228625
H -1.877802 -2.368265 -1.634789
H -4.215178 -2.516056 -2.494128
H -4.787120 1.537723 -1.203500
C 2.297860 -2.479590 0.471276
C -0.181733 1.165787 3.100550
C -2.254251 -1.168487 2.532000
C -0.691239 -3.466484 0.976246
C 2.597759 0.367884 1.840930

O	0.371733	-0.887865	-1.691018
O	3.274372	2.757817	-0.074369
H	3.607242	3.496037	-0.587007
H	3.733761	1.964339	-0.425329
O	4.411025	0.403606	-0.880561
H	5.365067	0.304025	-1.034201
H	3.954844	-0.095813	-1.588816
O	2.912431	-1.111450	-2.583241
H	1.981550	-1.057774	-2.271802
H	2.880989	-1.021645	-3.537564
O	7.164245	0.157208	-1.379501
H	7.716454	0.837514	-1.770485
H	7.760480	-0.525033	-1.064047
H	1.935374	-3.050546	-0.383909
H	3.109851	-1.841952	0.123549
H	2.703746	-3.183685	1.204522
H	2.449145	1.446495	1.834938
H	3.027400	0.098420	2.813065
H	3.327366	0.133031	1.065026
H	-1.772580	-3.458902	0.841543
H	-0.226354	-3.889628	0.086034
H	-0.473719	-4.137554	1.814215
H	-2.890284	-1.733012	1.849310
H	-2.279342	-1.675832	3.501278
H	-2.692222	-0.179105	2.663375
H	-1.226733	1.473397	3.083609
H	0.084942	0.933926	4.137219
H	0.430511	2.008122	2.783437

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L2_R_T_4w Energy E=-1353.07419108 A.U.

Ir	-0.269896	-0.397593	-0.102103
C	-0.898889	-1.796519	1.627785
C	-0.065578	-0.779656	2.153708
C	-0.136619	-2.573644	0.670535
C	1.223050	-0.877316	1.500329
C	1.170431	-2.008745	0.604481
C	-2.323560	3.339916	0.178146
C	-1.398296	4.248331	0.658734
C	-0.087797	3.845369	0.883747
C	0.302607	2.527242	0.667938
C	-0.628712	1.602206	0.225164
C	-1.942145	2.017545	-0.052526
H	-3.335557	3.668861	-0.029130
H	-1.692245	5.275332	0.838773
H	0.650530	4.562297	1.224581
H	1.346454	2.271668	0.820101
C	-2.854376	-1.160893	-1.506839
C	-4.144714	-1.011404	-1.962908
C	-4.786837	0.202339	-1.741017
C	-4.113965	1.220079	-1.097905
C	-2.803286	1.023222	-0.665946
N	-2.213316	-0.177785	-0.864499
H	-5.804448	0.353494	-2.081195
H	-2.297201	-2.075787	-1.660491
H	-4.630132	-1.825492	-2.484367
H	-4.591270	2.176789	-0.934874
C	2.312853	-2.510699	-0.201774
C	-0.392231	0.165522	3.252579
C	-2.294126	-2.094431	2.048267
C	-0.589172	-3.826458	0.008280
C	2.456541	-0.154455	1.893863
O	0.494747	-0.137081	-1.737935
O	3.570928	2.629910	0.828184
H	4.112198	3.413049	0.718452
H	3.958406	1.951362	0.237891
O	4.363822	0.538086	-0.773517
H	5.283996	0.264428	-0.926149
H	3.941239	0.618100	-1.650615
O	2.874508	0.644533	-3.081759
H	1.981506	0.440639	-2.764583
H	2.786782	1.406324	-3.658294

O	7.029669	-0.269566	-1.164610
H	7.782564	0.149686	-0.742077
H	7.370268	-0.695607	-1.954263
H	1.978929	-2.986167	-1.124149
H	3.008018	-1.707688	-0.452719
H	2.862383	-3.257846	0.380060
H	2.259745	0.859500	2.236890
H	2.927815	-0.697148	2.721291
H	3.171893	-0.096081	1.073547
H	-1.671816	-3.852886	-0.119922
H	-0.119967	-3.965115	-0.966195
H	-0.321521	-4.690351	0.625538
H	-2.905750	-2.448901	1.217675
H	-2.287019	-2.882958	2.807040
H	-2.780512	-1.222007	2.483178
H	-1.464883	0.336491	3.338291
H	-0.039864	-0.246495	4.203161
H	0.094202	1.129293	3.105211

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L2_TS_4w Energy E=-1353.03536887 A.U.

Ir	0.023278	-0.336362	-0.168944
C	0.248174	-1.993308	-1.636972
C	-0.402098	-0.908626	-2.293238
C	-0.628428	-2.471579	-0.581426
C	-1.644871	-0.647203	-1.609613
C	-1.782017	-1.641739	-0.574518
C	2.859303	2.863395	-0.363014
C	2.253987	3.874788	-1.089615
C	0.964859	3.697773	-1.573277
C	0.289159	2.502299	-1.348435
C	0.884576	1.461400	-0.638601
C	2.181635	1.668345	-0.129944
H	3.858433	3.018963	0.027951
H	2.781723	4.803532	-1.269203
H	0.481723	4.493325	-2.129578
H	-0.718826	2.391668	-1.732917
C	2.183236	-1.481636	1.625097
C	3.397450	-1.553731	2.275561
C	4.299534	-0.511673	2.109518
C	3.948371	0.562435	1.316507
C	2.707214	0.583353	0.686518
N	1.855785	-0.455171	0.836141
H	5.263856	-0.533760	2.602911
H	1.437970	-2.258242	1.731281
H	3.622061	-2.405901	2.903294
H	4.628927	1.393164	1.187103
C	-2.962973	-1.787133	0.314480
C	0.075540	-0.219903	-3.521289
C	1.524032	-2.640885	-2.045887
C	-0.420741	-3.704237	0.227413
C	-2.714782	0.287092	-2.055737
O	-0.622008	0.226211	1.577789
O	-0.815317	1.926829	1.909482
H	-0.476264	2.295580	1.077943
H	-1.858817	1.998440	1.935423
O	-3.273084	1.923885	2.255490
H	-3.989209	1.907895	1.594340
H	-3.312019	1.096872	2.781560
O	-2.579361	-0.404103	3.408208
H	-1.762039	-0.307482	2.881810
H	-2.312981	-0.471610	4.327924
H	-2.306815	1.129020	-2.615484
H	-3.410000	-0.233740	-2.722337
H	-3.293718	0.678802	-1.218817
H	-3.432867	-0.824498	0.513068
H	-3.706419	-2.429287	-0.168548
H	-2.705456	-2.232917	1.274387
H	0.638028	-3.934039	0.353468
H	-0.877918	-3.626640	1.214625
H	-0.873337	-4.564263	-0.276557
H	2.096008	-2.983956	-1.182442

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L2_P_4w Energy E=-1353.05171541 A.U.

Ir	-0.692482	-0.074811	-0.033601
C	-2.412652	0.396417	1.215064
C	-1.947621	-0.921551	1.538985
C	-2.958398	0.360314	-0.137227
C	-2.056315	-1.728547	0.355176
C	-2.727994	-0.922099	-0.657395
C	3.087689	0.855754	1.730111
C	3.526117	-0.307038	2.346537
C	2.772385	-1.473586	2.218465
C	1.579917	-1.466706	1.507556
C	1.087167	-0.299174	0.920796
C	1.889816	0.857990	1.014693
H	3.680434	1.759274	1.822913
H	4.430573	-0.299300	2.944967
H	3.113917	-2.390194	2.687843
H	1.023003	-2.392238	1.416322
C	-0.359484	2.792014	-1.036145
C	0.226200	4.032143	-1.181444
C	1.439625	4.267164	-0.547641
C	2.018474	3.255238	0.191009
C	1.380584	2.021737	0.301575
N	0.191504	1.816527	-0.307798
H	1.929188	5.229957	-0.633804
H	-1.302274	2.554261	-1.511038
H	-0.260963	4.792460	-1.777710
H	2.968557	3.414462	0.683280
C	-3.056814	-1.413057	-2.021478
C	-1.521371	-1.385161	2.884807
C	-2.555476	1.531058	2.169230
C	-3.700750	1.474558	-0.788121
C	-1.828238	-3.197329	0.256316
O	0.228780	-0.770320	-1.812451
O	1.287236	0.058338	-2.364617
H	0.880483	0.392856	-3.172635
H	2.658889	-0.791422	-2.394691
O	3.294924	-1.563987	-2.293151
H	3.963190	-1.376300	-1.550243
H	2.633645	-2.351959	-2.056847
O	1.425845	-3.049892	-1.737977
H	0.815945	-2.242446	-1.741393
H	1.086710	-3.699482	-2.358656
O	4.924880	-0.995134	-0.433630
H	5.784671	-1.400940	-0.298551
H	4.539881	-0.812632	0.439514
H	-3.505239	-0.632646	-2.635261
H	-2.157988	-1.768068	-2.533262
H	-3.762819	-2.246384	-1.968708
H	-1.038445	-3.532244	0.929104
H	-2.738888	-3.746722	0.516390
H	-1.546879	-3.489780	-0.756120
H	-1.008735	-0.601039	3.441360
H	-2.403566	-1.685792	3.458653
H	-0.856189	-2.245645	2.827150
H	-2.421270	2.494559	1.675498
H	-3.553321	1.527124	2.619199
H	-1.825506	1.465404	2.975693
H	-3.348590	2.449810	-0.449153
H	-3.624773	1.440176	-1.875811
H	-4.763549	1.416750	-0.532753

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L2_R_S Energy E= -1276.67540950 A.U.

Ir -0.020093 -0.422688 -0.143172
C -0.108400 -0.907782 2.070300
C 1.146359 -0.272779 1.884703
C -0.103296 -2.105267 1.257395
C 1.945631 -1.055502 0.962117
C 1.192236 -2.205939 0.614151
C -2.047092 3.318503 0.124579
C -1.057265 4.271208 0.302562
C 0.275243 3.885757 0.341858
C 0.629760 2.542425 0.263493
C -0.357272 1.579215 0.127165
C -1.704132 1.973891 0.018537
H -3.080875 3.632029 0.035162
H -1.324740 5.318112 0.381164
H 1.057548 4.629868 0.436862
H 1.683018 2.289614 0.300368
C -2.698395 -1.264965 -1.178855
C -4.052244 -1.178979 -1.428035
C -4.713382 -0.000275 -1.108135
C -3.997233 1.060764 -0.588774
C -2.628871 0.929614 -0.377291
N -2.022616 -0.248404 -0.637672
H -5.778528 0.095471 -1.281840
H -2.119339 -2.143095 -1.428534
H -4.570008 -2.018118 -1.873186
H -4.486494 1.998949 -0.363715
C 1.664818 -3.319988 -0.243459
C 1.651079 0.894326 2.642911
C -1.172659 -0.505695 3.028954
C -1.148404 -3.159736 1.277174
C 3.363251 -0.811395 0.602761
O 0.166875 -0.890951 -1.892373
O 3.826661 2.389921 0.164359
H 4.623257 2.890586 0.349622
H 3.894626 2.105327 -0.773079
O 3.846169 1.407780 -2.364848
H 3.709505 1.931324 -3.156136
H 3.460040 0.525185 -2.544087
O 2.694379 -1.067530 -2.735233
H 1.733558 -1.055069 -2.498128
H 2.762814 -1.497411 -3.590611
H -0.976730 -0.940296 4.014076
H -1.215248 0.577140 3.145977
H -2.156788 -0.849113 2.709304
H -0.964726 -3.825875 2.126586
H -2.146737 -2.740978 1.401925
H -1.133289 -3.769504 0.374248
H 2.238065 -4.024303 0.368390
H 0.838250 -3.865478 -0.697234
H 2.316896 -2.953604 -1.036763
H 3.585872 -1.184460 -0.397105
H 3.622515 0.247195 0.645003
H 4.004212 -1.345787 1.313293
H 2.432503 1.429758 2.104058
H 0.856511 1.590906 2.907069
H 2.088758 0.519253 3.575329

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L2_R_T Energy E= -1276.67892542 A.U.

Ir -0.110053 -0.411197 -0.157960
C -0.364710 -1.309685 1.905096
C 0.992980 -0.883936 1.785711
C -0.568792 -2.392021 0.963916
C 1.595302 -1.614242 0.701393
C 0.631637 -2.588032 0.234959
C -1.544836 3.573494 0.412933
C -0.444162 4.323039 0.785993
C 0.805756 3.721815 0.865655
C 0.963402 2.365202 0.601704
C -0.138733 1.600541 0.257126
C -1.397009 2.214089 0.135742

H -2.512627 4.053827 0.325312
H -0.556672 5.378897 1.000477
H 1.676218 4.310722 1.131756
H 1.957798 1.938708 0.670555
C -2.930319 -0.754157 -1.231928
C -4.227031 -0.404580 -1.534536
C -4.653631 0.881994 -1.223576
C -3.768930 1.771280 -0.650513
C -2.461915 1.372993 -0.376533
N -2.082726 0.103653 -0.652050
H -5.669296 1.189995 -1.441855
H -2.537057 -1.735662 -1.460695
H -4.882531 -1.123323 -2.007779
H -4.077089 2.782973 -0.424141
C 0.905395 -3.619892 -0.798621
C 1.702544 0.047794 2.693485
C -1.330445 -0.875036 2.953451
C -1.797655 -3.222720 0.881210
C 3.019118 -1.549684 0.281280
O 0.470603 -0.201394 -1.882227
O 4.150362 1.554810 0.858939
H 4.943240 1.802631 1.338329
H 4.395535 1.582948 -0.092025
O 4.700006 1.476124 -1.791512
H 4.869604 2.239160 -2.346374
H 4.141171 0.868500 -2.314118
O 2.999188 -0.265852 -3.083513
H 2.066129 -0.145412 -2.843126
H 3.017549 -0.481371 -4.018457
H -1.212441 -1.485127 3.854206
H -1.170337 0.165795 3.234377
H -2.363825 -0.978345 2.620662
H -1.772031 -3.978670 1.672552
H -2.703108 -2.633842 1.031273
H -1.874480 -3.751531 -0.068834
H 1.426152 -4.468596 -0.343557
H -0.008259 -3.999039 -1.255821
H 1.549115 -3.229050 -1.587444
H 3.127424 -1.664505 -0.798148
H 3.484077 -0.607037 0.573073
H 3.571358 -2.364796 0.761364
H 2.551842 0.528487 2.206640
H 1.040459 0.815265 3.092757
H 2.086165 -0.534015 3.539136

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L2_TS Energy E= -1276.63659817 A.U.

Ir -0.526966 -0.024558 0.037417
C -2.127123 -0.156352 -1.482514
C -2.332537 1.047377 -0.739885
C -2.332020 -1.275261 -0.571075
C -2.535941 0.697337 0.637149
C -2.576158 -0.749204 0.718364
C 2.962697 2.138678 -1.177135
C 2.772074 3.444805 -0.761957
C 1.607221 3.788428 -0.087758
C 0.625241 2.832874 0.152473
C 0.781743 1.515083 -0.275163
C 1.982810 1.177396 -0.930859
H 3.883264 1.874135 -1.685038
H 3.533041 4.191537 -0.953057
H 1.460413 4.807302 0.252916
H -0.272338 3.128666 0.684167
C 1.122675 -2.322571 -1.077466
C 2.177432 -2.945955 -1.710495
C 3.242248 -2.166488 -2.146998
C 3.215328 -0.805984 -1.920087
C 2.125340 -0.228676 -1.271125
N 1.085743 -0.999923 -0.876655
H 4.085075 -2.619579 -2.655261
H 0.271470 -2.883706 -0.716021
H 2.158798 -4.018001 -1.857490
H 4.037672 -0.181335 -2.241981

C -2.823202 -1.505405 1.973653
C -2.401992 2.414555 -1.317757
C -1.981650 -0.262882 -2.960706
C -2.407814 -2.704172 -0.979536
C -2.880210 1.620332 1.753175
O 0.308070 -0.553285 1.736473
O 0.922377 0.710572 2.702512
H 1.280595 1.289529 2.007419
H 1.718458 0.267730 3.209569
O 2.845215 -0.436207 3.817839
H 2.926186 -0.512827 4.771510
H 2.803234 -1.343462 3.427923
O 2.152696 -2.506418 2.383059
H 1.465930 -1.928553 1.992972
H 2.629306 -2.916638 1.658506
H -2.515674 2.630842 1.569414
H -3.966674 1.680907 1.872006
H -2.459919 1.276401 2.698588
H -2.140073 -1.181052 2.761425
H -3.845537 -1.333597 2.322027
H -2.692436 -2.577753 1.833705
H -1.766099 -2.917777 -1.835080
H -2.141655 -3.379850 -0.165953
H -3.431207 -2.946117 -1.283179
H -1.379241 -1.126305 -3.245532
H -2.962575 -0.374932 -3.433217
H -1.509752 0.625807 -3.379138
H -1.717396 2.541325 -2.155660
H -3.418048 2.591904 -1.684381
H -2.182467 3.185087 -0.580535

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L2_P Energy E= -1276.66223268 A.U.

Ir 0.573857 0.004513 0.023428
C 2.250325 0.595172 -1.172924
C 2.368687 -0.818489 -0.906255
C 2.453428 1.300302 0.090449
C 2.460762 -0.989451 0.507813
C 2.549976 0.339414 1.109168
C -2.954503 -1.215410 -2.080541
C -2.860247 -2.587388 -2.240336
C -1.758087 -3.260937 -1.732818
C -0.742742 -2.562288 -1.085077
C -0.799019 -1.176685 -0.928000
C -1.943377 -0.516314 -1.422903
H -3.825824 -0.698424 -2.466800
H -3.645986 -2.130255 -2.751296
H -1.683257 -4.336979 -1.844611
H 0.109783 -3.116769 -0.707513
C -0.924182 2.671395 -0.064586
C -1.914304 3.566129 -0.412124
C -2.983397 3.106101 -1.169824
C -3.027666 1.774440 -1.532773
C -2.000936 0.913442 -1.150826
N -0.952828 1.385920 -0.434003
H -3.776364 3.780666 -1.470504
H -0.075334 2.975904 0.532237
H -1.844953 4.597117 -0.091440
H -3.856208 1.394300 -2.115143
C 2.714015 0.577748 2.566626
C 2.450611 -1.879660 -1.942137
C 2.242405 1.225696 -2.521251
C 2.604972 2.773725 0.228960
C 2.663291 -2.266910 1.245292
O -0.580539 -0.387774 1.860471
O -1.089787 -1.712144 2.056096
H -1.256284 -2.003216 1.139614
H -2.503687 -1.747126 3.660090
O -3.185560 -1.179381 4.040147
H -3.259538 -1.395228 4.972164
H -2.989994 0.302776 3.229241
O -2.633474 0.933224 2.559659

H	-1.401389	0.194985	2.032670	C	1.575394	0.704387	1.514436	H	-4.490036	-2.269797	-1.725704
H	-3.366250	1.189835	1.995226	C	2.204613	-1.161237	0.277905	H	-4.567276	1.731072	-0.183176
H	3.729991	-2.440363	1.418735	C	2.204443	1.161426	0.278061	C	1.910522	-3.210242	-0.384151
H	2.166089	-2.250230	2.215495	C	2.653056	0.000185	-0.439939	C	1.759825	0.955709	2.565713
H	2.277516	-3.119946	0.687065	C	-3.572056	1.513347	0.184246	C	-0.945901	-0.655166	3.062813
H	3.723217	0.296685	2.882451	C	-3.471143	2.891467	0.087178	C	-0.814641	-3.267088	1.252779
H	2.561580	1.624301	2.828089	C	-2.233970	3.463125	-0.164436	C	3.487375	-0.597566	0.430494
H	2.008447	-0.023250	3.143120	C	-1.134340	2.636447	-0.288630	O	0.157886	-1.199818	-1.764203
H	3.649994	3.053823	0.063077	C	-2.434748	0.732789	0.042286	O	3.489317	2.648076	0.066532
H	2.011039	3.316870	-0.507258	H	-4.535177	1.053045	0.358065	H	4.250372	3.217335	0.202666
H	2.330152	3.124206	1.224641	H	-4.353932	3.510735	0.193268	H	3.418790	2.477327	-0.896937
H	3.266810	1.423194	-2.852714	H	-2.114771	4.533692	-0.271590	O	2.703903	1.901059	-2.394847
H	1.771241	0.577013	-3.259322	H	-0.151038	3.032970	-0.502625	H	2.773050	2.425984	-3.196103
H	1.707149	2.175746	-2.520196	C	-1.134148	-2.636485	-0.288776	H	2.793851	0.965614	-2.668858
H	3.473609	-1.919171	-2.329275	C	-2.233704	-3.463255	-0.164532	O	2.700405	-0.810720	-2.889944
H	2.214152	-2.863875	-1.540689	C	-3.470901	-2.891703	0.087196	H	1.788642	-1.098243	-2.711036
H	1.781910	-1.683092	-2.779715	C	-3.571923	-1.513595	0.184319	H	2.966433	-1.208752	-3.723652

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L3_CAT_S Energy E=-1063.77710366 A.U.

lr	0.418852	-0.127691	-0.411775
C	1.276125	-0.269311	1.686919
C	1.564936	1.053472	1.282401
C	1.948724	-1.162962	0.743213
C	2.379677	1.014377	0.077679
C	2.676874	-0.347403	0.208841
C	-3.350568	1.823884	0.104463
C	-3.114343	3.166436	-0.141775
C	-1.836596	3.575903	-0.493984
C	-0.828120	2.636730	-0.536681
C	-2.306230	0.917308	0.023523
H	-4.351005	1.481554	0.332852
H	-3.927143	3.881149	-0.087636
H	-1.617399	4.608100	-0.735565
H	0.181751	2.904924	-0.813979
C	-1.384454	-2.547232	-0.368870
C	-2.551045	-3.260752	-0.153258
C	-3.695858	-2.577377	0.221139
C	-3.654365	-1.195468	0.333485
C	-2.462509	-0.532971	0.091417
H	-4.621036	-3.110374	0.405246
H	-0.468472	-3.022804	-0.691201
H	-2.551382	-4.334903	-0.287880
H	-4.548886	-0.643802	0.590424
C	3.509662	-0.872541	-1.307130
C	1.182323	2.280183	2.018351
C	0.576594	-0.697638	2.923501
C	2.072218	-2.632995	0.878625
C	2.975193	2.186291	-0.611088
O	0.623498	-1.108941	-1.898750
H	1.312666	-0.853571	3.719416
H	-0.130988	0.052273	3.275330
H	0.045071	-1.639592	2.786853
H	2.947892	-2.849809	1.501591
H	1.210195	-3.077774	1.375305
H	2.225099	-3.116013	-0.086374
H	4.058325	-0.081680	-1.815304
H	4.226466	-1.603178	-0.925785
H	2.866379	-1.373741	-2.043285
H	3.070017	2.024239	-1.684412
H	2.414093	3.104365	-0.439699
H	3.982235	2.355271	-0.213724
H	1.126390	3.159867	1.379086
H	0.242147	2.168610	2.557530
H	1.960734	2.483124	2.763468
N	-1.345638	-1.223022	-0.219571
N	-1.048964	1.343003	-0.258161

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L3_CAT_T Energy E=-1063.80030198 A.U.

lr	0.423363	0.000010	-0.366005
C	1.575527	-0.704468	1.514349

C	1.575394	0.704387	1.514436
C	2.204613	-1.161237	0.277905
C	2.204443	1.161426	0.278061
C	2.653056	0.000185	-0.439939
C	-3.572056	1.513347	0.184246
C	-3.471143	2.891467	0.087178
C	-2.233970	3.463125	-0.164436
C	-1.134340	2.636447	-0.288630
C	-2.434748	0.732789	0.042286
H	-4.535177	1.053045	0.358065
H	-4.353932	3.510735	0.193268
H	-2.114771	4.533692	-0.271590
H	-0.151038	3.032970	-0.502625
C	-1.134148	-2.636485	-0.288776
C	-2.233704	-3.463255	-0.164532
C	-3.470901	-2.891703	0.087196
C	-3.571923	-1.513595	0.184319
C	-2.434698	-0.732935	0.042272
H	-4.353632	-3.511045	0.193346
H	-0.150821	-3.032916	-0.502835
H	-2.114429	-4.533810	-0.271733
H	-4.535068	-1.053387	0.358258
C	3.449962	0.000305	-1.689603
C	1.091976	1.595068	2.598361
C	1.092385	-1.595406	2.598179
C	2.569186	-2.566343	-0.038196
C	2.568784	2.566632	-0.037869
O	0.264472	0.000135	-2.181200
H	1.944173	-1.893930	3.218382
H	0.370982	-1.101330	3.247209
H	0.643453	-2.510455	2.211219
H	3.576133	-2.764035	0.344705
H	1.905497	-3.284511	0.442647
H	2.586789	-2.758437	-1.110943
H	3.259884	0.884726	-2.296577
H	4.512946	0.000450	-1.425165
H	3.260122	-0.884169	-2.296574
H	2.586694	2.758751	-1.110604
H	1.904778	3.284639	0.442776
H	3.575554	2.764547	0.345381
H	0.643766	2.510511	2.211507
H	0.369871	1.101053	3.246662
H	1.943482	1.892878	3.219294
N	-1.232255	-1.308943	-0.170977
N	-1.232338	1.308898	-0.170867

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-1293.20165384 A.U.

lr	0.045867	-0.426813	-0.132264
C	0.092852	-0.952567	2.043020
C	1.306476	-0.239324	1.824618
C	0.147192	-2.143273	1.209019
C	2.116884	-0.954696	0.856835
C	1.422042	-2.144975	0.513102
C	-2.216523	3.179111	0.226689
C	-1.282545	4.192856	0.389193
C	0.063776	3.876199	0.367425
C	0.443631	2.552463	0.242985
N	-0.462803	1.572253	0.131944
C	-1.788323	1.873595	0.078635
H	-3.272168	3.412183	0.187772
H	-1.609690	5.219769	0.502323
H	0.834629	4.631620	0.447674
H	1.495236	2.292309	0.227414
C	-2.629393	-1.423147	-1.107156
C	-3.999558	-1.405743	-1.296101
C	-4.711624	-0.273112	-0.935475
C	-4.030894	0.825976	-0.435124
C	-2.655244	0.757383	-0.283019
N	-1.990594	-0.375303	-0.585434
H	-5.787143	-0.235337	-1.061055
H	-2.013166	-2.263429	-1.395188

L3_R_S Energy E=-1292.99061421 A.U.

lr	0.046136	-0.426500	-0.132154
C	0.092139	-0.950923	2.043306
C	1.305933	-0.237878	1.824876
C	0.146844	-2.142237	1.210245
C	2.116759	-0.954023	0.858025
C	1.421963	-2.144510	0.514831
C	-2.218313	3.178320	0.225093
C	-1.284939	4.192679	0.387233
C	0.061569	3.876777	0.365682
C	0.442203	2.553206	0.241873
N	-0.463662	1.572419	0.131243
C	-1.789330	1.872982	0.077692
H	-3.274090	3.410736	0.185869
H	-1.612672	5.219464	0.499825
H	0.831981	4.632685	0.445608
H	1.494006	2.293738	0.226429
C	-2.628240	-1.424170	-1.108398
C	-3.998429	-1.407659	-1.297276
C	-4.711280	-0.275656	-0.936226
C	-4.031287	0.823813	-0.435685
C	-2.655568	0.756171	-0.283810
N	-1.990164	-0.376011	-0.586453
H	-5.786848	-0.238659	-1.061622
H	-2.011393	-2.263925	-1.396662
H	-4.488326	-2.271920	-1.727128
H	-4.568288	1.728453	-0.183414
C	1.910186	-3.210340	-0.381926
C	1.759145	0.957584	2.567152
C	-0.946854	-0.652719	3.062623
C	-0.815117	-3.265923	1.254233
C	3.487418	-0.597135	0.432054
O	0.159216	-1.200189	-1.763674
O	3.487377	2.648730	0.066697
H	4.249686	3.216240	0.203118
H	3.418189	2.476274	-0.896648
O	2.708602	1.899092	-2.395395
H	2.779619	2.423403	-3.196882
H	2.797805	0.963323	-2.668551

O	2.702673	-0.812907	-2.888689	H	3.129898	-0.400575	0.146711	C	-1.166608	-2.217070	0.368480
H	1.790832	-1.099271	-2.708344	H	3.352687	-2.144245	0.122808	C	-2.152678	-1.176562	0.416231
H	2.967265	-1.212061	-3.722307	H	2.189073	0.400176	1.978840	C	3.919035	0.156770	-1.192597
H	-0.692378	-1.153434	4.002442	H	0.771203	0.338408	3.061559	C	4.219367	-1.001819	-1.888591
H	-1.017071	0.414588	3.271027	H	2.019209	-0.900408	3.148273	C	3.244114	-1.976670	-2.023850
H	-1.930855	-1.010643	2.759987					C	2.008156	-1.764242	-1.442747
H	-0.512204	-3.937410	2.066389					N	1.724632	-0.655177	-0.753415
H	-1.829329	-2.934856	1.474272					C	2.658032	0.311975	-0.634715
H	-0.814709	-3.850219	0.334887					H	4.665125	0.932829	-1.089439
H	2.414920	-3.971938	0.223531					H	5.201781	-1.137488	-2.324699
H	1.096177	-3.695941	-0.919748					H	3.430450	-2.892709	-2.569590
H	2.628013	-2.825486	-1.104733					H	1.211799	-2.490684	-1.529951
H	3.690116	-0.945311	-0.580905					C	0.441034	2.553546	1.151597
H	3.664606	0.478573	0.476302					C	1.191006	3.687745	1.397624
H	4.199126	-1.086629	1.107654					C	2.510561	3.717837	0.975543
H	2.460524	1.565104	1.993948					C	3.027499	2.620305	0.308915
H	0.932604	1.572823	2.921424					C	2.222581	1.511460	0.089426
H	2.295245	0.599999	3.455427					N	0.945538	1.485479	0.525880

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L3_R_T Energy E= -1293.0112171 A.U.

Ir	-0.529053	-0.468727	-0.323048								
C	-0.531427	-1.682793	1.624063								
C	0.757672	-1.121728	1.487345								
C	-0.775732	-2.533769	0.463637								
C	1.326829	-1.573500	0.224993								
C	0.394275	-2.498703	-0.364531								
C	-1.208010	3.754490	0.149431								
C	0.050561	4.335052	0.198532								
C	1.168818	3.526626	0.102816								
C	0.998334	2.161346	-0.039963								
N	-0.215780	1.607634	-0.080668								
C	-1.321355	2.381926	0.005862								
H	-2.092309	4.373249	0.217446								
H	0.149175	5.408393	0.308875								
H	2.176769	3.918539	0.136434								
H	1.864442	1.516551	-0.101004								
C	-3.596138	-0.404812	-0.443242								
C	-4.858935	0.153518	-0.444076								
C	-4.981261	1.521084	-0.254167								
C	-3.838795	2.284456	-0.087104								
C	-2.595626	1.668545	-0.099748								
N	-2.496843	0.332233	-0.258493								
H	-5.956758	1.992525	-0.248699								
H	-3.448371	-1.463297	-0.606060								
H	-5.724248	-0.477767	-0.599601								
H	-3.917856	3.355317	0.040960								
C	0.622796	-3.288360	-1.597992								
C	1.460689	-0.254392	2.461281								
C	-1.442497	-1.550572	2.791163								
C	-1.923215	-3.462355	0.304340								
C	2.714742	-1.331287	-0.241089								
O	-0.519015	-0.321116	-2.142103								
O	3.891908	1.668916	0.768589								
H	4.313486	2.099563	1.515868								
H	4.630160	1.445385	0.150256								
O	5.787049	0.926219	-0.961313								
H	5.998042	1.456547	-1.732910								
H	6.632930	0.523397	-0.674374								
O	8.150849	-0.172290	-0.153296								
H	8.584418	-0.918136	-0.575594								
H	8.837780	0.300607	0.323411								
H	-1.318615	-2.418766	3.446220								
H	-1.222204	-0.662070	3.381271								
H	-2.491606	-1.517113	2.495330								
H	-1.654320	-4.429495	0.742347								
H	-2.811977	-3.115396	0.830679								
H	-2.169285	-3.641252	-0.742702								
H	1.171998	-4.198685	-1.335791								
H	-0.310771	-3.587025	-2.072569								
H	1.221152	-2.739727	-2.324958								
H	2.784675	-1.324234	-1.328528								

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L3_TS Energy E= -1292.97664257 A.U.

Ir	0.227546	-0.175471	0.112307								
C	0.420199	-1.441279	2.008666								
C	0.687804	-0.109292	2.390374								
C	1.398342	-1.813432	0.991027								
C	1.811460	0.384596	1.608298								
C	2.286280	-0.694073	0.797272								
C	-3.451667	1.990635	-0.077404								
C	-3.145631	3.277340	0.333336								
C	-1.837940	3.584774	0.674677								
C	-0.886966	2.585619	0.629605								
N	-1.193207	1.334510	0.269693								
C	-2.454308	1.029211	-0.114061								
H	-4.459147	1.743808	-0.383945								
H	-3.917559	4.036992	0.364824								
H	-1.548746	4.585538	0.968307								
H	0.149700	2.779313	0.864678								
C	-1.497000	-2.247611	-1.291745								
C	-2.661918	-2.818343	-1.770130								
C	-3.848862	-2.112666	-1.653288								
C	-3.828671	-0.848524	-1.088461								
C	-2.626311	-0.322950	-0.639522								
N	-1.487464	-1.041169	-0.721587								
H	-4.780499	-2.536393	-2.008621								
H	-0.544896	-2.754850	-1.367554								
H	-2.628804	-3.798508	-2.228274								
H	-4.742602	-0.275793	-1.006002								
C	3.501504	-0.672467	-0.045755								
C	-0.013791	0.657092	3.448806								
C	-0.587059	-2.355512	2.604746								
C	1.605860	-3.184848	0.460026								
C	2.507745	1.685343	1.789394								
O	0.795173	0.007016	-1.630113								
O	0.650385	2.063273	-2.253929								
H	0.389092	2.021827	-3.179864								
H	1.633244	2.219079	-2.245195								
O	3.291041	2.198410	-2.130838								
H	3.860629	2.912291	-2.430042								
H	3.509833	1.404504	-2.661633								
O	3.139064	-0.214198	-3.313977								
H	2.217711	-0.340034	-3.051669								
H	3.242015	-0.551201	-4.207673								
H	1.865557	2.440600	2.242355								
H	3.354766	1.545782	2.469159								
H	2.903022	2.067028	0.846934								
H	3.738205	0.335510	-0.383998								
H	4.345069	-1.040326	0.548182								
H	3.408202	-1.307753	-0.925547								
H	0.679576	-3.757800	0.420423								
H	2.066286	-3.176372	-0.527582								
H	2.283306	-3.723620	1.131107								
H	-0.975459	-3.067681	1.876527								
H	-0.120045	-2.935403	3.407205								
H	-1.426464	-1.812289	3.037061								
H	-1.012754	0.271491	3.647234								
H	0.561350	0.574478	4.377426								
H	-0.086631	1.719950	3.217472								

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L3_P Energy E= -1293.0169029 A.U.

Ir	-0.139608	-0.296296	0.172358								
C	-0.699582	-0.842524	2.196157								
C	-0.272478	-2.016758	1.490281								
C	-1.865353	-0.308993	1.520513								

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L4_CAT_S Energy E= -1123.64608652 A.U.

Ir	0.685215	-0.134403	-0.424002								
C	1.566927	-0.298350	1.702275								
C	1.684846	1.062019	1.363378								
C	2.318059	-1.066386	0.718696								
C	2.472319	1.166997	0.145548								
C	2.916112	-0.139851	-0.212361								
C	-3.226093	1.548764	0.010212								
C	-1.881887	2.934340	-0.173988								
C	-3.841117	3.464972	-0.448654								
C	-0										

C	-3.409095	-2.690069	0.092076	H	4.856979	-0.055789	-1.218756	H	-4.927262	2.971616	0.189507
C	-3.410737	-1.288414	0.141209	H	3.755264	-1.225339	-1.951223				
C	-2.174443	-0.644050	-0.014333	H	2.929750	2.570046	-1.299716				
N	-1.021719	-1.321575	-0.215639	H	2.204484	3.269077	0.152304	58			
H	-4.338065	-3.237075	0.209171	H	3.872550	2.714354	0.184834	L4_R_T Energy E=	-1352.85443139	A.U.	
H	-0.106525	-3.132358	-0.534244	H	0.792815	2.701643	1.911025	lr	0.264283	-0.542572	-0.171340
H	-2.202059	-4.439646	-0.214382	H	0.437081	1.413122	3.057621	C	0.420287	-1.544856	1.854353
C	3.795374	-0.501235	-1.352776	H	2.026613	2.180288	3.061388	C	1.487852	-0.605311	1.757842
C	1.193003	2.205797	2.169648	C	-4.578311	-0.659451	0.225010	C	0.651394	-2.577686	0.861402
C	0.886733	-0.869673	2.893560	C	-4.553225	0.697556	0.235337	C	2.316552	-0.983097	0.640570
C	2.604996	-2.523085	0.789193	H	-5.515974	-1.192938	0.329622	C	1.818760	-2.242609	0.129407
C	2.944407	2.430337	-0.480925	H	-5.477468	1.253427	0.348652	C	-2.596769	2.595760	0.402298
O	0.791086	-0.902629	-2.046332					C	-1.867914	3.724546	0.808866
H	1.603423	-0.997445	3.710686	58				C	-0.497359	3.649317	0.919365
H	0.087390	-0.220241	3.248718	L4_R_S Energy E=	-1352.85013672	A.U.		C	0.209128	2.461051	0.656314
H	0.456239	-1.848426	2.678709	lr	0.335965	-0.493459	-0.145397	C	-0.479342	1.327856	0.288188
H	3.504400	-2.682749	1.393780	C	0.520116	-1.064265	2.046033	C	-1.876836	1.412458	0.150295
H	1.796288	-3.076816	1.265812	C	1.471290	-0.030748	1.854125	H	-2.386705	4.653369	1.017723
H	2.787919	-2.944932	-0.198719	C	0.893768	-2.154824	1.169861	H	0.066395	4.528133	1.211610
H	4.309982	0.373747	-1.747634	C	2.443285	-0.454403	0.863663	H	1.289175	2.480981	0.752708
H	4.548772	-1.227324	-1.042186	C	2.113329	-1.780537	0.481471	C	-2.343216	-1.891246	-1.130176
H	3.197200	-0.939745	-2.159844	C	-2.858207	2.322089	0.223210	C	-3.710004	-1.963636	-1.382014
H	2.961368	2.362563	-1.568394	C	-2.255224	3.568617	0.465086	C	-4.515076	-0.882578	-1.088778
H	2.331488	3.283030	-0.193554	C	-0.883045	3.667401	0.516022	C	-3.947319	0.282366	-0.558694
H	3.964478	2.639857	-0.143152	C	-0.048152	2.540747	0.394872	C	-2.559274	0.274687	-0.330938
H	0.876769	3.044303	1.551033	C	-0.609993	1.296855	0.209479	N	-1.789823	-0.806495	-0.602584
H	0.356139	1.923558	2.807142	C	-2.011622	1.208301	0.093713	H	-5.581734	-0.924606	-1.280299
H	2.003583	2.557327	2.816391	H	-2.873655	4.452020	0.578470	H	-1.681779	-2.715132	-1.363478
C	-4.570299	-0.464473	0.290026	H	-0.417583	4.635994	0.658311	H	-4.119140	-2.868406	-1.811997
C	-4.479632	0.888715	0.220869	H	1.023280	2.700290	0.441070	C	2.464910	-3.030515	-0.951537
H	-5.532437	-0.943277	0.431062	C	-2.035608	-2.149413	-1.080820	C	1.773135	0.499942	2.702739
H	-5.375101	1.494948	0.301609	C	-3.385355	-2.414838	-1.312055	C	-0.626545	-1.576227	2.913851
				C	-3.385355	-2.414838	-1.312055	C	-0.138737	-3.829879	0.738550
				C	-4.330764	-1.450754	-1.037330	C	3.593058	-0.339860	0.235628
				C	-3.923370	-0.202210	-0.545997	O	0.653237	-0.116549	-1.908102
				C	-2.549600	-0.024685	-0.319476	O	3.444262	2.931711	0.942224
				N	-1.641064	-0.994028	-0.568710	H	4.094369	3.446533	1.424042
				H	-5.381456	-1.641961	-1.225661	H	3.632275	3.087215	-0.009379
				H	-1.262491	-2.864185	-1.328065	O	3.885376	3.160218	-1.719289
				H	-3.667374	-3.374019	-1.726022	H	3.730892	3.946440	-2.245423
				C	2.899580	-2.632452	-0.443772	H	3.591852	2.399947	-2.258224
				C	1.581848	1.210229	2.654126	O	2.977535	0.933467	-3.067790
				C	-0.575087	-1.087685	3.052538	H	2.081128	0.648680	-2.825846
				C	0.275327	-3.505131	1.170290	H	3.069442	0.778334	-4.010394
				C	3.674786	0.273636	0.473630	H	-0.274785	-2.149067	3.777352
				O	0.581288	-0.793313	-1.923313	H	-0.870967	-0.571719	3.258742
				O	3.007060	3.468110	0.224177	H	-1.546519	-2.044055	2.562018
				H	3.604475	4.193413	0.415579	H	0.239413	-4.564790	1.456475
				H	3.128949	3.258343	-0.727518	H	-1.193052	-3.672885	0.967253
				O	3.267993	2.650638	-2.350839	H	-0.055412	-4.274311	-0.253500
				H	2.954131	3.135070	-3.116151	H	3.300989	-3.604240	-0.538964
				H	3.180216	1.699066	-2.567890	H	1.775478	-3.734850	-1.416009
				O	2.976574	-0.045776	-2.830686	H	2.868707	-2.380242	-1.728366
				H	2.080711	-0.374450	-2.567047	H	3.736400	-0.370070	-0.845311
				H	3.148808	-0.389935	-3.709920	H	3.642917	0.700783	0.558733
				H	-0.217836	-1.521879	3.991432	H	4.426741	-0.878994	0.698667
				H	-0.937384	-0.082644	3.267373	H	2.353754	1.297082	2.237550
				H	-1.422488	-1.684850	2.714748	H	0.862345	0.922908	3.124832
				H	0.740109	-4.108184	1.957316	H	2.366160	0.092240	3.528986
				H	-0.792828	-3.462816	1.381297	C	-4.663767	1.480723	-0.251505
				H	0.427861	-4.027144	0.225772	C	-4.015143	2.581797	0.206412
				H	3.709125	-3.113679	0.114973	H	-5.736240	1.498009	-0.407236
				H	2.291904	-3.415892	-0.895060	H	-4.573064	3.487442	0.418044
				H	3.347398	-2.036126	-1.239204				
				H	3.956876	0.047082	-0.554838	58			
				H	3.563254	1.353899	0.573827	L4_TS Energy E=	-1352.81222062	A.U.	
				H	4.494915	-0.044299	1.127520	lr	-0.753733	0.000435	0.002040
				H	2.128295	1.991484	2.126474	C	-2.065071	0.223464	-1.764010
				H	0.608460	1.595430	2.955119	C	-2.286596	1.348946	-0.912942
				H	2.142144	0.970038	3.564984	C	-2.522845	-0.963253	-1.051230
				C	-4.779378	0.917630	-0.306807	C	-2.756282	0.868564	0.357146
				C	-4.266089	2.122999	0.052564	C	-2.943819	-0.563479	0.238497
				H	-5.846705	0.796230	-0.451150	C	3.133743	1.787670	-0.353688

C	3.028767	3.082962	0.179536	C	-2.906950	2.126020	-0.183204	C	0.948419	2.260295	2.756650
C	1.823246	3.515846	0.684358	C	-1.833965	1.217439	-0.205189	O	0.743201	-0.108733	-0.628419
C	0.678120	2.698065	0.661902	N	-0.602234	1.534747	0.267195	H	5.815764	3.046757	0.135297
C	1.422749	1.422847	0.123992	H	-3.461204	4.132624	0.385342	H	5.837396	1.359666	0.659196
C	1.975582	0.988299	-0.362107	H	0.585242	2.939840	1.179642	H	5.437793	1.749090	-1.006511
H	3.898429	3.729833	0.201191	H	-1.197929	4.665361	1.281238	H	3.292276	4.314799	-1.760759
H	1.748753	4.511266	1.108059	C	3.739728	-0.072352	1.821305	H	3.845438	2.746166	-2.342000
H	-0.242631	3.094360	1.076714	C	1.782029	-1.586092	-2.688071	H	2.131016	3.167646	-2.432762
C	0.910908	-2.326339	-1.151280	C	1.779441	1.581056	-2.636621	H	-0.462358	2.453083	0.015875
C	2.057688	-2.938419	-1.656138	C	3.151512	2.532451	0.064455	H	-0.025553	4.119340	0.430505
C	3.229793	-2.218707	-1.749632	C	2.907248	-2.607006	0.150353	H	0.284977	3.500005	-1.194705
C	3.252564	-0.883527	-1.326261	O	0.172647	-0.427925	2.122123	H	-0.024232	1.895050	2.424612
C	2.050611	-0.340657	-0.837012	O	0.669908	-1.664426	2.643731	H	1.298671	1.621482	3.567964
N	0.901723	-1.056686	-0.765581	H	0.800127	-1.434510	3.574469	H	0.816671	3.267375	3.168538
H	4.130699	-2.678880	-2.140569	H	-3.535961	-2.717719	0.645934	H	3.446619	0.868003	3.523580
H	-0.019831	-2.870208	-1.054700	O	-3.692520	-2.660443	1.598215	H	4.959128	0.973339	2.634969
H	2.008406	-3.974141	-1.966917	H	-3.753375	-3.561451	1.924383	H	4.335620	2.394720	3.481718
C	-3.477262	-1.429107	1.321997	H	-2.785986	-1.481122	2.359330	lr	-2.301924	-0.551937	-0.078206
C	-2.126071	2.772277	-1.306935	O	-2.250928	-0.755106	2.761644	C	-3.310957	-1.947515	-1.674808
C	-1.670410	0.269069	-3.199084	H	-0.833139	-0.524115	2.268738	C	-3.877749	-2.183934	-0.397022
C	-2.645849	-2.321535	-1.647367	H	-2.856003	-0.054186	3.011114	C	-1.914831	-2.288597	-1.624801
C	-3.198731	1.690872	1.516372	H	3.955988	-2.866912	-0.024540	C	-2.828378	-2.700875	0.455859
O	-0.277270	-0.819299	1.719801	H	2.688731	-2.758953	1.207327	C	-1.621731	-2.766807	-0.313583
O	0.252540	0.253654	2.947298	H	2.294508	-3.306394	-0.418305	C	-4.937961	2.395583	1.570497
H	0.751564	0.887044	2.402568	H	4.799845	-0.318034	1.703238	C	-5.140835	2.014606	2.887374
H	0.929053	-0.315570	3.496916	H	3.675534	0.880798	2.354748	C	-4.477117	0.3903810	3.933028
O	1.906046	-1.183662	4.160728	H	3.293822	-0.844749	2.448564	C	-3.630380	0.160370	2.576276
H	1.818842	-1.408264	5.090141	H	4.124580	2.783357	-0.369357	C	-3.436611	0.513801	1.245727
H	1.886529	-2.016893	3.629818	H	2.429715	3.240567	-0.344650	C	-4.081638	1.662981	0.750907
O	1.360697	-2.964799	2.327827	H	3.223930	2.694909	1.140674	H	-5.441532	3.275275	1.182550
H	0.770788	-2.291066	1.932987	H	2.663997	1.776189	-3.251241	H	-5.805421	2.588926	3.523135
H	1.927548	-3.295752	1.628019	H	1.022908	1.125612	-3.275126	H	-4.610859	0.617796	4.431181
H	-2.714141	2.667139	1.528112	H	1.396270	2.543742	-2.296232	H	-3.104330	-0.689748	2.996392
H	-4.279019	1.861170	1.469996	H	2.631825	-1.625631	-3.376709	C	-2.280966	1.324780	-2.447190
H	-2.979232	1.193583	2.461487	H	1.544547	-2.608215	-2.398452	C	-2.663096	2.459579	-3.154138
H	-2.921073	-1.277913	2.249240	H	0.928089	-1.179794	-3.229062	C	-3.585647	3.344035	-2.607267
H	-4.526252	-1.187052	1.514507	C	-4.165786	1.685256	-0.699198	C	-4.102462	3.113493	-1.341247
H	-3.418575	-2.485068	1.060978	C	-4.324306	0.420961	-1.166151	C	-3.712872	1.988176	-0.618062
H	-1.905927	-2.487904	-2.430861	H	-4.996971	2.381297	-0.703567	H	-3.890691	4.223435	-3.163767
H	-2.546918	-3.110920	-0.901222	H	-5.289298	0.102171	-1.545270	H	-1.543889	0.652012	-2.873140
H	-3.630512	-2.432348	-2.112368					H	-2.239165	2.653595	-4.133877
H	-1.105964	-0.617536	-3.490031	94				H	-4.800560	3.823341	-0.909402
H	-2.558377	0.319317	-3.836985	L1-DIMERTs_S E= -2062.04017651 A.U.				C	-0.285695	-3.237529	0.136762
H	-1.054437	1.141535	-3.415603	lr	2.301899	0.551890	0.078150	C	-5.316459	-2.078177	-0.026168
H	-1.323423	2.907641	-2.030861	C	3.877646	2.183925	0.397044	C	-4.050952	-1.517841	-2.890693
H	-3.056405	3.119092	-1.767942	C	3.310716	1.947591	1.674785	C	-0.948768	-2.260178	-2.756933
H	-1.925192	3.415916	-0.452173	C	2.828359	2.700796	-0.455981	C	-3.031233	-3.252654	1.823230
C	4.347554	1.233347	-0.873585	C	1.914597	2.288669	1.624614	O	-0.743150	0.108577	0.628303
C	4.406936	-0.039701	-1.340360	C	1.621627	2.766767	0.313332	H	-4.336122	-2.394463	-3.481645
H	5.236965	1.853971	-0.882090	C	4.102652	-3.113318	1.341518	H	-4.959419	-0.973090	-2.634725
H	5.337674	-0.441250	-1.724650	C	3.585796	-3.343820	2.607530	H	-3.447016	-0.867804	-3.523518
				C	2.663126	-2.459417	3.154287	H	-0.817122	-3.267229	-3.168925
58				C	2.280928	-1.324702	2.447242	H	-1.299059	-1.621272	-3.568156
L4_P Energy E= -1352.83616963 A.U.				C	2.809754	-1.069998	1.186079	H	0.023939	-1.895026	-2.424952
lr	0.841065	-0.015610	0.056522	C	3.713018	-1.988072	0.618250	H	0.025465	-4.119347	-0.430985
C	2.133786	0.694467	-1.494758	H	4.800846	-3.823125	0.909761	H	0.462276	-2.453100	-0.016319
C	2.147684	-0.746203	-1.519046	H	3.890885	-4.223160	3.164098	H	-0.284920	-3.500095	1.194285
C	2.795613	1.126180	-0.266173	H	2.239141	-2.653419	4.134006	H	-2.130823	-3.167848	2.432536
C	2.644032	-1.199123	-0.254937	H	1.543777	-0.651966	2.873117	H	-3.845254	-2.746359	2.341987
C	3.083534	-0.020605	0.488917	C	3.630517	-0.160505	-2.576224	H	-3.292160	-4.314957	1.760593
C	-3.247485	-0.522823	-1.159855	C	4.477345	-0.903941	-3.392885	H	-5.437730	-1.749160	1.006739
C	-3.376190	-1.857750	-1.582816	C	5.141147	-2.014636	-2.887116	H	-5.837502	-1.359593	-0.658892
C	-2.290697	-2.705791	-1.487961	C	4.938247	-2.395529	-1.570218	H	-5.815866	-3.046727	-0.135131
C	-1.048705	-2.265066	-0.996670	C	4.081819	-1.662945	-0.750726	C	-2.809730	1.070052	-1.186005
C	-0.856143	-0.949602	-0.612790	H	5.805818	-2.588940	-3.522801	C	3.436714	-0.513856	-1.245658
C	-1.986734	-0.104302	-0.692883	H	3.104411	0.689532	-2.996432				
H	-4.321482	-2.210417	-1.980952	H	4.611114	-0.617987	-4.431051	94			
H	-2.391679	-3.736919	-1.811451	H	5.441875	-3.275151	-1.182186	L1-DIMERTs_SU E= -2062.04864146 A.U.			
H	-0.241210	-2.984823	-0.924603	C	0.285646	3.237489	-0.137170	lr	2.307331	0.554980	0.077993
C	-0.404955	2.736701	0.792344	C	4.050588	1.518040	2.890787	C	3.842848	2.226554	0.327973
C	-1.414044	3.697066	0.848854	C	5.316399	2.078184	0.026357	C	3.274873	2.027394	1.616546
C	-2.664421	3.397359	0.354347	C	3.031360	3.252491	-1.823363	C	2.794562	2.710922	-0.540844

C	1.877327	2.342748	1.552596	O	-0.770815	0.264311	0.538276	C	3.459849	1.940247	1.172896
C	1.586787	2.774477	0.220228	H	-4.344522	-2.565673	-3.369833	C	2.814806	2.513844	0.029781
C	4.297665	-3.016669	1.333732	H	-4.914264	-1.072092	-2.614513	C	2.252058	-3.800015	1.427769
C	3.854424	-3.240267	2.628550	H	-3.416126	-1.072063	-3.533690	C	2.299378	-3.718684	2.810821
C	2.926172	-2.380708	3.203563	H	-0.798544	-3.361433	-3.087969	C	2.340747	-2.473881	3.427876
C	2.462373	-1.279297	2.492111	H	-1.248928	-1.709916	-3.502465	C	2.357000	-1.314169	2.660607
C	2.917404	-1.030521	1.202693	H	0.068674	-1.998290	-2.361138	C	2.323870	-1.374644	1.269503
C	3.828541	-1.922736	0.609244	H	-0.046897	-4.245405	-0.180976	C	2.257412	-2.640834	0.653825
H	5.002568	-3.707050	0.881971	H	0.531822	-2.574342	-0.053179	H	2.205553	-4.773773	0.950255
H	4.222179	-4.094621	3.186080	H	-0.226072	-3.354658	1.333083	H	2.296074	-4.623561	3.408683
H	2.560925	-2.568146	4.207885	H	-2.098225	-3.118783	2.531169	H	2.357848	-2.404932	4.510741
H	1.723713	-0.624029	2.942216	H	-3.815901	-2.717802	2.425764	H	2.373711	-0.351629	3.161623
C	3.550708	-0.174686	-2.624050	H	-3.244484	-4.295913	1.888679	C	1.901388	-1.081169	-2.667543
C	4.386829	-0.910734	-3.459195	H	-5.419656	-1.785299	1.056432	C	1.749040	-2.171560	-3.517941
C	5.104449	-1.987976	-2.956413	H	-5.811267	-1.428275	-0.618800	C	1.808090	-3.465317	-3.013251
C	4.968716	-2.342836	-1.623144	H	-5.774546	-3.105421	-0.066372	C	1.994646	-3.665489	-1.654147
C	4.126898	-1.615811	-0.784148	C	-2.916876	1.030432	-1.202797	C	2.136913	-2.576923	-0.795313
H	5.759456	-2.557797	-3.606027	C	3.427143	-0.500656	-1.279576	C	2.109273	-1.261579	-1.302470
H	2.981092	0.648985	-3.040138					H	1.700566	-4.315504	-3.678088
H	4.469526	-0.644845	-4.507934	94				H	1.832003	-0.080083	-3.079185
H	5.514357	-3.198234	-1.237973	L1-DIMER_S E=-2062.08577254 A.U.				H	1.582237	-2.009347	-4.578004
C	0.260896	3.260539	-0.247576	lr	-2.346289	-0.252985	0.043931	H	2.023344	-4.676936	-1.261140
C	4.025165	1.658570	2.846315	C	-4.325193	-0.938919	-0.737221	C	1.771168	3.575135	0.073249
C	5.286073	2.130547	-0.030032	C	-4.385724	-0.951961	0.693230	C	5.339245	0.179730	1.536173
C	2.994995	3.229670	-1.921475	C	-3.367895	-1.935758	-1.152181	C	5.213014	0.162104	-1.646385
C	0.911387	2.347781	2.685400	C	-3.460016	-1.940044	1.172970	C	3.106650	2.373468	-2.550787
O	0.771075	-0.264938	-0.538116	C	-2.814798	-2.513832	0.030052	C	3.293027	2.382204	2.584749
H	5.773683	3.106460	0.066251	C	-2.252135	3.800039	1.427687	O	0.411773	0.508584	0.172271
H	5.811070	1.429434	0.618980	C	-2.299501	3.718731	2.810739	H	6.081338	0.762862	-1.936575
H	5.419244	1.786005	-1.056311	C	-2.340865	2.473938	3.427814	H	5.576709	-0.746159	-1.166112
H	3.242971	4.296357	-1.888288	C	-2.357070	1.314212	2.660565	H	4.688856	-0.138253	-2.554332
H	3.815239	2.718609	-2.425532	C	-2.323903	1.374662	1.269461	H	3.736503	3.233125	-2.806669
H	2.097345	3.118704	-2.530924	C	-2.257440	2.640843	0.653764	H	3.334623	1.582013	-3.265201
H	-0.532598	2.574042	0.054602	H	-2.205634	4.773788	0.950156	H	2.066732	2.670785	-2.694996
H	0.046400	4.245191	0.180333	H	-2.296236	4.623619	3.408586	H	1.101394	3.441285	0.924123
H	0.224734	3.352733	-1.332825	H	-2.357995	2.405007	4.510679	H	2.232623	4.564350	0.159420
H	-0.069048	1.997338	2.361422	H	-2.373771	0.351680	3.161595	H	1.156510	3.565579	-0.827041
H	1.248663	1.709122	3.502652	C	-1.901327	1.081121	-2.667569	H	2.265450	2.682453	2.795235
H	0.797881	3.360589	3.088404	C	-1.748936	2.171496	-3.517980	H	3.564727	1.592348	3.286119
H	3.415956	1.072782	3.534150	C	-1.807986	3.465261	-3.013312	H	3.938978	3.241636	2.798440
H	4.913790	1.071806	2.614477	C	-1.994586	3.665460	-1.654218	H	4.884755	-0.127838	2.478670
H	4.344954	2.565914	3.369426	C	-2.136895	2.576910	-0.795370	H	5.676792	-0.723607	1.028816
lr	-2.307322	-0.555107	-0.077891	C	-2.109246	1.261560	-1.302505	H	6.219301	0.789811	1.764526
C	-3.275257	-2.027332	-1.616403	H	-1.700426	4.315436	-3.678159				
C	-3.843360	-2.226213	-0.327849	H	-1.831948	0.080025	-3.079191	94			
C	-1.877814	-2.343123	-1.552350	H	-1.582104	2.009263	-4.578036	L1-DIMER_SU E=-2062.08577254 A.U.			
C	-2.795265	-2.710833	0.541065	H	-2.023284	4.676914	1.261230	lr	-2.346289	-0.252985	0.043931
C	-1.587483	-2.774869	-0.219955	C	-1.771152	-3.575104	0.073818	C	-4.325193	-0.938919	-0.737221
C	-4.968483	2.343285	1.622573	C	-5.339464	-0.179459	1.535666	C	-4.385724	-0.951961	0.693230
C	-5.104291	1.988712	2.955913	C	-5.212763	-0.162394	-1.646881	C	-3.367895	-1.935758	-1.152181
C	-4.386727	0.911557	3.458960	C	-3.106232	-2.373899	-2.550584	C	-3.460016	-1.940044	1.172970
C	-3.550610	0.175285	2.624007	C	-3.293454	-2.381772	2.584926	C	-2.814798	-2.513832	0.030052
C	-3.426994	0.500946	1.279461	O	-0.411776	-0.508565	0.172261	C	-2.252135	3.800039	1.427687
C	-4.126655	1.616049	0.783772	H	-6.081042	-0.763201	-1.937106	C	-2.299501	3.718731	2.810739
H	-5.514059	3.198634	1.237201	H	-5.576531	0.745947	-1.166813	C	-2.340865	2.473938	3.427814
H	-5.759303	2.558699	3.605377	H	-4.688468	0.137818	-2.554797	C	-2.357070	1.314212	2.660565
H	-4.469467	0.645909	4.507757	H	-3.736029	-3.233608	-2.806435	C	-2.323903	1.374662	1.269461
H	-2.981045	-0.648322	3.040296	H	-3.334087	-1.582568	-3.265171	C	-2.257440	2.640843	0.653764
C	-2.461474	1.279093	-2.492105	H	-2.066285	-2.671233	-2.694558	H	-2.205634	4.773788	0.950156
C	-2.925007	2.380494	-3.203749	H	-1.101894	-3.441498	0.925131	H	-2.296236	4.623619	3.408586
C	-3.853366	3.240142	-2.629041	H	-2.232625	-4.564362	0.159397	H	-2.357995	2.405007	4.510679
C	-4.296954	3.016668	-1.334319	H	-1.155954	-3.565244	-0.826104	H	-2.373771	0.351680	3.161595
C	-3.828078	1.922764	-0.609625	H	-2.265888	-2.681851	2.795707	C	-1.901327	1.081121	-2.667569
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H	-1.722711	0.623761	-2.941954	H	-3.939341	-3.241258	2.798592	C	-1.807986	3.465261	-3.013312
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H	-5.001918	3.707137	-0.882787	H	-5.677003	0.723750	1.028074	C	-2.136895	2.576910	-0.795370
C	-0.261730	-3.261260	0.247922	H	-6.219516	-0.789527	1.764070	C	-2.109246	1.261560	-1.302505
C	-5.286566	-2.129712	0.030101	lr	2.346290	0.252984	0.043950	H	-1.700426	4.315436	-3.678159
C	-4.025309	-1.658382	-2.846281	C	4.325298	0.938778	-0.736991	H	-1.831948	0.080025	-3.079191
C	-0.911831	-2.348542	-2.685112	C	4.385628	0.952088	0.693469	H	-1.582104	2.009263	-4.578036
C	-2.995940	-3.229355	1.921746	C	3.368069	1.935557	-1.152266	H	-2.023284	4.676914	-1.261230

C	-1.771152	-3.575104	0.073818	C	-4.249201	1.013787	0.847447	C	1.773457	-3.595366	-0.314533
C	-5.339464	-0.179459	1.535666	C	-4.431036	0.948932	-0.568641	C	5.452750	-0.139735	-1.287915
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O	-0.411776	-0.508565	0.172261	C	-2.448623	-3.810276	-1.338462	O	0.409252	-0.554359	-0.404093
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H	-5.576531	0.745947	-1.166813	C	-2.603881	-2.535839	-3.368261	H	5.437887	0.654874	1.471542
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H	-3.334087	-1.582568	-3.265171	C	-2.361743	-2.631513	-0.600272	H	3.084618	-1.789347	3.246352
H	-2.066285	-2.671233	-2.694558	H	-2.409384	-4.771636	-0.835831	H	1.791690	-2.747788	2.519861
H	-1.101894	-3.441498	0.925131	H	-2.641448	-4.683925	-3.288785	H	1.177535	-3.417477	-1.210891
H	-2.232625	-4.564362	0.159397	H	-2.679846	-2.495574	-4.450019	H	2.241389	-4.580791	-0.408227
H	-1.155954	-3.565244	-0.826104	H	-2.534986	-0.406215	-3.161172	H	1.084378	-3.625664	0.529687
H	-2.265888	-2.681851	2.795707	C	-1.740163	-0.975556	2.631641	H	2.507602	-2.563196	-2.936615
H	-3.565430	-1.591848	3.286111	C	-1.572984	-2.040773	3.511370	H	3.845885	-1.453964	-3.252082
H	-3.939341	-3.241258	2.798592	C	-1.708292	-3.348425	3.059928	H	4.174433	-3.128472	-2.819136
H	-4.885076	0.128341	2.478138	C	-1.988902	-3.589632	1.723371	H	5.069678	0.238963	-2.236445
H	-5.677003	0.723750	1.028074	C	-2.146519	-2.527522	0.835012	H	5.767163	0.721026	-0.698136
H	-6.219516	-0.789527	1.764070	C	-2.036867	-1.198963	1.290777	H	6.338435	-0.749001	-1.495994
Ir	2.346290	0.252984	0.043950	H	-1.589439	-4.177978	3.748486				
C	4.325298	0.938778	-0.736991	H	-1.608777	0.037098	2.997387	94			
C	4.385628	0.952088	0.693469	H	-1.335625	-1.847798	4.552707	L2-DIMERTs_S E=	-2094.88768398	A.U.	
C	3.368069	1.935557	-1.152266	H	-2.079947	-4.612371	1.370865	Ir	-2.338796	0.501283	0.283144
C	3.459849	1.940247	-1.172896	C	-1.773479	3.595383	-0.314952	C	-4.209223	1.531063	1.149797
C	2.814806	2.513844	0.029781	C	-5.452845	0.139561	-1.287473	C	-3.905549	2.224460	-0.041327
C	2.252058	-3.800015	1.427769	C	-5.047140	0.281939	1.869389	C	-3.074608	1.665328	2.050096
C	2.299378	-3.718684	2.810821	C	-2.857493	2.519737	2.468954	C	-2.556446	2.741526	0.063704
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H	2.205553	-4.773773	0.950255	H	-4.444516	0.036278	2.744291	C	-2.631735	0.561970	-2.762853
H	2.296074	-4.623561	3.408683	H	-3.405048	3.436819	2.714072	C	-2.848942	-0.138145	-1.583279
H	2.357848	-2.404932	4.510741	H	-3.084199	1.789802	3.246298	C	-3.397998	-1.431954	-1.649387
H	2.373711	-0.351629	3.161623	H	-1.791349	2.748130	2.519529	H	-4.187039	-2.974378	-2.974378
C	1.901388	-1.081169	-2.667543	H	-1.177900	3.417647	-1.211566	H	-3.861058	-1.676988	-4.996410
C	1.749040	-2.171560	-3.517941	H	-2.241436	4.580830	-0.408296	H	-2.811733	0.561224	-4.900191
C	1.808090	-3.465317	-3.013251	H	-1.084079	3.625535	0.529013	H	-2.173982	1.543176	-2.740963
C	1.994646	-3.665489	-1.654147	H	-2.507941	2.562802	-2.936875	C	-2.744309	-2.052211	1.836813
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C	2.109273	-1.261579	-1.302470	H	-4.174712	3.128204	-2.819191	C	-3.837601	-4.019592	1.062186
H	1.700566	-4.315504	-3.678088	H	-5.069893	-0.239255	-2.236004	C	-3.942268	-3.434459	-0.184530
H	1.832003	-0.080083	-3.079185	H	-5.767186	-0.721129	-0.697552	C	-3.438584	-2.153842	-0.390570
H	1.582237	-2.009347	-4.578004	H	-6.338556	0.748802	-1.495511	H	-4.231908	-5.014403	1.232340
H	2.023344	-4.676936	-1.261140	Ir	2.320554	-0.283083	-0.080107	H	-2.240528	-1.466885	2.594414
C	1.771168	3.575135	0.073249	C	4.249373	-1.013678	0.847270	H	-3.091284	-3.755868	3.074937
C	5.339245	0.179730	1.536173	C	4.431037	-0.949021	-0.568853	H	-4.412625	-3.963939	-1.002418
C	5.213014	0.162104	-1.646385	C	3.257046	-2.020769	1.124163	C	-0.754246	2.867228	1.916671
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C	3.293027	2.382204	2.584749	C	2.807279	-2.538814	-0.130770	C	-5.503744	0.884687	1.493603
O	0.411773	0.508584	0.172271	C	2.448285	3.810250	-1.338564	C	-3.059635	1.243079	3.475394
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H	5.576709	-0.746159	-1.166112	C	2.603702	2.535753	-3.368315	O	-0.613965	-0.038599	0.566936
H	4.688856	-0.138253	-2.554332	C	2.530534	1.355601	-2.635779	H	-6.137620	1.587279	2.043277
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H	3.334623	1.582013	-3.265201	C	2.361554	2.631505	-0.600327	H	-5.364880	0.007561	2.126536
H	2.066732	2.670785	-2.694996	H	2.408938	4.771626	-0.835970	H	-3.465618	2.048827	4.096034
H	1.101394	3.441285	0.924123	H	2.641002	4.683847	-3.288920	H	-3.684252	0.366234	3.646092
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H	1.156510	3.565579	-0.827041	H	2.535071	0.406125	-3.161138	H	0.044239	2.592704	1.222798
H	2.265450	2.682453	2.795235	C	1.740250	0.975606	2.631667	H	-0.742388	3.951214	2.068869
H	3.564727	1.592348	3.286119	C	1.572984	2.040842	3.511359	H	-0.544486	2.395231	2.875490
H	3.938978	3.241636	2.798440	C	1.708128	3.348490	3.059859	H	-0.810097	3.460788	-0.940365
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H	5.676792	-0.723607	1.028816	C	2.146368	2.527538	0.834965	H	-2.032314	4.689419	-0.588462
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H -2.461060 0.300533 -3.046180
H -2.661376 2.311045 -4.491733
H -2.520268 4.704639 -0.933505
C -1.704781 -3.570985 -0.363438
C -5.027077 -0.420732 1.969678
C -5.531281 -0.229745 -1.159416
C -3.603327 -2.304924 -2.598265
C -2.673057 -2.528997 2.448620
O -0.397119 -0.517498 -0.202182
H -6.419584 -0.858565 -1.273918
H -5.818845 0.643380 -0.575020
H -5.239787 0.105562 -2.155097
H -4.248979 -3.148551 -2.748701
H -3.974484 -1.488263 -3.218398
H -2.624286 -2.607638 -2.970927
H -0.875671 -3.446091 0.334041
H -2.134289 -4.563583 -0.195897
H -1.309717 -3.545535 -1.378769
H -1.597996 -2.711994 2.459613
H -2.915908 -1.843820 3.259773
H -3.174797 -3.477005 2.668086
H -4.428095 -0.178315 2.846613
H -5.488199 0.499500 1.613534
H -5.828394 -1.095491 2.286466
Ir 2.362618 0.312303 -0.063064
C 4.454788 1.010402 -0.494150
C 4.220704 1.083173 0.912815
C 3.565705 1.938072 -1.157345
C 3.137775 2.012815 1.133115
C 2.747579 2.534396 -0.152817
C 2.107885 -3.617172 1.599236
C 1.884870 -3.445649 2.953388
C 1.766080 -2.161739 3.474817
C 1.896426 -1.049189 2.651854
C 2.141431 -1.200208 1.292202
C 2.230682 -2.503126 0.767298
H 2.188072 -4.620855 1.196777
H 1.803221 -4.308065 3.603798
H 1.579914 -0.261888 4.534587
H 1.794080 -0.061370 3.085228
C 2.481704 -1.296703 -2.623362
C 2.589776 -2.416833 -3.417073
C 2.611688 -3.664892 -2.802833
C 2.504532 -3.743653 -1.429860
C 2.388374 -2.579195 -0.672410
H 2.713277 -4.566581 -3.395155
H 2.461269 -0.300700 -3.046159
H 2.661657 -2.311282 -4.491598

94

L2-DIMERTs_SU E=-2094.89510058 A.U.

Ir -2.312056 0.553214 0.194231
C -4.165049 1.797862 0.805893
C -3.720993 2.297418 -0.439355
C -3.105280 1.988313 1.779049
C -2.351005 2.741873 -0.282463
C -1.999709 2.593227 1.104950
C -3.522848 -2.216918 -2.816729
C -3.138389 -1.658603 -4.023154
C -2.474200 -0.437836 -4.040432
C -2.217836 0.241243 -2.854959
C -2.621040 -0.294599 -1.640503
C -3.262451 -1.544800 -1.622931
H -4.019555 -3.180495 -2.811291
H -3.349925 -2.176491 -4.950764
H -2.159366 -0.008259 -4.984924
H -1.691001 1.187071 -2.888222
C -3.207437 -1.725038 1.979672
C -3.820961 -2.914672 2.308613
C -4.326093 -3.705877 1.283766
C -4.178555 -3.293299 -0.025428
C -3.541160 -2.087444 -0.304413
H -4.826851 -4.640351 1.507599
H -2.786835 -1.073242 2.734040

H	2.520308	-4.704697	-0.933260	H	-5.955394	-0.954957	2.102286	C	2.399051	-2.587997	-0.609704
C	1.705004	3.570931	-0.364974	Ir	2.346534	0.319276	-0.081579	H	2.750108	-4.640786	-3.279818
C	5.026224	0.421582	1.970847	C	4.438387	1.031128	-0.598863	H	2.463504	-0.369264	-3.039811
C	5.531732	0.229227	-1.157971	C	4.269842	1.028310	0.818882	H	2.682807	-2.415115	-4.434009
C	3.604487	2.303873	-2.598482	C	3.518845	1.980990	-1.173132	H	2.548068	-4.718414	-0.815947
C	2.671915	2.529949	2.447894	C	3.209967	1.958804	1.137720	C	1.702507	3.578738	-0.216571
O	0.397142	0.517471	-0.202239	C	2.748647	2.530357	-0.100709	C	5.122799	0.311038	1.802937
H	6.420101	0.857978	-1.272334	C	2.105265	-3.565259	1.686827	C	5.472315	0.273357	-1.350495
H	5.819022	-0.643686	-0.573123	C	1.854786	-3.358693	3.031176	C	3.474305	2.404281	-2.597588
H	5.240650	-0.106455	-2.153648	C	1.703627	-2.062609	3.512152	C	2.831192	2.429686	2.496865
H	4.286296	3.147366	-2.748949	C	1.829883	-0.971880	2.659412	O	0.396587	0.541463	-0.284476
H	3.975842	1.486924	-3.218114	C	2.106533	-1.158812	1.311328	H	6.358830	0.902035	-1.479423
H	2.625646	2.606542	-2.971712	C	2.224281	-2.473749	0.825049	H	5.781689	-0.627031	-0.821321
H	0.875295	3.445929	0.331779	H	2.208291	-4.578474	1.314585	H	5.130383	-0.012596	-2.345445
H	2.134288	4.563548	-0.196980	H	1.775989	-4.203243	3.704969	H	4.132208	3.266213	-2.750264
H	1.310833	3.545517	-1.380650	H	1.494008	-1.899714	4.563692	H	3.824860	1.618959	-3.268198
H	1.596875	2.713106	2.458229	H	1.697898	0.025854	3.059508	H	2.471654	2.701469	-2.905911
H	2.914199	1.844986	3.259400	C	2.491150	-1.354863	-2.592658	H	0.929081	3.452143	0.541521
H	3.173677	3.477948	2.667349	C	2.609064	-2.493901	-3.357396	H	2.153091	4.565998	-0.075247
H	4.426858	0.179467	2.847602	C	2.639783	-3.725398	-2.710898	H	1.227240	3.566409	-1.197312
H	5.487581	-0.498749	1.615267	C	2.528497	-3.770427	-1.336576	H	1.763106	2.635367	2.577226
H	5.827342	1.096530	2.287739	C	2.399126	-2.588071	-0.609762	H	3.107496	1.709803	3.265780
N	2.393100	-1.372983	-1.288524	H	2.749982	-4.641113	-3.279709	H	3.365316	3.359155	2.719388
N	-2.393004	1.372910	-1.288596	H	2.463139	-0.369586	-3.040106	H	4.567370	0.042184	2.700712

94

L2-DIMER_SU E=-2094.94550136 A.U.

Ir	-2.346572	-0.319299	-0.081240
C	-4.438463	-1.031182	-0.598405
C	-4.269909	-1.028033	0.819343
C	-3.518968	-1.981208	-1.172455
C	-3.210097	-1.958529	1.138396
C	-2.748786	-2.530362	-0.099903
C	-2.104836	3.565396	1.686748
C	-1.854212	3.358951	3.031088
C	-1.703092	2.062905	3.512178
C	-1.829527	0.972096	2.659565
C	-2.106332	1.158909	1.311497
C	-2.224039	2.473806	0.825098
H	-2.207828	4.578580	1.314412
H	-1.775268	4.203564	3.704784
H	-1.493352	1.900102	4.563708
H	-1.697553	-0.025604	3.059750
C	-2.491399	1.354591	-2.592463
C	-2.609336	2.493558	-3.357302
C	-2.639897	3.725123	-2.710927
C	-2.528438	3.770286	-1.336623
C	-2.399051	2.587997	-0.609704
H	-2.750108	4.640786	-3.279818
H	-2.463504	0.369264	-3.039811
H	-2.682807	2.415115	-4.434009
H	-2.548068	4.718414	-0.815947
C	-1.702507	-3.578738	-0.216571
C	-5.122799	-0.311038	1.802937
C	-5.472315	-0.273357	-1.350495
C	-3.474305	-2.404281	-2.597588
C	-2.831192	-2.429686	2.496865
O	-0.396587	-0.541463	-0.284476
H	-6.358830	-0.902035	-1.479423
H	-5.781689	0.627031	-0.821321
H	-5.130383	0.012596	-2.345445
H	-4.132208	-3.266213	-2.750264
H	-3.824860	-1.618959	-3.268198
H	-2.471654	-2.701469	-2.905911
H	-0.929081	-3.452143	0.541521
H	-2.153091	-4.565998	-0.075247
H	-1.227240	-3.566409	-1.197312
H	-1.763106	-2.635367	2.577226
H	-3.107496	-1.709803	3.265780
H	-3.365316	-3.359155	2.719388
H	-4.567370	-0.042184	2.700712
H	-5.543005	0.602705	1.384279

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L2-DIMER_T E=-2094.94550136 A.U.

Ir	2.346572	0.319299	-0.081240
C	4.438463	1.031182	-0.598405
C	4.269909	1.028033	0.819343
C	3.518968	1.981208	-1.172455
C	3.210097	1.958529	1.138396
C	2.748786	2.530362	-0.099903
C	2.104836	-3.565396	1.686748
C	1.854212	-3.358951	3.031088
C	1.703092	-2.062905	3.512178
C	1.829527	-0.972096	2.659565
C	2.106332	-1.158909	1.311497
C	2.224039	-2.473806	0.825098
H	2.207828	-4.578580	1.314412
H	1.775268	-4.203564	3.704784
H	1.493352	-1.900102	4.563708
H	1.697553	0.025604	3.059750
C	2.491399	-1.354591	-2.592463
C	2.609336	-2.493558	-3.357302
C	2.639897	-3.725123	-2.710927
C	2.528438	-3.770286	-1.336623

N -2.399422 1.399282 -1.257074
N 2.399502 -1.399142 -1.256895

94

L3-DIMERTs_S E=-2127.32556059 A.U.

lr -2.536715 -0.473713 -0.141178
C -4.296362 -1.283187 -1.349926
C -4.580384 -1.632196 -0.008051
C -3.035532 -1.924888 -1.714711
C -3.495727 -2.458098 0.497596
C -2.575535 -2.678888 -0.573077
C -4.120426 3.026245 1.748652
C -4.427351 2.649207 3.047126
C -4.128463 1.359911 3.464997
C -3.576764 0.478224 2.557808
C -3.551301 2.105039 0.883575
H -4.322014 4.036585 1.417200
H -4.881615 3.359407 3.728961
H -4.329685 1.032472 4.477647
H -3.333254 -0.538431 2.835332
C -1.911683 1.569087 -2.293303
C -2.049386 2.762184 -2.979773
C -2.752693 3.800391 -2.387392
C -3.270948 3.623849 -1.113913
C -3.098750 2.406218 -0.472810
H -2.897465 4.739511 -2.909267
H -1.373006 0.727308 -2.706954
H -1.623521 2.864637 -3.970251
H -3.814339 4.427182 -0.633540
C -1.372609 -3.538865 -0.553769
C -5.818623 -1.295020 0.729564
C -5.181957 -0.543216 -2.279887
C -2.472011 -2.008156 -3.082669
C -3.478758 -3.150406 1.809654
O -0.697635 -0.569881 -0.278792
H -5.830302 -1.261902 -2.794508
H -5.831069 0.162284 -1.762540
H -4.622991 -0.010934 -3.049127
H -2.909868 -2.880514 -3.582768
H -2.723718 -1.141212 -3.692466
H -1.391111 -2.144843 -3.070225
H -1.242844 -4.027514 0.410191
H -1.459739 -4.315010 -1.318710
H -0.482590 -2.938595 -0.767226
H -2.469123 -3.275836 2.199608
H -4.092378 -2.648484 2.556702
H -3.906586 -4.151722 1.682019
H -5.668809 -1.224013 1.806363
H -6.284125 -0.378170 0.370062
H -6.539644 -2.105846 0.566110
lr 2.552670 0.484165 0.094104
C 4.602053 1.529177 -0.376843
C 4.424188 1.395859 1.021051
C 3.499347 2.308050 -0.915519
C 3.217582 2.135002 1.383179
C 2.680469 2.723194 0.180535
C 3.191289 -3.409246 1.741107
C 2.742446 -3.336073 3.050665
C 2.114944 -2.178251 3.485000
C 1.984993 -1.117261 2.606548
C 3.028165 -2.315463 0.904126
H 3.673692 -4.309551 1.383267
H 2.880793 -4.175883 3.722028
H 1.741014 -2.086331 4.497199
H 1.505393 -0.191365 2.894018
C 3.386729 -0.981328 -2.446506
C 3.867289 -2.029749 -3.204856
C 4.153764 -2.333148 -2.575431
C 3.906862 -3.360225 -1.217261
C 3.408270 -2.279280 -0.506812
H 4.554775 -4.068794 -3.137977
H 3.157295 -0.021895 -2.890237

H 4.025779 -1.895624 -4.267883
H 4.103116 -4.300091 -0.717888
C 1.505473 3.620614 0.128534
C 5.366409 0.772127 1.981689
C 5.763421 1.039184 -1.152510
C 3.388164 2.793539 -2.313319
C 2.781948 2.450116 2.764383
O 0.719508 0.659831 0.286488
H 6.520142 1.833608 -1.162770
H 6.229496 0.162650 -0.704077
H 5.522079 0.825644 -2.193095
H 3.871870 3.774553 -2.384597
H 3.900313 2.145975 -3.024099
H 2.351957 2.917704 -2.625959
H 1.287430 3.940718 -0.888719
H 0.625443 3.112865 0.533849
H 1.697428 4.513184 0.730161
H 1.710331 2.638612 2.823844
H 3.056840 1.673545 3.477321
H 3.294798 3.364794 3.085502
H 4.854852 0.335594 2.839851
H 5.987666 0.008059 1.516263
H 6.039605 1.545210 2.369309
N 3.177121 -1.095775 -1.126899
N -2.442123 1.393916 -1.080821
N -3.310410 0.834711 1.292371
N 2.450111 -1.181370 1.356849

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L3-DIMERTs_SU E=-2127.33535526 A.U.

lr 2.572032 0.434740 -0.006251
C 4.647873 1.148535 -0.739900
C 4.661936 1.160355 0.672442
C 3.580133 2.032508 -1.192787
C 3.605562 2.054688 1.131497
C 2.979754 2.626000 -0.029184
C 3.012198 -3.541772 1.564680
C 2.950051 -3.413374 2.943268
C 2.673884 -2.170293 3.493889
C 2.504325 -1.091147 2.647574
C 2.823755 -2.424207 0.764449
H 3.217709 -4.507449 1.121763
H 3.113365 -4.275833 3.579589
H 2.606021 -2.029644 4.565641
H 2.296132 -0.100316 3.029245
C 2.498301 -1.160681 -2.617047
C 2.667920 -2.261414 -3.435045
C 2.946182 -3.489342 -2.852457
C 3.010620 -3.581493 -1.471044
C 2.822120 -2.443576 -0.700018
H 3.109676 -4.368008 -3.466160
H 2.288888 -0.180513 -3.024791
H 2.598541 -2.148861 -4.510019
H 3.218045 -4.534893 -1.003117
C 1.953534 3.694065 -0.029744
C 5.639827 0.479499 1.553922
C 5.607427 0.450006 -1.627372
C 3.346783 2.452041 -2.596904
C 3.410489 2.500621 2.533033
O 0.728836 0.729023 -0.002320
H 6.412532 1.148237 -1.884542
H 6.070316 -0.410669 -1.146681
H 5.153999 0.131265 -2.566073
H 3.941805 3.350644 -2.796981
H 3.670758 1.700193 -3.315721
H 2.303888 2.705965 -2.785685
H 1.338627 3.664889 0.868985
H 2.457488 4.666286 -0.056118
H 1.307517 3.632980 -0.904924
H 2.384518 2.808074 2.733360
H 3.708466 1.743079 3.257245

H 4.051945 3.371173 2.713230
H 5.199760 0.159687 2.498692
H 6.109467 -0.377405 1.073233
H 6.437852 1.189737 1.799901
lr -2.572683 -0.434280 -0.006726
C -4.658437 -1.141585 -0.712869
C -4.649252 -1.173821 0.699303
C -3.598280 -2.019219 -1.195598
C -3.582471 -2.070297 1.128649
C -2.976191 -2.625802 -0.050497
C -3.003458 3.538797 1.575611
C -2.934753 3.406850 2.953534
C -2.656765 2.162195 3.499637
C -2.491609 1.085245 2.649712
C -2.819246 2.423259 0.771586
H -3.210972 4.505634 1.136191
H -3.094767 4.267723 3.592832
H -2.584272 2.018662 4.570699
H -2.282088 0.093279 3.027701
C -2.517501 1.167512 -2.614841
C -2.690899 2.270423 -3.429117
C -2.962893 3.497478 -2.841779
C -3.017826 3.586430 -1.459744
C -2.826319 2.446296 -0.692731
H -3.128799 4.377924 -3.452278
H -2.312619 0.188021 -3.026394
H -2.629089 2.160233 -4.504799
H -3.220218 4.539115 -0.988173
C -1.947348 -3.690888 -0.081952
C -5.614157 -0.507066 1.605347
C -5.633831 -0.431399 -1.573793
C -3.391554 -2.421061 -2.608945
C -3.360454 -2.533570 2.520540
O -0.728964 -0.725649 -0.016529
H -6.450922 -1.121303 -1.814869
H -6.077425 0.430908 -1.077918
H -5.200121 -0.111378 -2.521266
H -3.994487 -3.314248 -2.809657
H -3.725242 -1.658681 -3.311996
H -2.353626 -2.677471 -2.820179
H -1.305111 -3.658950 0.797491
H -2.449005 -4.664618 -0.092255
H -1.328839 -3.628610 -0.976556
H -2.331348 -2.846065 2.695280
H -3.640498 -1.783823 3.259897
H -4.000807 -3.404245 2.703890
H -5.162044 -0.204790 2.550170
H -6.089334 0.358416 1.145916
H -6.409779 -1.221021 1.848658
N -2.597846 1.251798 -1.282373
N 2.587972 -1.248005 -1.285367
N 2.592167 -1.213326 1.318564
N -2.585334 1.210893 1.321429

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L3-DIMERTs_T E=-2127.34941698 A.U.

lr -2.517179 -0.434491 0.000152
C -4.586260 -1.167822 -0.709001
C -4.587754 -1.166986 0.705084
C -3.519630 -2.050786 -1.163467
C -3.522368 -2.049857 1.162760
C -2.905256 -2.628241 0.000626
C -2.946085 3.564749 1.518805
C -2.890392 3.454531 2.899189
C -2.621754 2.217676 3.467014
C -2.451189 1.127441 2.635154
C -2.758072 2.436053 0.733943
H -3.147825 4.524945 1.062486
H -3.054156 4.325721 3.523385
H -2.561093 2.090187 4.540851
H -2.250020 0.140900 3.031423
C -2.451035 1.129784 -2.633392

H	-0.825302	-3.391681	-1.377326	H	-2.623493	1.529562	4.738549	H	3.298771	2.326896	3.046459
H	-1.798543	-3.110957	2.387602	H	-2.201020	-0.222100	3.027803	H	3.474343	3.887157	2.271510
H	-3.227738	-2.315567	3.080137	C	-2.376028	1.374407	-2.487415	H	4.915342	0.793552	2.583666
H	-3.374738	-3.892065	2.332585	C	-2.588564	2.540104	-3.199208	H	5.835463	0.023786	1.275631
H	-4.896443	-0.845765	2.591991	C	-2.925980	3.693889	-2.506363	H	6.127023	1.705127	1.698796
H	-5.831029	-0.113191	1.272137	C	-3.005377	3.649255	-1.123777	N	2.479349	-1.327417	-1.154848
H	-6.082654	-1.796269	1.713800	C	-2.772956	2.451312	-0.462877	N	-2.479322	1.327448	-1.154857
Ir	2.388235	0.472983	-0.037105	H	-3.124700	4.619026	-3.035643	N	-2.509685	1.040646	1.426362
C	4.356967	1.286257	-0.784336	H	-2.121923	0.447991	-2.985129	N	2.509631	-1.040672	1.426378
C	4.314740	1.491020	0.624078	H	-2.507285	2.533214	-4.279292				
C	3.251175	2.017289	-1.379508	H	-3.260132	4.542766	-0.568885				
C	3.172001	2.329452	0.929717	C	-1.501846	-3.611462	-0.533953	98			
C	2.537908	2.669832	-0.315487	C	-5.345589	-0.943095	1.593672	L4-DIMERts-S E=	-2247.26109464	A.U.	
C	3.144340	-3.314256	1.831275	C	-5.431783	-0.446178	-1.533887	Ir	-2.386016	-0.549454	-0.122267
C	3.104464	-3.078089	3.196184	C	-3.109693	-2.171053	-2.861660	C	-4.557552	-1.214285	-0.502601
C	2.755993	-1.814722	3.652011	C	-2.944108	-2.929322	2.210476	C	-4.280711	-1.348262	0.879549
C	2.492854	-0.823118	2.726494	O	-0.370908	-0.571255	-0.133443	C	-3.679269	-2.102375	-1.241025
C	2.860814	-2.281459	0.948907	H	-6.229943	-1.141245	-1.819037	C	-3.176413	-2.275802	1.022757
H	3.407366	-4.296868	1.461910	H	-5.886633	0.333534	-0.924344	C	-2.844218	-2.762453	-0.295423
H	3.341317	-3.872378	3.895112	H	-5.053971	-0.000220	-2.453703	C	-2.158588	3.346165	1.647848
H	2.703758	-1.590845	4.710444	H	-3.641988	-3.083219	-3.155811	C	-1.925057	3.145747	3.018322
H	2.228630	0.180309	3.033616	H	-3.527394	-1.363473	-3.461710	C	-1.783681	1.864956	3.506891
C	2.389457	-1.323888	-2.512599	H	-2.061114	-2.312151	-3.124171	C	-1.888231	0.738189	2.671218
C	2.628404	-2.472116	-3.243860	H	-0.844960	-3.641194	0.334865	C	-2.144511	0.892994	1.326704
C	3.003250	-3.626520	-2.571504	H	-1.927440	-4.612772	-0.661676	C	-2.264900	2.204346	0.831797
C	3.093630	-3.600231	-1.189087	H	-0.910366	-3.389218	-1.421568	H	-1.855915	3.998161	3.684790
C	2.833266	-2.419577	-0.507814	H	-1.883047	-3.139818	2.342592	H	-1.594413	1.717111	4.564523
H	3.223096	-4.537743	-3.116364	H	-3.298770	-2.326942	3.046372	H	-1.752192	-0.245287	3.105253
H	2.108818	-0.397186	-2.995473	H	-3.474334	-3.887188	2.271391	C	-2.604928	1.270408	-2.599245
H	2.539016	-2.451004	-4.323127	H	-4.915399	-0.793636	2.583581	C	-2.712762	2.486374	-3.269404
H	3.378347	-4.494502	-0.650295	H	-5.835539	-0.023896	1.275541	C	-2.688459	3.664711	-2.552585
C	1.404337	3.609305	-0.480173	H	-6.127016	-1.705260	1.698673	C	-2.539533	3.624875	-1.160150
C	5.319736	1.016265	1.602750	Ir	2.394640	0.457771	-0.043945	C	-2.439988	2.357607	-0.560333
C	5.420063	0.571750	-1.531260	C	4.390191	1.202244	-0.798175	N	-2.484725	1.210623	-1.278962
C	3.048660	2.246886	-2.831996	C	4.354485	1.429889	0.606443	H	-2.780430	4.618635	-3.060558
C	2.863962	2.925460	2.253873	C	3.306657	1.957804	-1.406562	H	-2.609764	0.328496	-3.132790
O	0.379854	0.547237	-0.026436	C	3.238327	2.306811	0.896846	H	-2.817148	2.487421	-4.346620
H	6.200672	1.292182	-1.801169	C	2.607971	2.641979	-0.354227	C	-1.835746	-3.812345	-0.589651
H	5.893643	-0.207272	-0.935201	C	3.044323	-3.313530	1.893450	C	-5.043509	-0.735343	1.997280
H	5.055447	0.133507	-2.459885	C	2.999748	-3.052420	3.253581	C	-5.643650	-0.397614	-1.106688
H	3.566686	3.170223	-3.115614	C	2.677325	-1.773378	3.684619	C	-3.759987	-2.387562	-2.698748
H	3.477327	1.452887	-3.442471	C	2.443835	-0.792527	2.739976	C	-2.674647	-2.846521	2.301511
H	1.997863	2.374569	-3.092287	C	2.790856	-2.290207	0.991144	O	-0.567647	-0.788928	-0.405915
H	0.742043	3.600571	0.385154	H	3.288424	-4.307878	1.542922	H	-6.530978	-1.021496	-1.252077
H	1.801401	4.625337	-0.581238	H	3.213903	-3.839171	3.968190	H	-5.928586	0.436478	-0.466731
H	0.825318	3.391718	-1.377156	H	2.623222	-1.529676	4.738559	H	-5.363591	-0.000373	-2.082791
H	1.798535	3.110898	2.387777	H	2.200941	0.222052	3.027832	H	-4.458038	-3.211848	-2.877365
H	3.227725	2.315487	3.080301	C	2.376126	-1.374341	-2.487412	H	-4.132844	-1.531637	-3.262180
H	3.374732	3.892004	2.332787	C	2.588730	-2.540013	-3.199227	H	-2.794599	-2.681291	-3.111562
H	4.896425	0.845685	2.592127	C	2.926150	-3.693805	-2.506398	H	-0.985828	-3.753148	0.090595
H	5.831030	0.113159	1.272261	C	3.005473	-3.649208	-1.123806	H	-2.291021	-4.800318	-0.469461
H	6.082641	1.796224	1.713980	C	2.772967	-2.451295	-0.462883	H	-1.463598	-3.738532	-1.610994
N	2.500790	-1.293555	-1.179430	H	3.124934	-4.618919	-3.035694	H	-1.605278	-3.055539	2.263307
N	-2.500779	1.293580	-1.179513	H	2.122022	-0.447918	-2.985113	H	-2.866947	-2.180924	3.141867
N	-2.555231	1.046148	1.408045	H	2.507500	-2.533095	-4.279314	H	-3.192904	-3.787980	2.510131
N	2.555213	-1.046176	1.408134	H	3.260237	-4.542726	-0.568928	H	-4.404710	-0.511231	2.850685
				C	1.501898	3.611494	-0.533869	H	-5.537134	0.187492	1.695395
94				C	5.345557	0.943006	1.593768	H	-5.817078	-1.433674	2.331460
L3-DIMER_T E=	-2127.38546559	A.U.		C	5.431803	0.446173	-1.533800	C	-2.472557	4.770528	-0.305685
Ir	-2.394630	-0.457764	-0.044000	C	3.109779	2.171127	-2.861576	C	-2.291178	4.633842	1.033092
C	-4.390173	-1.202250	-0.798259	C	2.944117	2.929291	2.210571	H	-2.570786	5.754891	-0.749053
C	-4.354480	-1.429918	0.606356	O	0.370920	0.571241	-0.133384	H	-2.240852	5.515272	1.663241
C	-3.306621	-1.957782	-1.406645	H	6.229991	1.141231	-1.818894	Ir	2.386029	0.549456	-0.122240
C	-3.238305	-2.306818	0.896759	H	5.886615	-0.333575	-0.924273	C	4.557594	1.214282	-0.503386
C	-2.607932	-2.641961	-0.354313	H	5.054011	0.000262	-2.453647	C	4.280627	1.348265	0.879736
C	-3.044536	3.313462	1.893461	H	3.642146	3.083265	-3.155683	C	3.679394	2.102384	-1.240898
C	-3.000031	3.052320	3.253588	H	3.527438	1.363536	-3.461640	C	3.176329	2.275818	1.022844
C	-2.677554	1.773287	3.684612	H	2.061217	2.312306	-3.124110	C	2.844256	2.762465	-0.295376
C	-2.443954	0.792473	2.739957	H	0.845020	3.641250	0.334954	C	2.158382	-3.346138	1.647909
C	-2.790943	2.290181	0.991144	H	1.927504	4.612796	-0.661610	C	1.924681	-3.145697	3.018350
H	-3.288683	4.307802	1.542943	H	0.910407	3.389244	-1.421475	C	1.783259	-1.864897	3.506882
H	-3.214283	3.839038	3.968204	H	1.883055	3.139788	2.342680	C	1.887928	-0.738144	2.671205

C	2.144376	-0.892972	1.326727	H	-6.675777	-0.762466	-0.961362	C	-4.568084	-1.222047	-0.352699
C	2.264841	-2.204331	0.831860	H	-5.930714	0.667934	-0.249416	C	-4.209384	-1.353348	1.009107
H	1.855437	-3.998100	3.684821	H	-5.507688	0.170159	-1.890105	C	-3.715444	-2.094562	-1.138401
H	1.593860	-1.717034	4.564488	H	-4.787456	-3.062174	-2.707514	C	-3.086821	-2.268367	1.091475
H	1.751829	0.245340	3.105200	H	-4.402501	-1.401413	-3.121918	C	-2.818606	-2.749231	-0.238734
C	2.605207	-1.270449	-2.599162	H	-3.115772	-2.616128	-3.038549	C	-2.176773	3.381457	1.586122
C	2.713106	-2.486425	-3.269292	H	-1.205511	-3.796264	0.081497	C	-1.908187	3.201965	2.953350
C	2.688736	-3.664751	-2.552456	H	-2.588975	-4.756004	-0.448093	C	-1.738182	1.930142	3.456041
C	2.539676	-3.624892	-1.160036	H	-1.738347	-3.724472	-1.600920	C	-1.850877	0.790784	2.639091
C	2.440066	-2.357615	-0.560249	H	-1.646831	-3.026480	2.259440	C	-2.141310	0.925728	1.299260
N	2.484888	-1.210644	-1.278891	H	-2.820038	-2.098918	3.204044	C	-2.290163	2.227847	0.788701
H	2.780752	-4.618682	-3.060405	H	-3.245949	-3.693450	2.600899	H	-1.833003	4.064212	3.606415
H	2.610089	-0.328544	-3.132720	H	-4.299975	-0.363498	2.988909	H	-1.520133	1.799418	4.510326
H	2.817592	-2.487490	-4.346497	H	-5.466022	0.375963	1.893688	H	-1.691391	-0.184745	3.082894
C	1.835813	3.812365	-0.589682	H	-5.773261	-1.231303	2.552954	C	-2.673256	1.238675	-2.620144
C	5.043322	0.735303	1.997515	C	-2.312906	4.799124	-0.459817	C	-2.811459	2.443536	-3.305825
C	5.643734	0.397573	-1.106345	C	-2.123653	4.696154	0.880884	C	-2.791068	3.632728	-2.607658
C	3.760258	2.387559	-2.698615	H	-2.375420	5.772785	-0.932330	C	-2.617331	3.615713	-1.217265
C	2.674496	2.846577	2.301546	H	-2.030577	5.593463	1.483105	C	-2.491213	2.359095	-0.601628
O	0.567675	0.788854	-0.406046	Ir	2.437149	0.509964	-0.114686	N	-2.531655	1.201191	-1.301891
H	6.531230	1.021323	-1.251270	C	4.667535	1.061546	-0.344501	H	-2.903127	4.577538	-3.128359
H	5.928307	-0.436748	-0.466522	C	4.320906	1.211300	1.017951	H	-2.669576	0.289418	-3.140496
H	5.363912	0.000655	-2.082647	C	3.867470	1.986974	-1.125994	H	-2.932518	2.426870	-4.381161
H	4.458413	3.211767	-2.877182	C	3.252807	2.189180	1.105400	C	-1.821939	-3.792723	-0.590435
H	4.133067	1.531592	-3.262017	C	3.015847	2.692760	-0.223064	C	-4.917335	-0.751439	2.167588
H	2.794934	2.681383	-3.111508	C	2.035824	-3.423023	1.533391	C	-5.695697	-0.420401	-0.896673
H	0.985604	3.752855	0.090175	C	1.791641	-3.254162	2.906527	C	-3.876695	-2.384187	-2.587924
H	2.290938	4.800342	-0.468960	C	1.692873	-1.984280	3.432681	C	-2.497866	-2.822983	2.339253
H	1.464112	3.738862	-1.611209	C	1.856769	-0.838311	2.633892	O	-0.602477	-0.737032	-0.598097
H	1.605249	3.056152	2.263066	C	2.127259	-0.963808	1.288877	H	-6.579637	-1.056430	-1.004910
H	2.866209	2.180757	3.141859	C	2.200039	-2.262917	0.754172	H	-5.961710	0.405629	-0.238486
H	3.193183	3.787736	2.510460	H	1.679712	-4.122856	3.545688	H	-5.467052	-0.012036	-1.881563
H	4.404518	0.511566	2.851016	H	1.493566	-1.861012	4.491603	H	-4.575869	-3.216442	-2.720607
H	5.536617	-0.187751	1.695757	H	1.754443	0.136383	3.096281	H	-4.291696	-1.534284	-3.130357
H	5.817154	1.433437	2.331499	C	2.600194	-1.238235	-2.642956	H	-2.934782	-2.670967	-3.055786
C	2.472578	-4.770533	-0.305564	C	2.665392	-2.436941	-3.349914	H	-0.950049	-3.749545	0.062159
C	2.291046	-4.633825	1.033191	C	2.590095	-3.634713	-2.670732	H	-2.274872	-4.782787	-0.478653
H	2.570853	-5.754903	-0.748905	C	2.432665	-3.631667	-1.278284	H	-1.482562	-3.694864	-1.621215
H	2.240628	-5.515245	1.663345	C	2.380160	-2.380750	-0.640810	H	-1.422726	-2.979797	2.247113
				N	2.476140	-1.215311	-1.322828	H	-2.681644	-2.174407	3.194608
				H	2.647065	-4.575395	-3.207640	H	-2.960190	-3.789923	2.562389
				H	2.642809	-0.281647	-3.147713	H	-4.234719	-0.502587	2.978995
				H	2.775465	-2.408645	-4.426183	H	-5.454303	0.154588	1.889936
				C	2.081890	3.794622	-0.569521	H	-5.649041	-1.468433	2.552838
				C	4.992703	0.564081	2.173333	C	-2.546762	4.773965	-0.380213
				C	5.743942	0.191869	-0.888924	C	-2.336204	4.658690	0.956366
				C	4.042077	2.271449	-2.575116	H	-2.663890	5.750858	-0.835309
				C	2.703483	2.775020	2.357260	H	-2.280549	5.549622	1.572474
				O	0.673398	0.821505	-0.532325	Ir	2.406284	0.551316	-0.111612
				H	6.676412	0.760268	-0.959736	C	4.604547	1.148383	-0.442186
				H	5.929670	-0.669778	-0.248834	C	4.307508	1.293618	0.934756
				H	5.508268	-0.171104	-1.889669	C	3.766546	2.063801	-1.195076
				H	4.789351	3.060705	-2.707678	C	3.226193	2.250754	1.058349
				H	4.403443	1.400105	-3.121819	C	2.936426	2.750460	-0.264592
				H	3.117446	2.615616	-3.038885	C	2.090765	-3.375630	1.571831
				H	1.206459	3.796165	0.079964	C	1.871335	-3.200872	2.948408
				H	2.590461	4.756084	-0.447896	C	1.761276	-1.928539	3.466398
				H	1.740815	3.725180	-1.602011	C	1.886030	-0.786248	2.654917
				H	1.647570	3.027689	2.258527	C	2.130572	-0.915969	1.305196
				H	2.819843	2.099504	3.203666	C	2.216818	-2.218529	0.780418
				H	3.246973	3.693707	2.600492	H	1.789091	-4.066382	3.596329
				H	4.299793	0.364411	2.989640	H	1.583467	-1.800321	4.528606
				H	5.464589	-0.377176	1.894532	H	1.777234	0.190465	3.111793
				H	5.773969	1.230158	2.552639	C	2.551801	-1.216691	-2.631579
				C	2.311743	-4.798983	-0.459693	C	2.625277	-2.419921	-3.329693
				C	2.122484	-4.695948	0.881003	C	2.580378	-3.612783	-2.639175
				H	2.374078	-5.772666	-0.932183	C	2.443945	-3.600020	-1.244668
				H	2.029234	-5.593227	1.483243	C	2.378494	-2.344582	-0.616675
								N	2.445865	-1.183345	-1.309836
								H	2.646380	-4.557174	-3.168547
								H	2.573499	-0.263797	-3.144740
								H	2.720099	-2.399127	-4.407590

98

L4-DIMERTs_SU E= -2247.24591630 A.U.

Ir	-2.436918	-0.509860	-0.114757
C	-4.667138	-1.062372	-0.344751
C	-4.320691	-1.211684	1.017784
C	-3.866484	-1.987571	-1.125901
C	-3.252193	-2.189110	1.105639
C	-3.014726	-2.692839	-0.222650
C	-2.036767	3.423262	1.533301
C	-1.792608	3.254480	2.906452
C	-1.693615	1.984634	3.432644
C	-1.857243	0.838613	2.633872
C	-2.127684	0.964030	1.288841
C	-2.200719	2.263109	0.754100
H	-1.680865	4.123212	3.545593
H	-1.494323	1.861428	4.491575
H	-1.754732	-0.136042	3.096298
C	-2.600542	1.238271	-2.643013
C	-2.666037	2.436949	-3.349992
C	-2.591007	3.634751	-2.670836
C	-2.433578	3.631769	-1.278386
C	-2.380799	2.380876	-0.640888
N	-2.476485	1.215404	-1.322886
H	-2.648180	4.575409	-3.207764
H	-2.642905	0.281665	-3.147759
H	-2.776100	2.408606	-4.426262
C	-2.080353	-3.794448	-0.568772
C	-4.992918	-0.564538	2.172960
C	-5.743817	-0.193344	-0.889656
C	-4.040686	-2.272432	-2.574995
C	-2.702937	-2.774457	2.357760
O	-0.673276	-0.820624	-0.532962

98

L4-DIMERTs_T E= -2247.25393449 A.U.

Ir	-2.375841	-0.539584	-0.127941
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C	1.964113	3.829544	-0.574899	H	-5.407798	-2.155845	2.455870	C	2.722695	-0.986629	-2.613928
C	5.031122	0.659033	2.065999	C	-3.200464	4.463072	-0.688234	C	3.004204	-2.157678	-3.312708
C	5.675525	0.297916	-1.026030	C	-3.041485	4.468327	0.660356	C	3.154800	-3.344663	-2.625509
C	3.883704	2.346021	-2.650903	H	-3.441488	5.378751	-1.216050	C	3.012698	-3.358194	-1.232319
C	2.714975	2.833723	2.327928	H	-3.150596	5.395515	1.212497	C	2.733482	-2.132565	-0.602153
O	0.604896	0.858354	-0.418435	Ir	2.268528	0.737770	-0.049063	N	2.597972	-0.972758	-1.291383
H	6.584390	0.892763	-1.159075	C	4.211297	1.796985	-0.378950	H	3.381304	-4.262718	-3.156735
H	5.923173	-0.542990	-0.379488	C	3.898420	1.839312	1.013095	H	2.591218	-0.042173	-3.126547
H	5.398130	-0.094070	-2.005091	C	3.202891	2.550112	-1.097894	H	3.102736	-2.117623	-4.389779
H	4.603953	3.153964	-2.815214	C	2.649871	2.548094	1.166359	C	1.091396	3.812359	-0.547801
H	4.248587	1.481071	-3.205568	C	2.243922	2.996306	-0.145009	C	4.807644	1.342787	2.005150
H	2.933950	2.661170	-3.083769	C	2.726914	-3.273354	1.386269	C	5.441797	1.119757	-1.093165
H	1.083729	3.770833	0.065904	C	2.514744	-3.223178	2.773523	C	3.245435	2.789734	-2.673301
H	2.433664	4.804015	-0.408694	C	2.195480	-2.022768	3.372491	C	2.105907	3.028943	2.330245
H	1.635373	3.790048	-1.612788	C	2.101862	-0.829095	2.635429	O	0.296743	0.599755	-0.292974
H	1.655167	3.081311	2.263855	C	2.324653	-0.829340	1.273135	H	6.226118	1.875279	-1.200885
H	2.861019	2.157363	3.169154	C	2.625761	-2.066326	0.668790	H	5.837352	0.319409	-0.469047
H	3.261165	3.754812	2.555305	H	2.602078	-4.126358	3.366889	H	5.243153	0.712160	-2.084880
H	4.371024	0.454064	2.907836	H	2.023966	-1.992558	4.443006	H	3.754423	3.744610	-2.840324
H	5.503693	-0.277530	1.773016	H	1.847232	0.085222	3.159544	H	3.793780	2.037928	-3.241377
H	5.817816	1.335594	2.414153	C	2.708211	-0.810130	-2.672749	H	2.241865	2.877521	-3.090558
C	2.358112	-4.762627	-0.414978	C	2.996522	-1.931950	-3.445523	H	0.255306	3.550960	0.101934
C	2.190238	-4.652047	0.927992	C	3.176777	-3.155707	-2.834276	H	1.334496	4.864258	-0.368787
H	2.431493	-5.738848	-0.880663	C	3.057556	-3.255715	-1.442629	H	0.765761	3.716303	-1.583147
H	2.125780	-5.545972	1.539005	C	2.770739	-2.074938	-0.734288	H	1.015902	3.026270	2.294546
				N	2.605262	-0.877203	-1.349560	H	2.425494	2.418931	3.174059
98				H	3.408913	-4.036038	-3.423746	H	2.431144	4.054570	2.532486
L4-DIMER_S E=-2247.29294952 A.U.				H	2.553088	0.160831	-3.125457	H	4.230679	1.050115	2.881322
Ir	-2.268516	-0.737765	-0.049059	H	3.076123	-1.825290	-4.519632	H	5.414619	0.490101	1.703394
C	-4.211287	-1.796985	-0.378928	C	1.042511	3.825294	-0.419202	H	5.486241	2.148107	2.303113
C	-3.898393	-1.839328	1.013112	C	4.758530	1.342638	2.116505	C	3.124800	-4.518968	-0.402949
C	-3.202886	-2.550100	-1.097893	C	5.443896	1.220330	-0.978971	C	2.946316	-4.438515	0.940889
C	-2.649838	-2.548104	1.166351	C	3.253230	2.913508	-2.539260	H	3.359165	-5.468986	-0.869506
C	-2.243903	-2.996302	-0.145026	C	2.019266	2.960614	2.448786	H	3.033734	-5.331172	1.550810
C	-2.726946	3.273354	1.386267	O	0.296905	0.579422	-0.183182	Ir	-2.256986	-0.722814	-0.102204
C	-2.514771	3.223183	2.773520	H	6.212403	1.995594	-1.055660	C	-4.231732	-1.740748	-0.492378
C	-2.195493	2.022778	3.372489	H	5.848824	0.412115	-0.371226	C	-3.938949	-1.822848	0.900568
C	-2.101865	0.829105	2.635429	H	5.267433	0.835098	-1.983658	C	-3.221386	-2.479765	-1.218888
C	-2.324660	0.829345	1.273136	H	3.765140	3.873828	-2.659860	C	-2.704982	-2.560134	1.052143
C	-2.625782	2.066327	0.668789	H	3.813948	2.184290	-3.124305	C	-2.281228	-2.969618	-0.264230
H	-2.602113	4.126364	3.366885	H	2.258401	3.018083	-2.973315	C	-2.639713	3.196679	1.587270
H	-2.023975	1.992572	4.443003	H	0.198517	3.518988	0.200411	C	-2.411714	3.057084	2.965687
H	-1.847223	-0.085209	3.159545	H	1.258277	4.873140	-0.188514	C	-2.104856	1.816986	3.484588
C	-2.708222	0.810125	-2.672748	H	0.741360	3.768939	-1.464807	C	-2.035970	0.670576	2.673228
C	-2.996547	1.931941	-3.445523	H	0.930602	2.958374	2.385962	C	-2.273743	0.760466	1.317170
C	-3.176817	3.155696	-2.834278	H	2.317609	2.312114	3.271697	C	-2.564194	2.035600	0.794598
C	-3.057595	3.255707	-1.442630	H	2.337515	3.976022	2.706353	H	-2.478456	3.922608	3.615213
C	-2.770764	2.074935	-0.734288	H	4.173974	1.003578	2.970692	H	-1.922188	1.717157	4.548998
N	-2.605274	0.877201	-1.349560	H	5.395610	0.519088	1.796745	H	-1.786759	-0.277431	3.135766
H	-3.408963	4.036024	-3.423749	H	5.407824	2.155812	2.455859	C	-2.722652	0.986631	-2.613940
H	-2.553089	-0.160834	-3.125456	C	3.200413	-4.463080	-0.688230	C	-3.004153	2.157680	-3.312723
H	-3.076148	1.825279	-4.519632	C	3.041437	-4.468330	0.660360	C	-3.154764	3.344663	-2.625526
C	-1.042492	-3.825283	-0.419242	H	3.441426	-5.378763	-1.216046	C	-3.012687	3.358194	-1.232334
C	-4.758493	-1.342671	2.116537	H	3.150540	-5.395519	1.212502	C	-2.733477	2.132566	-0.602164
C	-5.443902	-1.220341	-0.978926					N	-2.597952	0.972759	-1.291392
C	-3.253247	-2.913485	-2.539261	98				H	-3.381263	4.262718	-3.156756
C	-2.019206	-2.960628	2.448765	L4-DIMER_SU E=-2247.29623974 A.U.				H	-2.591165	0.042175	-3.126557
O	-0.296898	-0.579420	-0.183181	Ir	2.256988	0.722816	-0.102199	H	-3.102667	2.117624	-4.389796
H	-6.212397	-1.995616	-1.055614	C	4.231739	1.740747	-0.492359	C	-1.091383	-3.812353	-0.547826
H	-5.848835	-0.412138	-0.371168	C	3.938951	1.822837	0.900587	C	-4.807649	-1.342808	2.005131
H	-5.267458	-0.835094	-1.983612	C	3.221397	2.479770	-1.218868	C	-5.441789	-1.119757	-1.093185
H	-3.765165	-3.873801	-2.659860	C	2.704985	2.560127	1.052163	C	-3.245419	-2.789718	-2.673324
H	-3.813969	-2.184260	-3.124294	C	2.281236	2.969619	-0.264208	C	-2.105906	-3.028954	2.330225
H	-2.258425	-3.018063	-2.973332	C	2.639678	-3.196680	1.587278	O	-0.296735	-0.599752	-0.292942
H	-0.198488	-3.518970	0.200354	C	2.411657	-3.057084	2.965692	H	-6.226106	-1.875282	-1.200918
H	-1.258247	-4.873130	-0.188548	C	2.104795	-1.816985	3.484589	H	-5.837352	-0.319419	-0.469060
H	-0.741363	-3.768927	-1.464852	C	2.035928	-0.670575	2.673229	H	-5.243142	-0.712148	-2.084893
H	-0.930543	-2.958367	2.385925	C	2.273724	-0.760464	1.317175	H	-3.754410	-3.744591	-2.840357
H	-2.317549	-2.312142	3.271687	C	2.564176	-2.035607	0.794606	H	-3.793758	-2.037906	-3.241397
H	-2.337434	-3.976044	2.706326	H	2.478382	-3.922608	3.615217	H	-2.241848	-2.877506	-3.090577
H	-4.173932	-1.003643	2.970732	H	1.922107	-1.717158	4.548996	H	-0.255299	-3.550962	0.101922
H	-5.395562	-0.519104	1.796799	H	1.786709	0.277433	3.135763	H	-1.334483	-4.864254	-0.368830

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H -3.111165 2.265252 -4.323329
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H -4.118815 -1.048636 2.915352
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H -5.389403 -2.153699 2.385842
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L4-DIMER_T E= -2247.29132080 A.U.

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C 2.266500 -2.998141 3.037099
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